

# A VIRTUAL DIELECTRIC EIGENMODE EXPANSION OF HIGH-GAIN FEL RADIATION FOR STUDY OF PARAXIAL WAVE MODE COUPLING\*

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## Abstract

An analytic formulation that uses eigenmodes of a dielectric wave guide to describe the signal field of an FEL is presented. This formulation can provide an efficient characterization of the FEL self-similar eigenmodes and enables a clear descriptive connection to free-space propagation of the input and output radiation. The entire evolution of the radiation wave through the linear gain regime is described with arbitrary initial conditions. By virtue of the flexibility in the expansion basis, this technique can be used to find the direct coupling and amplification of specific modes of interest. A simple transformation converts the derived coupled differential evolution equations into a set of coupled algebraic equations and yields a matrix determinant equation for the FEL eigenmodes. Laguerre-Gaussian modes used as an expansion basis allows investigation of coupling and amplification of optical modes that contain orbital angular momentum, suggesting new regimes of operation for future FELs.

## INTRODUCTION

The electromagnetic (EM) signal field in a free-electron laser (FEL) is optically guided within the source electron beam (e-beam) during exponential gain(1; 2; 3). In this regime, it can be useful to describe the FEL light as a sum over eigenmodes of a virtual waveguide structure(4; 5; 6; 7). This permits investigation of the coupling and propagation characteristics of specific EM mode structures during the interaction. There can also be flexibility in the form of the expansion mode basis such that a specific basis set can be chosen to optimally suit a given FEL geometry. The eigenmodes of a quadratic index fiber as presented here, for example, are particularly useful because they are composed of composite gaussian functions (typically Hermite-Gaussian or Laguerre Gaussian functions) that also arise in the solutions to the paraxial wave equation for free-space propagation(8; 9). This correspondence establishes a useful connection between free-space modes and the optically guided modes of the FEL, providing a model that not only can describe optical mode propagation from startup through high-gain, but also both the input (seeding) and output radiation characteristics.

This framework is motivated in particular by the desire to explore the coupling and propagation characteristics of well-known Laguerre-Gaussian (LG) modes. These modes are of interest since, for the higher-order azimuthal modes, they are known to possess a well-defined value  $l\hbar$  of orbital angular momentum (OAM) as a result of a azimuthal component of the linear momentum(10). Light that carries OAM is a subject of intense research for current and potential applications in microscopy(11), information encoding(12), quantum entanglement schemes(13), Bose-Einstein condensates(14), and molecular transitions(15). Coherent OAM modes allow the possibility of light-driven micro-mechanical devices or the use of torque from photons as a exploratory tool(16). Modes of this type may be particularly relevant for study with modern optical and next-generation x-ray FELs with the ability to probe the structure of matter down to Å length and attosecond time scales. For future FEL light sources with, for example, flexibility in the field polarization (which varies the spin angular momentum of the emitted photons), the ability to directly generate intense higher-order LG modes in situ would further extend the experimental and operational capabilities.

## MODE DESCRIPTION

The radiation fields in the FEL can be expanded in terms of transverse radiation modes of a guiding structure, with slowly-growing amplitudes that vary only as a function of the axis and e-beam propagation coordinate,  $z$ . The electric field is assumed to be dominantly transverse and is given by the modal expansion

$$\mathbf{E}_{\perp}(\mathbf{r}, t) = \text{Re} \left[ \sum_q C_q(z) \tilde{\mathcal{E}}_{\perp q}(\mathbf{r}_{\perp}) e^{i[k_{zq}(\omega)z - \omega t]} \right] \quad (1)$$

where  $\tilde{\mathcal{E}}_{\perp q} = \tilde{\mathcal{E}}_{\perp q} \hat{\mathbf{e}}_{\perp}$  is an eigenfunction of an infinite, ideal wave guide (or optical fiber),  $C_q(z)$  is the mode amplitude,  $\hat{\mathbf{e}}_{\perp}$  is the field polarization vector and  $k_{zq}(\omega)$  is the axial wavenumber of the mode  $q$  at the frequency  $\omega$ . The modes are orthogonal and normalized, with mode power:  $P_q \delta_{q,q'} = (k_{zq}(\omega)/2\mu_0\omega) \text{Re} \left[ \iint \tilde{\mathcal{E}}_{\perp q} \tilde{\mathcal{E}}_{\perp q'}^* d^2\mathbf{r}_{\perp} \right]$ . The total power in the input field is then  $P_T = \sum_q |C_q(0)|^2 P_q$ .

