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# Maxwell-consistent, symmetry- and energy-preserving solutions for ultrashort laser pulse propagation beyond the paraxial approximation

P. González de Alaiza Martínez,<sup>\*</sup> G. Duchateau, B. Chimier, and R. Nuter  
*Centre Lasers Intenses et Applications, Université de Bordeaux - CNRS - CEA, UMR 5107, F-33405 Talence, France*

I. Thiele

*Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*

S. Skupin

*Institut Lumière Matière, Université Lyon - CNRS, UMR 5306, 69622 Villeurbanne, France*

V. T. Tikhonchuk<sup>†</sup>

*ELI-Beamlines, Institute of Physics, Czech Academy of Sciences, 25241 Dolní Brežany, Czech Republic*

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We analytically and numerically investigate the propagation of ultrashort tightly focused laser pulses in vacuum, with particular emphasis on Hermite-Gaussian and Laguerre-Gaussian modes. We revisit the Lax series approach for forward-propagating linearly-polarized laser pulses, in order to obtain Maxwell-consistent, symmetry- and energy-preserving analytical solutions for the propagation of all field components beyond the paraxial approximation in four-dimensional geometry (space and time). Our solution converges towards an exact solution of the wave equation. Three-dimensional numerical simulations of ultrashort tightly-focused pulses validate our analytical development.

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## I. INTRODUCTION

Spatial and temporal pulse shaping makes the laser a highly versatile tool for a large number of applications such as micromachining and material processing [12, 17, 29], Terahertz generation [19, 35], or biological imaging and non-invasive surgeries [10, 41]. Paraxial approximation, which assumes that the light angular spectrum is sufficiently narrow, is widely used to study the propagation of laser beams in weak focusing conditions. However, the applications mentioned above usually require tightly focused ultrashort laser pulses. Modeling the propagation of such laser pulses is a complex problem because the deviation from the principal propagation direction is large and the paraxial approximation is no longer valid.

Electromagnetic codes, such as Particle-In-Cell codes [7, 20] or codes based on the Unidirectional Pulse Propagation Equation [21, 22], are powerful tools for understanding experiments on laser-matter interaction, where laser field components are commonly known in the far field. In these simulations external electromagnetic waves that enter the computational domain are usually prescribed as paraxial modes on the boundaries, which is not adequate for strongly focused ultrashort laser pulses because the initial distortion may be increased in the course of propagation, leading eventually to nonphysical

fields in the simulation box. Therefore, there is a need to determine analytical solutions of Maxwell equations for tightly focused laser pulses.

Different analytical models, restricted to specific beam shapes or spatial symmetry conditions, have been developed to describe nonparaxial laser beam propagation in several physical contexts, such as perturbative expansions of the wave equation [14, 26], the angular spectrum method [32], transformation optics [16] or laser-driven electron acceleration based on Helmholtz equation [27, 28]. Lax *et al.* [24] proposed a simple method which paved the way to introduce the nonparaxial corrections to a given paraxial solution in more general situations. They demonstrated that the paraxial solution is actually the zeroth-order consistent solution to the Maxwell equations, obtained by expanding the wave equation (in their case, for Gaussian linearly-polarized vector potential) using a power series in the beam divergence angle.

The nonparaxial perturbative equations proposed by Lax *et al.* were subsequently analyzed in more detail, always on the basis of the wave equation applied to the vector potential, by several authors for either Gaussian beams [11, 13, 30, 33, 34] or Hermite-Gaussian and Laguerre-Gaussian beams [1, 2, 23, 37]. More recently, Favier *et al.* took into account spatio-temporal couplings in the wave equation in order to extend Lax perturbative equations to few-cycle pulses [15]. In the transverse-spatial and temporal Fourier domain, they linked the Lax series with a Taylor expansion of the exact solution of the wave equation but their proposed high-order corrections hinged on an arbitrary number of integration constants, which were chosen to match some known nonparaxial solutions.

<sup>\*</sup>Electronic address: pedro.gonzalez@u-bordeaux.fr

<sup>†</sup>Also at Centre Lasers Intenses et Applications, Université Bordeaux - CNRS - CEA, UMR 5107, F-33405 Talence, France

This paper aims at addressing two problems which remain open despite the advances made in the previous works. The first problem is that all the previous approaches solely dealt with the wave equation (in the cited papers, applied to the vector potential) split into a Lax series, and not with the full set of Maxwell equations when calculating high-order corrections. However, the electric and magnetic field components derived from a vector potential that is a rigorous solution of the wave equation do not necessarily satisfy the whole set of Maxwell equations. In other words, since each component of the electric, magnetic and vector potential fields verifies the scalar wave equation, we expect to obtain a unique solution to the Maxwell equations whatever the component chosen to calculate high-order corrections. The second problem is that, when calculating high-order terms of the Lax series from the solutions at lower orders, spurious homogeneous solutions that are not compatible with Maxwell equations may be added through integration constants. We demonstrate in this paper that removing those spurious homogeneous solutions implies preserving the laser energy through transverse planes. Conservation of energy is a fundamental physical principle that, to the best of our knowledge, had never been considered before in the context of nonparaxial corrections. Indeed, determining these integration constants by making *ad hoc* assumptions on the nonparaxial corrections at the focal point [11, 37] or on the beam axis [30], as done in previous works, may be incompatible with the Maxwell equations [25].

In Sec. II our Lax-series-based analytical solution for all electromagnetic field components is presented. Maxwell equations are satisfied and thus each electromagnetic field component verifies the scalar wave equation. The total energy through transverse planes and the existing symmetry between electric and magnetic fields are preserved. Recursive relations to obtain the terms of our Lax series are given and the resulting solution is successfully compared with a numerically exact Maxwell solver [38]. In Sec. III we calculate the leading term of the asymptotic limit of our Lax-series-based analytical solution far from the focal plane, for both monochromatic beams and ultrashort laser pulses, which results in paraxial-like expressions. These analytical expressions are a baseline for further developments aiming at obtaining an easy and low-computational-cost means of computing the near fields related to those assumed-known paraxial far fields. Thanks to three-dimensional Maxwell-consistent numerical simulations carried out with the code ARCTIC, based on the Yee scheme [40], we discuss the adequacy of prescribing ultrashort laser pulses by the leading term of the asymptotic limit at a finite distance from the focal plane. Conclusions and outlooks are drawn in Sec. IV.

## II. ANALYTICAL SOLUTIONS OF MAXWELL EQUATIONS

### A. Maxwell equations and their properties

Maxwell equations in vacuum read as follows:

$$\nabla \cdot \mathbf{E} = 0, \quad (1)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (2)$$

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0, \quad (3)$$

$$\partial_t \mathbf{E} - c^2 \nabla \times \mathbf{B} = 0, \quad (4)$$

where  $\mathbf{E}$  and  $\mathbf{B}$  are the electric and magnetic fields, respectively, and  $c$  is the speed of light in vacuum. Maxwell's equations are highly symmetrical and they place the electric and magnetic fields on equal footing [9]. Indeed, both electric and magnetic fields verify the wave equation:

$$(c^{-2} \partial_t^2 - \nabla^2) \mathbf{E} = \mathbf{0}, \quad (5)$$

$$(c^{-2} \partial_t^2 - \nabla^2) \mathbf{B} = \mathbf{0}. \quad (6)$$

Note that in this paper we formally present our results in vacuum. For monochromatic or narrow-bandwidth pulses, by replacing  $c$  by  $c/n_0$ , where  $n_0$  is a constant refractive index, our results generalize to homogeneous dielectric media. Because our solutions are derived in the Fourier space, it would be straightforward to extend it to shorter pulses with linear dispersion.

### B. The wave equation

Throughout this paper we shall work in Cartesian coordinates  $(x, y, z)$ , where  $x$  is the optical propagation axis (also referred to as longitudinal axis) and  $y$  and  $z$  are the transverse coordinates. The beam focus position is placed at  $x = 0$ .

We seek solutions of Maxwell equations that are waves propagating along longitudinal axis according to the following Ansatz:

$$\mathbf{E}(x, y, z, t) = E_0 \begin{pmatrix} \psi_{E_x}(x, y, z, t) \\ \psi_{E_y}(x, y, z, t) \\ \psi_{E_z}(x, y, z, t) \end{pmatrix} e^{i(k_0 x - \omega_0 t)}, \quad (7)$$

$$\mathbf{B}(x, y, z, t) = \frac{E_0}{c} \begin{pmatrix} \psi_{B_x}(x, y, z, t) \\ \psi_{B_y}(x, y, z, t) \\ \psi_{B_z}(x, y, z, t) \end{pmatrix} e^{i(k_0 x - \omega_0 t)}, \quad (8)$$

where  $\omega_0 = 2\pi c/\lambda_0$  is the angular frequency of the laser field,  $\lambda_0$  is the wavelength,  $k_0 = \omega_0/c$  is the wavenumber,  $\psi_{E_x}$ ,  $\psi_{E_y}$ ,  $\psi_{E_z}$ ,  $\psi_{B_x}$ ,  $\psi_{B_y}$  and  $\psi_{B_z}$  are the spatio-temporal envelopes of  $E_x$ ,  $E_y$ ,  $E_z$ ,  $B_x$ ,  $B_y$  and  $B_z$ , respectively, and  $E_0$  represents the electric field amplitude. Note that in this paper we only seek forward-propagating solutions along  $x$  axis, as stated by Ansätze (7) and (8), although Eqs. (5) and (6) admit, in general, bidirectional solutions. Implicitly, we require that  $\mathbf{E}$  and  $\mathbf{B}$  have no evanescent components. Moreover, because they are complex fields, their temporal bandwidth must be restricted to the positive frequency range.

By substituting Eq. (7) into Eq. (5) and Eq. (8) into Eq. (6), each of the six spatial envelopes, generically denoted as  $\psi$ , verifies the so-called wave equation:

$$\nabla_{\perp}^2 \psi + 2ik_0 \left[ \partial_x + \frac{\partial t}{c} \right] \psi = -\partial_x^2 \psi + \frac{\partial_t^2 \psi}{c^2}, \quad (9)$$

where  $\nabla_{\perp}^2 = \partial_y^2 + \partial_z^2$ . It is useful to express Eq. (9) in the laser co-moving reference system  $x' = x$  and  $t' = t - x/c$ :

$$\nabla_{\perp}^2 \psi + 2ik_0 \left( 1 + \frac{i\partial_{t'}}{\omega_0} \right) \partial_{x'} \psi = -\partial_{x'}^2 \psi. \quad (10)$$

The paraxial approximation neglects the term on right-hand side of Eq. (10) by claiming that field variations along  $x$  axis are small compared to the wavelength  $\lambda_0$  (i.e., the wavefront is considered to be almost perpendicular to  $x$  axis) and to the transverse variations along  $y$  and  $z$  axes (i.e., the transverse profile is supposed to remain almost unchanged over a distance of the order of  $\lambda_0$ ). Considering  $D_0$  the  $1/e$  diameter of the Gaussian solution at beam focus (we assume that the diameter is the same along  $y$  and  $z$  axis) and  $x_R = \pi D_0^2/(4\lambda_0)$  the associated Rayleigh length, we reformulate Eq. (10) in the dimensionless coordinates  $\xi = x'/x_R$ ,  $\tau = \omega_0 t'$ ,  $v = 2y/D_0$  and  $\zeta = 2z/D_0$  as follows:

$$\partial_{\perp}^2 \psi + 4iT \partial_{\xi} \psi = -\varepsilon^2 \partial_{\xi}^2 \psi, \quad (11)$$

where  $\partial_{\perp}^2 = \partial_v^2 + \partial_{\zeta}^2$  and the operator  $T = 1 + i\partial_{\tau}$  introduces the space-time focusing [6, 8]. Equation (11) reveals that the term on right-hand side is actually a small correction of order of  $\varepsilon^2$ , where  $\varepsilon = D_0/(2x_R)$  is the tangent of the beam divergence angle and is assumed to be small in the paraxial limit. For arbitrary spatial beam shapes, for which the Gaussian  $1/e$  beam diameter  $D_0$  does not apply, one can define  $\varepsilon$  as the angular spectral width divided by  $k_0$ . Note that monochromatic solutions are given by Eq. (11) in the limit  $T \rightarrow 1$ , which means that time variations of the envelopes are negligible.

