Some Sample Calculations for the Far Field Harmonic Power and Angular Pattern in LCLS-1 and LCLS-2

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ABSTRACT

Calculations with the GINGER FEL simulation code are given for the predicted harmonic content for LCLS-1 operating in SASE mode both at 8 keV and 800 eV photon energy, and also for the soft x-ray undulator line of LCLS-2 at 238 eV ($\lambda \sim 5.0$ nm), near the upper wavelength limit. With detailed transverse and longitudinal knowledge of the harmonic microbunching content, one can estimate the far field angular intensity for both odd and even harmonics. Comparison to previous LCLS-1 experimental results for the second and third harmonic fractional power shows good agreement. When run at the strongest undulator K parameter, LCLS-2 will have extremely high harmonic levels, greater than 0.4% in the 2nd harmonic relative to the fundamental, even for perfectly aligned electron beams and greater than 10% in the third harmonic if run deep into saturation.

INTRODUCTION

In response to a request by Z. Huang and M. Rowen to look at the expected even harmonic radiation power from LCLS-2, in fall 2012 I upgraded the GINGER numerical FEL simulation code to have this capability. Previously, the code could calculate the near- and far-field radiation patterns for odd harmonics only (including the fundamental). The new extension to the code relies upon the fact that if the electron beam microbunching at a given harmonic is known as a function of (x,y,z,t) , one can directly calculate the far field radiation in that harmonic without having to follow the details of the interaction with the particles in the undulator (*i.e.*, the near-field emission). Consequently, so long as the harmonic coupling coefficients between the microbunching and electric field emission are accurately known, it is possible to calculate the far field emission for both odd *and* even harmonics.

GINGER, as is true for essentially all commonly used FEL simulation codes, makes the assumption that the emission of even harmonic radiation does NOT affect the energy loss of the individual particles (and thus ignores any true gain). Rather, the microbunching at even harmonics is overwhelmingly due to the particle interaction with the fundamental radiation field. This interaction can lead to very strong microbunching that also contains strong harmonic “overtones” at all harmonic numbers $h > 1$. In recent FEL literature this phenomenon has been called “nonlinear harmonic generation” (NHG), in contrast to “coherent harmonic generation” (CHG) that is associated with true FEL gain at higher harmonics (*i.e.*, the harmonic radiation non-negligibly affects the particle microbunching *and* the energy loss). For all $h > 1$, including odd harmonics, the neglect of CHG and limitation to NHG effects only is an excellent approximation so long as the gain at the fundamental is significantly larger than that at higher harmonics (more specifically, greater than that at the 3rd harmonic which typically will have the highest gain of all higher harmonics). For the second and fourth harmonics, CHG is *extremely* small, due both to the small bunching $\leftrightarrow$ emission coupling factors and to the fact that the on-axis emission is suppressed for a well-centered e-beam in the undulator (as appears to be true at LCLS). For $h=6$, it is conceivable that a situation involving strong CHG at $h=3$ could lead to a relatively significant $h=6$ microbunching component relative to that associated with NHG for the fundamental component at $h=1$.

Although GINGER now also can follow the self-consistent interaction (*i.e.*, energy loss and true CHG with gain) between the code macroparticles and the third harmonic in addition to that with the fundamental,

Fund. and Harmonic Rad. Power vs. Z

Harmonic Bunching vs. Z

Figure 1 --- LCLS-1 Case-1 comprised of a 14.3 GeV energy, 0.4 mm-mrad emittance, 3-kA e-beam radiating at a resonant wavelength of 0.15 nm (8 keV). The left plot shows the time-averaged radiation power at the fundamental, 3rd, and 5th harmonics while the right plot shows the time-averaged, macroparticle bunching factor for harmonics 1 through 5.

the calculations presented in this note were performed using the NHG approximation and allowed only the fundamental wavelength radiation component to act back upon the particles. In the absence of any special effort to suppress fundamental gain (and associated energy spread increase) via phase shifters and/or attenuators, it is a good assumption that the third harmonic microbunching component in LCLS-1 and LCLS-2 will be nearly all due to the electron beam interaction with the fundamental radiation.