One significant advantage of the orthogonal mode expansion approach is the ability to simplify the 3D excitation equations by writing the field evolution in terms of 1D mode amplitudes, and by integrating over the transverse di-

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mensions to quantify the effective coupling at each position along the interaction. This can be done irrespective of the analytic formalism used to describe the e-beam evolution (ie, Vlasov approach, plasma fluid, etc).

In this paper, we focus on an expansion where  $\tilde{\mathcal{E}}_{\perp q}$  is an eigenmode of a dielectric waveguide with refractive index  $n(\mathbf{r}_{\perp})$ . Assuming small transverse variation,  $\nabla n(\mathbf{r}_{\perp})^2 \ll k$  the dielectric eigenmode equation that defines the expansion basis is

$$\nabla_{\perp}^2 \tilde{\mathcal{E}}_{\perp q}(\mathbf{r}_{\perp}) + [n(\mathbf{r}_{\perp})^2 k^2 - k_{zq}^2] \tilde{\mathcal{E}}_{\perp q}(\mathbf{r}_{\perp}) = 0, \quad (2)$$

where  $k = \omega/c$ . With the expansion fields from Eq. (1) and the dielectric eigenmode equation in Eq. (2), the paraxial wave equation in the presence of a local source current is written in terms of the evolution the mode amplitude  $C_q(z)$  via,

$$\frac{d}{dz} C_q(z) = -\frac{1}{4\mathcal{P}_q} e^{-ik_{zq}z} \iint \tilde{\mathbf{J}}_{\perp}(\mathbf{r}) \cdot \tilde{\mathcal{E}}_{\perp q'}^*(\mathbf{r}_{\perp}) d^2\mathbf{r}_{\perp} \quad (3)$$

$$-i \sum_{q'} \kappa_{q,q'}^d C_{q'}(z) e^{-i(k_{zq} - k_{zq'})z}$$

where

$$\kappa_{q,q'}^d = \frac{\omega\epsilon_0}{4\mathcal{P}_q} \iint [n(\mathbf{r}_{\perp})^2 - 1] \tilde{\mathcal{E}}_{\perp q'}(\mathbf{r}_{\perp}) \cdot \tilde{\mathcal{E}}_{\perp q}^*(\mathbf{r}_{\perp}) d^2\mathbf{r}_{\perp}. \quad (4)$$

This term characterizes the mode overlap in the dielectric, and physically represents the virtual polarization currents that are necessarily subtracted when using eigenmodes of a virtual dielectric waveguide. In the absence of the current term, Eq. (4) describes the propagation of paraxial waves in terms of waveguide eigenmodes.

Guided Laguerre-Gaussian eigenfunctions of an optical fiber are obtained with the refractive index:

$$n(\mathbf{r}_{\perp})^2 = 1 - \left(\frac{r}{z_R}\right)^2, \quad (5)$$

where  $z_R = kw_0^2/2$  is the Rayleigh length and  $w_0$  is the characteristic waist size of a transversely gaussian mode profile. By inserting Eq. (5) into Eq. (2) we obtain(17; 18),

$$\tilde{\mathcal{E}}_{\perp;p,l}(r, \phi) = \tilde{\mathcal{A}}_{p,l} \sqrt{\frac{2}{\pi w_0^2} \frac{p!}{(p+|l|)!}} (-1)^p e^{il\phi} \quad (6)$$

$$e^{-\frac{r^2}{w_0^2}} \left(\frac{r\sqrt{2}}{w_0}\right)^{|l|} L_p^{|l|} \left(\frac{2r^2}{w_0^2}\right)$$