Equation (11) in the transverse-spatial and temporal Fourier domain (see Appendix A) reads:

$$\left( \frac{i\kappa_{\perp}^2}{4\hat{T}} + \partial_{\xi} - \frac{i\varepsilon^2}{4\hat{T}} \partial_{\xi}^2 \right) \hat{\psi} = 0, \quad (12)$$

where  $\kappa_{\perp}^2 = \kappa_y^2 + \kappa_z^2$ ,  $\kappa_y = D_0 k_y/2$ ,  $\kappa_z = D_0 k_z/2$ ,  $\hat{T} = 1 + \Omega$ , and  $\Omega = \omega/\omega_0$ . Restricting the temporal

bandwidth of the complex fields  $\mathbf{E}$  and  $\mathbf{B}$  to the positive frequency range implies that  $\Omega \ll 1$ . The exact forward-propagating solution of Eq. (12), with the boundary condition placed at  $\xi = 0$ , reads:

$$\hat{\psi}(\xi, \kappa_y, \kappa_z, \Omega) = \hat{\psi}(0, \kappa_y, \kappa_z, \Omega) e^{-\frac{2i\xi\hat{T}}{\varepsilon^2} \left( 1 - \sqrt{1 - \frac{\varepsilon^2 \kappa_{\perp}^2}{4\hat{T}^2}} \right) \xi}, \quad (13)$$

which, by abuse of language, will be called *general solution of the wave equation* all through this paper in spite of its lack of bidirectionality.

Equation (13) discloses that the exact forward-propagating solution preserves its complex module in all transverse planes:

$$|\hat{\psi}(\xi, \kappa_y, \kappa_z, \Omega)| = |\hat{\psi}(0, \kappa_y, \kappa_z, \Omega)|, \quad (14)$$

whenever  $\varepsilon\kappa_{\perp}/(2\hat{T}) \leq 1$  (i.e., for propagating modes).

### C. The Lax series approach

A Taylor expansion of Eq. (13) in powers of  $\kappa_{\perp}$  (around  $\kappa_{\perp} = 0$ ) and  $\xi$  (around  $\xi = 0$ ), reveals that the general solution of the wave equation depends on powers of  $\varepsilon$  [15]. Motivated from this fact, in order to solve Eq. (12) one can express  $\hat{\psi}$  in a series using  $\varepsilon$  as expansion parameter [24]. Because this perturbative approach is a rearrangement of a Taylor expansion, its convergence is thus guaranteed by Taylor's theorem for any  $\varepsilon$  if high-order terms are calculated as explained below (i.e., satisfying Maxwell consistency, energy preservation, symmetry between electric and magnetic fields and absence of evanescent modes). For linearly-polarized laser pulses, the transverse components (i.e.,  $\hat{\psi}_{E_y}$ ,  $\hat{\psi}_{E_z}$ ,  $\hat{\psi}_{B_y}$  and  $\hat{\psi}_{B_z}$ , generically denoted as  $\hat{\psi}_{\perp}$ ) expand in even powers of  $\varepsilon$  [13]:

$$\hat{\psi}_{\perp}(\xi, \kappa_y, \kappa_z, \Omega) = \sum_{j=0}^{\infty} \varepsilon^{2j} \hat{\psi}_{\perp}^{(2j)}(\xi, \kappa_y, \kappa_z, \Omega), \quad (15)$$

whereas the longitudinal components (i.e.,  $\hat{\psi}_{E_x}$  and  $\hat{\psi}_{B_x}$ , generically denoted as  $\hat{\psi}_{\parallel}$ ) expand in odd powers of  $\varepsilon$ :

$$\hat{\psi}_{\parallel}(\xi, \kappa_y, \kappa_z, \Omega) = \sum_{j=0}^{\infty} \varepsilon^{2j+1} \hat{\psi}_{\parallel}^{(2j+1)}(\xi, \kappa_y, \kappa_z, \Omega), \quad (16)$$

where the functions  $\hat{\psi}_{\perp}^{(2j)}$  and  $\hat{\psi}_{\parallel}^{(2j+1)}$  have to be determined.

### D. Lax series: Splitting the wave equation

If we substitute Eqs. (15) and (16) into Eq. (12), the wave equation is split into recursive equations.

The lowest order ( $j = 0$ ) corresponds to the paraxial equation:

$$\left(\frac{i\kappa_{\perp}^2}{4\hat{T}} + \partial_{\xi}\right)\hat{\psi}_{\perp}^{(0)} = 0, \quad (17)$$

$$\left(\frac{i\kappa_{\parallel}^2}{4\hat{T}} + \partial_{\xi}\right)\hat{\psi}_{\parallel}^{(1)} = 0, \quad (18)$$

where  $\hat{\psi}_{\perp}^{(0)} = C_{0,\perp}^{(0)}e^{-i\frac{\kappa_{\perp}^2}{4\hat{T}}\xi}$  and  $\hat{\psi}_{\parallel}^{(1)} = C_{0,\parallel}^{(1)}e^{-i\frac{\kappa_{\parallel}^2}{4\hat{T}}\xi}$  are, respectively, their solutions. The coefficients  $C_{0,\perp}^{(0)} = C_{0,\perp}^{(0)}(\kappa_y, \kappa_z, \Omega)$  and  $C_{0,\parallel}^{(1)} = C_{0,\parallel}^{(1)}(\kappa_y, \kappa_z, \Omega)$  do not depend on  $\xi$  (see their expressions for Hermite-Gaussian and Laguerre-Gaussian beams in Appendix B).

High-order corrections ( $j > 0$ ) verify:

$$\left(\frac{i\kappa_{\perp}^2}{4\hat{T}} + \partial_{\xi}\right)\hat{\psi}_{\perp}^{(2j)} = \frac{i}{4\hat{T}}\partial_{\xi}^2\hat{\psi}_{\perp}^{(2j-2)}, \quad (19)$$

$$\left(\frac{i\kappa_{\parallel}^2}{4\hat{T}} + \partial_{\xi}\right)\hat{\psi}_{\parallel}^{(2j+1)} = \frac{i}{4\hat{T}}\partial_{\xi}^2\hat{\psi}_{\parallel}^{(2j-1)}, \quad (20)$$

with the paraxial differential operator in the left-hand side. We choose to express the solution to Eqs. (19) and (20) as the sum of a homogeneous solution  $\hat{H}$  and a particular solution  $\hat{P}$ :

$$\hat{\psi}_{\perp}^{(2j)} = \hat{H}_{\perp}^{(2j)} + \hat{P}_{\perp}^{(2j)}, \quad (21)$$

$$\hat{\psi}_{\parallel}^{(2j+1)} = \hat{H}_{\parallel}^{(2j+1)} + \hat{P}_{\parallel}^{(2j+1)}, \quad (22)$$

where the homogenous solutions are, respectively:

$$\hat{H}_{\perp}^{(2j)} = C_{0,\perp}^{(2j)}e^{-i\frac{\kappa_{\perp}^2}{4\hat{T}}\xi}, \quad (23)$$

$$\hat{H}_{\parallel}^{(2j+1)} = C_{0,\parallel}^{(2j+1)}e^{-i\frac{\kappa_{\parallel}^2}{4\hat{T}}\xi}, \quad (24)$$

where the coefficients  $C_{0,\perp}^{(2j)} = C_{0,\perp}^{(2j)}(\kappa_y, \kappa_z, \Omega)$  and  $C_{0,\parallel}^{(2j+1)} = C_{0,\parallel}^{(2j+1)}(\kappa_y, \kappa_z, \Omega)$  do not depend on  $\xi$ . It is important to note that even though  $\hat{H}_{\perp}^{(2j)}$  and  $\hat{H}_{\parallel}^{(2j+1)}$  formally obey the paraxial equation, they are part of the nonparaxial higher-order corrections.

The particular solutions can be written as:

$$\hat{P}_{\perp}^{(2j)} = \mathcal{P}_{\perp}^{(2j)}(\xi)e^{-i\frac{\kappa_{\perp}^2}{4\hat{T}}\xi}, \quad (25)$$

$$\hat{P}_{\parallel}^{(2j+1)} = \mathcal{P}_{\parallel}^{(2j+1)}(\xi)e^{-i\frac{\kappa_{\parallel}^2}{4\hat{T}}\xi}, \quad (26)$$

where the coefficients  $\mathcal{P}_{\perp}^{(2j)}(\xi)$  and  $\mathcal{P}_{\parallel}^{(2j+1)}(\xi)$  do depend on  $\xi$ . Since in the neighborhood of the focal plane the

form  $\hat{\psi} \sim e^{-i\frac{\kappa_{\perp}^2}{4\hat{T}}\xi}$  dominates, the particular solutions must vanish in that plane, i.e.,  $\mathcal{P}_{\perp}^{(2j)}(0) = \mathcal{P}_{\parallel}^{(2j+1)}(0) = 0$ . To evaluate them through a recursive procedure as shown below, they can be constructed as  $j$ -order polynomials in  $\xi$ :

$$\mathcal{P}_{\perp}^{(2j)}(\xi) = \sum_{k=1}^j C_{k,\perp}^{(2j)}\xi^k, \quad (27)$$

$$\mathcal{P}_{\parallel}^{(2j+1)}(\xi) = \sum_{k=1}^j C_{k,\parallel}^{(2j+1)}\xi^k, \quad (28)$$

where the coefficients  $C_{k,\perp}^{(2j)}$  and  $C_{k,\parallel}^{(2j+1)}$  have to be determined.

From the point of view of Lax recursive equations, homogeneous solutions  $\hat{H}$  are simply arbitrary integration constants and hence Eqs. (19) and (20) do not suffice to determine them. These homogenous solutions *must* be determined from Maxwell equations (see Sec. II E). We demonstrate in this paper that such Maxwell-consistent calculation of the high-order corrections ensures that the overall laser energy through transverse planes is not modified by the Lax series terms of order  $j > 0$  and that the Lax series converges towards an exact solution of the wave equation for all electromagnetic components (see Sec. II F). This is a fundamental difference with respect to previous works, where, for example, in order to determine the high-order corrections, some authors had considered *ad hoc* assumptions such that they are zero at the beam focal point [11, 37], they follow the structure of a spherical wave emanating from such beam focal point [30] or they must match some known nonparaxial solutions [15]. Indeed, in the particular solutions proposed by most of these works dealing with Hermite-Gaussian and Laguerre-Gaussian paraxial families, spurious homogeneous solutions are found when a Gram-Schmidt orthogonalization process is applied in the focal plane [18, 31]. These spurious modes make the total power through transverse planes increase exponentially with  $\varepsilon$  [30], which is not physical.

When substituting Eq. (21) into Eq. (19), and Eq. (22) into Eq. (20), the following recursion relations are obtained for the coefficients of the particular solutions for all  $1 \leq k \leq j$  and  $j > 0$ :

$$C_{k,\perp}^{(2j)} = -\frac{i\kappa_{\perp}^4}{64\hat{T}^3}\frac{C_{k-1,\perp}^{(2j-2)}}{k} + \frac{\kappa_{\perp}^2}{8\hat{T}^2}C_{k,\perp}^{(2j-2)} + \frac{i}{4\hat{T}}(k+1)C_{k+1,\perp}^{(2j-2)}, \quad (29)$$

$$C_{k,\parallel}^{(2j+1)} = -\frac{i\kappa_{\parallel}^4}{64\hat{T}^3}\frac{C_{k-1,\parallel}^{(2j-1)}}{k} + \frac{\kappa_{\parallel}^2}{8\hat{T}^2}C_{k,\parallel}^{(2j-1)} + \frac{i}{4\hat{T}}(k+1)C_{k+1,\parallel}^{(2j-1)}, \quad (30)$$

