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A virtual dielectric eigenmode expansion of high-gain FEL radiation for study of paraxial wave mode coupling

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ABSTRACT

An expansion of guided free-electron laser radiation is presented in terms of eigenmodes of a transversely varying dielectric waveguide. For a particular quadratic distribution of the refractive index, the constituent eigenmode expansion basis is equivalent to a free-space paraxial basis evaluated at the mode waist, which facilitates investigations of guided coupling to naturally diffracting Gaussian modes over many Rayleigh lengths. A set of coupled differential equations is derived for the slowly varying field mode amplitude coefficients and the longitudinal electron density bunching in the cold-beam fluid approximation. Preliminary results calculated in this formulation show that selective amplification of dominant higher-order modes, particularly azimuthal modes, can be achieved by seeding with higher-order spatial modes and by selective density pre-bunching of the electron beam.

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1. Introduction

High-gain free-electron lasers (FELs) exhibit radiation gainguiding, a well-known phenomena that occurs during light amplification when the coherent interaction between the source electron beam (e-beam) and the electromagnetic (EM) field introduces an inward curvature in the phase front of the light, refracting it back towards the lasing core of the e-beam [1–3]. The e-beam behaves like an optical guide for the EM field, which eventually settles into a selfsimilar eigenmode of the FEL system (supermode) that propagates with a fixed transverse profile and spot size [4,5].

Guided modes have been previously explored analytically by direct derivation of the eigenmode equations from the coupled Maxwell–Vlasov equations [4,6–9], and through expansions of the FEL signal fields in terms of step-index fiber modes [3], eigenmodes of a hollow conducting-boundary waveguide [5], and free-space paraxial waves [10,11]. Since, in an FEL, the e-beam operates simultaneously as an optical source and as a guiding structure, an EM mode description of the FEL light permits investigation of the guiding characteristics, amplification and coupling of individual EM modes to the e-beam. In the case of an FEL that lacks an external waveguide structure (beyond the e-beam), it is natural to explore the coupling to the ubiquitous Hermite–Gaussian (HG) or Laguerre–Gaussian (LG) modes that describe free-space wave propagation in the paraxial limit. However, since these modes naturally diffract, we show that the propagation and gain-guiding of these modes over many Rayleigh lengths in an FEL interaction can be better investigated by an expansion of the radiation field in terms of guided eigenmodes of a quadratic index medium (QIM). These modes are described by an eigenmode basis that is equivalent to the free-space paraxial mode basis evaluated at the waist [12]. This connection to freespace modes is useful for characterizing the propagating radiation fields emitted from the FEL and for understanding input radiation coupling, as in the case of seed radiation injection. Even though the guiding mechanism in the FEL is different than in a QIM, the FEL modes may be very similar in spatial profile to a simple combination of QIM eigenmodes. In such cases, the LG or HG eigenmodes of a QIM, with slowly growing amplitude coefficients, serve as an excellent basis set for the FEL signal field.

The coupling of higher-order spatial modes to the e-beam in an FEL is of increasing recent interest, particularly due to the development of high-brightness, X-ray FELs for investigations of molecular and atomic scale processes relevant to both physics and biology. Spatial structure in the transverse intensity distribution of such a coherent light source can be used to reveal specific information about a target sample. Precise combinations of Gaussian and hollow (donut) modes have been used, for example, in Stimulated Emission Depletion (STED) microscopy as a tool for sub-diffraction limited fluorescence imaging [13]. Hollow modes, in the form of higher-order azimuthal LG modes, have recently been a topic of intense research since such modes are known to possess orbital angular momentum (OAM) as a consequence of an azimuthal component of the linear momentum [14]. For nextgeneration X-ray FELs that will have the ability to probe the structure of matter on short length and time scales, the generation

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of such modes may be relevant, since the OAM can be transferred from the photon field to the sample material. Such interactions using conventional laser sources have been previously shown to drive target particles to rotate or orbit the EM beam axis, allowing the possibility of light driven mechanical devices, or the use of torque from photons as a exploratory tool [15]. Though most OAM modes in the longer wavelengths can be readily generated using optical mode-conversion elements placed in the beam path, modern high power X-ray FELs may render such extrinsic methods impractical due to size constraints (if optical elements are needed with feature sizes that scale as the wavelength) or damage constraints. For this reason, it is of interest to explore the possibility of generating dominant OAM modes through intrinsic coupling to the source e-beam. The coupling to these modes, as well as to other higher-order paraxial modes, can be investigated directly by an expansion of the high-gain FEL radiation field in terms of guided eigenmodes of a QIM.

