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Analytical studies of constraints on the performance for EEHG FEL seed lasers

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Abstract

Laser seeding technique have been envisioned to produce nearly transform-limited pulses at soft X-ray FELs. Echo-Enabled Harmonic Generation (EEHG) is a promising, recent technique for harmonic generation with an excellent up-conversion to very high harmonics, from the standpoint of electron beam physics. This paper explores the constraints on seed laser performance for reaching wavelengths of 1 nm. We show that the main challenge in implementing the EEHG scheme at extreme harmonic factors is the requirement for accurate control of temporal and spatial quality of the seed laser pulse. For example, if the phase of the laser pulse is chirped before conversion to an UV seed pulse, the chirp in the electron beam microbunch turns out to be roughly multiplied by the harmonic factor. In the case of a Ti:Sa seed laser, such factor is about 800. For such large harmonic numbers, generation of nearly transform-limited soft X-ray pulses results in challenging constraints on the Ti:Sa laser. In fact, the relative discrepancy of the time-bandwidth product of the seed-laser pulse from the ideal transform-limited performance should be no more than one in a million. The generated electron beam microbunching is also very sensitive to distortions of the seed laser wavefront, which are also multiplied by the harmonic factor. In order to have minimal reduction of the FEL input coupling factor, it is desirable that the size-angular bandwidth product of the UV seed laser beam be very close to the ideal i.e. diffraction-limited performance in the waist plane at the middle of the modulator undulator.

1 Introduction

An important goal for any advanced X-ray FEL is the production of X-ray pulses with the minimum allowed photon energy width for given pulse

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length, which defines the transform-limit. A well-known approach to obtain fully coherent radiation in the soft X-ray region relies on frequency multiplication, a scheme known as high-gain-harmonic-generation (HGHG) [1, 2]. In a HGHG FEL, the radiation output is obtained from a coherent subharmonic seed laser pulse. Consequently, the optical properties of HGHG FELs are expected to reflect the characteristics of the high-quality seed laser. Echo-enabled harmonic generation (EEHG) is a recent, promising technique for efficient harmonic generation [3, 4]. The key advantage of EEHG over HGHG is that the amplitude of the achieved microbunching factor decays slowly with an increasing harmonic number. Consequently, as concerns electron beam physics issues, EEHG allows for the generation of fully coherent radiation at soft X-ray wavelengths with a single upshift stage, and using a conventional optical laser system. The remarkable up-frequency conversion efficiency of the method has stimulated wide interest to generate near transform-limited soft X-ray pulses. Several EEHG FEL projects are now under development [5]-[7]. A typical EEHG setup consists of two stages for electron beam phase space manipulation, followed by a radiator. Each stage includes an undulator, which is used to modulate the electron beam in energy with the help of a seed laser, and a chicane following the modulator, which is used to apply energy-dependent slippage to the electrons. The radiator is composed by a sequence of undulators tuned to the desired output wavelength. This final section is similar to that used for SASE FELs. However it is shorter, and produces coherent radiation only because the beam has been coherently prebunched. The seed laser is assumed to be tuned at 200 nm (or 270 nm) corresponding to the fourth harmonic (or the third) of a Ti:Sapphire laser.

Limitations on the performance of EEHG schemes related with electron beam dynamics issues, as the beam goes through the various undulators and chicanes, has been extensively discussed in literature [8, 9, 10] and goes beyond the scope of this paper. Here we will focus our attention on the first part of the harmonic generation process, discussing the constraints on the seed laser performance needed for reaching wavelengths of about 1 nm. In fact, in chirped-pulse amplification systems (CPA) systems, both temporal and spatial quality of the beam can be degraded due to the propagation through the optical components, non-linear effects or inhomogeneous doping concentration in the amplifying media, and thermal effects linked to the pumping process. In particular, the aim of this work is to evaluate the impact of variations of the characteristics of output radiation when the FEL is seeded by a laser with non-ideal properties, including effects such as linear and nonlinear frequency chirp and wavefront distortion.