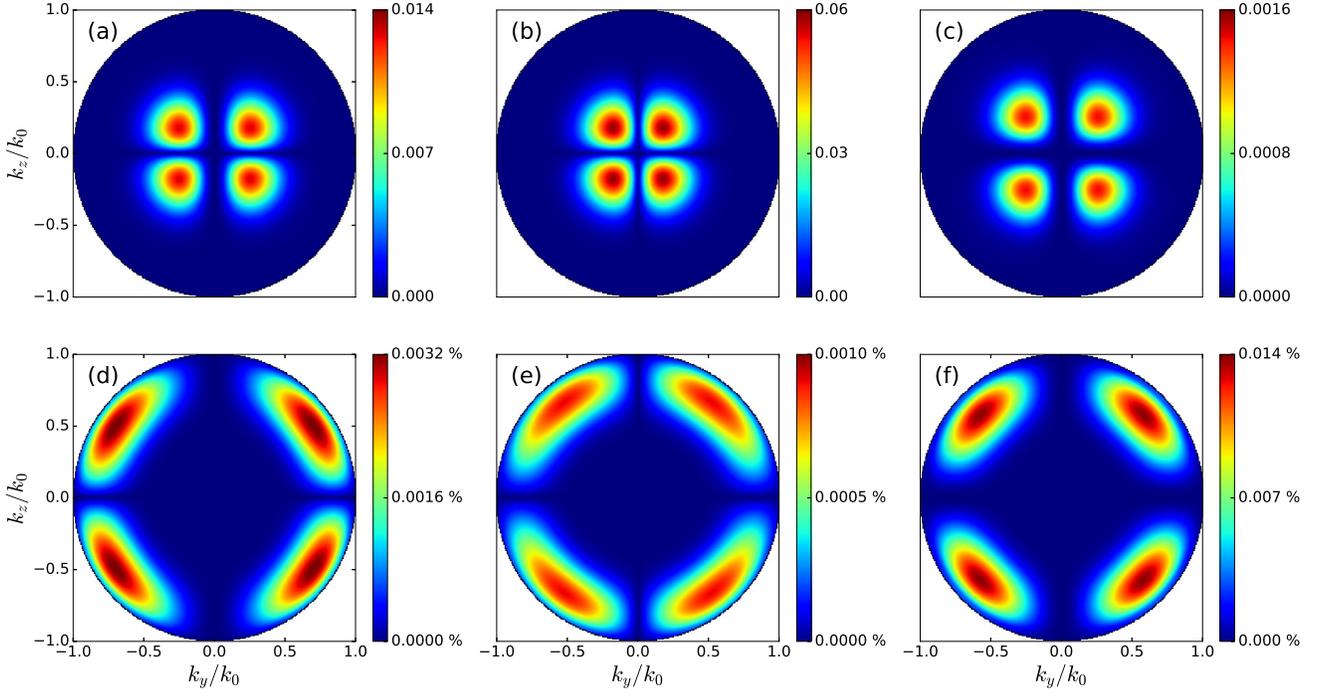


FIG. 1: Lax-series-based analytical solution  $\hat{\psi}$  constructed from the (1,1)-order Hermite-Gaussian mode, truncated at order  $j = 5$ . We consider  $\lambda_0 = 800$  nm and  $\varepsilon = 0.25$ . The results are plotted in the transverse plane placed at  $\xi = 1$ . We show the spatial envelopes for (a)  $E_x$ , (b)  $E_y$ , and (c)  $E_z$ . The corresponding local relative errors, given by Eq. (73), are shown in (d), (e) and (f), respectively.

where, by notation convention,  $C_{k,\perp}^{(2j-2)} = C_{k,\parallel}^{(2j-1)} = 0$  if  $k = j$  and  $C_{k+1,\perp}^{(2j-2)} = C_{k+1,\parallel}^{(2j-1)} = 0$  if  $k \geq j - 1$ .

It is important to note that the above recursive relations involve the coefficients  $C_{0,\perp}^{(2j-2)}$  and  $C_{0,\parallel}^{(2j-1)}$  of the homogeneous solution, which will be determined from the Maxwell equations in the following subsection.

### E. Lax series: Splitting Maxwell equations

We split Maxwell equations by substituting the Lax expansions (15) and (16), together with the Ansätze (7) and (8), into Eqs. (1)-(4).

The envelopes of all the electromagnetic components at paraxial order ( $j = 0$ ) must verify simultaneously the following overdetermined system of equations:

$$\hat{T} \hat{\psi}_{E_x}^{(1)} + \frac{\kappa_y}{2} \hat{\psi}_{E_y}^{(0)} + \frac{\kappa_z}{2} \hat{\psi}_{E_z}^{(0)} = 0, \quad (31)$$

$$\hat{T} \hat{\psi}_{B_x}^{(1)} + \frac{\kappa_y}{2} \hat{\psi}_{B_y}^{(0)} + \frac{\kappa_z}{2} \hat{\psi}_{B_z}^{(0)} = 0, \quad (32)$$

$$\hat{T} \hat{\psi}_{B_x}^{(1)} - \frac{\kappa_y}{2} \hat{\psi}_{E_z}^{(0)} + \frac{\kappa_z}{2} \hat{\psi}_{E_y}^{(0)} = 0, \quad (33)$$

$$\hat{\psi}_{B_y}^{(0)} + \hat{\psi}_{E_z}^{(0)} = 0, \quad (34)$$

$$\hat{\psi}_{B_z}^{(0)} - \hat{\psi}_{E_y}^{(0)} = 0, \quad (35)$$

$$\hat{T} \hat{\psi}_{E_x}^{(1)} + \frac{\kappa_y}{2} \hat{\psi}_{B_z}^{(0)} - \frac{\kappa_z}{2} \hat{\psi}_{B_y}^{(0)} = 0, \quad (36)$$

which has a unique solution whatever two components are prescribed [38]. In this paper, without loss of generality, we choose the paraxial-order field polarized along  $y$  axis (note that the solution for any other polarization angle can be obtained by applying a rotation transformation):

$$\hat{\psi}_{E_y}^{(0)} = C e^{-i \frac{\kappa_z}{4\hat{T}} \xi}, \quad (37)$$

$$\hat{\psi}_{E_z}^{(0)} = 0, \quad (38)$$

where  $C(\kappa_y, \kappa_z, \Omega)$  is a coefficient not depending on  $\xi$ . The rest of the components are then calculated from the system (31)-(36):

$$\hat{\psi}_{E_x}^{(1)} = -\frac{\kappa_y}{2\hat{T}} C e^{-i \frac{\kappa_z}{4\hat{T}} \xi}, \quad (39)$$

$$\hat{\psi}_{B_x}^{(1)} = -\frac{\kappa_z}{2\hat{T}} C e^{-i \frac{\kappa_z}{4\hat{T}} \xi}, \quad (40)$$

$$\hat{\psi}_{B_y}^{(0)} = 0, \quad (41)$$

$$\hat{\psi}_{B_z}^{(0)} = C e^{-i\frac{\kappa_{\perp}^2}{4\hat{T}}\xi}. \quad (42)$$

Similarly, the envelopes at high orders ( $j > 0$ ) must verify simultaneously the following overdetermined system of recursive equations:

$$2i\hat{T}\hat{\psi}_{E_x}^{(2j+1)} + i\kappa_y\hat{\psi}_{E_y}^{(2j)} + i\kappa_z\hat{\psi}_{E_z}^{(2j)} = -\partial_{\xi}\hat{\psi}_{E_x}^{(2j-1)}, \quad (43)$$

$$2i\hat{T}\hat{\psi}_{B_x}^{(2j+1)} + i\kappa_y\hat{\psi}_{B_y}^{(2j)} + i\kappa_z\hat{\psi}_{B_z}^{(2j)} = -\partial_{\xi}\hat{\psi}_{B_x}^{(2j-1)}, \quad (44)$$

$$\hat{T}\hat{\psi}_{B_x}^{(2j+1)} - \frac{\kappa_y}{2}\hat{\psi}_{E_z}^{(2j)} + \frac{\kappa_z}{2}\hat{\psi}_{E_y}^{(2j)} = 0, \quad (45)$$

$$\hat{\psi}_{B_y}^{(2j)} + \hat{\psi}_{E_z}^{(2j)} = \frac{\kappa_z}{2\hat{T}}\hat{\psi}_{E_x}^{(2j-1)} + \frac{i}{2\hat{T}}\partial_{\xi}\hat{\psi}_{E_z}^{(2j-2)}, \quad (46)$$

$$\hat{\psi}_{B_z}^{(2j)} - \hat{\psi}_{E_y}^{(2j)} = -\frac{\kappa_y}{2\hat{T}}\hat{\psi}_{E_x}^{(2j-1)} - \frac{i}{2\hat{T}}\partial_{\xi}\hat{\psi}_{E_y}^{(2j-2)}, \quad (47)$$

$$\hat{T}\hat{\psi}_{E_x}^{(2j+1)} + \frac{\kappa_y}{2}\hat{\psi}_{B_z}^{(2j)} - \frac{\kappa_z}{2}\hat{\psi}_{B_y}^{(2j)} = 0, \quad (48)$$

$$\hat{\psi}_{B_z}^{(2j)} - \hat{\psi}_{E_y}^{(2j)} = \frac{\kappa_z}{2\hat{T}}\hat{\psi}_{B_x}^{(2j-1)} + \frac{i}{2\hat{T}}\partial_{\xi}\hat{\psi}_{B_z}^{(2j-2)}, \quad (49)$$

$$\hat{\psi}_{B_y}^{(2j)} + \hat{\psi}_{E_z}^{(2j)} = \frac{\kappa_y}{2\hat{T}}\hat{\psi}_{B_x}^{(2j-1)} + \frac{i}{2\hat{T}}\partial_{\xi}\hat{\psi}_{B_y}^{(2j-2)}, \quad (50)$$

which allows us to calculate the homogeneous parts in Eqs. (21) and (22). Note that the particular solutions calculated in Sec. IID satisfy all equations (43)-(50). In order to determine a unique homogeneous solution, we have to account for the symmetry existing between the electric and magnetic fields. For forward-propagating linearly-polarized pulses, by observing Eqs. (46) and (50) and Eqs. (47) and (49), we require that:

$$\hat{H}_{E_z}^{(2j)} = \hat{H}_{B_y}^{(2j)}, \quad (51)$$

$$\hat{H}_{E_y}^{(2j)} = -\hat{H}_{B_z}^{(2j)}, \quad (52)$$

which indeed is the opposite situation to the paraxial order (compare to Eqs. (34) and (35)). *A posteriori*, we will demonstrate in Sec. IIF that this symmetry condition prevents high-order corrections from modifying the total laser energy.

After some manipulations, taking into account that we have prescribed the transverse electric field as in Eqs. (37) and (38), we get the following homogeneous solution for orders  $j > 0$ :

$$C_{0,E_x}^{(2j+1)} = \frac{\kappa_{\perp}^2}{16\hat{T}^2}C_{0,E_x}^{(2j-1)} + \frac{i}{4\hat{T}}C_{1,E_x}^{(2j-1)}, \quad (53)$$

$$C_{0,E_y}^{(2j)} = \frac{\kappa_z^2}{8\hat{T}^2}C_{0,E_y}^{(2j-2)} - \frac{\kappa_{\perp}^2}{16\hat{T}^2}C_{0,B_z}^{(2j-2)} - \frac{\kappa_y\kappa_z}{8\hat{T}^2}C_{0,E_z}^{(2j-2)} - \frac{i}{4\hat{T}}C_{1,B_z}^{(2j-2)}, \quad (54)$$

$$C_{0,E_z}^{(2j)} = \frac{\kappa_y^2}{8\hat{T}^2}C_{0,E_z}^{(2j-2)} + \frac{\kappa_{\perp}^2}{16\hat{T}^2}C_{0,B_y}^{(2j-2)} - \frac{\kappa_y\kappa_z}{8\hat{T}^2}C_{0,E_y}^{(2j-2)} + \frac{i}{4\hat{T}}C_{1,B_y}^{(2j-2)}, \quad (55)$$

$$C_{0,B_x}^{(2j+1)} = \frac{\kappa_{\perp}^2}{16\hat{T}^2}C_{0,B_x}^{(2j-1)} + \frac{i}{4\hat{T}}C_{1,B_x}^{(2j-1)}, \quad (56)$$

$$C_{0,B_y}^{(2j+1)} = C_{0,E_z}^{(2j)}, \quad (57)$$

$$C_{0,B_z}^{(2j+1)} = -C_{0,E_y}^{(2j)}, \quad (58)$$

where  $C_{1,E_x}^{(1)} = C_{1,B_x}^{(1)} = C_{1,B_y}^{(0)} = C_{1,B_z}^{(0)} = 0$  by notation convention.