In this work, we present a description of guided FEL light through an expansion of the radiation field in terms of dielectric waveguide eigenmodes. From the general expression for the slowly varying field amplitudes, a quadratic form is taken for the distribution of the virtual refractive index, yielding a set of guided LG paraxial modes as a basis for the FEL radiation. A cold-beam approximation is used to describe the e-beam current density, and a set of coupled excitation equations is obtained for the FEL field amplitudes and the axial e-beam density bunching. The coupling to higher-order modes is discussed and preliminary results are given from calculations of radiation seeding (FEL amplifier) and helical pre-bunching of the e-beam to generate and amplify higher-order spatial modes.

2. Field expansion and waveguide mode excitation

In a structure of axial translational symmetry, the radiation fields can be expanded in terms of transverse radiation modes with amplitudes that vary only as a function of the symmetry axis, *z*. Neglecting backward propagating waves and approximating the fields as dominantly transverse, the radiation field expansion in terms of waveguide modes is

$$\underline{\tilde{E}}_{\perp}(\underline{r}) = \sum_{q} C_{q}(z) \underline{\tilde{\mathscr{E}}}_{\perp q}(r_{\perp}) \mathbf{e}^{ik_{zq}z}$$
⁽¹⁾

and similarly for the magnetic field $\underline{\mathscr{H}}_{\perp q} = (1/Z_q)\hat{e}_z \times \underline{\mathscr{E}}_{\perp q}$, where k_{zq} is the *q*th mode axial wavenumber, and $Z_q = (k/k_{zq})\sqrt{\mu_0/\varepsilon_0}$ for TE modes. The modes form a complete orthogonal set and are normalized to the mode power

$$\mathscr{P}_{q}\delta_{q,q'} = \frac{1}{2}\operatorname{Re} \iint [\underline{\tilde{\mathscr{E}}}_{\perp q}(r_{\perp}) \times \underline{\tilde{\mathscr{H}}}_{\perp q'}^{*}(r_{\perp})] \cdot \hat{e}_{z} \, \mathrm{d}^{2}\mathbf{r}.$$
⁽²⁾

The expansion mode $\tilde{\mathscr{E}}_{\perp q}$ is an eigenmode of a dielectric medium with transverse variation in the refractive index $n(r_{\perp})$. Assuming $\nabla n^2 \ll k$, the eigenmode equation is

$$\nabla_{\perp}^{2} \underline{\tilde{\mathscr{E}}}_{\perp q}(r_{\perp}) + [n(r_{\perp})^{2}k^{2} - k_{zq}^{2}]\underline{\tilde{\mathscr{E}}}_{\perp q}(r_{\perp}) = 0$$
(3)

where $k = \omega/c$. With Eqs. (1) and (3) the excitation equation for the mode *q* in the presence of a source current is given by

$$\frac{\mathrm{d}}{\mathrm{d}z}C_{q}(z) = -\frac{1}{4\mathscr{P}_{q}}\mathrm{e}^{-\mathrm{i}k_{zq}z} \iiint_{\underline{j}_{\perp}} (\mathbf{r}) \cdot \underbrace{\tilde{\mathscr{E}}_{\perp q}^{*}}_{\mathcal{E}_{\perp}}(r_{\perp}) \,\mathrm{d}^{2}\mathbf{r}
-\mathrm{i}\sum_{q'} C_{q'}(z)\mathrm{e}^{-\mathrm{i}\Delta k_{zqq'}z}\kappa_{q,q'}^{d}$$
(4)

where

$$\kappa_{q,q'}^{d} = \frac{\omega \varepsilon_{0}}{4 \mathscr{P}_{q}} \iint [n(r_{\perp})^{2} - 1] \underline{\tilde{\mathscr{E}}}_{\perp q'} \cdot \underline{\tilde{\mathscr{E}}}_{\perp q}^{*} d^{2} \mathbf{r}$$
(5)

and $\Delta k_{zqq'} = k_{zq} - k_{zq'}$ is the difference between the axial wavenumbers of the modes q and q'. The term $\kappa_{q,q'}^d$ characterizes the mode overlap in the dielectric and represents the virtual polarization currents and charges that must be subtracted when using eigenmodes of a dielectric waveguide, since here no such structure exists in the physical system.

