Theoretical and numerical investigation of internal conical refraction of structured light beams

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1. INTRODUCTION

The conical refraction of light in a biaxial crystal is an interesting phenomena that has attracted much attention since it was theoretically predicted, almost two centuries ago, by Hamilton [1] and confirmed experimentally shortly afterwards by Lloyd [2] and Poggendorff [3]. In more recent times, many works have been devoted to both the theoretical [4–8, 10–16] as well as the experimental aspects of this phenomena [17–21]. The basic problem, however, is that the equations describing the phenomena are quite cumbersome and cannot be solved without assuming some approximations. For instance, the wave-vectors inside the crystal are given by the Fresnel equation, which is of fourth-order, and although analytic solutions can be obtained [13], they are too cumbersome to be used and most authors prefer to resort to some kind of approximations for the two modes that appear due to the anisotropic refraction. This latter approximation, in particular, could lead to the production of higher order Bessel beams from a lower order one [22–25].

In order to elucidate the validity of the approximate methods used so far, we present in this paper an ab-initio calculation of the evolution of a structured light beam of arbitrary shape along the optical axis inside a biaxial crystal. Our purpose is to obtain a set of equations given in such a form that they can be solved numerically. Section 3, the boundary conditions are used to obtain the complete set of equations to be solved numerically. Section 4 is devoted to two important applications of our formalism: we study the evolution of circularly and linearly polarized Gaussian and Bessel beams inside a KTP crystal. The results are presented in a series of graph obtained by numerical calculation in which the evolution of the refraction cone is clearly seen at various depths inside the crystal. In Section 5, we outline our procedure for the numerical simulations. In Section 6, we present some brief conclusions of our study.

2. GEOMETRY

Maxwell’s equations imply for the electric field $E$ inside the crystal

$$\nabla \times (\nabla \times E) - \omega^2 \hat{\epsilon} \cdot E = 0, \quad (1)$$

where $\hat{\epsilon}$ is the dielectric tensor. Let the principal axis of $\hat{\epsilon}$ be $e_i$ ($i = 1, 2, 3$) and choose them as the coordinates axis. Thus

$$\hat{\epsilon} = \text{diag}\{e_1, e_2, e_3\}$$

with the convention $e_1 < e_2 < e_3$.

For a plane wave $\propto \exp(ik \cdot x)$:

$$K \cdot E = 0, \quad (2)$$

where

$$K = \hat{k}k - k^2 \hat{i} + \omega^2 \hat{\epsilon}. \quad (3)$$
Eq. 2 has non-trivial solution if the determinant of the matrix $K$ is zero:

$$\Delta \equiv \left[ k^2 - \omega^2 (e_1 + e_2 + e_3) \right] (k \cdot k') + \omega^2 \left[ k^2 + \omega^2 e_1 e_2 e_3 \right] = 0,$$

which is the Fresnel equation [26]. Here and in the following we use the convention

$$k' = \hat{e} \cdot k, \quad k'' = \hat{e}^2 \cdot k.$$

To the vector $k$ is associated another vector $s$ such that $k \cdot s = \omega$. Explicitly,

$$s = N^{-1}(k) \left\{ (k \cdot k') k + \left[ k^2 - \omega^2 (e_1 + e_2 + e_3) \right] k' + \omega^2 k'' \right\},$$  

where

$$N(k) = (k \cdot k') k^2 - \omega^2 e_1 e_2 e_3.$$

The optical axis is given by $k = \omega n$, where

$$n_1 = \frac{\sqrt{e_3 (e_2 - e_1)}}{e_3 - e_1}, \quad n_2 = 0, \quad n_3 = \frac{\sqrt{e_1 (e_3 - e_2)}}{e_3 - e_1},$$

and thus

$$n^2 = e_2, \quad \mathbf{n} \cdot \mathbf{n}' = e_1 e_3, \quad n^2 = e_1 e_3 (e_1 - e_2 + e_3).$$

It can be seen with some simple algebra that the Fresnel determinant can also be written in the form

$$\Delta = (k^2 - \omega^2 e_2) (k \cdot k') - \omega^2 (e_1 + e_2 + e_3) - \omega^2 (e_2 - e_1) (e_3 - e_2) k_2^2.$$

At the optical axis, both the function $N(k)$ and the vector term in curly brackets in Eq. (5) are zero and this equation is undefined. This corresponds to the case of internal conical refraction. In this case, the vector $s$ must be recalculated setting $k = \omega n + \delta k$ in the Fresnel equation (4) and then taking the limit $\delta k \to 0$. Explicitly, setting $\Delta(k) \equiv \text{Det} K$, we find:

$$\Delta(\omega n + \delta k) = 2 \omega^3 \left\{ (\mathbf{n} \cdot \mathbf{n}') n + \left[ n^2 - (e_1 + e_2 + e_3) \right] n' \right\}$$

$$+ n'' \cdot \delta k + \omega^2 \delta k \cdot \left\{ (\mathbf{n} \cdot \mathbf{n}') \hat{e} + 2 (\mathbf{n} \cdot \mathbf{n}')(\mathbf{n} \cdot \mathbf{n}') \right\} \cdot \delta k + \omega O(\delta k^3) = 0.$$

