

AXIAL SYMMETRY IN SPONTANEOUS UNDULATOR RADIATION FOR XFELO TWO-BUNCH EXPERIMENT*

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Abstract

A well known discrepancy exists between 2D and 3D FEL simulation codes with respect to the radiation field intensity prior to the exponential gain regime [1]. This can be qualitatively explained by the fact that the 3D field representation preserves many more modes than does the axisymmetric field solved for by a 2D code. In this paper, we seek to develop an analytical model that quantifies this difference. We begin by expanding the spontaneous undulator radiation field as a multipole series, whose lowest order mode is axisymmetric. This allows us to calculate the difference in predicted intensity. Next, we confirm these results with numerical calculation and existing FEL codes GINGER and GENESIS. Finally, we discuss the implications of this study with respect to the XFELO two-bunch experiment to be conducted at LCLS-II.

INTRODUCTION

The x-ray FEL oscillator (XFELO) has the potential to be a new source of bright x-rays with unprecedented spectral purity [2–4]. Over the last decade, there have been separate experiments demonstrating the necessary technologies to meet the stringent operational demands of the XFELO: diamond Bragg crystal reflectors with high reflectivity [5], low thermal conductivity [6], and sufficient resilience to high-intensity x-rays [7]; availability of suitable compound refractive mirrors [8]; feedback system for the stabilization of x-ray components [9]. The next logical step is a holistic experiment integrating these technologies together into a proof-of-concept for the XFELO.

To this end, a collaboration between Argonne and SLAC has recently proposed a cavity-based XFELO (CBXFELO) experiment to be performed at the hard x-ray line at LCLS-II [10, 11]. The goal is to test whether we can sufficiently stabilize a large-scale x-ray cavity so as to observe FEL gain. Specifically, we plan to send two electron bunches separated longitudinally by about 2 ns into an undulator, such that the first bunch generates spontaneous undulator radiation (SUR) that is then returned by the x-ray cavity to be amplified by the second bunch. Doing this requires coordinating a number of engineering and physics efforts.

This paper is focused on one aspect of the physics – the symmetry of SUR and its impact on subsequent gain. This is important to our numerical modelling process, specifically

in comparing 2D vs 3D FEL codes. To clarify, 2D codes, such as GINGER [12], assumes cylindrical symmetry in the electric field, such that there is only one transverse dimension. 3D codes, such as GENESIS [13], preserve the full two dimensional transverse space, but at the cost of significantly larger computational complexity. Previous literature [14] have shown that 2D and 3D codes agree well in the exponential gain and nonlinear saturation regime, for both high-gain FELs and low-gain oscillators. This is because axisymmetric modes typically experience the largest FEL gain, so that they eventually overwhelm all other transverse modes.

On the other hand, this situation does not apply early in the gain process, where the two-bunch CBXFELO experiment is expected to operate. In this case, we expect significantly lower field intensity predicted from a 2D code vs the 3D version. Understanding and quantifying this difference is an important step in the numerical modeling process, which in the bigger picture, will allow us to better predict and optimize the number of photons measurable in the experimental setup.

THEORY

We begin by investigating the degree to which SUR can be described by an axisymmetric mode most suitable for amplification. Consider the SUR from a collection of electrons: any single electron j with 6D coordinates $(t_j, \eta_j, \mathbf{x}_j, \mathbf{x}'_j)$ contributes the field [14]

$$\mathcal{E}_{\nu,j}(\vec{\phi}) = e^{i\omega t_j} e^{-ik\vec{\phi}\cdot\vec{x}_j} \int_0^{L_u} dz e^{i(\Delta\nu-2\eta_j)k_u z} \times e^{\frac{1}{2}ik(\vec{\phi}-\vec{x}'_j)^2(z-L_u/2)}, \quad (1)$$

where for simplicity we neglect constant prefactors in this discussion. The field in (1) is in frequency-angular representation, with $\nu \equiv \omega/\omega_1$ being the scaled frequency relative to the resonant FEL frequency $\omega_1 = 2\pi c/\lambda_1$, and $\vec{\phi}$ being the 2D angular coordinate. Furthermore, let $\Delta\nu \equiv \nu - 1$ be the detuning and L_u be the undulator length.

Next, we write in polar coordinates $\vec{\phi} \equiv (\phi, \psi)$, where ϕ, ψ are the magnitude and phase of the angle vector respectively. Using the Jacobi-Anger identity, we perform a multipole expansion to obtain

$$\mathcal{E}_{\nu,j}(\phi, \psi) = e^{i\omega t_j} \sum_{n=-\infty}^{\infty} \int_{-L_u/2}^{L_u/2} dz i^n e^{in(\psi-\theta(z))} \times J_n(k\phi|\vec{x}_j + z\vec{x}'_j|) e^{ik(\phi^2+\vec{x}'_j^2)z/2} \times e^{ik_u(\Delta\nu-2\eta_j)(z-L_u/2)}. \quad (2)$$

* This work is supported by U.S. Dept. of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357, and U.S. National Science Foundation under Award No. PHY-1549132, the Center for Bright Beams.