3. E-beam fluid model and coupled excitation equations

A linear plasma fluid model for a cold e-beam (negligible energy spread) can be used to describe the signal excitation in an FEL interaction [5]. A relativistic e-beam in an FEL experiences transverse oscillations driven by the interaction with the periodic structure. This motion drives an axial ponderomotive force that modulates the axial electron velocity such that, to first-order, the axial velocity of a cold beam within a static undulator can be expanded as $v_z(\underline{r}, t) = v_{z0} + \text{Re}[\tilde{v}_{z1}(\underline{r})e^{-i\omega t}]$ where $v_{z0} = \beta_z c$ is the d.c. component and \tilde{v}_{z1} is the perturbation oscillating at signal frequency ω . Longitudinal variations in the velocity, like those found in planar undulator systems, are ignored for the moment. The velocity modulation \tilde{v}_{z1} develops a density bunching modulation that is similarly described in a linear model as n(r, t) = $n_0 f(r_{\perp}) + \text{Re}[\tilde{n}_1(\underline{r})e^{-i\omega t}]$ where n_0 is the on-axis electron density and $f(r_{\perp})$ is the transverse density profile of the e-beam. The a.c. component of the longitudinal current density results from both the axial velocity and density perturbations and is $\tilde{J}_{z}(\underline{r}) = -e[n_{0}f(r_{\perp})\tilde{v}_{z1}(\underline{r}) + v_{z0}\tilde{n}_{1}(\underline{r})].$ If the transverse divergence of the current perturbation is assumed small $\nabla_{\perp} \cdot \tilde{J}_{\perp} \ll \partial \tilde{J}_{z} / \partial z$, the continuity equation can be written as $d\tilde{J}_z/dz = -i\omega e\tilde{n}_1(\underline{r})$. The transverse component of the current density that excites the signal wave is written in terms of the density perturbation as

$$\tilde{J}_{\perp}(\underline{r}) = -\frac{1}{2}e\tilde{n}_{1}(\underline{r})\tilde{\underline{\nu}}_{\perp w}e^{-ik_{w}z}$$
(6)

where $\underline{\tilde{v}}_{\perp w}$ is the transverse velocity vector and k_w is the axial wavenumber of the periodic undulator lattice.

From the expressions for the current density and the relativistic force equation for the axial velocity perturbation, the density bunching can be expressed as a second-order differential equation [5]. It is useful to define the density bunching parameter

$$\tilde{\mathbf{i}}_{q}(z) = \frac{e}{8\mathscr{P}_{q}} e^{-\mathrm{i}(\omega/\nu_{z0})z} \iint \tilde{\mathbf{n}}_{1}(\underline{r}) \underline{\tilde{\nu}}_{\perp w} \cdot \underline{\tilde{\mathscr{E}}}_{\perp q}^{*}(r_{\perp}) \, \mathrm{d}^{2}\mathbf{r}.$$
(7)

By combining the density modulation equation from Ref. [5] with Eqs. (4) and (7) we obtain a coupled form for the mode excitation evolution equations:

$$\frac{d}{dz}C_{q}(z) = \tilde{\mathbf{i}}_{q}(z)e^{i\theta_{q}z} - i\sum_{q'}\kappa^{d}_{q,q'}C_{q'}(z)e^{-i\Delta k_{z,qq'}z} \left[\frac{d^{2}}{dz^{2}} + \theta^{2}_{pr}\right]\tilde{\mathbf{i}}_{q}(z) = i\sum_{q'}Q_{q,q'}C_{q'}(z)e^{-i\theta_{q'}z}$$
(8)