This equation can be rewritten in the form

$$2 N(\omega n + \delta k) \mathbf{s} \cdot \delta k + \omega^2 \delta k \cdot \mathbf{M} \cdot \delta k = 0,$$

where

$$N(\omega n + \delta k) = 2 \omega^3 \left[ e_1 (e_2 + e_3) n_1 \delta k_1 + e_3 (e_1 + e_2) n_2 \delta k_3 \right].$$

and the matrix $\mathbf{M}$ is given by

$$\mathbf{M} = 2 (\mathbf{n} \cdot \mathbf{n}') - (e_2 - e_1)(e_3 - e_2) \mathbf{e}_2 \mathbf{e}_2.$$

It then follows that

$$\mathbf{s} = \lim_{\delta k \to 0} \frac{\mathbf{M} \cdot \delta k}{\delta k \cdot \mathbf{M} \cdot \delta k}$$

and clearly

$$\mathbf{s} \cdot \delta k = 0 = \delta k \cdot \mathbf{M} \cdot \delta k.$$

Therefore

$$\mathbf{s} = \frac{2 \left[ (\mathbf{n} \cdot \delta k) n + (\mathbf{n} \cdot \delta k)n' \right] - (e_2 - e_1)(e_3 - e_2) \delta k_2}{2 \left[ e_2 (\mathbf{n} \cdot \mathbf{n}') \delta k + e_3 \delta k_3 (\mathbf{n} \cdot \delta k) \right]},$$

with the conditions

$$4 (\mathbf{n} \cdot \delta k) (\mathbf{n}' \cdot \delta k) = (e_2 - e_1)(e_3 - e_2) (\delta k_2)^2.$$

Notice that the absolute magnitude of $\delta k$ does not appear in these last expressions defining the vector $s$.

**A. Geometry of refraction cone**

Eqs. (15) and (16) define the vector $s$ that sweeps the internal refraction cone. It follows from these equations that the intersections of the cone with the plane $(3, 1)$ is given by two vectors that bound it:

$$s_1 = \frac{1}{e_2} \mathbf{n} \quad \text{and} \quad s_2 = \frac{1}{e_1 e_3} n',$$

corresponding to $\delta k_2 = 0$.

Since

$$s_1^2 = \frac{1}{e_2} = s_1 \cdot s_2,$$

$$s_2^2 = \frac{1}{e_3} + \frac{1}{e_1} - \frac{e_2}{e_1 e_3},$$

it follows that $(s_2 - s_1) \cdot s_1 = 0$.

Consider a cone as depicted in Fig. 1. Choose the z axis in the $s$ direction and the y axis in the $e_2$ direction. Let $\beta$ be the angle between $s_1$ and $s_2$ that is

$$\tan \beta = \sqrt{\frac{(e_2 - e_1)(e_3 - e_2)}{e_1 e_3}}.$$

The cone is given by the equation

$$f(r) \equiv x^2 + \tan \beta \ z x + y^2 = 0,$$

and the vector normal to the cone is

$$\mathbf{p} \equiv \{x + \frac{1}{2} \tan \beta \ z, \ y, \ \frac{1}{2} \tan \beta \ x\}.$$

It satisfies the condition

$$\mathbf{p} \cdot \mathbf{s} = 0$$

everywhere on the cone, in accordance with Eq. 15.

In this new system of coordinates

$$\mathbf{n} = \{0, 0, n\},$$

and

$$\mathbf{n}' = \{-n' \sin \beta, 0, n' \cos \beta\},$$

where $n$ and $n'$ are given by Eq. 7. It then follows that

$$4 (\mathbf{n} \cdot \mathbf{p}) (\mathbf{n}' \cdot \mathbf{p}) = nn' \sin \beta \tan \beta \ p_y^2,$$

in accordance with Eq. 16. This last equation implies

$$p_z = \frac{1}{2} \tan \beta \left(p_x \pm \sqrt{p_x^2 + p_y^2}\right).$$

Notice also that the angle $\alpha$ between $\mathbf{n}$ and the $e_3$ axis is given by

$$\tan \alpha = \sqrt{\frac{e_3 (e_2 - e_1)}{e_1 (e_3 - e_2)}}.$$

Accordingly, the matrix $\hat{e}$ in this system of coordinates is

$$\hat{e} = \begin{pmatrix} e_1 \cos^2 \alpha + e_3 \sin^2 \alpha & 0 & -(e_3 - e_1) \sin \alpha \cos \alpha \\ 0 & e_2 & 0 \\ -(e_3 - e_1) \sin \alpha \cos \alpha & 0 & e_1 \sin^2 \alpha + e_3 \cos^2 \alpha \end{pmatrix}.$$