A description of the impact of phase chirp of the EEHG (or HGHG) FEL output can be made without numerical simulation codes. In fact, as is well-known, if the phase of the seed laser is chirped, the chirp is simply multiplied by the frequency multiplication factor N. In this case, the method used to describe the output field perturbation is independent of the specific kind of harmonic generation technique: it only depends on the frequency multiplication factor N. It follows that both EEHG and HGHG FELs starting from a Ti:Sa laser with a wavelength around 800 nm can produce transform-limited radiation down to wavelengths of 1 nm only when the relative discrepancy of the time-bandwidth product of the compressed 800 nm laser pulse from the ideal, transform-limited performance is no more than one in a million, roughly corresponding to the squared of the harmonic number. However, pulses from a commercially available Ti:Sapphire chirped pulse amplifiers are usually limited in such discrepancy to around 1%, due to non-ideal effects. Therefore, research and development activities must be performed in order to reach the required temporal quality. To the best of our knowledge, there is only one article [2] reporting on the impact of temporal variations in seed laser pulses on EEHG FEL output radiation characteristics, [10]. The analysis in [10] is based on numerical simulations in the case of 1.2 nm output radiation wavelength. According to results of the sensitivity study in [10], the phase of the 202 nm seed laser pulse (corresponding to the fourth harmonic of a Ti:Sa laser) must to be controlled to within 0.5 degrees. Consequently, the phase of the Ti:Sa laser output must to be controlled to within roughly 0.1 degrees. This result is consistent with our analysis, which is performed at a very elementary level.

We also evaluate the impact on the EEHG FEL output of wavefront errors in the seed laser. In the case of ideal performance, the seed (UV) laser beam must be characterized by a flat (i.e. diffraction-limited) wavefront in the waist plane in the middle of the modulator undulator. If the wavefront exhibits errors, errors in the microbuch wavefront follow, which are multiplied by the frequency multiplication factor. These microbunch wavefront errors do not affect the spatial quality of the FEL output radiation, which is the same for both perturbed and unperturbed wavefront cases. They only affect the input signal value at the target harmonic. However, because of the exponential dependence of the signal suppression factor on the wavefront errors, one obtains an appreciable FEL output only when phase errors are sufficiently small to give appreciable input signal. As a result, the seed UV laser beam must exhibit a nearly diffraction-limited wavefront in the waist plane, with very little phase variation. In particular for a target harmonic with wavelengths of about 1 nm, the wavefront of the UV beam must be controlled to within a fraction of a degree across the electron beam area. These relatively small phase variations cause the signal at the entrance of

[2] The issue was also discussed during the preparation of this work in [11]. There HGHG was mainly considered but, as noted above, the method used to describe the output field perturbation is independent of the specific kind of harmonic generation technique.

the FEL amplifier to drop of a quantity of order of the ideal (diffraction-limited) performance. In contrast with phase variation in time, the spatial quality of UV seed laser beam can be improved by means of active optics and spatial filtering. However, these manipulations with laser beam usually cause significant losses in beam power.

To the best of our knowledge, the crucially important problem of seeding with beam wavefront distortions was only recently reported in workshops [12, 13], where the impact of wavefront errors on the EEHG performance was discussed, based on numerical simulations, in the case of the highest target harmonic at 13 nm. Results of [12, 13] are consistent with our analysis, which has been performed purely analytically.

The suppression of the output signal due to phase variations in space seems somehow in contrast with the effects of phase variations in time, where phase errors affect the temporal quality of the output radiation, but not the FEL output power. From this viewpoint, it should be noted that the radiation field is characterized by notions such as temporal and spatial coherence. The transverse coherence of FEL radiation develops automatically, without laser seeding. This happens due to transverse eigenmode selection: due to different gains of the FEL transverse eigenmodes, only one survives at the end of the FEL process. The coherence time is defined by the inverse FEL amplification bandwidth. For conventional soft X-ray FELs the typical amplification bandwidth is much wider than the Fourier transform limited value corresponding to the radiation pulse duration, meaning that the coherence time is much shorter than the pulse duration. Consequently, microbunch phase variations in time only lead to phase variations in the output radiation pulse, without suppression of the output power level.

2 Issues affecting the performance of EEHG FEL

Phase control is an important aspect in the development of all FEL sources based on harmonic generation. Methods for dealing with issues concerning temporal phase variations in frequency multipliers are based on the same general principle [14]: the effect of frequency multiplication by a harmonic factor N, is to multiply the phase variation by N. The EEHG scheme is obviously based on harmonic generation, but is more complicated than other schemes, and consists of two modulators, two dispersion sections, and one radiator undulator. A unique feature of EEHG scheme is the utilization of two different seed laser pulses which can have different temporal and spatial quality. It is thus natural to investigate the question whether the general principle above can also be applied to EEHG. Analytical results [4] refer to the specific model an of infinitely long, uniform electron bunch only. This steady state model proved to be very fruitful, allowing for simple analytical expressions describing the main characteristics of EEHG scheme. However, as discussed above, the seed laser pulses and, consequently the electron beam microbunching, are always characterized by phase variations in time and space (wavefront distortions). We will therefore extend analytical description of EEHG scheme in [4], following the line of derivations in that reference, to the time dependent case and account for finite duration and transverse size of the electron bunch.