where $\theta_q = \omega/v_{z0} - (k_{zq} + k_w)$ is the characteristic detuning parameter for a given mode. The coupling between the e-beam and the FEL radiation field is given by the parameter $Q_{q,q'} = \theta_p^2 \kappa_{q,q'}$ in Eq. (8) where $\theta_p = (e^2 n_0 / \gamma \gamma_z^2 \varepsilon_0 m_e v_{z0}^2)^{1/2}$ is the longitudinal plasma wavenumber of a uniformly distributed e-beam profile used in a 1D model. The e-beam mode-coupling coefficient $\kappa_{q,q'}$ is

$$\kappa_{q,q'} = \frac{\varepsilon_0(k_{zq'} + k_w)}{8\mathscr{P}_q} \iint f(r_\perp) \tilde{\mathscr{E}}_{pm,q'} \underline{\tilde{\nu}}_{\perp w} \cdot \underline{\tilde{\mathscr{E}}}_{\perp q}^* \, \mathrm{d}^2 \mathbf{r}. \tag{9}$$

The polarization of the radiation field and the transverse electron motion in the undulator are assumed to be in the same direction (in FEL seeding scenarios this may not be a given). The axial ponderomotive field is $\tilde{\mathscr{E}}_{pm,q}(r_{\perp}) = \frac{1}{2} [\tilde{\mathcal{V}}_{\perp q} \times \underline{\mathscr{D}}_{\perp w}^* + \underline{\widetilde{\mathcal{V}}}_{\perp w}^* \times \underline{\mathscr{D}}_{\perp q}] \cdot \hat{e}_z$ where $\tilde{v}_{\perp q}$ is the transverse electron velocity due to the

Lorentz force of the *q*th mode of the signal field, $\tilde{\mathscr{B}}_{\perp W}$ is the transverse magnetic field of the undulator and $\tilde{\mathscr{B}}_{\perp q} = \mu_0 \tilde{\mathscr{H}}_{\perp q}$. The term $JJ = [J_0(\alpha) - J_1(\alpha)]^2$ can be included in the coupling parameter $\kappa_{q,q'}$ for a strong planar undulator (JJ = 1 for a helical undulator geometry), where J_0 and J_1 are the first- and second-order Bessel functions and $\alpha = K^2/(4 + 2K^2)$ where $K = e|\tilde{\mathscr{B}}_{\perp W}|/mck_W$ is the undulator parameter. The relativistic factor is $\gamma = \gamma_z \sqrt{1 + K^2/2}$ with $\gamma_z^2 = 1/(1 - \beta_z^2)$.

The effects of longitudinal space charge in the beam are consolidated into the finite-width beam parameter $\theta_{pr} = \bar{r}\theta_p$, which assumes a single plasma mode. The plasma reduction factor satisfies $|\bar{r}| \leq 1$, and can be calculated numerically for a specific e-beam geometry [10]. In the limit that the e-beam radius is large compared to the bunching wavelength, $\lambda \gamma_z \ll r_0$, one can make the approximation $\bar{r} \simeq 1$.

The first equation in Eqs. (8) describes the excitation of the mode amplitude C_q due to the density perturbation and transverse wiggling motion of the electrons throughout the FEL interaction. The second equation in Eqs. (8) describes the evolution of the modal density bunching \mathbf{i}_q through the e-beam coupling to the expansion modes.

The initial conditions for Eqs. (8) specify the operating characteristic of the FEL. For example, when operating as a single-pass amplifier (seeded FEL) there is negligible initial density and velocity modulation $\tilde{\mathbf{i}}_q(0), d\tilde{\mathbf{i}}_q(z)/dz|_{z=0} = 0$ and the initial seed field is non-zero $C_q(0) \neq 0$. Alternately, for a self-amplified spontaneous emission FEL (SASE), the amplified shot noise can be related to the pre-bunching conditions $\tilde{\mathbf{i}}_q(0) \neq 0$, $d\tilde{\mathbf{i}}_q(z)/dz|_{z=0} = 0$ and the input signal field vanishes $C_q(0) = 0$.