This note presents three particular e-beam/undulator cases relevant to LCLS. The first case employs a 14.3-GeV, 3-kA, 0.4 mm-mrad emittance, $\sigma_\gamma/\gamma = 1.E-4$, e-beam passing through the LCLS-1 undulator “as built” (*e.g.*, with the actual short-short-long break and quadrupole configuration as provided by H.-D. Nuhn) radiating at 8.3 keV photon energy ($\lambda=0.15$ nm). The second case also corresponds to LCLS-1 but with the e-beam energy reduced to 4.3 GeV, the relative incoherent energy spread increased to $3.0E-4$, and the fundamental radiation wavelength increased to 1.5 nm (826 eV). For these two cases, I chose these particular parameters in order to make a direct comparison to results in Ratner *et al.* [PRSTAB **14**, 060701 (2011)]; in particular, see Table III but note that there is an important typographical error that misstates the current as 1 kA rather than the correct 3 kA current]. That paper has measurements for both second and third harmonic emission from LCLS-1; for $h=3$, the paper also presents GENESIS simulation predictions. The third and last case studied here is an “LCLS-2”, 3-kA, 0.4 mm-mrad, 8.5-GeV, $\sigma_\gamma/\gamma = 1.5E-4$, e-beam passing through the “soft x-ray”, 55-mm undulator whose strength is tuned for FEL radiation resonance at 238 eV (5.0 nm). Because this case has a very large undulator parameter ($K \sim 10.0$) compared that of LCLS1 ($K \sim 3.7$), there is a much greater harmonic radiation power fraction.

In all cases the results were obtained for “simple” SASE configurations with e-beam shot noise initiated with the standard GINGER algorithm. The runs employed periodic boundary conditions with a time window equivalent to at least 1.5 slippage lengths subdivided into 256 or greater time slices. In the frequency domain, the full bandwidth is ~ 10 times the FEL gain bandwidth. At the end of this note, Table 1 compares the GINGER predictions with the experimental results obtained by Ratner *et al.* for LCLS-1 and finds good agreement in terms of the P_2/P_1 and P_3/P_1 ratios. Please note that only one or two runs were done for each case. For more accurate results in terms of averages over many virtual shots

Fundamental Far Field Intensity from e- Bunching at Z=62.2 m

2nd Harm. Far Field Intensity from e- Bunching at Z=62.2 m

Figure 2: Far field intensity emitted by z=62 m for the fundamental and second harmonics for LCLS-1 Case 1. This position has both high harmonic power and good spectral bandwidth.

and more realistic LCLS e-beam phase spaces, one should do many such simulation runs with different random number seeds and, moreover, use a full “start-to-end”, time-resolved model electron beam.

Case 1: LCLS1- 14.3 GeV - 8keV - 3kA - 0.4 mm-mrad:

Here SASE power saturation is reached by $z \sim 50$ m in the undulator. Powered by nonlinear microbunching associated with the fundamental FEL interaction, the third harmonic radiation power and bunching come up strongly by the end of the simulation at $z=84$ m (see the two plots of Fig. 1).). The peak bunching for the fundamental is about 0.4 while that of the third harmonic only reaches ~ 0.08 . Evaluated at $z=62$ m where the spectral bandwidth and mode quality remains excellent, the third harmonic fractional power is 1.3% that of the fundamental. The equivalent value for the 2nd harmonic is

3rd Harm. Far Field Intensity from e- Bunching at Z=62.2 m

5th Harm. Far Field Intensity from e- Bunching at Z=62.2 m

Figure 3: Far field intensity emitted by z=62 m for the third and fifth harmonics for LCLS-1 Case 1

Overall TEM Mode Fit at Z=62.19 m

Overall TEM Mode Fit at Z=84.33 m

Figure 4 –Near-field intensity pattern at z=62 m (left) and much farther into saturation at z=84 m (right) for the 8 keV, LCLS-1 Case I. Decomposition into TEM modes and calculation of the far field M^2 shows that as the FEL goes deeper into saturation, a higher fraction of power goes into higher order modes and, likewise, the downstream focusability decreases.