To this aim, we assume that the temporal profile of the electron beam can be modeled as a Gaussian, and that the initial electron beam distribution can be factorized as a product of energy, $f_{0p}(p)$, and density, $f_{0\zeta}(\zeta)$ distributions as

$$f_0(\zeta, p) = f_{0p}(p) f_{0\zeta}(\zeta) = \frac{N_0}{2\pi\sigma_\zeta} \exp\left[-\frac{p^2}{2} - \frac{\zeta^2}{2\sigma_\zeta^2}\right] . \tag{1}$$

Here $p = (E - E_0)/\sigma_E$ is the dimensionless energy deviation of a particle from the average energy E_0, and the rms spread is given by σ_E. Similarly, $\zeta = \omega_l t$ is the dimensionless time, with ω_l the laser frequency, assumed to be the same in both stages, and σ_ζ is the rms spread of the density distribution. Finally N_0 is the total number of particles in the beam. The longitudinal phase space is described by the variables (ζ, p). Passing through the first modulator and dispersive section the phase space variables transform to (ζ', p'), which are given by

$$p' = p + A_1 \sin(\zeta + \phi_1) \ , \quad \zeta' = \zeta + B_1 p' \ , \tag{2}$$

where $A_1 = \Delta E_1/\sigma_E$, ΔE_1 being the energy modulation imposed by the seed laser, $\phi_1 = \phi_1(\zeta)$ is the phase of the laser pulse, which depends on the time ζ, and $B_1 = R_{56}^{(1)}\sigma_E\omega_l/(E_0 c)$, $R_{56}^{(1)}$ is the strength of the first chicane. Substituting Eq. (2) into Eq. (1) one can obtain the distribution after the first modulator and dispersive section. The new phase space variables (ζ', p') will transform after the passage through the second modulator and dispersive section, to (ζ'', p''), which are given, in a similar way, by

$$p'' = p' + A_2 \sin(\zeta' + \phi_2) \ , \quad \zeta'' = \zeta' + B_2 p'' \ , \tag{3}$$

the subscript '2' referring to the second stage [3]. Using Eq. (1)-(3) one can obtain an explicit expression for the phase space distribution after the second

[3] We kept our notation similar to that of [4]. However, we chose $\omega_l \equiv \omega_1 = \omega_2$ from the very beginning. Therefore $K = \omega_2/\omega_1 = 1$ for us. Also note that, since reference [4] deals with the steady state case, the phases of the two laser pulses are constant.

stage, $f_2(\zeta'', p'')$, which will not be reported here. In order to analyze the harmonic composition of the current density we first need to project the phase space distribution onto the real space-time coordinates by performing an integration along p''. This leads to the density distribution function ρ, that can be Fourier-analyzed further to give

$$\bar{\rho}(\Omega) = \int_{-\infty}^{\infty} dp'' d\zeta'' \exp[-i\Omega\zeta''] f_2(\zeta'', p'') \ , \tag{4}$$

where $\Omega = \omega/\omega_l$ is the conjugate variable of ζ, whose meaning is that of normalized frequency.

The integrals in Eq. (4) cannot be easily performed, directly. As customary, one can transform the final variables (ζ'', p'') back to the initial variables (ζ, p) and perform the required integrations with respect to the old variables. This allows to use the fact that $f_2(\zeta'', p'') = f_0(\zeta, p)$. Since $d\zeta'' dp'' = d\zeta dp$ one obtains

$$\begin{aligned} \bar{\rho}(\Omega) &= \int_{-\infty}^{\infty} dp d\zeta \exp[-i\Omega\zeta''(\zeta, p)] f_0(\zeta, p) \\ &= \frac{N_0}{2\pi\sigma_\zeta} \int_{-\infty}^{\infty} dp d\zeta \exp[-i\Omega\zeta''(\zeta, p)] \exp\left[-\frac{p^2}{2} - \frac{\zeta^2}{2\sigma_\zeta^2}\right] , \end{aligned} \tag{5}$$

where $\zeta''(\zeta, p)$ can be obtained from Eq. (2) and Eq. (3), and reads

$$\begin{aligned} \zeta''(\zeta, p) = \ & \zeta + (B_1 + B_2)p + A_1(B_1 + B_2)\sin(\zeta + \phi_1) \\ & + A_2 B_2 \sin\Big(\zeta + B_1 p + A_1 B_1 \sin(\zeta + \phi_1) + \phi_2\Big) \ . \end{aligned} \tag{6}$$

Substituting Eq. (6) into Eq. (5) we find, explicitly:

$$\bar{\rho}(\Omega) = \frac{N_0}{2\pi\sigma_\zeta} \int_{-\infty}^{\infty} dp d\zeta \exp\left[-\frac{p^2}{2} - \frac{\zeta^2}{2\sigma_\zeta^2}\right] ,$$