The following relation is useful:

$$e_1 \sin^2 \alpha + e_3 \cos^2 \alpha = \frac{e_1 e_3}{e_2}. \quad (28)$$
Thus, for any vector \( \mathbf{k} \), the scalar product \( \mathbf{k} \cdot \mathbf{k}' = k_x'^2 + k_y'^2 + k_z'^2 \) and we also have

\[
\mathbf{k} \cdot \mathbf{k}' = \left( \epsilon_1 + \epsilon_3 - \frac{\epsilon_1 \epsilon_3}{\epsilon_2} \right) k_x'^2 + k_y'^2 + \frac{\epsilon_1 \epsilon_3}{\epsilon_2} k_z'^2 - 2 \frac{\epsilon_1 \epsilon_3}{\epsilon_2} \sqrt{\epsilon_1 \epsilon_3 (\epsilon_2 - \epsilon_1)} (\epsilon_3 - \epsilon_2) k_x' k_z' = \frac{\epsilon_1 \epsilon_3}{\epsilon_2} \left( k_z' - \tan \beta k_x' \right)^2 + \epsilon_2 (k_x'^2 + k_y'^2). \tag{29}
\]

Accordingly, the Fresnel equation implies

\[
\left[ k_x'^2 + k_y'^2 - \epsilon_2 \omega^2 \right] \left[ (k_z' - \tan \beta k_x')^2 - \epsilon_2 \left( \omega^2 - \frac{\epsilon_2}{\epsilon_1} k_\perp^2 \right) \right] - \epsilon_2 \omega^2 \tan^2 \beta k_\perp^2 = 0. \tag{29}
\]

As a polynomial in \( k_z' \), it has four (real) roots: two positive and two negative ones.

Notice that for \( \beta \ll 1 \), the above equation has the following four solutions for \( k_z' \):

\[
K_- = \pm \sqrt{\epsilon_2 \omega^2 - k_\perp^2 + O(\beta^2)}
\]

\[
K_+ = \pm \sqrt{\epsilon_2 \omega^2 - \frac{\epsilon_2}{\epsilon_1} k_\perp^2 + \beta k_x + O(\beta^2)}. \tag{30}
\]

In the particular case of a uniaxial crystal such as, say, \( \epsilon_1 = \epsilon_2 \equiv \epsilon \), we have \( \beta = 0 \) and the four roots are given by

\[
k_x'^2 = \epsilon \omega^2 - k_\perp^2
\]

and

\[
k_z'^2 = \epsilon (\omega^2 - \epsilon^{-1} k_\perp^2).
\]

The first root corresponds to the ordinary wave and the second to the extraordinary wave.

In the following, we take \( K_+ \) and \( K_- \) as the two positive roots of Eq. (29), corresponding to propagation in the positive \( z \) direction inside the crystal.

**B. Fourier transform**

The general solution of Eq. (33) can be written in the form (the term \( e^{i\omega t} \) is not included for simplicity)

\[
E(r) = \frac{1}{(2\pi)^{3/2}} \int e^{iK \cdot r + i\Delta} \tilde{E}(K) \, dK, \tag{31}
\]

where \( \Delta \) is the Fresnel determinant and \( \tilde{E}(K) \) are functions to be determined by boundary conditions, as shown in the following.

Accordingly the Fourier transform Eq. (31) reduces to a two-dimensional integral:

\[
E(r) = \frac{1}{2\pi} \int e^{iK_x x + iK_y y} \bigg[ e^{iK_z z} \tilde{E}^+(k_x, k_y) + e^{-iK_z z} \tilde{E}^-(k_x, k_y) \bigg] \, dk_x \, dk_y, \tag{32}
\]

where \( \tilde{E}^\pm(k_x, k_y) \) are to be determined by the boundary conditions. A similar equation applies to \( \mathbf{D} \) with \( \hat{D}^\pm = \hat{e} \cdot \tilde{E}^\pm \). As for the magnetic field, it is

\[
B(r) = \frac{1}{2\pi \omega} \int e^{i(k_x x + k_y y)} \bigg[ e^{iK_z z} \mathbf{B}^+(k_x + K_z \hat{e}_z) \times \tilde{E}^+ + e^{-iK_z z} \mathbf{B}^-(k_x - K_z \hat{e}_z) \times \tilde{E}^- \bigg] \, dk_x \, dk_y. \tag{33}
\]