less than 0.01% (see right plot of Fig. 2). Far field, angle-resolved calculations for the fundamental through 3rd harmonic (Figs. 2 and 3) show typical angles of ~ 1 microradian or less. The scaling with harmonic number appears to be $\sim h^{-1/2}$; the less than inverse linear dependence suggests that the active bunching area decreases as the harmonic number increases. TEM mode decomposition of the time-dependent, near-field power shows that at z=62 m (see left plot of Fig. 4) the M^2 is below 1.1 and more than 97% of the power is contained in the time-integrated, best-fit TEM00 mode. Deeper into saturation (z=84 as shown on the right plot of Fig. 4) the fraction drops to $\sim 85\%$ and the M^2 increases above 1.4. The type of behavior appears to be quite prototypical --- namely, even though the power continues to increase beyond that at minimal spectral bandwidth, much of that power “leaks” out radially in the near-field beyond the e-beam radius causing the transverse mode quality to decrease. On the other hand, the far field angle appears to be little changed (1.1 microradians both at z=64 m and z=84 m.).

Case 2: LCLS1 - 4.3 GeV - 3kA - 1.5nm/826 eV

The much lower low photon energy in this case leads to a significantly shorter gain length and rapid saturation (by z ~ 20 m; see Fig. 5) relative to the previous 8-keV case. The undulator strength K is $\sim 6\%$ smaller than in Case 1; this reduction should have negligible effect on the coupling strength to FEL harmonic emission. The integrated third harmonic intensity is about 2% that of the fundamental while that of the second harmonic is $\sim 0.05\%$ (Figs. 6 and 7). As shown in the left plot of Fig. 8, although the M^2 of the near-field intensity profile evaluated at z=23.6 m is quite good (1.14), there is actually 7% of the intensity contained in higher order modes. By z=32 m (Fig. 8 right plot), the M^2 has increased to greater than 2.0 and only 62% of the field is in the lowest order mode. As in the higher energy case, there is a significant intensity “halo” extending to greater than 3X the RMS radius of the core region. Presumably this is an observable effect at LCLS and it would be interesting to measure the effective M^2 as a function of undulator length in the saturation regime and beyond, especially for lower resonant photon energies.

Fund. and Harmonic Rad. Power vs. Z

Harmonic Bunching vs. Z

Figure 5 – Time-averaged power and microbunching for the LCLS-1 Case-2 at 4.3 GeV and 1.5 nm fundamental output wavelength. As evident in the left plot, the power at the 3rd and 5th harmonics comes up rapidly just before saturation of the fundamental. The bunching fraction (right plot) reaches a fairly well-defined maximum and then decrease significantly as the FEL goes deeper into saturation.

Fundamental Far Field Intensity from e- Bunching at Z=23.6 m

2nd Harm. Far Field Intensity from e- Bunching at Z=23.6 m

Figure 6 – Angular far-field emission patterns evaluated for a 23.6 m long undulator (near the saturation point) for the fundamental and second harmonic for the LCLS-1 Case-2 at 4.3 GeV and 1.5 nm fundamental output wavelength.

Figure 7 – Third and fifth harmonic far-field, angular emission patterns evaluated for an undulator length of 23.6 m for the LCLS-1 Case-2 at 4.3 GeV photon energy.

Figure 8 – Near-field intensity patterns evaluated at z=23.6 m near saturation and at z=32.2 m for the LCLS-1 Case-2 at 4.3 GeV and 1.5 nm fundamental output wavelength. Mode decomposition shows that the fraction in the lowest order TEM00 mode drops significantly as the FEL goes deeper into saturation.

Fund. and Harmonic Rad. Power vs. Z

Harmonic Bunching vs. Z

Figure 9 – Average power and bunching for a hypothetical LCLS-2 tuned to 248 eV resonant photon energy (5.0 nm). As evident in the left plot, the power in the 3rd and 5th harmonics come up rapidly just before saturation of the fundamental. The odd harmonic power continues to grow with z beyond this saturation point, despite the bunching oscillating strongly with z.