where  $L_p^l(x) = \sum_{j=0}^p (p+l)!(-x)^j/j!(p-j)!(l+j)!$  is an associated Laguerre polynomial and  $\tilde{\mathcal{A}}_{p,l}$  is a normalization constant such that the mode power is  $P_{p,l} = (k_{z;p,l}(\omega)/2\mu_0\omega)|\tilde{\mathcal{A}}_{p,l}|^2$ . The mode index is double-valued:  $q = (p, l)$ , with  $p$  corresponding to the radial modes and  $l$  to the azimuthal modes. (The different indices are used interchangeably throughout.) The eigenmodes in Eq (7) are identical in the transverse dependence FEL Theory

to free-space LG fields that satisfy the paraxial wave equation when the free-space modes are evaluated at the optical beam waist. The explicit dependence on the Rayleigh length  $z_R$  in Eq. (5) defines a specific form for the dielectric profile in which a free-space Laguerre-Gaussian mode with waist size  $w_0$  at frequency  $\omega$  will propagate as a guided eigenmode of the virtual dielectric. The axial wavenumbers determined by Eq. (2) are,

$$k_{z;p,l}^2 = k^2 - \frac{4}{w_0^2} (2p + |l| + 1). \quad (7)$$

With Eq. (7) the dielectric mode overlap parameter  $\kappa_{q,q'}^d$  can be solved analytically(6).

## E-BEAM EVOLUTION

The e-beam evolution is solved in a linear cold plasma fluid model with the density given by

$$n(\mathbf{r}, t) = n_0 f(\mathbf{r}_{\perp}) + \text{Re}[\tilde{n}_1(\mathbf{r}) e^{i\omega(z/v_0 - t)}] \quad (8)$$

where  $n_0$  is the electron density,  $f(\mathbf{r}_{\perp})$  is the transverse density profile of the e-beam,  $\tilde{n}_1(\mathbf{r})$  is the spatial density perturbation and  $v_0$  is the axial velocity. The transverse divergence of the current density modulation is assumed to be small compared with the longitudinal variation such that the continuity equation is  $\partial \tilde{J}_z / \partial z = -i\omega e \tilde{n}_1(\mathbf{r})$ . With the longitudinal Lorentz force equation in the presence of both the magnetostatic undulator field and the electromagnetic input fields, the density evolution equation is written as(5)

$$\left[\frac{d^2}{dz^2} + \theta_p^2 f(\mathbf{r}_{\perp})\right] \tilde{n}_1(\mathbf{r}) = -g_{\perp} k_p^2 f(\mathbf{r}_{\perp}) \frac{\epsilon_0 c K}{2\gamma e \omega} \sum_{q'} C_{q'}(z)$$

$$\times [k_{zq'} + k_w]^2 \mathcal{E}_{\perp q'}(\mathbf{r}_{\perp}) e^{-i\theta_{q'} z}, \quad (9)$$

where  $\theta_p = \sqrt{e^2 n_0 / \gamma \gamma_z^2 \epsilon_0 m_e v_0^2}$  is the longitudinal plasma wave number,  $\theta_{q'} = \omega/v_0 - (k_{zq'}(\omega) + k_w)$  is the detuning of the input mode relative to the e-beam energy,  $\gamma_z^2 = (1 - \beta_z^2)^{-1}$ ,  $\gamma^2 = \gamma_z^2 (1 + K^2)$ ,  $K = e|\tilde{\mathcal{B}}_w|/m_e c k_w$  is the undulator parameter,  $|\tilde{\mathcal{B}}_w|$  is the field amplitude of the undulator and  $\lambda_w = 2\pi/k_w$  is the undulator wavelength. The undulator field is  $\mathbf{B}_w = \text{Re}\{|\tilde{\mathcal{B}}_w| \hat{\mathbf{e}}_w e^{-ik_w z}\}$  with polarization vector  $\hat{\mathbf{e}}_w$ . The transverse velocity due to the magnetic undulator field is  $\tilde{\mathbf{v}}_{\perp w} = (-icK/\gamma) \hat{\mathbf{e}}_z \times \hat{\mathbf{e}}_w$ . Polarization alignment between input field and the electron motion in the undulator is given by  $g_{\perp} = \hat{\mathbf{e}}_{\perp} \cdot (\hat{\mathbf{e}}_z \times \hat{\mathbf{e}}_w^*)$ . The transverse component of the current density that excites the signal wave is written in terms of the density modulation as