This explains why only a relative phase ϕ was introduced in [4]. At variance, in this paper we treat the time-dependent case, where the two laser phases can exhibit different time variations. As a result, here we include the phases ϕ_1 and ϕ_2 of both lasers.

$$\times \exp\Bigg\{ -i\Omega\Bigg[\zeta + (B_1 + B_2)p + A_1(B_1 + B_2)\sin(\zeta + \phi_1)$$
$$+A_2B_2 \sin\Big(\zeta + B_1p + A_1B_1 \sin(\zeta + \phi_1) + \phi_2\Big)\Bigg]\Bigg\} \tag{7}$$

The following step consists in expanding the exponential factors containing trigonometric expressions according to [4]:

$$\exp[-i\Omega A_1(B_1 + B_2)\sin(\zeta + \phi_1)] = \sum_{k=-\infty}^{\infty} \exp[ik(\zeta + \phi_1)]J_k\left[-\Omega A_1(B_1 + B_2)\right] \tag{8}$$

and

$$\exp\Big[-i\Omega A_2B_2 \sin\Big(\zeta + B_1p + A_1B_1 \sin(\zeta + \phi_1) + \phi_2\Big)\Big] =$$
$$\sum_{m=-\infty}^{\infty} \exp\Big[im\Big(\zeta + B_1p + A_1B_1 \sin(\zeta + \phi_1) + \phi_2\Big)\Big] J_m\left[-\Omega A_2B_2\right] \ , \tag{9}$$

where one can still expand

$$\exp[imA_1B_1 \sin(\zeta + \phi_1)] = \sum_{l=-\infty}^{\infty} \exp[il(\zeta + \phi_1)]J_l\left[mA_1B_1\right] \ . \tag{10}$$

Assuming, for the moment, a dependence of the laser phases ϕ_1 and ϕ_2 on ζ, and collecting terms that have a dependence on ζ we can define

$$\bar{f_\zeta}(k + l + m - \Omega) = \int_{-\infty}^{\infty} d\zeta f_{0\zeta}(\zeta) \exp[i(k + l + m - \Omega)\zeta] \exp[i(k + l)\phi_1 + im\phi_2] \tag{11}$$

and obtain from Eq. (7):

$$\bar{\rho}(\Omega) = \frac{1}{\sqrt{2\pi}} \sum_{m,k,l} \bar{f_\zeta}(k + l + m - \Omega)J_k\left[-\Omega A_1(B_1 + B_2)\right] J_m\left[-\Omega A_2B_2\right] J_l\left[mA_1B_1\right]$$
$$\times \int_{-\infty}^{\infty} dp \exp\left[-\frac{p^2}{2}\right] \exp[-i\Omega(B_1 + B_2)p + imB_1p] \ . \tag{12}$$

[4] In the following k is just an index, without the meaning of wavenumber.

The integration over p can be carried out using

$$\frac{1}{N_0}\int_{-\infty}^{\infty} dp \exp[-i\Omega p(B_1+B_2)+impB_1] f_{0p}(p) = \exp[(\Omega(B_1+B_2)-mB_1)^2/2] \tag{13}$$

which yields

$$\begin{aligned}\bar{\rho}(\Omega) = &\sum_{m,k,l} \bar{f_\zeta}(k+l+m-\Omega) J_k\left[-\Omega A_1(B_1+B_2)\right] J_m\left[-\Omega A_2 B_2\right] J_l\left[mA_1B_1\right] \\ &\times \exp[(\Omega(B_1+B_2)-mB_1)^2/2]\,. \end{aligned} \tag{14}$$

Setting $n = k+l$ and using

$$J_{k+l}(\alpha+\beta) = \sum_{l=-\infty}^{\infty} J_l(\beta) J_k(\alpha)\,, \tag{15}$$

Eq. (14) can be re-written as

$$\begin{aligned}\bar{\rho}(\Omega) = &\sum_{m,n} \bar{f_\zeta}(n+m-\Omega) J_n\left[-\Omega A_1(B_1+B_2)+mA_1B_1\right] J_m\left[-\Omega A_2 B_2\right] \\ &\times \exp[(\Omega(B_1+B_2)-mB_1)^2/2]\,. \end{aligned} \tag{16}$$