In conclusion, by setting  $C$  in Eqs. (37) and (38) the nonparaxial solution can be calculated in the whole space thanks to the recursive formulae Eqs. (29)-(30) and Eqs. (53)-(58). By way of example, the correction at order  $j = 1$  reads:

$$\hat{\psi}_{E_x}^{(3)} = \left[ \frac{\kappa_{\perp}^2}{16\hat{T}^2} - \frac{i\kappa_{\perp}^4}{64\hat{T}^3}\xi \right] \hat{\psi}_{E_x}^{(1)}, \quad (59)$$

$$\hat{\psi}_{E_y}^{(2)} = \left[ \frac{\kappa_z^2 - \kappa_y^2}{16\hat{T}^2} - \frac{i\kappa_{\perp}^4}{64\hat{T}^3}\xi \right] \hat{\psi}_{E_y}^{(0)} - \frac{\kappa_y\kappa_z}{8\hat{T}^2}\hat{\psi}_{E_z}^{(0)}, \quad (60)$$

$$\hat{\psi}_{E_z}^{(2)} = \left[ \frac{\kappa_y^2 - \kappa_z^2}{16\hat{T}^2} - \frac{i\kappa_{\perp}^4}{64\hat{T}^3}\xi \right] \hat{\psi}_{E_z}^{(0)} - \frac{\kappa_y\kappa_z}{8\hat{T}^2}\hat{\psi}_{E_y}^{(0)}, \quad (61)$$

$$\hat{\psi}_{B_x}^{(3)} = \left[ \frac{\kappa_{\perp}^2}{16\hat{T}^2} - \frac{i\kappa_{\perp}^4}{64\hat{T}^3}\xi \right] \hat{\psi}_{B_x}^{(1)}, \quad (62)$$

$$\hat{\psi}_{B_y}^{(2)} = \left[ \frac{\kappa_y^2 - \kappa_z^2}{16\hat{T}^2} + \frac{i\kappa_{\perp}^4}{64\hat{T}^3}\xi \right] \hat{\psi}_{E_z}^{(0)} - \frac{\kappa_y\kappa_z}{8\hat{T}^2}\hat{\psi}_{E_y}^{(0)}, \quad (63)$$

$$\hat{\psi}_{B_z}^{(2)} = \left[ -\frac{\kappa_z^2 - \kappa_y^2}{16\hat{T}^2} - \frac{i\kappa_{\perp}^4}{64\hat{T}^3}\xi \right] \hat{\psi}_{E_y}^{(0)} + \frac{\kappa_y\kappa_z}{8\hat{T}^2}\hat{\psi}_{E_z}^{(0)}. \quad (64)$$

## F. Properties of the solution

The overall laser energy is calculated by integrating the longitudinal component of the Poynting vector ( $\Pi_x$ ) over transverse coordinates and time (see Appendix C):

$$U = \frac{D_0^2}{4\omega_0} \int_{-\infty}^{+\infty} \Pi_x dv d\zeta d\tau, \quad (65)$$

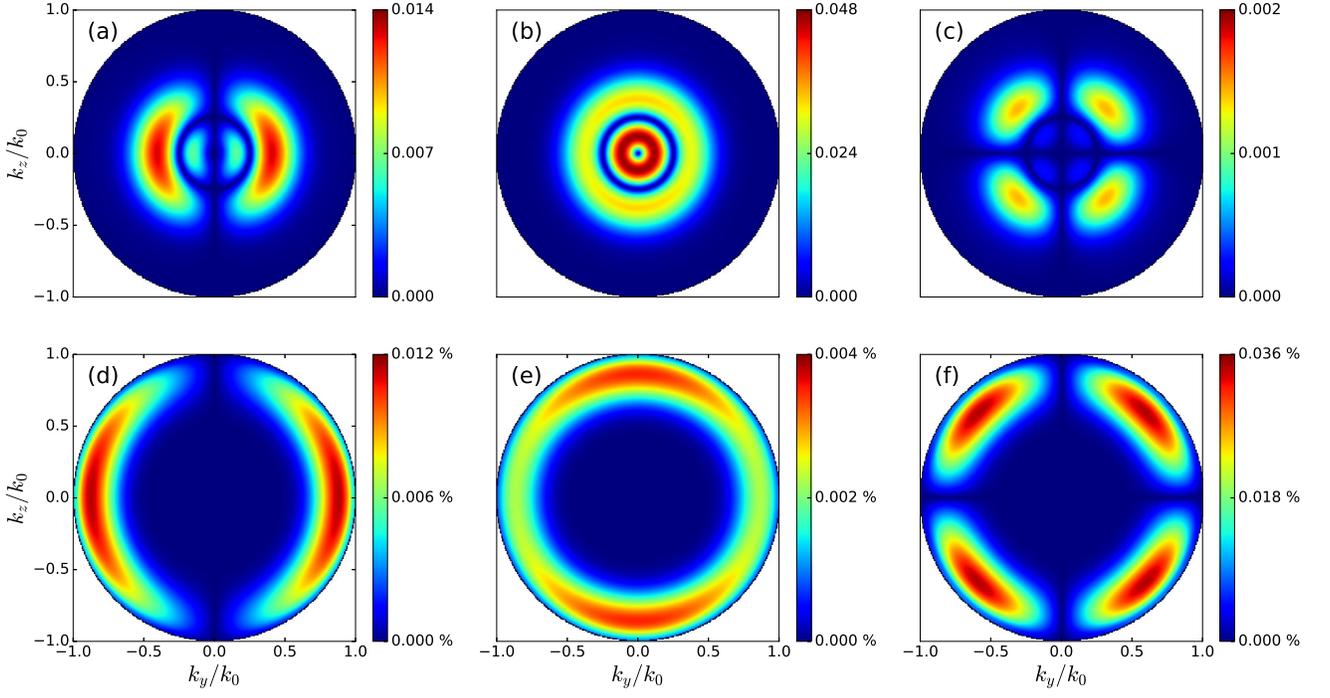


FIG. 2: Lax-series-based analytical solution  $\hat{\psi}$  constructed from the (1,1)-order Laguerre-Gaussian mode, truncated at order  $j = 5$ . We consider  $\lambda_0 = 800$  nm and  $\varepsilon = 0.25$ . The results are plotted in the transverse plane placed at  $\xi = 1$ . We show the spatial envelopes for (a)  $E_x$ , (b)  $E_y$ , and (c)  $E_z$ . The corresponding local relative errors, given by Eq. (73), are shown in (d), (e) and (f), respectively.

where  $\Pi_x = c^2 \varepsilon_0 (E_y \bar{B}_z - E_z \bar{B}_y)$ . In terms of the inner product between envelopes defined by Eq. (C5), the normalized total energy  $4\omega_0 U / (c\varepsilon_0 E_0^2 D_0^2)$  can be expanded in powers of  $\varepsilon$  as follows:

$$\begin{aligned} & \langle \psi_{E_y}, \psi_{B_z} \rangle - \langle \psi_{E_z}, \psi_{B_y} \rangle = \\ & \sum_{j=0}^{\infty} \varepsilon^{2j} \sum_{\alpha=0}^j \langle \psi_{E_y}^{(2\alpha)}, \psi_{B_z}^{(2j-2\alpha)} \rangle - \\ & \sum_{j=0}^{\infty} \varepsilon^{2j} \sum_{\alpha=0}^j \langle \psi_{E_z}^{(2\alpha)}, \psi_{B_y}^{(2j-2\alpha)} \rangle. \end{aligned} \quad (66)$$

We shall demonstrate that our solution, calculated according to Secs. IID and IIE, conserves this total energy. That is to say, the paraxial level sets the energy and high-order corrections do not modify it:

$$\begin{aligned} & \langle \psi_{E_y}, \psi_{B_z} \rangle - \langle \psi_{E_z}, \psi_{B_y} \rangle = \\ & \langle \psi_{E_y}^{(0)}, \psi_{B_z}^{(0)} \rangle - \langle \psi_{E_z}^{(0)}, \psi_{B_y}^{(0)} \rangle. \end{aligned} \quad (67)$$

Proving Eq. (67) is equivalent to prove that all the  $\varepsilon^{(2j)}$ -order terms of Eq. (66) are zero, for  $j \geq 1$ . Using Fourier-backtransformed Eqs. (60), (61), (63) and (64), we verify that the  $\varepsilon^2$ -order term is zero:

$$\begin{aligned} & \left( \langle \psi_{E_y}^{(0)}, \psi_{B_z}^{(2)} \rangle + \langle \psi_{E_y}^{(2)}, \psi_{B_z}^{(0)} \rangle \right) - \\ & \left( \langle \psi_{E_z}^{(0)}, \psi_{B_y}^{(2)} \rangle + \langle \psi_{E_z}^{(2)}, \psi_{B_y}^{(0)} \rangle \right) = 0, \end{aligned} \quad (68)$$

because, in virtue of the properties of the inner product given by Eqs. (C9), (C10) and (C12), the first two terms cancel one another:

$$\begin{aligned} & \langle \psi_{E_y}^{(0)}, \psi_{B_z}^{(2)} \rangle + \langle \psi_{E_y}^{(2)}, \psi_{B_z}^{(0)} \rangle = \\ & - \underbrace{\langle \psi_{E_y}^{(0)}, \frac{\partial_{v\zeta}^2}{8T^2} \psi_{E_z}^{(0)} \rangle + \langle \frac{\partial_{v\zeta}^2}{8T^2} \psi_{E_z}^{(0)}, \psi_{E_y}^{(0)} \rangle}_{=0} \\ & + \underbrace{\langle \psi_{E_y}^{(0)}, \frac{\partial_{\zeta}^2 - \partial_v^2}{16T^2} \psi_{E_y}^{(0)} \rangle - \langle \frac{\partial_{\zeta}^2 - \partial_v^2}{16T^2} \psi_{E_y}^{(0)}, \psi_{E_y}^{(0)} \rangle}_{=0} \\ & + \underbrace{\langle \psi_{E_y}^{(0)}, -\frac{i\xi \partial_{\perp}^4}{64T^3} \psi_{E_y}^{(0)} \rangle + \langle -\frac{i\xi \partial_{\perp}^4}{64T^3} \psi_{E_y}^{(0)}, \psi_{E_y}^{(0)} \rangle}_{=0} = 0, \end{aligned} \quad (69)$$

as well as the last two terms (not shown).

We have checked that the higher-order terms of Eq. (66) are also zero, suggesting that Eq. (67) is satisfied. Indeed, numerical simulations confirm this energy conservation.

Moreover, as already explained in Sec. IIC, the Taylor theorem guarantees us that our  $j$ -order solution, for any laser component ( $E_x$ ,  $E_y$ ,  $E_z$ ,  $B_x$ ,  $B_y$  or  $B_z$ ), converges, up to an error  $\mathcal{O}(\varepsilon^{2j+2})$ , towards the exact solution of the wave equation, given by Eq. (13), in complex module and complex argument. The former is invariant according to Eq. (14) and the later, by doing a Taylor series of Eq. (13)

in  $\kappa_{\perp}/\hat{T}$ , expands in powers of  $\varepsilon$  as follows:

$$\begin{aligned} \arg \left[ \hat{\psi}(\xi, \kappa_y, \kappa_z) \right] - \arg \left[ \hat{\psi}(0, \kappa_y, \kappa_z) \right] = \\ - \frac{\kappa_{\perp}^2 \xi}{4 \hat{T}} - \frac{\kappa_{\perp}^4 \xi}{64 \hat{T}^3} \varepsilon^2 + \mathcal{O}(\varepsilon^4). \end{aligned} \quad (70)$$

For instance, we verify the convergence for  $E_y$  component at order  $j = 1$ . From Eqs. (15), (37), (38) and (60), on the one hand we have that:

$$\frac{|\hat{\psi}_{E_y}(\xi)|}{|\hat{\psi}_{E_y}(0)|} = \left| 1 + \frac{-i\xi\kappa_{\perp}^4\varepsilon^2}{64\hat{T}^3} \right| = 1 + \mathcal{O}(\varepsilon^4), \quad (71)$$

and on the other hand we have:

$$\begin{aligned} \arg \left[ \hat{\psi}_{E_y}(\xi) \right] - \arg \left[ \hat{\psi}_{E_y}(0) \right] = \\ - \frac{\kappa_{\perp}^2}{4\hat{T}}\xi + \arctan \left[ \frac{-\xi\kappa_{\perp}^4\varepsilon^2}{64\hat{T}^3} \right] = \\ - \frac{\kappa_{\perp}^2}{4\hat{T}}\xi - \frac{\kappa_{\perp}^4\xi}{64\hat{T}^3}\varepsilon^2 + \mathcal{O}(\varepsilon^4). \end{aligned} \quad (72)$$

The previous developments have shown the reliability of the proposed analytical solution.

Finally, it is worth mentioning that our solution does converge in the propagating region, given by  $\varepsilon\kappa_{\perp}/(2\hat{T}) \leq 1$ , but it may diverge in the evanescent one. This comes from the fact that the quotient between a high-order correction and the previous one depends on power of  $\varepsilon\kappa_{\perp}/(2\hat{T})$ , as one observes from the recursive formulae (29)-(30) and (53)-(58). This ratio is  $\leq 1$  in the propagating region and hence the convergence of the series is guaranteed.