$$\tilde{\mathbf{J}}_{\perp}(\mathbf{r}) = -\frac{1}{2} e \tilde{n}_1(\mathbf{r}) \tilde{\mathbf{v}}_{\perp w} e^{-ik_w z}. \quad (10)$$

Equation (9) describes the evolution of the density modulation in the presence of longitudinal space charge effects (second term, left hand side) and the ponderomotive fields (right hand side). In the mode expansion approach, it is convenient to express the density perturbation  $\tilde{n}_1(\mathbf{r})$  as a

sum over the expansion eigenmodes such that the orthogonality of the basis can be used to compactly write the density evolution equation (9) in terms of spatial modulation amplitudes. We write,

$$\tilde{n}_1(\mathbf{r}) = \frac{k\epsilon_0}{e} \sum_q a_q(z) \tilde{\mathcal{E}}_{\perp q}(\mathbf{r}_{\perp}). \quad (11)$$

Plugging this expansion into Eq. (9), both sides are then multiplied by  $\tilde{\mathcal{E}}_{\perp q}^*$  and integrated over the transverse coordinate. With Eq. (10) and Eq. (4), the coupled FEL excitation equations are

$$\begin{aligned} \frac{d}{dz} C_q(z) &= -i\xi_q g_{\perp}^* a_q(z) e^{i\theta_q z} \\ &\quad - i \sum_{q'} \kappa_{q,q'}^d C_{q'}(z) e^{i(\theta_{q'} - \theta_q)z}, \\ \frac{d^2}{dz^2} a_q(z) + \theta_p^2 \sum_j \mathbb{F}_{q,j} a_j(z) &= \\ &\quad - \frac{1}{\xi_q} \sum_{q'} Q_{q,q'} C_{q'}(z) e^{-i\theta_{q'} z}, \end{aligned} \quad (12)$$

where  $\xi_q = Kk^2/4\gamma k_{zq}$ . The coupling between the e-beam and the signal field is given by the mode coupling coefficient:

$$Q_{q,q'} = g_{\perp} \theta_p^2 \frac{(k_{zq'} + k_w)^2}{8k_{zq}} \left(\frac{K}{\gamma}\right)^2 \mathbb{F}_{q,q'}. \quad (13)$$

where  $\mathbb{F}_{q,q'}$  is the beam profile overlap coefficient and quantifies the spatial overlap of the e-beam profile with the expansion modes:

$$\mathbb{F}_{q,q'} = \frac{\iint f(\mathbf{r}_{\perp}) \tilde{\mathcal{E}}_{\perp q'}(\mathbf{r}_{\perp}) \tilde{\mathcal{E}}_{\perp q}^*(\mathbf{r}_{\perp}) d^2\mathbf{r}_{\perp}}{\iint |\tilde{\mathcal{E}}_{\perp q}(\mathbf{r}_{\perp})|^2 d^2\mathbf{r}_{\perp}}. \quad (14)$$

The coupling to any arbitrary transverse e-beam profile can be computed using Eq. (14), with analytic solutions available in the LG basis for several analytic forms including flat (“beer-can”), parabolic and gaussian distributions(6). Equation (12) fully describes the field evolution and density bunching evolution of the e-beam with arbitrary initial conditions on the bunching  $a_q(0)$ , velocity modulation  $da_q(0)/dz$  and input field amplitudes  $C_{q'}(0)$ . Note that with the coupling turned off ( $Q_{q,q'} = 0$ ), Eq. (12) describes the evolution due only to longitudinal space-charge oscillations, with the density mode amplitudes coupled to each other through  $\mathbb{F}_{q,q'}$ . This contribution is valid when the characteristic e-beam radius satisfies  $r_0 \gtrsim \lambda\gamma_z$ , and is useful for calculation of the overall density and velocity bunching amplitudes of the e-beam over a drift. Longitudinal space-charge can also have a significant contribution to the e-beam dynamics during the FEL interaction.