We now apply the adiabatic approximation imposing that the width of the peaks in $\bar{f_\zeta}$ is much narrower than the harmonic separation ω_l between peaks. Analysis of Eq. (16) and Eq. (11) shows that due to the adiabatic approximation, the contribution to $\bar{f}(\Omega)$ for a given value of $m+n$, is peaked around $\Omega \simeq m+n$. This means that the terms in the sum over m in Eq. (16) can be analyzed separately for a fixed value of $m+n$, and one obtains

$$\begin{aligned}\bar{\rho}(\Omega, m+n) = &\sum_{n} \bar{f_\zeta}(n+m-\Omega) J_n\left[-\Omega A_1(B_1+B_2)+mA_1B_1\right] J_m\left[-\Omega A_2 B_2\right] \\ &\times \exp[(\Omega(B_1+B_2)-mB_1)^2/2]\,. \end{aligned} \tag{17}$$

It should be remarked that due to the adiabatic approximation, and to non-resonant behavior of Bessel functions, in Eq. (16) we can replace Ω with $m+n$ under the Bessel functions. In this way, $\bar{f_\zeta}$ can be interpreted as the Fourier transform of the electron bunch density. The physical meaning of all this, is that $\bar{f_\zeta}$ is peaked at frequencies Ω near to multiples $n+m$ of the laser frequency. In [4] it is reported that, in order to maximize the modulus of the bunching factor one should impose $n = \pm 1$. This can be seen directly by inspecting the right hand side of Eq. (13). In fact, for values of Ω near to $n+m$, the argument in the exponential function can be written as $p^2(B_1 n + B_2(n+m))^2/2$. When $n = -1$ and m is positive and large for example, one sees that that $B_1 n$ is large and negative, while $B_2 m$ is large and positive. Therefore, m can be chosen such that $-B_1 + B_2(m-1) \simeq 0$. This is guarantees remarkable up-frequency conversion efficiency, almost independently on the energy spread and constitutes one of the great advantages of the EEHG scheme. We will restrict our investigation to the case $n = -1$ and $m > 0$, thus obtaining

$$
\begin{aligned}
\bar{\rho}(\Omega, m-1) = {} & \bar{f}_\zeta(m-1-\Omega) J_{-1}\left[-\Omega A_1(B_1+B_2) + m A_1 B_1\right] \\
& \times J_m\left[-\Omega A_2 B_2\right] \exp[(\Omega(B_1+B_2) - m B_1)^2/2] \,.
\end{aligned} \tag{18}
$$

Note that if the laser phases would not depend on ζ, which is not true in general, one could separately calculate

$$
\begin{aligned}
& \int_{-\infty}^{\infty} d\zeta f_{0\zeta}(\zeta) \exp[i(m-1-\Omega)\zeta] = \\
& \frac{1}{\sqrt{2\pi}\sigma_\zeta} \int_{-\infty}^{\infty} d\zeta \exp\left[-\frac{\zeta^2}{2\sigma_\zeta^2}\right] \exp[i(m-1-\Omega)\zeta] = \exp\left[-\frac{\sigma_\zeta^2}{2}(m-1-\Omega)^2\right] .
\end{aligned} \tag{19}
$$

In this case, the adiabatic approximation can be simply enforced imposing that $\sigma_\zeta \gg 1$. Finally, it should be noted that the initial electron density distribution and laser phases ϕ_1 and ϕ_2 are not only functions of ζ, but also of the transverse position $\vec{r}$. It should be understood that the transverse direction can be factorized, which is a simplifying but not principal assumption, and that therefore, all the expressions above are considered valid at any fixed transverse position.

To conclude, let us consider our initial question, whether the general principle of the frequency multiplier chains is valid or not for EEHG. The answer is affirmative, and can be seen by inspecting Eq. (18) and Eq. (11). In the case when $\phi_1 = \phi_2$ such principle can be applied strictly. In case ϕ_1 and ϕ_2 differ, but are still of the same order of magnitude, we can conclude that, since $n = -1$ and m is large, only ϕ_2 is important and the principle is applicable with accuracy roughly $1/N$.

3 Temporal quality of the seed laser beam

Nowadays, high peak power laser systems are capable of producing very high intensities, thus fulfilling the requirements for many high field applications including EEHG FELs. In particular, femtosecond laser systems have become the primary method to deal with these applications. The reasons for this are the availability of broadband, efficient lasing media such as titanium-doped sapphire (Ti:Sa), and of techniques like Kerr-lens mode locking and chirp pulse amplification (CPA). In CPA systems, light passes through a number of optical components. Moreover, non-linear effects take place in the amplifying medium. This can degrade the temporal quality of the output pulse, which can be appropriately modeled in a slowly-varying real field envelope and time-dependent carrier frequency approximation. The time-bandwidth product constitutes a proper measure of the departure from the ideal case, in which there are no temporal variations of the carrier frequency. In this Section we quantitatively describe the relation between carrier frequency chirp and corresponding broadening of the spectrum. This leads to a time-bandwidth product exceeding the Fourier limit.