4. LG mode expansion

The choice of the refractive index $n(r_{\perp})$ in Eq. (3) determines the form of the basis expansion used in the excitation equations (8). For example, a step-profile optical fiber model yields Bessel and Hankel functions for the field inside and outside, respectively, [3]. For a continuous, weakly guiding QIM of the form $n^2(r) = n_0^2 - (r/z_R)^2$, where $z_R = kw_0^2/2$ is the Rayleigh length and w_0 is the characteristic waist size of the fundamental mode, the expansion basis consists of a complete orthogonal set of LG functions [16–18]. Since LG modes also occur as solutions to the cylindrical paraxial wave equation, this choice for the refractive index identifies the desired connection between the guided mode expansion and a description of the FEL system using paraxial, diffracting modes of free-space [12].

LG modes provide a convenient working basis to model the FEL radiation for geometries that are largely axisymmetric over the interaction length. The complete LG mode basis can also be readily transformed into a basis of HG functions, suitable for rectilinear geometries. The LG modes have the form

$$\tilde{\mathscr{E}}_{\perp;p,l}(r,\phi) \propto e^{-il\phi} e^{-r^2/w_0^2} \left(\frac{r\sqrt{2}}{w_0}\right)^{|l|} L_p^{|l|} \left(\frac{2r^2}{w_0^2}\right)$$
(10)

where L_p^l is an associated Laguerre polynomial. The mode index q takes on two values (p, l) corresponding to the radial and azimuthal mode indices, respectively. The axial wavenumber associated with each mode $k_{zq} = k_{z;p,l}$ is given by

$$k_{z;p,l}^2 = k^2 n_0^2 - \frac{4}{w_0^2} (2p+l+1).$$
(11)

The refractive index on axis of the virtual dielectric can be taken as $n_0^2 \simeq 1$. The expansion waist size w_0 is arbitrary, but can be chosen to be on the order of the transverse e-beam size r_0 to facilitate efficiency in modeling the beam evolution with only a finite number of expansion modes.

It is noted that the LG modes of Eq. (10), as well as those of a free-space paraxial system, possess an axial field component for both the electric and magnetic fields. The magnitude of each respective axial field component is on the order of λ/w_0 relative to the principle transverse component, and can be suitably neglected, validating the approximation made in deriving the amplitude evolution equation for transverse fields in Eq. (4) [19].

5. OAM mode amplification in a cold beam

The coupling of the e-beam to azimuthal modes can be shown by inspection of Eq. (9) if the coupling coefficient $\kappa_{p,l,p',f'}$ yields a non-zero value for modes with |l| > 0. In general, a transverse ebeam distribution given by the real function $f(r_{\perp})$ will couple to both +l and -l modes equally. The resulting signal field may have azimuthal structure, but will not possess a net value of OAM. Generation of a dominant OAM mode can occur if a preferential geometric chirality is intrinsic to the system. Such is the case if, for example, either the seed laser contains OAM or if the e-beam has a strong helical perturbation along the longitudinal axis that will excite a helical phase structure in the radiation field.

It is noted that, in the LG mode description, since each photon generated by the e-beam with azimuthal mode number *l* has *lh* units of OAM, the source e-beam will experience an opposing torque. This small effect on the transverse velocity can be included in the expression for the transverse current through the term $\tilde{v}_{\perp q}$. It is typically small compared to the transverse velocity due to the undulator $(|\tilde{v}_{\perp q}/\tilde{v}_{\perp w}| \sim |\hat{\mathscr{B}}_{\perp q}/2\gamma_z^2 \hat{\mathscr{B}}_{\perp w}|)$ and is presently neglected.

Amplification of a pure OAM input mode (OAM seeding with SASE effects turned off) can be examined with the injection of a $l_s > 0$ LG mode at the undulator entrance. The mode couples to the e-beam at the characteristic mode detuning value $\theta = \theta_{p_s, l_s} + k_{z;p_s, l_s} - k_z$. The calculated evolution of both the radiation spot size and the differential power gain for three LG seed modes is shown in Fig. 1. Input parameters from the Visible to Infrared SASE or Seeded Amplifier (VISA) FEL at Brookhaven National Laboratory are used in the calculations [21–23]. The VISA FEL is ideal for investigations of LG mode amplification since it has previously produced both hollow and spiral transverse EM intensity patterns that are suggestive of single or multiple interfering OAM modes [24].