## SUPERMODES

During exponential gain, the eigensolutions to Eqs. (12) are the combinations of the expansion mode profiles that

propagate self-similarly, i.e., with constant amplitude coefficients and with distinct complex wavenumbers(19). In the presence of gain, each supermode wavenumber will be different from the wavenumber of free-space and can be written with a complex valued perturbation  $\tilde{\delta}k$  that is due to the FEL interaction  $k_{SM} = k + \tilde{\delta}k$ , where  $\text{Re}\{\tilde{\delta}k\}$  anticipates an effective modified refractive index to that of free-space (guiding), and  $\text{Im}\{\tilde{\delta}k\}$  is related to the exponential gain. Since the supermodes evolve after the initial startup period and have fixed transverse profiles along  $z$ , one can substitute  $C_q(z) = b_q e^{i(k_{SM} - k_{zq})z}$  for the mode amplitude coefficients Eq. (1). Inserting this transformation into Eq. (12) converts the coupled second-order differential equations into a set of coupled algebraic equations written in matrix form,

$$\left[ \left[ \underline{\mathbf{I}}(\tilde{\delta}k - \theta)^2 - \theta_p^2 \underline{\mathbf{M}} \right] \left[ \underline{\mathbf{I}}\tilde{\delta}k + \underline{\kappa}^d - \underline{\Delta}k \right] + \underline{\mathbf{Q}} \right] \underline{b} = 0. \quad (15)$$

The matrix elements of  $\underline{\mathbf{M}}$  are given by  $\mathbb{M}_{q,q'} = (k_{zq'}/k_{zq})\mathbb{F}_{q,q'}$ , and similarly for  $\underline{\kappa}^d = \{\kappa_{q,q'}^d\}$ ,  $\underline{\mathbf{Q}} = \{Q_{q,q'}\}$ , and  $\underline{\Delta}k = \{\Delta k_q \delta_{q,q'}\}$ . The matrix  $\underline{\mathbf{I}}$  is the identity. The supermode coefficients  $b_q$ , which are elements of the column vector  $\underline{b}$  are given by solutions to Eq. (15). The dominant, or highest gain supermode coefficients correspond to the solution that yields the most negative value of  $\text{Im}\{\tilde{\delta}k\}$ , defined to be  $\delta k_i$ . The full complex valued solution  $\tilde{\delta}k = \tilde{\delta}k_r + i\tilde{\delta}k_i$ , with the corresponding set of eigenvalue coefficients  $b_q$  define the dominant supermode field of the FEL. The 3D power gain length, or e-folding length is given by  $L_G = 1/|2\tilde{\delta}k_i|$ . Solutions to Eq. (15) have been shown to be equivalent(7) to solutions in the cold beam limit given by an alternate formulation which describes the interaction through the coupled Maxwell-Vlasov equations(19).

In the 1D limit the matrix elements are degenerate:  $\underline{\mathbf{F}} \rightarrow \underline{\mathbf{I}}$  and  $\underline{\kappa}^d, \underline{\Delta}k \rightarrow \underline{\mathbf{0}}$ , and Eq. (15) effectively reduces to the familiar FEL cubic equation with gain parameter  $\underline{\mathbf{Q}} \rightarrow \underline{\mathbf{I}}\underline{\mathbf{Q}} = \underline{\mathbf{I}}(\theta_p \theta_s)^2 k/4 = \underline{\mathbf{I}}(2k_w \rho)^3$  where  $\rho$  is the well-known Pierce parameter often used in FEL theory(20).