### G. Example: Monochromatic Hermite-Gaussian and Laguerre-Gaussian beams

We confront our Lax-series-based analytical solution to a numerical algorithm computing Maxwell-consistent solutions [38] (see Appendix D). To do so, monochromatic beams are considered (i.e.,  $\hat{T} \rightarrow 1$ ) and the coefficient  $C(\kappa_y, \kappa_z, \Omega)$  in Eqs. (37)-(42) shall refer here to either a Hermite-Gaussian beam (see Eq. (B8)) or a Laguerre-Gaussian beam (see Eq. (B16)). Since the Lax series originates from a Taylor expansion around the beam focus, the best way to proceed is to prescribe our analytical solution in the focal plane, truncated at different orders  $j$ , and subsequently measure, for all electromagnetic components, the error between the solution of exact solver ( $\hat{\psi}^{\text{solver}}$ ) and our analytical solution ( $\hat{\psi}$ ) in different transverse planes. We compute errors using the standard Frobenius norm. The local relative error in a transverse

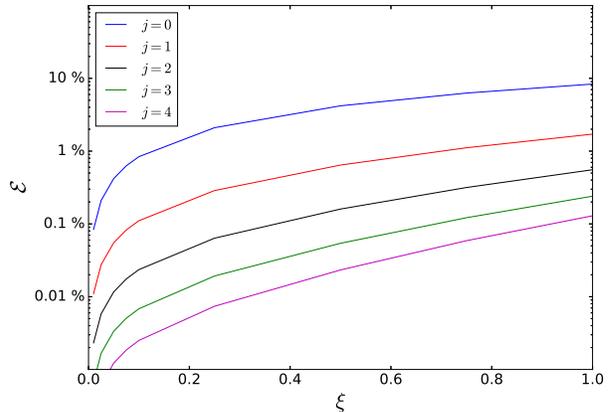


FIG. 3: Global relative error [Eq. (74)] between our analytical solution and the exact solution for  $E_y$  as a function of the longitudinal coordinate at different truncation orders. The Lax series is built from the (1,1)-order Hermite-Gaussian mode, taking  $\lambda_0 = 800$  nm and  $\varepsilon = 0.25$ .

plane is quantified as:

$$e = e(\xi, \kappa_y, \kappa_z) = \frac{k_0 \left| \hat{\psi}^{\text{solver}} - \hat{\psi} \right|}{\sqrt{\iint_{k_{\perp}^2 \leq k_0^2} \left| \hat{\psi}^{\text{solver}} \right|^2 dk_y dk_z}}, \quad (73)$$

and the global relative error in the same plane is:

$$\mathcal{E} = \mathcal{E}(\xi) = \sqrt{\frac{\iint_{k_{\perp}^2 \leq k_0^2} \left| \hat{\psi}^{\text{solver}} - \hat{\psi} \right|^2 dk_y dk_z}{\iint_{k_{\perp}^2 \leq k_0^2} \left| \hat{\psi}^{\text{solver}} \right|^2 dk_y dk_z}}. \quad (74)$$

Figures 1 and 2 show the analytical solution built from a (1,1)-order Hermite-Gaussian and (1,1)-order Laguerre-Gaussian modes, respectively, in the transverse plane placed at  $\xi = 1$ . We take  $\lambda_0 = 800$  nm and a moderate  $\varepsilon = 0.25$  (for which the evanescent power is negligible). The highest local relative error (see Eq. (73)) appear in a ring (i.e., high values of transverse wavenumbers). When increasing the truncation order of the Lax series, this ring becomes narrower and the errors reduce in absolute value (not shown). This confirms numerically the convergence of our Lax-series-based solution seen as a Taylor expansion in  $\kappa_y$  and  $\kappa_z$ . Figure 3 shows that the global relative error diminishes too in all transverse planes when increasing the truncation order. This also confirms numerically the convergence of our Lax-series-based solution seen as a Taylor expansion in  $\xi$ .

### III. ASYMPTOTIC BEHAVIOR FAR FROM FOCAL PLANE

Let us assume that, following Eqs. (37)-(42), the transverse field components at the paraxial order in the position space are:

$$\psi_{E_y}^{(0)} = \psi^{(0)}, \quad (75)$$

$$\psi_{E_z}^{(0)} = 0. \quad (76)$$

The paraxial mode  $\psi^{(0)}$  expands in the limit  $\xi \rightarrow \pm\infty$  as:

$$\psi^{(0)} = \frac{1}{\xi^N} \left[ a_0 + \frac{a_1}{\xi} + \frac{a_2}{\xi^2} + \dots \right], \quad (77)$$

where  $N > 0$  is the leading exponent of the asymptotic limit (in general,  $N$  is not necessarily an integer), which implies that  $a_0 \neq 0$ , and all coefficients  $a_j = a_j(\nu, \zeta, \tau)$  do not depend on  $\xi$ . Equation (77) verifies the paraxial equation (B1):

$$\begin{aligned} \frac{\partial_{\perp}^2 a_0}{\xi^N} + \frac{\partial_{\perp}^2 a_1 - 4iTNa_0}{\xi^{N+1}} + \\ \frac{\partial_{\perp}^2 a_2 - 4iT(N+1)a_1}{\xi^{N+2}} + \dots = 0, \end{aligned} \quad (78)$$

from where we deduce that:

$$\partial_{\perp}^{2(j+1)} a_j = 0, \quad (79)$$

for all  $j \geq 0$ .

In the scope of this paper, we aim at calculating the asymptotic limit where  $\xi \rightarrow \pm\infty$  of our solution, generically denoted as  $\psi^{\infty}$ , at the leading term  $\mathcal{O}(\xi^{-N})$ . The particular solutions of high-order corrections for  $E_y$  and  $E_z$  components, given by Eq. (29), vanish by virtue of Eq. (79) at the leading order  $\mathcal{O}(\xi^{-N})$ . Hence, only the homogenous solutions of high-order corrections may contribute to the limit  $\xi \rightarrow \pm\infty$ , given by Eqs. (54) and (55), at such leading order  $\mathcal{O}(\xi^{-N})$ . After some manipulations, the limits for the transverse components are, respectively:

$$\frac{\psi_{E_y}^{\infty}}{\psi^{(0)}} \sim 1 + \frac{1}{a_0} \sum_{j=1}^{\infty} \varepsilon^{2j} A_{E_y}^{(2j)}, \quad (80)$$

$$\frac{\psi_{E_z}^{\infty}}{\psi^{(0)}} \sim \frac{1}{a_0} \sum_{j=1}^{\infty} \varepsilon^{2j} A_{E_z}^{(2j)}, \quad (81)$$

where, from Eqs. (60) and (61) we obtain for  $j = 1$ :

$$A_{E_y}^{(2)} = \frac{(\partial_{\nu}^2 - \partial_{\zeta}^2)}{16T^2} a_0, \quad (82)$$

$$A_{E_z}^{(2)} = \frac{\partial_{\nu\zeta}^2}{8T^2} a_0, \quad (83)$$

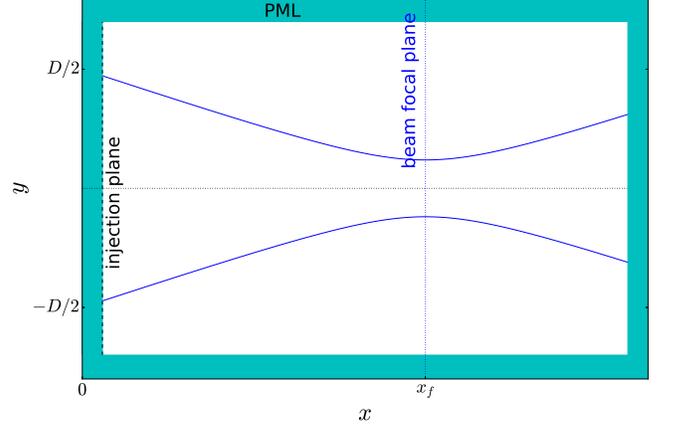


FIG. 4: Numerical box in ARCTIC (cut at  $z = 0$ ). The PML region is colored in cyan. The parameters of the laser beam are defined at  $x = 0$ , namely, the  $1/e$  diameter  $D$  and the numerical aperture. The injection plane for the Total-Field/Scattered-Field technique is placed right after the PML (vertical black dashed line). The beam focal plane (vertical blue dashed line) is at  $x = x_f$ . Solid blue lines illustrate the  $1/e$  beam diameter of the corresponding Gaussian pulse.

and, from Eqs. (54), (55) and (79) we obtain the following recursive formulae for  $j > 1$ :

$$A_{E_y}^{(2j)} = -\frac{1}{8T^2} \left[ \partial_{\zeta}^2 A_{E_y}^{(2j-2)} - \partial_{\nu\zeta}^2 A_{E_z}^{(2j-2)} \right], \quad (84)$$

$$A_{E_z}^{(2j)} = -\frac{1}{8T^2} \left[ \partial_{\nu}^2 A_{E_z}^{(2j-2)} - \partial_{\nu\zeta}^2 A_{E_y}^{(2j-2)} \right]. \quad (85)$$

From Eqs. (80)-(85) we see that the leading terms of the limits of  $E_y$  and  $E_z$  where  $\xi \rightarrow \pm\infty$  hinge upon the dominant coefficient  $a_0$  in Eq. (77). The series in Eqs. (80) and (81) must be truncated at order  $\sim \mathcal{O}(\xi^{-N})$ . These limits are first specified below for monochromatic (i.e.,  $T \rightarrow 1$ ) Hermite-Gaussian (Appendix E 1) and Laguerre-Gaussian (Appendix E 2) families. Then, these limits are calculated with a time envelope coupled to Hermite-Gaussian (Appendix E 3) and Laguerre-Gaussian beams (Appendix E 4).

Our analytical method is able to link the nonparaxial near fields to the far fields. These leading terms of the asymptotic expressions in many cases are simply the paraxial-level term of the Lax series, as shown in Appendices E 1-E 4, and usually mimic quite well experimental conditions, e.g., a broad beam on a focusing mirror.

In order to carry out accurate simulations under highly nonparaxial conditions using Finite-Difference-Time-Domain (FDTD) Maxwell codes, one should compute the fields on the focal plane (where the series converges faster) using our analytical approach and then propagate it to the boundaries using numerically exact Fourier solvers [38]. This would be less expensive than calculating directly the high-order corrections of the Lax series in a transverse plane far from the focal plane with

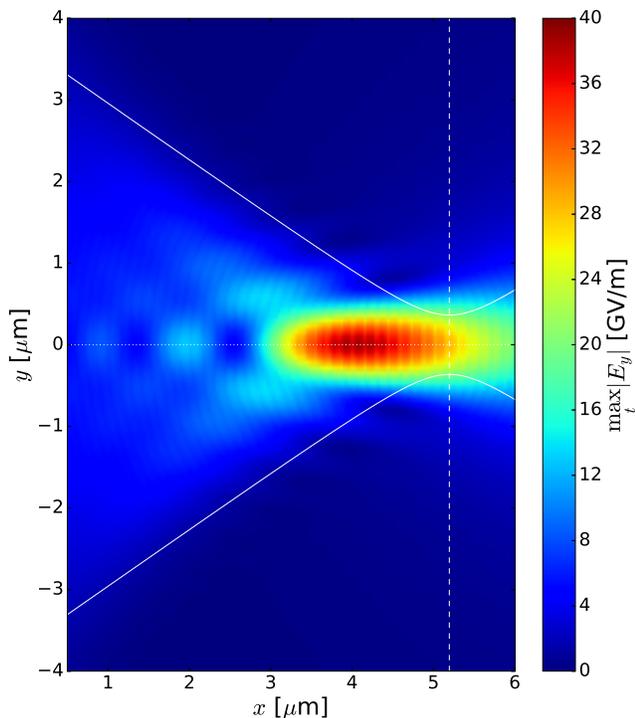


FIG. 5: Maximum value that  $|E_y|$  reaches on the  $XY$  plane, for a  $y$ -polarized  $0.8\text{-}\mu\text{m}$ -wavelength 20-fs-FWHM 36-nJ Gaussian laser beam prescribed at  $x = 0$  with  $\text{NA} = 0.57$  and  $D = 7.31\ \mu\text{m}$ . The horizontal white dotted line represents the optical axis. The length of the PML layer is  $0.32\ \mu\text{m}$  along  $x$  axis and hence the laser pulse is injected at  $x = 0.32\ \mu\text{m}$  using the paraxial-order term. The vertical white dashed line indicates the beam focal plane position ( $x_f = 5.20\ \mu\text{m}$ ) and the white solid lines depict the profile of the Gaussian pulse (paraxial-order term of the Lax series). The leading term of the asymptotic expansion, given by Eq. (E22), is employed to prescribe the laser pulse.

a sufficient precision, as one can see in Fig. 3. Nevertheless, if the boundaries where fields need to be prescribed are very distant from the focal plane (several Rayleigh lengths), which means that the transverse-spatial and temporal windows are very large, spectral algorithms would demand considerable computational resources. In this situation, prescribing directly the asymptotic limit of the Lax series on boundaries *far enough from the focal plane* may be computationally interesting.