**3. REFLECTION AND REFRACTION**

In order to study the reflection and refraction of the waves, we write the electric vector \( \mathbf{E} \) in vacuum (that is, for \( z < 0 \)) in the form

\[
E(x, y, z) = \frac{1}{2\pi} \int dk_x \, dk_y \, e^{ik_z z} \left[ e^{iK_z z} \tilde{E}^I(k_x, k_y) + e^{-iK_z z} \tilde{E}^R(k_x, k_y) \right], \tag{34}
\]

where \( k_z = (\omega^2 - k_x^2 - k_y^2)^{1/2} \) and \( \tilde{E}^{(LR)}(k_x, k_y) \) are the two-dimensional Fourier transforms of the electric field components of the incident and reflected waves, \( \tilde{E}^{(I,R)}(x, y, 0-) \) at the interface; similar equations apply to the magnetic field component.
The boundary conditions imply the continuity of $E_x$, $E_y$, $B_z$ and $B_y$ at the interface $z = 0$ (the continuity conditions on $D_x$ and $B_z$ are not independent since, from the Maxwell equations, $i\omega D_x = \partial_y B_z - \partial_z B_y$ and $i\omega B_z = \partial_y E_y - \partial_z E_z$). It is convenient to express each Fourier transformed component of $B$ and $E_z$ in the vacuum region in terms of only $E_x$ and $E_y$ using the Maxwell equations. For the incident field (see [26]):

$$E^I_z = -\frac{1}{k_z} \left( k_z E^I_x + k_y E^I_y \right)$$

$$B^I_z = -\frac{1}{k_z \omega} \left[ k_y k_z E^I_x + (k_y^2 + k_z^2) E^I_y \right]$$

$$B^I_y = \frac{1}{k_z \omega} \left[ (k_z^2 + k_y^2) E^I_z + k_y k_z E^I_y \right]$$

$$B^I_z = \frac{1}{\omega} \left( - k_y E^I_x + k_z E^I_y \right).$$

These equations can be rewritten in terms of a $2 \times 2$ dyad as

$$\mathbf{e}_z \times \mathbf{B}^I = -k_z \omega \left( \omega^2 \mathbf{I} - \mathbf{k}_z \mathbf{k}_z \right)^{-1} \tilde{\mathbf{E}}^I.$$

Here and in the following, $\mathbf{V}_\perp = (V_x, V_y)$ for any vector $\mathbf{V}$ and also

$$\mathbf{k}_\perp \cdot \mathbf{k}_\perp = \begin{pmatrix} k_x^2 & k_x k_y \\ k_y k_x & k_y^2 \end{pmatrix}.$$

For the reflected field, it is only necessary to change the sign of $k_z$. Accordingly

$$\mathbf{e}_z \times \left( \mathbf{B}^R + \mathbf{B}^R \right) = -k_z \omega \left( \omega^2 \mathbf{I} - \mathbf{k}_z \mathbf{k}_z \right)^{-1} \left( \tilde{\mathbf{E}}^I - \tilde{\mathbf{E}}^R \right),$$

and the boundary conditions take the form

$$\tilde{\mathbf{E}}^I + \tilde{\mathbf{E}}^R = \tilde{\mathbf{E}}^+ + \tilde{\mathbf{E}}^-,$$

and

$$\tilde{\mathbf{E}}^I - \tilde{\mathbf{E}}^R = -\frac{1}{k_z \omega} \left( \omega^2 \mathbf{I} - \mathbf{k}_z \mathbf{k}_z \right) \left[ \mathbf{e}_z \times \left( \mathbf{B}^I + \mathbf{B}^I \right) \right].$$

At this point, it is convenient to define

$$\mathbf{F} \equiv \tilde{\mathbf{E}}^+ + \tilde{\mathbf{E}}^-,$$

$$k_z \mathbf{G} \equiv K_+ \mathbf{E}^+ + K_- \mathbf{E}^-,$$

and accordingly,

$$\tilde{\mathbf{E}}^+ = \frac{1}{K_- - K_+} \left( K_+ \mathbf{F} - k_z \mathbf{G} \right),$$

$$\tilde{\mathbf{E}}^- = \frac{1}{K_- - K_+} \left( -K_+ \mathbf{F} + k_z \mathbf{G} \right);$$

also

$$k_z^2 \tilde{\mathbf{E}}^+ + k_z^2 \tilde{\mathbf{E}}^- = -K_+ K_- \mathbf{F} + (K_+ + K_-) k_z \mathbf{G}.$$

Since $i\omega \mathbf{B} = \nabla \times \mathbf{E}$, equation Eq. (42) takes the explicit form

$$\tilde{\mathbf{E}}^I - \tilde{\mathbf{E}}^R = -\frac{1}{\omega^2} \left[ k_z F_z k_\perp - (\omega^2 \mathbf{I} - \mathbf{k}_z \mathbf{k}_z) \mathbf{G}_\perp \right].$$