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The $n = 0$ term in this expansion yields the axisymmetric component of the SUR. We denote that by

$$\mathcal{E}^S(\phi) \equiv e^{i\omega t_j} \int_{-L_u/2}^{L_u/2} dz J_0(k\phi|\vec{x}_j + z\vec{x}'_j|) \times e^{ik(\phi^2 + \vec{x}'_j{}^2)z/2} e^{iku(\Delta\nu - 2\eta_j)(z + L_u/2)}. \quad (3)$$

Vanishing angular divergence

In the case of an electron beam with vanishing (or negligible) angular divergence, i.e., $\vec{x}'_j = 0$ for all electrons, we are able to simplify Eq. (3) into a more tractable form. Assume for simplicity that $\Delta\nu = \eta = 0$, and that the beam is round with a Gaussian spatial profile:

$$f(r) = \frac{1}{\sigma_x^2} e^{-r^2/2\sigma_x^2}, \quad (4)$$

where σ_x is the electron beam size. We define [14]

$$\sigma_{r'} = \sqrt{\lambda_1/2L_u}, \quad \sigma_r = \sqrt{2\lambda_1 L_u}/4\pi, \quad (5)$$

to be the natural angular divergence and beam size of the SUR respectively. Notice that $\sigma_{r'}\sigma_r = \lambda_1/4\pi \equiv \epsilon_r$, the emittance of the radiation beam. Now let us rescale the radial angular coordinate accordingly

$$\tilde{\phi} \equiv \frac{\phi}{\sqrt{2}\sigma_{r'}}, \quad (6)$$

such that full radial angular flux (integrated over angular phase ψ) is found to be

$$\begin{aligned} \mathcal{F}(\tilde{\phi}) &= \frac{\sin^2(\pi\tilde{\phi}^2/2)}{(\pi\tilde{\phi}^2/2)^2} \sum_{n=-\infty}^{\infty} I_n\left(\frac{\tilde{\phi}^2}{2\sigma^2}\right) e^{-\tilde{\phi}^2/2\sigma^2} \\ &= \frac{\sin^2(\pi\tilde{\phi}^2/2)}{(\pi\tilde{\phi}^2/2)^2}, \end{aligned} \quad (7)$$

where $\sigma \equiv \sigma_r/\sigma_x$, i.e., the ratio of natural radiation beam size to electron beam size. The symmetric radial angular flux, on the other hand, is

$$\mathcal{F}^S(\tilde{\phi}) = \frac{\sin^2(\pi\tilde{\phi}^2/2)}{(\pi\tilde{\phi}^2/2)^2} I_0\left(\frac{\tilde{\phi}^2}{2\sigma^2}\right) e^{-\tilde{\phi}^2/2\sigma^2}. \quad (8)$$

Figure 1 shows the plot of \mathcal{F} and \mathcal{F}^S with different σ . With decreasing σ , e.g. increasing electron beam size at fixed radiation beam size, the symmetric flux becomes narrower and represents a smaller portion of the full SUR angular spectrum.

NUMERICAL RESULTS

For a general electron beam, Equation 3 is difficult to solve analytically. We resort to numerical integration combined with random sampling of the desired electron distribution. Figure 2 shows the angular spectrum for a beam with parameters similar to the CBXFEL experiment. Here, $\sigma_x = 5.8\sigma_r$ and $\sigma_{x'} = 0.989\sigma_{r'}$. Compared to the case of vanishing

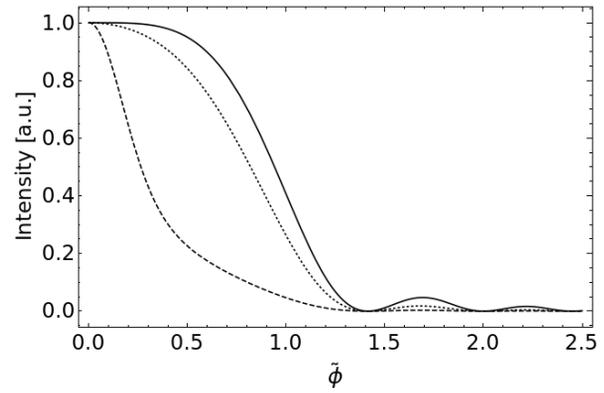


Figure 1: Angular flux for all modes (solid line), and symmetric mode only with $\sigma = 0.2$ (dashed) and $\sigma = 1$ (dotted).