We verify our analytical results with three-dimensional (3D) Maxwell-consistent numerical simulations performed using the code ARCTIC [39]. Maxwell equations are discretized by means of Yee scheme [40]. The simulation domain is delimited by Bérenger's Perfectly-Matched-Layer (PML) absorbing boundary condition [4, 5]. The laser is injected via  $E_y$ ,  $E_z$ ,  $B_y$  and  $B_z$  components in the transverse plane placed right after the PML according to the Total-Field/Scattered-Field technique [36], as shown in Fig. 4. This boundary is placed several Rayleigh lengths from the beam focus  $x = x_f$ .

The origin of the optical axis ( $x = 0$ ) is set at the position of the left boundary. The input paraxial-order Gaussian pulse at  $x = 0$  is characterized by its  $1/e$  beam diameter  $D$  and numerical aperture (NA). The numerical aperture ( $0 \leq \text{NA} \leq 1$ ) of a Gaussian beam is defined as the sine of its divergence angle. Our Lax series expansion parameter  $\varepsilon = (D_0/2)/x_R$ , that is, the ratio of the  $1/e$  beam radius at focus  $D_0/2$  and the Rayleigh length  $x_R$ , represents the tangent of the beam divergence angle. Thus, expressed in terms of  $\varepsilon$ , the numerical aperture reads:

$$\text{NA} = \frac{\varepsilon}{\sqrt{1 + \varepsilon^2}}. \quad (86)$$

The beam focal plane situates at  $x = x_f$ :

$$x_f = \frac{\lambda_0}{\pi\varepsilon^2} \sqrt{\left(\frac{\pi\varepsilon D}{2\lambda_0}\right)^2 - 1}. \quad (87)$$

If injecting the leading term of the asymptotic expansion of our solution at  $x = 0$  (i.e., a simple Gaussian beam) instead of directly injecting the full solution, then the position of the focal plane obtained with the full Maxwell solver may differ from  $x_f$ .

We simulate a  $y$ -polarized Gaussian laser beam at the wavelength  $\lambda_0 = 0.8\ \mu\text{m}$  coupled, according to Eq. (E22), with the Gaussian time envelope:

$$C_\tau(\Omega) = \frac{\tau_p}{2\sqrt{\pi}} e^{-\frac{\tau_p^2 \Omega^2}{4}} = \mathcal{F}_\tau \left[ e^{-\frac{t^2}{\tau_p^2}} \right], \quad (88)$$

where  $\tau_p = 16.99\ \text{fs}$  is the  $1/e$  duration and thus the Full-Width-at-Half-Maximum (FWHM) duration of the pulse (envelope of intensity) is 20 fs (i.e., 7.49 optical cycles). The  $1/e$  beam diameter at  $x = 0$  is  $D = 7.31\ \mu\text{m}$ . We take a numerical aperture of  $\text{NA} = 0.57$  in the vacuum, which gives  $\varepsilon = 0.7$  corresponding to strong focusing conditions where the nonparaxial regime is completely established [30]. The beam focal plane should situate at  $x_f = 5.20\ \mu\text{m}$  according to Eq. (87). Since  $x_R = 0.52\ \mu\text{m}$ , the prescription plane is  $x_f/x_R = 10$  Rayleigh lengths far from the beam focal plane. An overall input energy of 36 nJ is considered (which corresponds to  $E_0 = 55.36\ \text{GV/m}$ ). The resolution chosen in ARCTIC is  $\Delta x = 31.8\ \text{nm}$  (25 points per wavelength),  $\Delta y = \Delta z = 63.7\ \text{nm}$  (13 points per wavelength) and  $\Delta t = 84.9\ \text{as}$  (31 points per period). The PML layer is ten cells wide in each direction.

Figure 5 shows the maximum value of  $|E_y|$  over time in the  $XY$  plane (i.e.,  $z = 0$ ). The laser pulse is prescribed according to Eq. (E22). The temporal inverse Fourier transformed is computed from Eq. (A6) using the 64-points Gauss-Legendre quadrature formula in the frequency interval  $-10/\tau_p \leq \Omega \leq 10/\tau_p$ . The error of 22% between the position of the beam focal plane given by ARCTIC ( $x = 4.06\ \mu\text{m}$ ) and the theory ( $x_f = 5.20\ \mu\text{m}$ ) is due to the fact that only the leading term of the asymptotic solution is taken into consideration. The previous evaluations have been performed within conditions

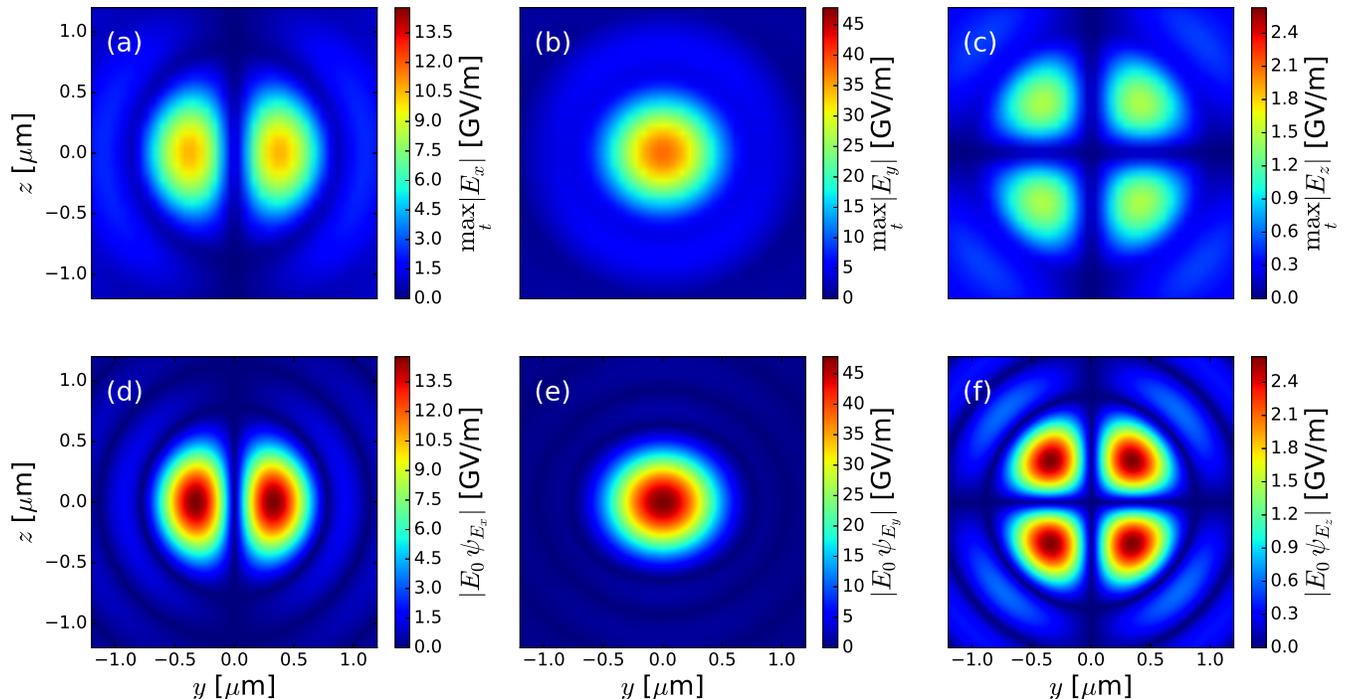


FIG. 6: Comparison of ARCTIC's results (maximum values that the module of the electric field components attain in the focal plane) with our analytical solution. Results corresponding to Fig. 5 in the beam focal plane at  $x = 4.06 \mu\text{m}$ : Maximum values of (a)  $|E_x|$ , (b)  $|E_y|$  and (c)  $|E_z|$ . Analytical solution in the focal plane at  $x_f = 5.20 \mu\text{m}$ , calculated from the homogeneous parts given by Eqs. (37)-(39) and (53)-(55) up to order  $j = 18$ , with  $T = 1$  and by filtering the evanescent modes: (d)  $|E_0 \psi_{E_x}|$ , (e)  $|E_0 \psi_{E_y}|$  and (f)  $|E_0 \psi_{E_z}|$ .

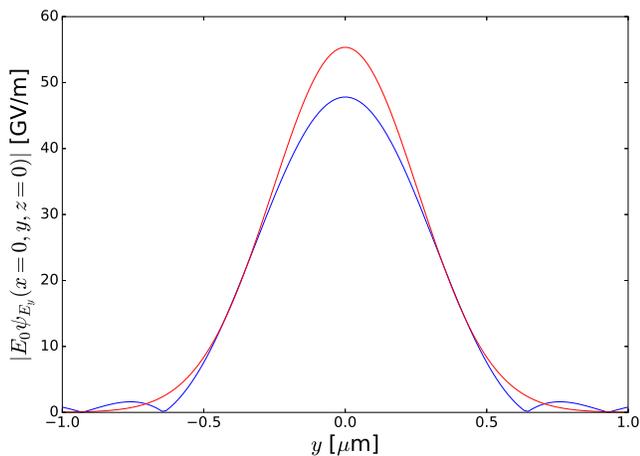


FIG. 7: Cut along  $y$  axis of  $|E_0 \psi_{E_y}|$  corresponding to Fig. 6(e) (blue solid line). The red solid line accounts for the paraxial-order term of the series.

of very tightly focused pulses ( $\varepsilon = 0.7$ ). By decreasing  $\varepsilon$  to 0.5, the error drops to roughly 10% (not shown), which is acceptable. Therefore, it turns out that prescribing the laser fields at a *finite* distance implies a contribution of next-to-leading orders of the asymptotic expansion: the

smaller  $\varepsilon$ , the smaller the next-to-leading order contribution.

The maximum values in the focal plane over time of the module of the electric field components are comparable with the module of the corresponding spatial envelopes with  $T \rightarrow 1$ . These latter values,  $|E_0 \psi|$ , computed up to order  $j = 18$  using the recursive formulae (37)-(39) and (53)-(55) in the position space, are depicted in Fig. 6(d-f). Note that one must apply a filter to the solution of the Lax series because it does not converge for evanescent modes (see Sec. II F). The peak of  $E_y$  predicted by our Lax-series-based solution is 47.80 GV/m, which is lower than the peak of the paraxial-order term of the series ( $E_0 = 55.36$  GV/m), as illustrated in Fig. 7, due to the strong focusing conditions. The cuts in the focal plane of the simulation corresponding to Fig. 5 are shown in Fig. 6(a-c). One observes that the results of ARCTIC and our analytical solution qualitatively agree but the amplitudes are  $\sim 20\%$  smaller (the peak of  $E_y$  is 37.80 GV/m).

#### IV. CONCLUSION AND OUTLOOKS

Both the wave equation and the paraxial equation possess an infinite number of solutions. In this pa-

per, we have demonstrated that from any paraxial solution we can build, in a self-consistent fashion, an exact solution of the wave equation for the six electromagnetic field components, assuming forward-propagating linearly-polarized laser pulses, which, by the first time to best of our knowledge, is consistent with Maxwell equations, conserves the energy transported through transverse planes and preserves the symmetry between the electric and magnetic fields. To do so, we have split, following the procedure by Lax *et al.* [24] and in the transverse-spatial and temporal Fourier space, both the scalar wave equations applied to each electromagnetic field component and to the Maxwell equations. High-order corrections have been separated in a *homogeneous* solution and a *particular* solution. The particular solution is integrated directly from the wave equation. The homogeneous solution, instead, must be calculated so that the whole set of Maxwell equations is satisfied and the existing symmetry between the electric and magnetic fields is preserved. Only then the total laser energy through transverse planes is conserved. We give simple recursive relations in order to obtain these Maxwell-consistent high-order corrections, which are polynomials on the longitudinal coordinate whose coefficients are paraxial modes related to transverse-spatial and temporal derivatives of the paraxial-order term of the Lax series. The convergence of our Lax-series-based solution towards the exact solution of the wave equation is demonstrated and then numerically illustrated.

Since in experiments fields are usually known far from the focal plane, we have derived the leading term if the asymptotic expansion of the full analytical solution of the Maxwell equations. In the case of a strongly focused 20-fs-FWHM Gaussian laser pulse, numerical simulations confirm the reliability of this asymptotic expression up to an accuracy of 10%. Further developments for next-to-leading orders are expected to decrease this error.