From this last equation and Eq. (41) and Eq. (42), we eliminate $\tilde{\mathbf{E}}^I$ and get

$$2\tilde{\mathbf{E}}_I = \mathbf{F}_I - \frac{1}{\omega^2} \left[ k_z F_z k_\perp - (\omega^2 \mathbf{I} - \mathbf{k}_z \mathbf{k}_z) \mathbf{G}_\perp \right].$$

This equation must be supplemented with Eq. (1), which now takes the form

$$(k_\perp \cdot \mathbf{F}_I + k_z \mathbf{G}_z) k_\perp + (K_+ K_- - k_z^2) \mathbf{F}_I$$

$$- (K_+ + K_-) k_z \mathbf{G}_\perp + \omega^2 (\hat{\mathbf{e}} \cdot \mathbf{F})_I = 0$$

$$k_z k_\perp \cdot \mathbf{G}_\perp - k_z^2 F_z + \omega^2 (\hat{\mathbf{e}} \cdot \mathbf{F})_z = 0.$$

We also have the condition $\nabla \cdot \mathbf{D} = 0$ which implies

$$k_\perp \cdot (\hat{\mathbf{e}} \cdot \mathbf{F}) + k_z (\hat{\mathbf{e}} \cdot \mathbf{G})_z = 0.$$

Thus we have a set of six equations for the six components of $\mathbf{F}$ and $\mathbf{G}$. It is convenient to rewrite Eq. (47) and Eq. (48) in the form

$$\mathbf{A} \left( \begin{array}{c} F_x \\ F_y \\ F_z \end{array} \right) + \mathbf{B} \left( \begin{array}{c} G_x \\ G_y \\ G_z \end{array} \right) = 0,$$

and Eq. (46) and Eq. (49) as

$$\mathbf{C} \left( \begin{array}{c} F_x \\ F_y \\ F_z \end{array} \right) + \mathbf{D} \left( \begin{array}{c} G_x \\ G_y \\ G_z \end{array} \right) = 2\omega^2 \left( \begin{array}{c} \tilde{E}_x \\ \tilde{E}_y \\ \tilde{E}_z \end{array} \right),$$

where $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$ are $3 \times 3$ matrices. Explicitly,

$$\mathbf{A} = \omega^2 \hat{\mathbf{e}} - k_z^2 \mathbf{I} + \begin{pmatrix} K_+ K_- + k_z^2 & k_z k_y & 0 \\ k_z k_y & K_+ K_- + k_z^2 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

where $\hat{\mathbf{e}}$ is given by Eq. (27) and $\mathbf{I}$ is the $3 \times 3$ unit matrix,

$$\mathbf{B} = \begin{pmatrix} -K_+ + K_- & 0 & k_z \\ 0 & -(K_+ + K_-) & k_y \\ k_x & k_y & 0 \end{pmatrix},$$

$$\mathbf{C} = \begin{pmatrix} \omega^2 & 0 & -k_x k_z \\ 0 & \omega^2 & -k_y k_z \\ k_x \epsilon_{xx} & k_y \epsilon_{yy} & k_z \epsilon_{zz} \end{pmatrix},$$

$$\mathbf{D} = \begin{pmatrix} \omega^2 - k_x^2 & -k_x k_y & 0 \\ -k_x k_y & \omega^2 - k_y^2 & 0 \\ k_z \epsilon_{xx} & 0 & k_z \epsilon_{zz} \end{pmatrix}.$$
It is worth noticing that in the particular case \( K^+ = K_- = K \), which may occur for \( k_\perp \sim \beta \), the determinant of \( \mathbf{A} + \mathbf{KB} \) is zero, and therefore equation Eq. (56) is undetermined; however, Eq. (57) yields the solution for \( \mathbf{E}^+ + \mathbf{E}^- \), which is the combination appearing in the Fourier transform Eq. (32) if \( K^+ = K_- \). In any case, we do not have this problem in the particular examples considered hereafter.

4. NUMERICAL EVALUATIONS

In this section, we present the numerical evaluations. For definiteness, we choose the parameters of a KTP crystal and perform the integrations for two Gaussian beams, linearly and circularly polarized, and a zero-order Bessel beams. The results are shown in figures 2, 3, and 4, where the unit of length is taken as \( k^{-1} = \lambda/2\pi = 1 \).

A. KTP crystal

For a KTP crystal, such as the one used in Ref. [21],
\[
\epsilon_1 = 3.1609, \quad \epsilon_2 = 3.1994, \quad \epsilon_3 = 3.5672,
\]
and therefore \( \tan \beta = 0.0354 \) (also \( \epsilon_2^2/(\epsilon_1\epsilon_3) = 0.9078 \) and \( \epsilon_2/(\epsilon_1\epsilon_3) = 0.2837 \)).