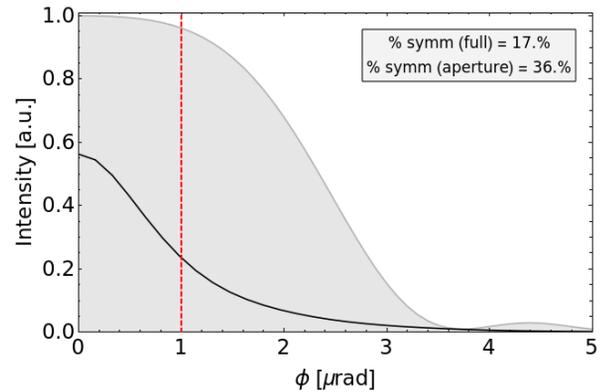


Figure 2: Angular flux with CBXFEL experimental parameters. Depicted are the full flux (gray background), and symmetric flux only (black). The total integrated flux ratio of the symmetric mode to all modes is about 17% over all angles, or 36% if we introduce an aperture of 1 μrad (indicated by dotted red line).

angular divergence, the inclusion of a finite divergence effectively reduces the “height” of the symmetric flux $\mathcal{F}^S(0)$ and results in a longer “tail” at larger angles.

Over repeated runs, the total integrated power of the symmetric mode comprises approximately 17% of that of all modes. If we introduce an aperture of 1 μrad however, we are able to improve this ratio to about 36%. A large ratio is crucial for the second pass in the XFEL experiment, since we expect only the symmetric part of the SUR to experience significant gain.

Comparison with FEL Codes

In the vanishing angular divergence case, we checked Eq. (3) with 2D FEL code GINGER and obtained good agreement. See Figure 3. The result from GINGER was averaged over multiple shots. In addition to Fig. 3, we also obtained good agreement for $\sigma_x \approx 2, 4$ and $8\sigma_r$ (not pictured).

With the inclusion of CBXFEL experiment parameters, it is not straightforward to perform a direct comparison between theory and FEL code. This is because the experimental setup involves electron beam focusing and undulator gaps,

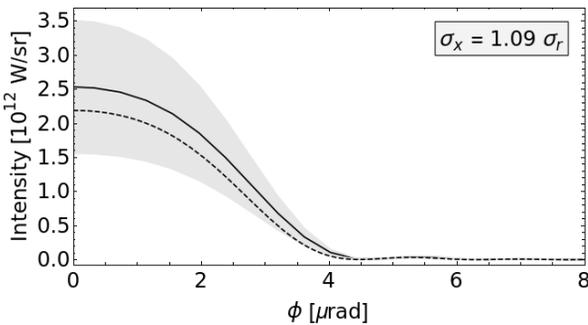


Figure 3: Comparison of angular flux between Eq. (8) (dashed) and 2D FEL code GINGER (solid) shows good agreement. Gray band shows 1σ of the shot-to-shot variation in GINGER. We set $\sigma_x \approx 1.1\sigma_r$.

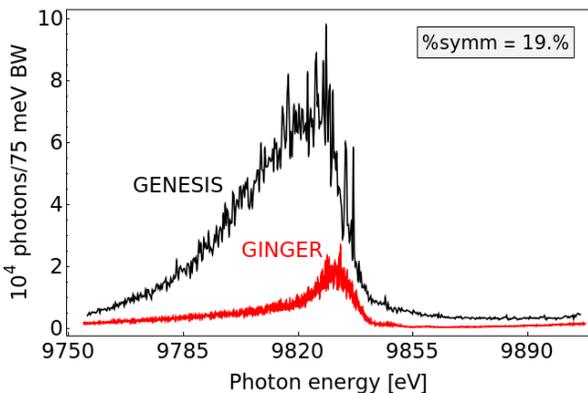


Figure 4: Spectral photon flux predicted by GINGER vs. GENESIS for CBXFEL parameters. Total integrated power ratio between GINGER and GENESIS is about 19%, which agrees well with theory.

which contradicts the assumption of no focusing and single undulator in deriving Eq. (3). However, we are able to directly compare the results of GINGER vs. GENESIS in terms of predicted photon flux. Should the discrepancy between 2D and 3D code be accurately described by Eqs. (2) and (3), the ratio of predicted flux should approach roughly $1/5$ as seen in the previous section (Fig. 2). We found this to be indeed the case (Fig. 4).

CONCLUSION

We have introduced analytical expressions representing the symmetric and non-symmetric modes of SUR, confirmed its accuracy with existing FEL codes, as well as demonstrated its ability to account for the difference between 2D and 3D FEL codes (before exponential gain regime). This will allow us to more confidently utilize both codes and provides a better basis for quantitative comparison.