### Acknowledgments

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### Appendix A: Definition of the transverse-spatial and temporal Fourier transform

Using the dimensionless coordinates  $\xi = x'/x_R$ ,  $v = 2y/D_0$ ,  $\zeta = 2z/D_0$ ,  $\kappa_y = D_0 k_y/2$ ,  $\kappa_z = D_0 k_z/2$ ,  $\tau = \omega_0 t'$  and  $\Omega = \omega/\omega_0$  we define the transverse-spatial and temporal Fourier transform of  $\psi$ , denoted as  $\hat{\psi}$ , as the combination of the transverse-spatial Fourier transform ( $\mathcal{F}_\perp$ ) and temporal Fourier transform ( $\mathcal{F}_\tau$ ):

$$\hat{\psi}(\xi, \kappa_y, \kappa_z, \Omega) = \mathcal{F}_\tau [\mathcal{F}_\perp [\psi(\xi, v, \zeta, \tau)]], \quad (\text{A1})$$

$$\psi(\xi, v, \zeta, \tau) = \mathcal{F}_\tau^{-1} \left[ \mathcal{F}_\perp^{-1} \left[ \hat{\psi}(\xi, \kappa_y, \kappa_z, \Omega) \right] \right], \quad (\text{A2})$$

where the transverse-spatial Fourier transform is:

$$\mathcal{F}_\perp [\psi] = \frac{1}{4\pi^2} \iint \psi e^{-i(\kappa_y v + \kappa_z \zeta)} dv d\zeta, \quad (\text{A3})$$

$$\psi = \iint \mathcal{F}_\perp [\psi] e^{i(\kappa_y v + \kappa_z \zeta)} d\kappa_y d\kappa_z, \quad (\text{A4})$$

and the temporal Fourier transform is:

$$\mathcal{F}_\tau [\psi] = \frac{1}{2\pi} \int \psi e^{i\Omega\tau} d\tau, \quad (\text{A5})$$

$$\psi = \int \mathcal{F}_\tau [\psi] e^{-i\Omega\tau} d\Omega. \quad (\text{A6})$$

For monochromatic pulses, the temporal Fourier transform defined in Eq. (A5) reduces to a multiplication by a Dirac delta function  $\delta(\Omega)$  in the temporal Fourier space.

### Appendix B: Solutions of the paraxial equations

The paraxial equation is:

$$(\partial_v^2 + \partial_\zeta^2 + 4iT\partial_\xi)\psi = (\partial_v^2 + \partial_\zeta^2 + 4F^2 T\partial_F)\psi = 0, \quad (\text{B1})$$

where the complex longitudinal variable  $F = i/(i-\xi)$  has already been introduced by Salamin [30]. By rewriting Eq. (B1) in the transverse-spatial and temporal Fourier space, we can see that the paraxial solution is of the form:

$$\hat{\psi} = C(\kappa_y, \kappa_z, \Omega) e^{-i\frac{\kappa_\perp^2}{4T}\xi}, \quad (\text{B2})$$

where  $\kappa_\perp^2 = \kappa_y^2 + \kappa_z^2$  and  $C(\kappa_y, \kappa_z, \Omega)$  is a coefficient independent of  $\xi$ .

Three families of exact solutions for Eq. (B1) are known when  $T \rightarrow 1$  (i.e., monochromatic pulses): Hermite-Gaussian modes (often called the *free-space eigenmodes*), Laguerre-Gaussian modes, and Ince-Gaussian modes [3]. Each of these families constitute a countably infinite set of orthogonal paraxial solutions, and they are complete [1].

## 1. Hermite-Gaussian modes

The Hermite-Gaussian modes are a well-known complete family of orthogonal paraxial solutions:

$$\psi_{n,m}^{(HG)}(F, v, \zeta) = \sqrt{\frac{(2F-1)^{m+n}}{n!m!2^{n+m}}} H_n\left(\frac{\sqrt{2}Fv}{\sqrt{2F-1}}\right) H_m\left(\frac{\sqrt{2}F\zeta}{\sqrt{2F-1}}\right) F e^{-F\rho^2}, \quad (\text{B3})$$

where  $n$  is the order of the Hermite polynomial  $H_n$  along  $y$  axis,  $m$  is the order along  $z$  axis,  $\rho^2 = v^2 + \zeta^2$ . Hermite polynomials verify:

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x), \quad (\text{B4})$$

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0, \quad (\text{B5})$$

where  $'$  accounts for the derivative with respect to the variable  $x$  and the first two polynomials are  $H_0(x) = 1$  and  $H_1(x) = 2x$ .

Hermite-Gaussian propagation modes are orthogonal between one another, with the inner product defined by Eq. (C7):

$$\langle \psi_{n,m}^{(HG)}, \psi_{p,q}^{(HG)} \rangle = \langle \psi_{p,q}^{(HG)}, \psi_{n,m}^{(HG)} \rangle = \frac{\pi}{2} \delta_n^q \delta_m^q, \quad (\text{B6})$$

where  $\delta_n^p$  refers to Kronecker delta function.

In the transverse-spatial Fourier space, the  $(n, m)$ -order Hermite-Gaussian mode reads:

$$\hat{\psi}_{n,m}^{(HG)} = C_{n,m}^{(HG)} e^{-i\frac{\kappa_y^2}{4}\xi}, \quad (\text{B7})$$

where:

$$C_{n,m}^{(HG)} = \frac{(-i)^{n+m}}{4\pi\sqrt{n!m!2^{n+m}}} H_n\left(\frac{\kappa_y}{\sqrt{2}}\right) H_m\left(\frac{\kappa_z}{\sqrt{2}}\right) e^{-\frac{\kappa_z^2}{4}}. \quad (\text{B8})$$

Transverse derivatives of Hermite-Gaussian modes can be expressed as a linear combination of Hermite-Gaussian modes:

$$i\kappa_y \hat{\psi}_{n,m}^{(HG)} = -\sqrt{n+1} \hat{\psi}_{n+1,m}^{(HG)} + \sqrt{n} \hat{\psi}_{n-1,m}^{(HG)}, \quad (\text{B9})$$

$$i\kappa_z \hat{\psi}_{n,m}^{(HG)} = -\sqrt{m+1} \hat{\psi}_{n,m+1}^{(HG)} + \sqrt{m} \hat{\psi}_{n,m-1}^{(HG)}, \quad (\text{B10})$$

where, by notation convention,  $\sqrt{n} H_{n-1}(x) = 0$  if  $n = 0$ .

## 2. Laguerre-Gaussian modes

The Laguerre-Gaussian modes are a well-known complete family of orthogonal paraxial solutions:

$$\psi_{p,l}^{(LG)}(F, v, \zeta) = \frac{(2F-1)^p (\sqrt{2}F)^{|l|}}{\sqrt{\frac{(p+|l|)!}{p!}}} (v + \text{sgn}(l) i\zeta)^{|l|} L_p^{|l|}\left(\frac{2\rho^2 F^2}{2F-1}\right) F e^{-F\rho^2}, \quad (\text{B11})$$

where  $p \geq 0$  is the radial index and  $l$  is the azimuthal index (it can be negative, zero or positive integer) of the generalized Laguerre polynomial  $L_p^{|l|}$ , and  $\text{sgn}(l)$  is the sign of  $l$ , i.e.,  $\text{sgn}(l) = 1$  if  $l \geq 0$  and  $\text{sgn}(l) = -1$  if  $l < 0$ . Generalized Laguerre polynomials verify:

$$L_p^{|l|}(x) = \frac{(2p+|l|-1-x)L_{p-1}^{|l|}(x) - (p+|l|-1)L_{p-2}^{|l|}(x)}{p}, \quad (\text{B12})$$

where the first two polynomials are  $L_0^{|l|}(x) = 1$  and  $L_1^{|l|}(x) = 1 + |l|x$ .

Laguerre-Gaussian propagation modes constitute an orthogonal set:

$$\langle \psi_{p,l}^{(LG)}, \psi_{q,r}^{(LG)} \rangle = \langle \psi_{q,r}^{(LG)}, \psi_{p,l}^{(LG)} \rangle = \frac{\pi}{2} \delta_p^q \delta_l^r. \quad (\text{B13})$$

The Gaussian beam belongs to both Hermite-Gaussian and Laguerre-Gaussian families:

$$\phi_{0,0}^{(HG)} = \phi_{0,0}^{(LG)}. \quad (\text{B14})$$

In the transverse-spatial Fourier space, the  $(p, l)$ -order Laguerre-Gaussian mode reads:

$$\hat{\psi}_{p,l}^{(LG)} = C_{l,p}^{(LG)} e^{-i\frac{\kappa_z^2}{4}\xi}, \quad (\text{B15})$$

where:

$$C_{p,l}^{(LG)} = \frac{(-i)^{2p+|l|} \sqrt{p!}}{4\pi \sqrt{2^{|l|}} (p+|l|)!} (\kappa_y + \text{sgn}(l) i\kappa_z)^{|l|} L_p^{|l|}\left(\frac{\kappa_z^2}{2}\right) e^{-\frac{\kappa_z^2}{4}}. \quad (\text{B16})$$

Transverse derivatives of Laguerre-Gaussian modes can be expressed as a linear combination of Laguerre-Gaussian modes:

$$\begin{aligned} -\kappa_z^2 \hat{\psi}_{p,l}^{(LG)} &= -2(2p+|l|+1) \hat{\psi}_{p,l}^{(LG)} \\ &\quad - 2\sqrt{(p+1)(p+1+|l|)} \hat{\psi}_{p+1,l}^{(LG)} \\ &\quad - 2\sqrt{p(p+|l|)} \hat{\psi}_{p-1,l}^{(LG)}, \end{aligned} \quad (\text{B17})$$

where, by notation convention,  $\sqrt{p} L_{p-1}^{|l|}(x) = 0$  if  $p = 0$ .

## Appendix C: Laser power and energy transported through a transverse plane and definition of the inner product between spatial envelopes

The Poynting vector is defined as:

$$\mathbf{\Pi} = c^2 \varepsilon_0 (\mathbf{E} \times \bar{\mathbf{B}}), \quad (\text{C1})$$

where the symbol  $\bar{\phantom{x}}$  denotes the complex conjugate. Its longitudinal component is:

$$\Pi_x = c^2 \varepsilon_0 (E_y \bar{B}_z - E_z \bar{B}_y), \quad (\text{C2})$$

whose integral over the transverse coordinates, calculated by employing Ansätze (7) and (8), gives the power flux through the transverse planes:

$$P = \frac{c\varepsilon_0 E_0^2 D_0^2}{4} \iint_{-\infty}^{+\infty} (\psi_{E_y} \bar{\psi}_{B_z} - \psi_{E_z} \bar{\psi}_{B_y}) dv d\zeta. \quad (\text{C3})$$

Integration of Eq. (C3) over time, assuming that there is a time-dependent envelope, gives the total laser energy, which should be the same through any transverse plane:

$$U = \frac{1}{\omega_0} \int_{-\infty}^{+\infty} P d\tau. \quad (\text{C4})$$

The form of the integral in Eq. (C4) suggests us to define the following inner product of spatial envelopes:

$$\langle a, b \rangle := \iiint_{-\infty}^{+\infty} a \bar{b} dv d\zeta d\tau, \quad (\text{C5})$$

which gives us the total energy of the laser pulse:

$$\frac{4\omega_0 U}{c\varepsilon_0 E_0^2 D_0^2} = \langle \psi_{E_y}, \psi_{B_z} \rangle - \langle \psi_{E_z}, \psi_{B_y} \rangle. \quad (\text{C6})$$

Note that for monochromatic beams (i.e., the envelopes do not depend on time) the inner product is defined as:

$$\langle a, b \rangle := \iint_{-\infty}^{+\infty} a \bar{b} dv d\zeta, \quad (\text{C7})$$

and, in this case,  $\langle \psi_{E_y}, \psi_{B_z} \rangle - \langle \psi_{E_z}, \psi_{B_y} \rangle$  represents the total power flux through transverse planes:

$$\frac{4P}{c\varepsilon_0 E_0^2 D_0^2} = \langle \psi_{E_y}, \psi_{B_z} \rangle - \langle \psi_{E_z}, \psi_{B_y} \rangle. \quad (\text{C8})$$

Following the definition of the inner product, if  $x$  is a scalar (i.e., it does not depend on  $v$  and  $\zeta$ ), we have that:

$$\langle xa, b \rangle = x \langle a, b \rangle, \quad (\text{C9})$$

$$\langle a, xb \rangle = \bar{x} \langle a, b \rangle. \quad (\text{C10})$$

Moreover, it follows from the theory of distributions that odd transverse-coordinate and time derivatives are anticommutative and even transverse-coordinate and time derivatives are commutative. For instance:

$$\langle \partial_v a, a \rangle = -\langle a, \partial_v a \rangle, \quad (\text{C11})$$

$$\langle \partial_v^2 a, a \rangle = \langle a, \partial_v^2 a \rangle, \quad (\text{C12})$$

provided that  $a(v \rightarrow \pm\infty) = 0$  and  $\partial_v a(v \rightarrow \pm\infty) = 0$ .