B. Gaussian beam

Consider a Gaussian beam polarized in the \( x \) direction and moving along the \( z \) axis. It has the form
\[
\mathbf{E} = E_0 G(r) \hat{e}_x, \quad (58)
\]
with
\[
G(r) = \frac{1}{\eta(z)} e^{i\omega z - i\omega r^2/2z(z)}, \quad (59)
\]
where \( E_0 \) is the amplitude, \( \eta(z) = z + iz_R \) and \( z_R \) is the Rayleigh range, defined as
\[
z_R = \omega w_0^2/2,
\]
in terms of the waist radius \( w_0 \).

As a Fourier transform, we have
\[
G(r) = \frac{1}{2\pi i\omega} \int \int dk \ e^{ik \cdot r - zk^2/2\omega} \delta(k_z - \omega - k^2/2\omega)
\]
\[
\equiv \frac{1}{2\pi i\omega} \int \int dk_x \ dk_y \ e^{ik_x x + ik_y y + i\omega z + ik^2/2\omega}. \quad (60)
\]
It then follows that
\[
\mathbf{E}^x = \frac{E_0}{i\omega} e^{-zk^2/2\omega}, \quad \mathbf{E}^y = 0. \quad (61)
\]

For simplicity, the waist of the beam is assumed to coincide with the surface of the crystal; thus, we set \( z = 0 \) in Eq. (60).

The above values must be substituted in Eqs. Eq. (56) and Eq. (57), and then the field inside the crystal can be calculated with Eq. (32). Explicitly, this integral is in polar coordinates \( r = (r, \phi, z) \)
\[
E(r, \phi, z) = \frac{1}{2\pi} \int_0^{2\pi} d\phi' \int_0^\omega \ d\mathbf{k}_\perp e^{i\mathbf{k}_\perp \cdot r \cos(\phi' - \phi)}
\]
\[
\times [e^{iK_z \cdot \mathbf{r}} \mathbf{E}^+(k_\perp, \phi') + e^{-iK_z \cdot \mathbf{r}} \mathbf{E}^-(k_\perp, \phi')], \quad (62)
\]
with
\[
k_z = \sqrt{\omega^2 - k^2_\perp}
\]
in all the formulas.

We can now use the equations in the previous section, with \( k_x = k_\perp \cos \phi', \ k_y = k_\perp \sin \phi' \), and \( \mathbf{E}^x \) given by Eq. (61) and \( \mathbf{E}^y = 0 \).

Another possibility is a circularly polarized beam:
\[
\mathbf{E} \propto (\hat{e}_x - i\hat{e}_y). \quad (63)
\]
The Fourier transform is then as Eq. (62), but with
\[
\mathbf{E}^x = -i\mathbf{E}^y, \quad (64)
\]
and therefore
\[
(k_x - ik_y)\mathbf{E}^x = -k_z\mathbf{E}^y.
\]

C. Bessel beam

For a Bessel beam of order 0, propagating along the \( z \) axis, we have [27] (at \( z = 0 \))
\[
\mathbf{E}^z(k) = \mathbf{E}^z(k_\perp, \phi, k_z) = \mathbf{e}^z(\phi) \delta(k_z - \omega \cos \phi) \delta(k_\perp - \omega \sin \phi),
\]
where
\[
\mathbf{e}^z(\phi) = \frac{i}{4\omega \sin \phi} \left[ (\mathbf{E} + iB \cos \phi) e^{-i\phi} (\hat{e}_x + i\hat{e}_y) \right.
\]
\[
- (\mathbf{E} - iB \cos \phi) e^{i\phi} (\hat{e}_x - i\hat{e}_y) - 2iB \sin \phi \mathbf{e} \right], \quad (65)
\]
and \( \phi \) is the axicon angle.

Accordingly, in the Fresnel equation Eq. (29) and all the above equations, it is enough to set
\[
k_x = \omega \sin \phi \cos \phi', \quad k_y = \omega \sin \phi \sin \phi',
\]
and solve the Fourier integral, with \( \phi' \) as the only variable.

In cylindrical coordinates,
\[
x = r \cos \phi, \quad y = r \sin \phi,
\]
we have inside the crystal, according to Eq. (32),
\[
\mathbf{E}^{in}(r) = \frac{\omega}{2\pi} \int_0^{2\pi} d\phi' e^{i\omega z \sin \phi \cos(\phi' - \phi)}
\]
\[
\times \left[ e^{iK_z \cdot \mathbf{r}} \mathbf{E}^+(\phi') + e^{-iK_z \cdot \mathbf{r}} \mathbf{E}^-(\phi') \right]. \quad (66)
\]
In this last integral, it is understood that \( k_\perp = \omega \sin \phi \) and \( k_z = \omega \cos \phi \), and therefore the functions in the integral depend on the integration variable \( \phi' \) only, and on the distance \( z \) inside the crystal through the exponents.