A Gaussian transverse e-beam density distribution, $f(r) = \exp(-r^2/r_0^2)$, is assumed. Results indicate a decrease in the differential power gain for an increase in the azimuthal mode number of the seed field mode. This is attributed to the reduction in the effective coupling between the e-beam and the field for increasing *l* values, as given by Eq. (9), since the radial profile of modes with $|l| \neq 0$ vanishes on axis. It is interesting to note that, in the cold-beam approximation with a axisymmetric Gaussian density distribution, there is no cross-coupling between modes where $l \neq l'$ in Eq. (9). As a result, the azimuthal mode number of the input beam is preserved and the characteristic spot size of the FEL supermode varies accordingly.

Generation of coherent OAM light without a seed field input can be investigated using a dominant helical density perturbation on the e-beam. The density term in Eq. (7) can be written as a sum over helical perturbations on the Gaussian e-beam,

$$\tilde{\mathsf{n}}_1 = \mathsf{n}_0 \mathrm{e}^{-r^2/r_0^2} \sum_l \tilde{\varepsilon}_l \mathrm{e}^{-\mathrm{i}l\phi} \tag{12}$$

where the perturbation amplitudes satisfy $|\tilde{\varepsilon}_l| \ll 1$. Non-zero values for $\tilde{\varepsilon}_0$ identify a pre-bunching perturbation at the fundamental



Fig. 1. (a) Calculated evolution of the seeded radiation spot size throughout the 4 m undulator for VISA FEL at $\lambda = 1064$ nm. Three LG modes (p, l) = (0, 0), (0, 1) and (0, 2) at $\theta = -6 \text{ m}^{-1}$ detuning with a $P = 0.1 \,\mu\text{W}$ seed are introduced at the undulator entrance. The Gaussian e-beam radius is $r_0 = 80 \,\mu\text{m}$. The seed waist is located at z = 0 and is $w_{s0} = 3r_0$ for the fundamental Gaussian. During the start-up period early on, the seed beam diffracts briefly until exponential gain develops. The self-focusing effects then guide the beam toward a fixed waist size. (b) Normalized differential power gain along undulator for each corresponding seed mode. The effects of space charge are neglected ($\theta_{pr} = 0$).



Fig. 2. Radiation intensity and phase at undulator exit, generated by a dominant (p, l) = (0, 1) initial helical density perturbation in the e-beam. A hollow mode structure is evident in the intensity distribution and is accompanied by a helical azimuthal phase variation.

that can be related to a SASE startup scenario. Fig. 2 shows the transverse intensity and phase at the undulator exit for a solution of the excitation equations with an initial density perturbation of $\tilde{\epsilon}_0 = 10^{-5}$ and $\tilde{\epsilon}_1 = 10^{-1}$ for the VISA FEL. The relative magnitude of each amplitude is determined by iteration, such that the higher-order hollow mode becomes visibly dominant in the transverse intensity profile. It is particularly clear from the phase that the structure is that of a dominant (p, l) = (0, 1) LG mode, and that the field is gain-guided from the appearance of inward curvature near the axis.

These results suggest that, since an initial bunching perturbation at the fundamental mode typically dominates the interaction, amplification of a dominant azimuthal mode requires a dominant azimuthal excitation at startup. We have shown that this can be achieved either by injection of an OAM seed mode with the appropriate intensity amplitude (if available at the operating frequency), or by introduction of the appropriate spatial perturbation that is not azimuthally symmetric to the injected beam. The magnitude of these respective initial conditions provides a guideline for required parameters needed to obtain OAM modes in the presence of SASE, and will be explored further in future work.

6. Conclusions

An expansion of the EM field of a high-gain FEL in terms of the eigenmodes of a weakly guiding virtual dielectric is shown. A quadratic dependence on the transverse refractive index yields guided LG eigenmodes of the paraxial wave equation, facilitating a description of FEL mode coupling to naturally occurring radiation fields. The amplification of higher-order LG modes with OAM is briefly investigated in this formalism and is suggested as a novel exploratory tool for future FEL light sources. Preliminary results show high-gain of a dominant OAM mode can be achieved in a cold beam either by OAM seeding or with a helical density perturbation in the e-beam.

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