The next step would be to investigate the gain in the radiation pulse after the second bunch. A potential complication comes from the cavity mirrors. Ironically, the pristine reflectivity of the diamond crystals, by its very nature, restricts the number of photons we are able to out-couple from the cavity. Therefore, the gain needs to be significant stronger than the

background SUR from the second pass and other sources of measurement noise. Since gain only occurs in the narrow frequency and angular bandwidth of the mirrors, we believe that a physical aperture could potentially restrict the phase space to allow the gain to dominate. This is supported by Fig. 2. By introducing a $1\ \mu\text{rad}$ aperture, we were able to improve the symmetric flux ratio to over one third. We hope to confirm this result with further, more detailed numerical calculation, taking into account the precise reflectivity curve of the diamond crystal.

ACKNOWLEDGEMENTS

We would like to thank Gabriel Marcus (SLAC) for his advice on using GENESIS. The FEL code GENESIS is written and maintained by Sven Reiche (PSI), while the code GINGER is created by William M. Fawley (SLAC). Funding for this project is provided in part by U.S. DOE, Office of Science, Office of BES, under Contract No. DE-AC02-06CH11357 and in part by the U.S. National Science Foundation under Award No. PHY-1549132, the Center for Bright Beams.

REFERENCES

- [1] Z. Huang and K.-J. Kim, "Review of X-ray free-electron laser theory," *Phys. Rev. STAB*, vol. 10, p. 034801, 2007. doi: 10.1103/PhysRevSTAB.10.034801
- [2] K.-J. Kim, Y. Shvyd'ko, and S. Reiche, "A proposal for an X-ray free-electron laser with an energy-recovery linac," *Phys. Rev. Lett.*, vol. 100, p. 244802, 2008. doi: 10.1103/PhysRevLett.100.244802
- [3] R. R. Lindberg, K.-J. Kim, Y. Shvyd'ko, and W. M. Fawley, "Performance of the X-ray free-electron laser with crystal Cavity," *Phys. Rev. STAB*, vol. 14, p. 010701, 2011. doi: 10.1103/PhysRevSTAB.14.010701
- [4] W. Qin *et al.*, "Start-to-End Simulations for an X-Ray FEL Oscillator at the LCLS-II and LCLS-II-HE", in *Proc. 38th Int. Free Electron Laser Conf. (FEL'17)*, Santa Fe, NM, USA, Aug. 2017, pp. 247–250. doi: 10.18429/JACoW-FEL2017-TUC05
- [5] Y. Shvyd'ko, S. Stoupin, V. Blank, and S. Terentyev, "Near 100% Bragg Reflectivity of X-rays," *Nature Photonics*, vol. 5, p. 539, 2011. doi: 10.1038/nphoton.2011.197
- [6] S. Stoupin, and Y. Shvyd'ko, "Ultraprecise studies of the thermal expansion coefficient of diamond using backscattering x-ray diffraction," *Phys. Rev. B*, vol. 83, p. 104102, 2011. doi: 10.1103/PhysRevB.83.104102
- [7] T. Kolodziej *et al.*, "High Bragg reflectivity of diamond crystals exposed to multi-kW/mm X-ray beams," *Journal of Synchrotron Radiation*, vol. 25, no. 4, p. 1022, 2018. doi: 10.1107/S1600577518007695
- [8] T. Kolodziej *et al.*, "Efficiency and coherence preservation studies of Be refractive lenses for XFEL application," *Journal of Synchrotron Radiation*, vol. 25, no. 2, p. 354, 2018. doi: 10.1107/S160057751701699X
- [9] S. Stoupin *et al.*, "Nanoradian angular stabilization of x-ray optical components," *Rev. Sci. Instrum.*, vol. 81, p. 055108, 2010. doi: 10.1063/1.3428722

- [10] K.-J. Kim *et al.*, “Test of an X-ray cavity using double bunches from the LCLS-II Cu-Linac,” in *Proc. IPAC 2019*, p. 1887, 2019. doi:10.18429/JACoW-IPAC2019-TUPRB096
- [11] G. Marcus *et al.*, “Cavity-Based Free-Electron Laser Research and Development: A Joint Argonne National Laboratory and SLAC National Laboratory Collaboration”, presented at the 39th Int. Free Electron Laser Conf. (FEL’19), Hamburg, Germany, Aug. 2019, paper TUD04.
- [12] GINGER code and documentation made available through private comm. with author W. Fawley (SLAC).
- [13] GENESIS version 2 code and documentation available at genesis.web.psi.ch.
- [14] K.-J. Kim, Z. Huang and R. R. Lindberg, *Synchrotron Lasers and Free-Electron Lasers*, 2017 (Cambridge University Press).