D. Simulation results

In order to see the propagation of the beams, we first solve Eq. (29) numerically with the parameters of the KTP crystal and obtain the solutions for \( K_\perp \). The numerical solutions are computed in the relevant interval of parameters, \( 0 \leq k_\perp \leq 1 \). The full numerical solution is needed, since a perturbation treatment of the equations leads to spurious zeros in \( \Delta K = K_+ - K_- \). However, as seen in figure 2, this quantity is small but always positive, which guarantees that the simultaneous numerical solutions of the systems Eq. (56) and Eq. (57) are well defined.

We integrate numerically by standard methods, using the Simpson’s rule [29]. In general, it is convenient to perform the integration in the \( k_\perp \) and \( \phi' \) variables. We implement the integration subroutine and solution of the systems Eq. (56) and Eq. (57) using a multithreaded code implemented in C++ in the case where angular integration is only needed, as for a Bessel incident beam.
beam. However, when integrals involve both $k_\perp$ and $\phi'$, the computational times increase dramatically even for multi-threaded implementations. To circumvent this, the numerical integration code was implemented using C++ with CUDA extensions[30] and it was run in Nvidia GPU's. The use of the GPU's substantially improved the computational times, reducing them several orders of magnitude from projected calculated times of weeks to minutes. This allowed to arbitrarily simulate the propagation to very long distances $L = 10^4$ with high numerical accuracy and very small grid spacing in the integrations. All the numerical simulations have machine precision error and for practical purposes are numerically exact. Simulations were run in a server with an Epyc AMD dual socket CPU with 96 cores and 2 Nvidia T4 GPU accelerators part of the LSCSC-LANMAC infrastructure. Results of the numerical simulations are presented in figures 3, 4, 5, 6, 7, 8, 9, and 10. Note that in these figures we have normalized the intensity $|E_{in}|^2$ with respect to its maximum value at each $L$. Typical parameters of the simulations for the integration in the Bessel case are grids of 1024 to 4096 points, and for the Gaussian case grids of 256 to 1024 points in $\phi'$ and 1024 to 4096 points in $k_\perp$.

In figures 3 and 4, we show the propagation inside the crystal of a Gaussian beam incident in the $\hat{e}_x$ direction. As shown in the scheme of figure 1. We find that the diffraction cone opens as the beam propagates inside the crystal. The cone opens asymmetrically, as shown in the transverse planes at different crystal lengths, figure 4. In contrast to this, when the beam is circularly polarized in figures refFig5 and 6, we find that the cone is symmetric. The reason for this is that both polarizations in the $\hat{e}_x$ and $\hat{e}_y$ are balanced. Thus, as one changes the proportion between polarizations, one can go from an asymmetric cone in the $\hat{e}_x$ axis to a symmetric one in the circularly polarized case. This process is symmetrical with respect to the change of the initial polarization axis to $\hat{e}_y$.

For the profile of the incident Bessel beam, we consider the linearly polarized case in figures 7 and 8 and the circularly polarized case in figures 9 and 10. Here, in contrast with the gaussian cases, we find that the diffraction cone does not occur. This is due to the property of Bessel beams of being diffraction free [31], and it could have been expected since we are considering a linear though birefringent medium. However, we find that there are formations of regions of minimal intensity in the center of the propagated beams. Interestingly, we find that the beam propagated in the crystal mixes several components of higher order Bessel functions, similar to what was reported in [23]. This leads to the formation of maxima around the dark region in the center of the intensity profile that rotates and mixes as the beam propagates, see Figs. 8 and 10. While a Bessel beam does not form a diffraction cone, we find that the beam gets deflected approximately following the directrix of the diffraction cone, but at a smaller slope than that of the gaussian case. The effect of the different chosen polarizations is that, for the linear case, one can observe that there are regions where the maxima in the center of the beam get strongly suppressed, with dark regions as in figure 7(a) and (c). In contrast to this, the maxima are approximately constant in the circularly polarized case, see figure 9(a) and (c). We verified this fact changing from right to left circularly polarized beams and we found that the results are essentially the same up to a rotation of 90° in the $x - y$ plane.