## SINGLE GAUSSIAN MODE

During high-gain, the proper balance between the natural diffraction of the coherent radiation and the guided focusing of the radiation due to the e-beam determines the eventual spot size  $w_{SM}$  of the EM supermode field. This can be obtained with the dielectric expansion formulation in a natural way, through the solutions to the excitation equations, or can be estimated by assuming that a single gaussian mode (SGM) structure closely approximates the supermode profile. An analytic form for the approximate SGM size  $w_g$  has been derived for a gaussian e-beam  $f(\mathbf{r}_{\perp}) = \exp(-r^2/r_0^2)$  in Ref. (5):

$$\left(1 + \frac{w_g^2}{2r_0^2}\right) \left[1 - \frac{1}{k w_g^2 k_w \rho}\right]^3 = 1 \quad (16)$$

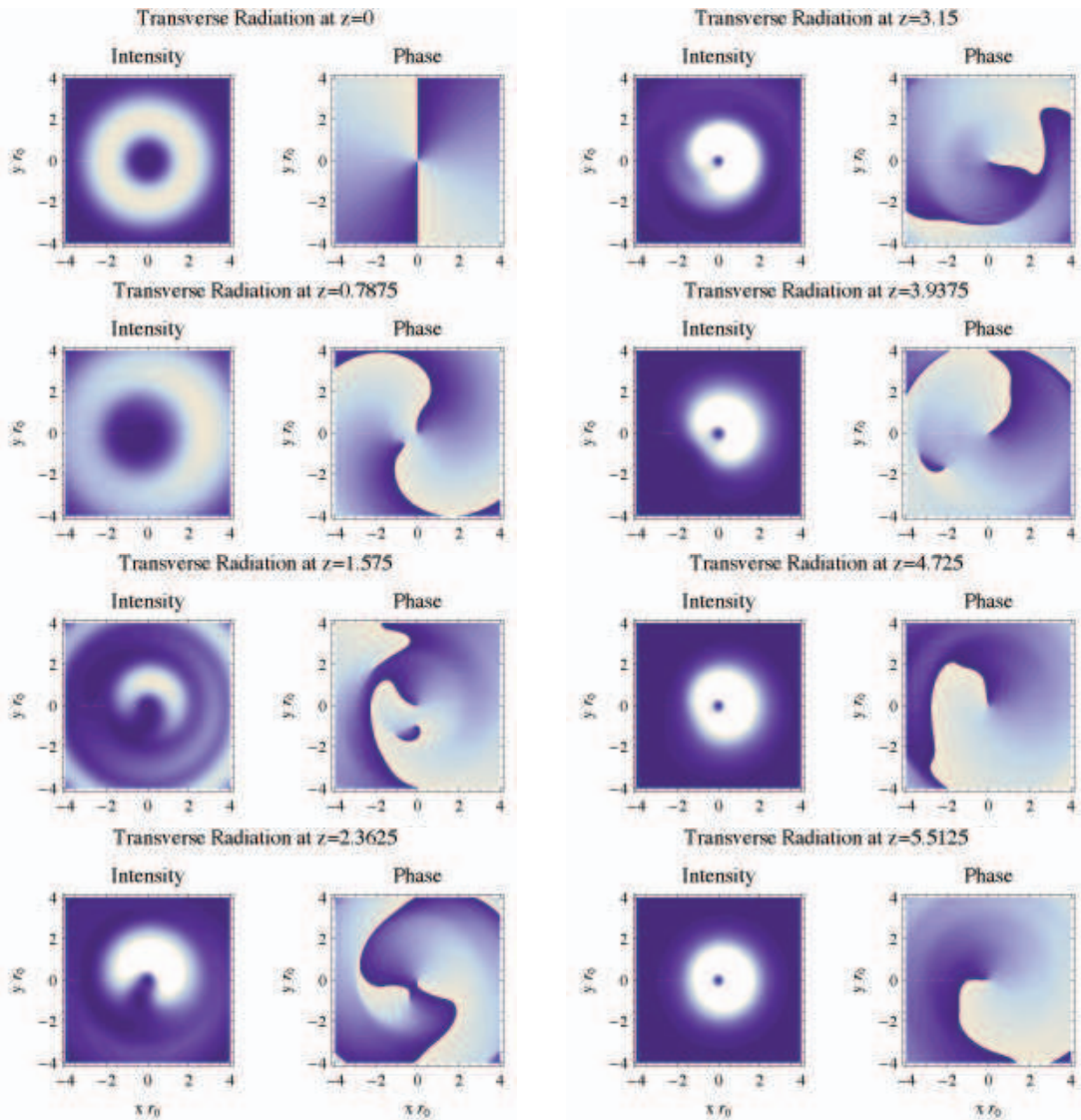


Figure 1: Intensity and phase along the undulator for an  $l = 2$  optical seed on a cold Gaussian e-beam, helically pre-punched for superradiant emission of an  $l = 1$  OAM mode. The  $l = 1$  mode has larger gain, and is the dominant mode at the end of the undulator.

and also provides a useful starting value for the expansion basis spot size  $w_0$  which can be used to streamline the computation of the full solutions.

## OAM COUPLING AND DISPERSION

It is interesting to note the form of the coupling in the case of an axisymmetric e-beam  $f(\mathbf{r}_\perp) = f(r)$ . With the simple azimuthal dependence of the LG basis in Eq. (7), the overlap integral in Eq. (14) is trivial and clearly demonstrates that the different azimuthal modes do not couple to each other:

$$\mathbb{F}_{(p,l),(p',l')} \propto 2\pi\delta_{l,l'}. \quad (17)$$

The excitations equations can therefore be solved for each azimuthal mode independently, allowing one to find the amplification and propagation of modes that contain OAM

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directly.

The presence of multiple azimuthal modes in the e-beam can reveal detailed information on the gain, guiding and microbunching characteristics that would otherwise be obscured with purely radial modes. Since each OAM mode couples to the electron bunch differently, they each have different gain curve and therefore different effective optical guiding. This leads to longitudinal mode dispersion where each OAM mode propagates at its own phase velocity, resulting in observable variation in the transverse intensity profile along the interaction length(7). Figure 1 shows the evolution of two simultaneous OAM modes – one excited by optical seeding, the other by superradiant emission. The on-axis topological singularity at the undulator entrance characteristic of the  $l = 2$  input optical mode is deformed and eventually replaced by a singularity with