3.1 Pulse duration and spectral width

For our purposes, it is convenient to consider a Gaussian pulse with a linear frequency chirp. This choice is one of analytical convenience only, and may be generalized. The slowly complex field envelope is given by

$$E(t) = A \exp\left[-\frac{t^2}{2\tau^2}\right] \exp\left[i\frac{\alpha t^2}{2\tau^2}\right] \tag{20}$$

where α is the chirp parameter, and the FWHM pulse duration is related to the rms duration τ by $\Delta\tau = \sqrt{4\ln 2} \cdot \tau$.

By Fourier transforming Eq. (20), it can be demonstrated (see e.g. [15]) that the spectral intensity is a Gaussian with a FWHM given by $\Delta\omega = (\sqrt{4\ln 2}/\tau)\sqrt{1+\alpha^2}$. The time-bandwidth product of the pulse is therefore

$$\Delta\omega \cdot \Delta\tau = 4\ln 2 \cdot \sqrt{1+\alpha^2} \tag{21}$$

This is larger than the time-bandwidth product of an unchirped Gaussian pulse, which is just $4\ln 2$. In other words, chirping increases the time-bandwidth product by broadening the pulse spectrum while preserving the pulse width. Note that $\Delta\omega \cdot \Delta\tau = 4 \ln 2$ is the smallest time-bandwidth product for a Gaussian pulse corresponding to the transform-limit (or bandwidth limit, or Fourier limit).

The temporal quality of the pulse can be defined by a quality factor M_t^2, defined as the ratio between the time-bandwidth product for real and transform-limited pulse. Hence, one can characterize pulse by specifying its quality through the M_t^2 factor and by giving the pulse shape. In our case of interest, $M_t^2 = \sqrt{1+\alpha^2} > 1$ for Gaussian pulses with linear frequency chirp.

Finally, it should be noted that considerations analogous to those just discussed above, can be proposed for the electron beam microbunching. For example the current envelope of a Gaussian, chirped electron beam can be described similarly as in Eq. (20), with a chirp parameter α_m. A time-bandwidth product can be defined, and a quality factor $M_{t,m}$ can be defined as well.

3.2 Constraint on temporal phase variation for the output Ti:Sa laser pulse

There are several simplifying assumptions that will be used in our analysis. As has been the case for the analysis presented in the previous paragraph, we restrict our attention to a microbunched electron beam with Gaussian shape. This is not a significant restriction, and extensions are not difficult to consider.

We introduce the following criterion: we consider the electron beam microbunching nearly transform-limited when the performance ratio $M_{t,m}^{-2}$ is down not more than $1/\sqrt{2}$. For a microbunching with Gaussian shape and linear frequency chirp, this criterion will be satisfied under the restriction that the microbunch chirp parameter $\alpha_m < 1$.

A specific example of a microbunched beam with Gaussian profile could be realized in the case when EEHG scheme uses an electron bunch with Gaussian temporal profile and a seed laser pulse with flat-top profile in time across the duration of the electron bunch. As demonstrated in e.g. [10], the generated bunching is not sensitive to the peak current. Therefore, EEHG can operate with a nonuniform electron bunch profile. In the next paragraph we will demonstrate that in any case, due to non-linear (self-phasing) effects in the Ti:Sa laser system and in the post-laser optics system, the seed laser must have flat-top profile in time with very little temporal variation. Therefore, the model of a seed pulse with flat-top profile and of an electron bunch with Gaussian profile is consistent with the EEHG scheme.

Now, if the phase of the seed laser is chirped, the microbunching chirp is simply multiplied by the frequency multiplication factor N. This can be seen by looking at the harmonic contents of the current density found in Eq. (16). That expression includes $\bar{f_\zeta}$, which in the case of $\phi_1 = \phi_2 = \alpha\zeta^2/(2\sigma_\zeta^2)$ is given by (see Eq. (11)):

$$\bar{f_\zeta}(m-1-\Omega) = \int_{-\infty}^{\infty} d\zeta f_{0\zeta}(\zeta) \exp[i(m-1-\Omega)\zeta] \exp[-i\phi_1 + im\phi_2]$$
$$= \frac{1}{\sqrt{2\pi}\sigma_\zeta} \int_{-\infty}^{\infty} d\zeta \exp[i(m-1-\Omega)\zeta] \exp\left[-\frac{\zeta^2}{2\sigma_\zeta^2}\right] \exp\left[i(m-1)\frac{\alpha\zeta^2}{2\tau_\zeta^2}\right] \tag{22}$$

The last phase factor under integral shows that the laser phase is indeed multiplied by $N = m - 1$.