5. DESCRIPTION OF THE NUMERICAL SCHEME USED FOR THE SIMULATIONS

The steps we follow, given the parameters of the KTP crystal are:

- We find numerically the real positive solutions Eq. (29), using standard methods, i.e. Newton-Raphson [29]
- We generate a high order interpolation polynomial (IP) with the solution of Eq. (29) for $K_{\perp}$
- With the IP, we construct the system of 12 equations (real and imaginary parts) given by Eq. (56) and Eq. (57), given an incident electric field profile in position space for each cartesian point at a crystal length $L_n$.
- We numerically solve the system of equations using standard Linear Algebra subroutines[29]
- With the solution of $E_{x,y,z}$ we integrate over momentum space (using Simpson’s rule), in the $k_x - k_y$ plane or for fixed $k_\perp$ for the Bessel incident beams.
Fig. 3. Propagation of the intensity $|E^{in}|^2$ and its projections for an incident gaussian beam polarized in the $x$ axis. (a) Propagation along the crystal length $L = L \times 10^{-3}$, $\bar{x} = x \times 10^{-2}$ and $\bar{y} = y \times 10^{-2}$. (b) Projection of the propagation for $\bar{y} = 0$. (c) Projection of the propagation for $\bar{x} = -2.5L \times 10^{-1}$, the approximate axis for the maxima in the intensity profile. Crystal parameters are the same as in figure 2. The waist of the gaussian beam is $w_0 = 10$.

Fig. 4. Transverse planes at different propagation distances $L$ for an incident gaussian beam polarized in the $x$ axis. The distance propagated along the crystal corresponds to the white lines in 3 (b) and (c). The distances are $L = 0.5(a), 1(b), 3(c), 5(d), 7(e), 9(f)$. Parameters are the same as in figure 3.

Fig. 5. Propagation of the intensity $|E^{in}|^2$ and its projections for an incident circularly polarized gaussian beam. (a) Propagation along the crystal length $L = L \times 10^{-3}$, $\bar{x} = x \times 10^{-2}$ and $\bar{y} = y \times 10^{-2}$. (b) Projection of the propagation for $\bar{y} = 0$. (c) Projection of the propagation for $\bar{x} = -2.5L \times 10^{-1}$, the approximate axis for the maxima in the intensity profile. Crystal parameters are the same as in figure 2. The waist of the gaussian beam is $w_0 = 10$. 
**Fig. 6.** Transverse planes at different propagation distances \( \tilde{L} \) for an incident gaussian beam circularly polarized. The distance propagated along the crystal corresponds to the white lines in Fig. 5 (b) and (c). The distances are \( \tilde{L} = 0.5(a), 1(b), 3(c), 5(d), 7(e), 9(f) \). Parameters are the same as in figure 5.

**Fig. 7.** Propagation of the intensity \( |E|^2 \) and its projections for an incident linearly polarized Bessel beam. (a) Propagation along the crystal length \( \tilde{L} = L \times 10^{-3}, \tilde{x} = x \times 10^{-2} \) and \( \tilde{y} = y \times 10^{-2} \). (b) Projection of the propagation for \( \tilde{y} = 0 \). (c) Projection of the propagation for \( \tilde{x} = -1.5\tilde{L} \times 10^{-1} \), the approximate axis for the maxima in the intensity profile. Crystal parameters are the same as in figure 2.

**Fig. 8.** Transverse planes at different propagation distances \( \tilde{L} \) for an incident linearly polarized Bessel beam. The distance propagated along the crystal corresponds to the white lines in Fig. 7 (b) and (c). The distances are \( \tilde{L} = 0.5(a), 1(b), 3(c), 5(d), 7(e), 9(f) \). Parameters are the same as in figure 7.
Fig. 9. Propagation of the intensity $|E|^2$ and its projections for an incident circularly polarized Bessel beam. (a) Propagation along the crystal length $\tilde{L} = L \times 10^{-3}$, $\tilde{x} = x \times 10^{-2}$ and $\tilde{y} = y \times 10^{-2}$. (b) Projection of the propagation for $\tilde{y} = 0$. (c) Projection of the propagation for $\tilde{x} = -1.5L \times 10^{-1}$, the approximate axis for the maxima in the intensity profile. Crystal parameters are the same as in figure 2.

Fig. 10. Transverse planes at different propagation distances $\tilde{L}$ for an incident circularly polarized Bessel beam. The distance propagated along the crystal corresponds to the white lines in Fig. 9 (b) and (c). The distances are $\tilde{L} = 0.5$ (a), 1 (b), 3 (c), 5 (d), 7 (e), 9 (f). Parameters are the same as in figure 9.
• We change the crystal length \( L_n \rightarrow L_{n+1} \) and repeat until we reach the desired length of the crystal \( L \).

As the algorithm is not dependent on previous steps in the propagation inside the crystal, therefore it can be fully parallelized.

6. CONCLUSIONS

Our methods and simulations can be extended to arbitrary incident profiles and linear crystals with more elaborated tensor parameters and less symmetry. Possible extensions of our methods include the analysis of propagation in nonlinear media and analogous systems, such as cold matter [32]. In any case, it is clear from our numerical results that the phenomenon of conic refraction is very sensitive to the initial conditions provided by the impinging beam on the crystal. Our study suggests that in practice a Gaussian beam is the best option for producing this very special effect in a laboratory.

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