topological charge 1, characteristic of the dominant  $l = 1$  mode. During the evolution, spiral intensity structures are observed in the intensity while isolated paired singularities are shown to appear (at  $z = 1.575$  and  $z = 3.9375$ ) and disappear in the transverse phase. Such structures demonstrate a complex interaction dynamic as the optical beam that carries  $2\hbar$  units of OAM per photon at the entrance is amplified and evolves into a dominant mode with  $\hbar$  units of OAM per photon. Future investigations could shed light on this issue in detail, showing exactly how much of the total orbital angular momentum may be transferred to, or extracted from the e-beam in this process, and how much may become coupled to the spin off-axis.

We note also that excitation of an  $l = l_0$  optical OAM mode at the fundamental frequency necessarily excites the same azimuthal mode structure in the e-beam [Eq. (11)]. Amplification of the pure OAM mode tends to bunch the e-beam into a continuous helix (or multiply twisted helices for  $|l| > 1$ ) longitudinally. The fundamental mode, which also may be present in the beam from shot noise, also tends to bunch the beam during gain, but into longitudinally separated microbunches. If two different azimuthal modes are present then both bunching processes will compete, the one corresponding to the larger coupling eventually dominating. During the mode competition, a portion of the e-beam along the transverse profile may therefore be resonant with both modes and amplify, while another portion may be out of phase with one mode and be suppressed. The peak intensity will therefore grow off-axis (Figure 1 at  $z = 1.575$ ) until the modal dispersion and asymmetric gain between the modes eventually leads to a dominant, single supermode ( $z = 5.5125$ ). Numerical simulations using GENESIS(21) with a cold-beam have confirmed this scenario, but more work remains to determine the full effects of emittance and betatron motion on the correlated bunching processes described here.

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