We will define the frequency chirp in the seed laser pulse only across the target duration of the electron bunch, and use the same time normalization as for the beam microbunching. The complex field envelope of a laser pulse with stepped profile and linear frequency chirp is given by

$$E(\zeta) = E_0 \exp\left[i\frac{\alpha\zeta^2}{2\sigma_\zeta^2}\right] , \tag{23}$$

where E_0 is a constant. As discussed above, the frequency multiplication yields a complex "microbunching" envelope with carrier frequency $\omega_0 = (m-1)\omega_l$

$$a(\zeta) = a_0 \exp\left[-\frac{\zeta^2}{2\sigma_\zeta^2}\right] \exp\left[i\frac{\alpha_m\zeta^2}{2\sigma_\zeta^2}\right] \tag{24}$$

where ρ_0 is a constant, and $\alpha_m = N\alpha$ is the microbunching chirp parameter. Note that what we loosely defined as "microbunching" is, more formally, the slowly-varying amplitude of the electron density modulation with carrier frequency $\Omega = N$. It follows from the previous analysis that the EEHG scheme can produce nearly transform-limited microbunching only under the restriction $\alpha_m \lesssim 1$, meaning that the laser chirp parameter must obey $\alpha \lesssim 1/N$. The EEHG seed laser is assumed to be a Ti:Sa laser. The actual seed laser beam consists in the third or in the fourth harmonic of the Ti:Sa laser beam. Usually, laser frequency multipliers are based on the use of Beta Barium Borate (BBO) crystals. The effect of frequency multiplication on phase variation amounts again to multiplication of the phase variations.

Therefore we may say that when we study constraints on the performance of Ti:Sa seed laser for EEHG schemes, the total frequency multiplication chain consists of two stages. The first stage is the BBO crystals with a frequency multiplication factor $N_1 = 3$ (or $N_1 = 4$). The second stage is the EEHG setup itself, with frequency multiplication factor up to $N_2 \sim 270$ (or $N_2 \sim 200$). If the final required output radiation is around wavelengths of 1 nm, the total frequency multiplication factor $N = N_1 N_2$ is about $N \sim 800$.

From the previously discussed condition $\alpha \lesssim 1/N$ it can be seen that the Ti:Sa laser produces nearly transform-limited microbunching at wavelengths around 1 nm only when the laser chirp parameter $\alpha \lesssim 10^{-3}$. Thus, for most purposes, if the total multiplication factor is around 800 or exceeds it, we may formulate the constraint on the Ti:Sa laser quality by requiring a quality factor M_t^2 departing from unity of no more than about 10^{-6}.

One can think that the above-discussed constraints on seed laser may be true only for the particular case of EEHG. However, we can show that these constraints are actually of more general validity. For example, HGHG schemes can produce nearly transform-limited radiation spanning down to wavelengths of 1 nm only under the same restrictions on temporal quality of the seed Ti:Sa laser. The key advantage of the EEHG scheme is that the amplitude of the achieved microbunching factor slowly decays with increasing harmonic number and that, consequently, generation of coherent soft X-ray emission within a single upshift stage becomes possible [3, 4]. However, considering constraints on the seed laser M_t^2 factor, all harmonic generation schemes are similar, and must obey the universal result

$$M_t^2 - 1 \lesssim \frac{1}{N^2} \ . \tag{25}$$

The requirement in the inequality (25) can be somehow relaxed if the requirement of near-Fourier limit is relaxed as well. For example, the operation of a EEHG FEL is characterized by two microbunch bandwidth scales of interest. One is associated with inverse electron bunch duration $\Delta\omega_b = 1/\tau_b$, τ_b being the electron bunch duration. The other is the FEL amplification bandwidth $\Delta\omega_a$. One can relax the requirement of near-Fourier limit substituting it by the requirement to achieve an output radiation bandwidth narrower than the SASE bandwidth $\Delta\omega_a$. On the one hand, the product of bunch duration by amplification bandwidth can be estimated in the order of $\tau_b\Delta\omega_a \sim 10^2$ in the soft X-ray wavelength range. On the other hand, the FEL radiation bandwidth broadening due to the effect of linear frequency chirp is about $\Delta\omega \sim |\alpha_m|/\tau_b$. Therefore, in the case when

$$|\alpha_m| > (\tau_b\Delta\omega_a) \sim 10^2 \ , \tag{26}$$

the output signal has a bandwidth larger than the SASE bandwidth, and harmonic generation techniques have no practical applications. However, if, for example, we have a microbunching chirp parameter $|\alpha_m| \sim 10$, the effective radiation bandwidth becomes ten times narrower than the SASE bandwidth, although is ten times wider compared to the ideal transform-limited bandwidth. Following this discussion, a weaker constraint on the temporal quality factor of seed laser is $M_t^2 - 1 < 10^2/N^2$. For a Ti:Sa laser seed and a radiation wavelength of 1 nm it is possible to discuss about harmonic generation techniques applications only when $M_t^2 - 1 < 10^{-4}$.