## Appendix D: The exact Maxwell solver in the transverse-spatial Fourier space

We shall adapt the exact Maxwell solver in transverse-spatial Fourier domain of Ref. [38] to the spatial envelopes given in Ansätze (7) and (8). Only the solver for monochromatic laser beams is presented here. To do so, those Ansätze are substituted into the Maxwell equations and we obtain the following overdetermined system:

$$\begin{pmatrix} k_x & k_y & k_z & 0 & 0 & 0 \\ 0 & 0 & 0 & k_x & k_y & k_z \\ 0 & -k_z & k_y & -k_0 & 0 & 0 \\ k_z & 0 & -k_x & 0 & -k_0 & 0 \\ k_y & -k_x & 0 & 0 & 0 & k_0 \\ k_0 & 0 & 0 & 0 & -k_z & k_y \\ 0 & -k_0 & 0 & -k_z & 0 & k_x \\ 0 & 0 & k_0 & -k_y & k_x & 0 \end{pmatrix} \begin{pmatrix} \hat{\psi}_{E_x} \\ \hat{\psi}_{E_y} \\ \hat{\psi}_{E_z} \\ \hat{\psi}_{B_x} \\ \hat{\psi}_{B_y} \\ \hat{\psi}_{B_z} \end{pmatrix} = \mathbf{0}, \quad (\text{D1})$$

where  $k_x = \sqrt{k_0^2 - k_y^2 - k_z^2}$  is the longitudinal component of the wavevector. We only consider forward-propagating modes (i.e.,  $k_x \geq 0$ ), and hence we require  $\hat{\psi}(x, k_y, k_z) = 0$  if  $k_y^2 + k_z^2 > k_0^2$ .

The system (D1) has a unique solution if we assume that the two transverse components of the electric field,  $E_y$  and  $E_z$ , are known:

$$\hat{\psi}_{E_x} = -\frac{k_y}{k_x} \hat{\psi}_{E_y} - \frac{k_z}{k_x} \hat{\psi}_{E_z}, \quad (\text{D2})$$

$$\hat{\psi}_{B_x} = -\frac{k_z}{k_0} \hat{\psi}_{E_y} + \frac{k_y}{k_0} \hat{\psi}_{E_z}, \quad (\text{D3})$$

$$\hat{\psi}_{B_y} = -\frac{k_y k_z}{k_0 k_x} \hat{\psi}_{E_y} - \frac{k_0^2 - k_y^2}{k_0 k_x} \hat{\psi}_{E_z}, \quad (\text{D4})$$

$$\hat{\psi}_{B_z} = \frac{k_0^2 - k_z^2}{k_0 k_x} \hat{\psi}_{E_y} + \frac{k_y k_z}{k_0 k_x} \hat{\psi}_{E_z}. \quad (\text{D5})$$

The transverse components of the electric field are prescribed in the transverse plane at  $x = x_0$  and propagated according the following expression:

$$\hat{\psi}_{E_y}(x, k_y, k_z) = \hat{\psi}_{E_y}(x_0, k_y, k_z) e^{-i(k_0 - k_x)(x - x_0)}, \quad (\text{D6})$$

$$\hat{\psi}_{E_z}(x, k_y, k_z) = \hat{\psi}_{E_z}(x_0, k_y, k_z) e^{-i(k_0 - k_x)(x - x_0)}, \quad (\text{D7})$$

which is the exact forward-propagating solution of Eq. (12).

## Appendix E: Examples of asymptotic expansions (leading term)

### 1. Monochromatic Hermite-Gaussian beams

If  $n$  and  $m$  are both even integers, the  $(n, m)$ -order Hermite-Gaussian mode (see Eq. (B3)) behaves asymp-

totically where  $\xi \rightarrow \pm\infty$  like:

$$\psi_{n,m}^{(HG)} \sim \frac{1}{\xi} [a_0 + \mathcal{O}(\xi^{-1})], \quad (\text{E1})$$

$$a_0 = -\frac{i\pi\sqrt{n!m!}}{2^{\frac{n+m}{2}} \left(\frac{n}{2}\right)! \left(\frac{m}{2}\right)!}. \quad (\text{E2})$$

If  $n$  is even and  $m$  is odd:

$$\psi_{n,m}^{(HG)} \sim \frac{1}{\xi^2} [a_0 + \mathcal{O}(\xi^{-1})], \quad (\text{E3})$$

$$a_0 = -\frac{2\sqrt{2}\sqrt{n!m!}}{2^{\frac{n+m}{2}} \left(\frac{n}{2}\right)! \left(\frac{m-1}{2}\right)!} \zeta. \quad (\text{E4})$$

If  $n$  is odd and  $m$  is even:

$$\psi_{n,m}^{(HG)} \sim \frac{1}{\xi^2} [a_0 + \mathcal{O}(\xi^{-1})], \quad (\text{E5})$$

$$a_0 = -\frac{2\sqrt{2}\sqrt{n!m!}}{2^{\frac{n+m}{2}} \left(\frac{n-1}{2}\right)! \left(\frac{m}{2}\right)!} v. \quad (\text{E6})$$

If both  $n$  and  $m$  are odd integers, then the asymptotic expansion is:

$$\psi_{n,m}^{(HG)} \sim \frac{1}{\xi^3} [a_0 + \mathcal{O}(\xi^{-1})], \quad (\text{E7})$$

$$a_0 = \frac{8i\sqrt{n!m!}}{2^{\frac{n+m}{2}} \left(\frac{n-1}{2}\right)! \left(\frac{m-1}{2}\right)!} v\zeta. \quad (\text{E8})$$

Whenever  $n$  and  $m$  are not simultaneously odd integers, by substituting Eqs. (E2), (E4) and (E6) into Eqs. (82) and (83) one deduces that the paraxial-order term dominates far from the focal plane:

$$\psi_{E_y}^\infty \sim \psi_{n,m}^{(HG)}, \quad (\text{E9})$$

$$\psi_{E_z}^\infty \sim 0. \quad (\text{E10})$$

When both  $n$  and  $m$  are odd integers, the substitution of Eq. (E8) into Eqs. (82) and (83) yields an extra term  $\sim \mathcal{O}(\xi^{-3})$  in the asymptotic limit of  $E_z$ :

$$\psi_{E_y}^\infty \sim \psi_{n,m}^{(HG)}, \quad (\text{E11})$$

$$\psi_{E_z}^\infty \sim \frac{\varepsilon^2}{8v\zeta} \psi_{n,m}^{(HG)}. \quad (\text{E12})$$

Following Eq. (67), it is straightforward to verify that these asymptotic limits contain all the power through the transverse plane of the solution.

## 2. Monochromatic Laguerre-Gaussian beams

Laguerre-Gaussian modes (see Eq. (B11)) behave asymptotically where  $\xi \rightarrow \pm\infty$  like:

$$\psi_{p,l}^{(LG)} \sim F^{|l|+1} [a_0 + \mathcal{O}(\xi^{-1})], \quad (\text{E13})$$

$$a_0 = \alpha_0 \rho^{|l|} e^{il\phi}, \quad (\text{E14})$$

$$\alpha_0 = (-1)^p \sqrt{\frac{2^{|l|} p!}{(p+|l|)!}} L_p^{|l|}(0), \quad (\text{E15})$$

where  $F = i/(i-\xi)$ ,  $\rho e^{\pm i\phi} = v \pm i\zeta$ , and, in the cylindrical coordinate system,  $\rho = \sqrt{v^2 + \zeta^2}$  represents the radial distance and  $\phi$  is the azimuth (such that  $v = \rho \cos \phi$  and  $\zeta = \rho \sin \phi$ ). Note that  $L_p^{|l|}(0) \neq 0$  for all  $p \geq 0$  and  $l$ . After some manipulations, when substituting Eq. (E14) into Eqs. (82) and (83) and Eqs. (84) and (85), we have:

$$A_{E_y}^{(2)} = \frac{|l|(|l|-1)}{8} \alpha_0 (v + i \operatorname{sgn}(l)\zeta)^{|l|-2}, \quad (\text{E16})$$

$$A_{E_z}^{(2)} = \operatorname{sgn}(l) i A_{E_y}^{(2)}, \quad (\text{E17})$$

which are zero if  $|l| \leq 1$ , and for  $j > 1$ :

$$A_{E_y}^{(2j)} = A_{E_z}^{(2j)} = 0. \quad (\text{E18})$$

Therefore, the limits for  $E_y$  and  $E_z$  are, respectively:

$$\psi_{E_y}^\infty \sim \left[ 1 + \frac{\varepsilon^2 |l| (|l|-1)}{8(v + i \operatorname{sgn}(l)\zeta)^2} \right] \psi_{p,l}^{(LG)}, \quad (\text{E19})$$

$$\psi_{E_z}^\infty \sim \frac{i\varepsilon^2 l (|l|-1)}{8(v + i \operatorname{sgn}(l)\zeta)^2} \psi_{p,l}^{(LG)}. \quad (\text{E20})$$

## 3. Hermite-Gaussian laser pulses

In the transverse-spatial and temporal Fourier space, we multiply the  $(n, m)$ -order Hermite-Gaussian mode in the focal plane ( $\xi = 0$ ) by a temporal envelope  $C_\tau(\Omega)$ , in order to prescribe the transverse fields according to Eqs. (75) and (76) with the following paraxial mode:

$$\hat{\psi}^{(0)} = C_\tau(\Omega) C_{n,m}^{(HG)}(\kappa_y, \kappa_z) e^{-i\frac{\kappa^2}{4T}\xi}, \quad (\text{E21})$$

which satisfies Eq. (B2) and where  $C_{n,m}^{(HG)}$  is given by Eq. (B8). Since by this choice the temporal and transverse-spatial envelopes are separated in the focal plane, the inverse transverse-spatial Fourier transform of

Eq. (E21) is straightforward and thus the paraxial mode in position space reads:

$$\psi^{(0)} = \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{n,m}^{(HG)}(\tilde{F}, v, \zeta) \right], \quad (\text{E22})$$

where  $\psi_{n,m}^{(HG)}$  is given by Eq. (B3) and:

$$\tilde{F} = \frac{i}{i - \xi/T}. \quad (\text{E23})$$

Following Sec. E1, whenever  $n$  and  $m$  are not simultaneously odd integers the asymptotic limits far from the focal plane are:

$$\psi_{E_y}^\infty \sim \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{n,m}^{(HG)}(\tilde{F}, v, \zeta) \right], \quad (\text{E24})$$

$$\psi_{E_z}^\infty \sim 0. \quad (\text{E25})$$

When both  $n$  and  $m$  are odd integers:

$$\psi_{E_y}^\infty \sim \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{n,m}^{(HG)}(\tilde{F}, v, \zeta) \right], \quad (\text{E26})$$

$$\psi_{E_z}^\infty \sim \frac{\varepsilon^2}{8T^2 v \zeta} \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{n,m}^{(HG)}(\tilde{F}, v, \zeta) \right]. \quad (\text{E27})$$

#### 4. Laguerre-Gaussian laser pulses

Analogously to Sec. E3, we prescribe laser field components based on the following paraxial mode that comes from multiplying a time envelope by a Laguerre-Gaussian mode in the focal plane:

$$\psi^{(0)} = \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{p,l}^{(LG)}(\tilde{F}, v, \zeta) \right], \quad (\text{E28})$$

where  $C_{p,l}^{(LG)}$  is given by Eq. (B16) and  $\tilde{F}$  is given by Eq. (E23).

Following Sec. E2, the asymptotic limits for each transverse laser components are, respectively:

$$\psi_{E_y}^\infty \sim \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{p,l}^{(LG)}(\tilde{F}, v, \zeta) \right] \times \left[ 1 + \frac{\varepsilon^2 |l| (|l| - 1)}{8T^2 (v + i \operatorname{sgn}(l) \zeta)^2} \right], \quad (\text{E29})$$

$$\psi_{E_z}^\infty \sim \mathcal{F}_\tau^{-1} \left[ C_\tau(\Omega) \psi_{p,l}^{(LG)}(\tilde{F}, v, \zeta) \right] \times \frac{i \varepsilon^2 l (|l| - 1)}{8T^2 (v + i \operatorname{sgn}(l) \zeta)^2}. \quad (\text{E30})$$

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