Fundamental Far Field Intensity from e- Bunching at Z=36.1 m

2nd Harm. Far Field Intensity from e- Bunching at Z=36.1 m

Figure 10 – Fundamental and second harmonic far field emission patterns for a hypothetical LCLS-2 radiating at 5.0 nm. The emission point of z=36 m lies approximately at the peak of the bunching at the fundamental wavelength but at a minimum in the oscillation of the higher harmonics.

Case 3: LCLS2 - 8.5 GeV - 3 kA - 0.4 mm-mrad - $\sigma_\gamma/\gamma = 1.5E-4$, 238 eV/5.0 nm

Here again the even lower photon energy compared to the LCLS-1 Case 2 leads to a very rapid power saturation occurring by $z \sim 30$ m. By the 43 m point in the undulator, the third harmonic power has reached greater than 10% of that of the fundamental and the 5th harmonic more than 1% (see Fig. 9). The output far field pattern for the fundamental and second harmonic (Fig. 10) strongly fluctuates with

Figure 11 – Third and fourth harmonic far field emission patterns for the 5-nm, LCLS-2 case.

angle suggesting that there is a large fraction of higher order modes. However, at higher harmonics (see Fig. 11 and 12 for harmonics 3, 4 and 5) there is essentially no evidence of a ripple. Examining the near field emission at $z=36$ m (right plot of Fig. 12), there is only an $\sim 84\%$ TEM00 content and the M^2 exceeds 2.2. By comparison, several gain lengths upstream of saturation at $z=24$ m, the TEM00 mode fraction is only slightly larger than 84% and the M^2 is 2.14. However, there is no ripple in the intensity with radial position as was seen at $z=36$ m. Significantly downstream of saturation at $z=42$ m (right plot of Fig. 13), the ripple is even stronger, the TEM00 fraction has dropped to $\sim 55\%$, and the M^2 exceeds 5. In general, even using basis functions through the TEM08 mode, the overall fit is poor, especially near the axis. Consequently, the transverse mode quality of the output radiation in these long wavelength cases can be quite sensitive to how deeply one goes into saturation. This behavior may have consequences for both for downstream users and possibly for self-seeding situations.

Figure 12 – 5th harmonic angular emission pattern (left) and near-field emission pattern and TEM mode decomposition evaluated for a 36-m undulator for a hypothetical LCLS-2 emitting at a 5-nm fundamental wavelength.

Overall TEM Mode Fit at Z=24.09 m

Overall TEM Mode Fit at Z=41.92 m

Figure 13 – Near-field emission patterns at z=24 m and z=42 m for LCLS-2 5 nm wavelength case.

In Table 1 below we summarize the various time-averaged, fundamental and relative harmonic output power levels for the different cases. The numbers in the double brackets are from Table IV of Ratner *et al.* and are based on experimental measurements at LCLS-1. The agreement is quite good, especially if one takes into account that the second harmonic measurements can be sensitive to e-beam misalignment in the undulator.

Table 1 --- Time-Averaged SASE Power at the Fundamental and Harmonics #2,3,5

	Fund. Pwr (P ₁) (GW)	P ₂ /P ₁	P ₃ /P ₁	P ₅ /P ₁
0.15 nm, 8keV, 3 kA, LCLS-1, 14 GeV; z=62 m	15	7.2E-5	1.3% {{ 0.2 – 2% }}	5.8E-4
1.5 nm, 800 eV, 3 kA, LCLS-1, 4.3GeV; z=24 m	18	5.0E-4 {{ 4 – 10 E-4 }}	1.9% {{ 2.0 – 2.5% }}	9.5E-4
5.0 nm, 248 eV, 3 kA, LCLS-2, 8.5GeV; z=36 m	48	3.9E-3	7.2%	1.1%
z=43 m	55	6.7E-3	12%	1.5%