To complete the picture, we should note that an alternative method to harmonic generation setups, called self-seeding [16, 17, 18], is available, and allows for the generation of temporally coherent radiation in XFELs. A self-seeded soft X-ray FEL consists of two undulators separated by a monochromator installed within a magnetic chicane. The remarkable temporal quality of the output radiation and the wavelength tunability of self-seeding schemes has stimulated interest in using this technique to generate nearly transform-limited soft- X-ray pulses. A project of self-seeding schemes with grating monochromator is now under development at LCLS II [19]-[21]. EEHG output will compete with self-seeding output only when the temporal quality of the seed laser beam obeys the mores stringent requirement (25).

3.3 Self-phasing and constraints on field amplitude variation

The seeding pulse from the Ti:Sa laser must necessarily propagate through vacuum window and BBO crystals without experiencing temporal phase distortions. Above a power density of 1GW/cm^2, the refractive index n becomes intensity-dependent according to the well-known expression

$$n = n_0 + n_2 I \,, \tag{27}$$

where n_0 is the index of refraction at low intensity and I is the laser intensity. Due to temporal variations of the laser pulse intensity, the pulse phase will then be distorted according to [15]

$$B = \frac{2\pi}{\lambda} \int_0^L dz n_2 I \,. \tag{28}$$

Here λ is the laser wavelength, and B represents the amount of phase distortions accumulated by the pulse over a length L. The dimensionless B parameter, also known as B integral, is often used as a measure of the strength of nonlinear effects due to the non-linear refractive index $n_2 I$. Field intensities, propagation distances, and values of $n_2 I$ such that $B > 1$ generally yield significant nonlinear effects, including self-phase modulation. Usually, in laser optics, when $B < 0.5$ pulse distortions should not be a problem.

Let us consider an optical setup behind the Ti:Sa laser with $B \sim 0.5$. In order to have minimal FEL output spectral broadening, the seed laser must have flat-top profile in time with very little temporal variation. The intensity variation must satisfy

$$\frac{\Delta I}{I} < \frac{2}{N} \tag{29}$$

For 1 nm wavelength mode of operation $N \sim 800$, and in the case of near transform-limited FEL output pulse, the intensity of Ti:Sa laser pulse must be controlled to about 0.3% across the target duration of the electron bunch.

4 Spatial quality of seed laser beam

In the last section we considered part of the constraints on the performance required for EEHG seed lasers. In particular, our discussion has been restricted to the temporal quality of laser beams. The former restriction allows one to obtain results which depend on the frequency multiplication factor only, so that the treatment discussed above applies not only to EEHG schemes, but to more general cases as well. In this section we discuss, instead, the influence of errors on the wavefront of the seed laser beam. A general principle discussed before states that the effect of frequency multiplication by a factor N is to multiply the phase variation in time by N. The same principle holds when dealing with phase variations in space. If the wavefront of the UV seed laser exhibits errors, the errors of the microbunching wavefront are multiplied by the frequency multiplication factor. This can be seen with an analysis similar to that in paragraph 3.2, based on the results in Section 2, which led to Eq. (22). However, now, the phase variations are to be considered as a function of spatial coordinates. In the case of variation in time, the temporal quality of the output FEL radiation is a replica of the temporal quality of the microbunching input. It seems natural to use the same principle for characterizing the spatial quality of the output FEL radiation. However, this cannot be done. The reason is that the transverse coherence of FEL radiation is settled without laser seeding. This is due to the transverse eigenmode selection mechanism: only the ground eigenmode survives at the end of the amplification process. It follows that the microbunching wavefront errors do not affect the spatial quality of the output radiation. They only affect the input signal value. The description of the influence of phase

Table 1
Analogy between temporal and spatial characteristics

Temporal (pulse)	Spatial (beam)
transform-limited pulse	diffraction-limited beam
temporal frequency	spatial frequency
bandwidth of amplification	bandwidth of amplification
temporal frequency shift (temporal linear phase chirp)	wavefront tilt (spatial linear phase chirp)
linear temporal frequency chirp (temporal quadratic phase chirp)	defocusing aberration (spatial quadratic phase chirp)
nonlinear temporal frequency chirps	high order wavefront aberrations
phase fluctuations in time	chaotic phase variation across the beam

errors depends in detail on the harmonic generation process. For example, in the case of HGHG, the seed laser directly produces microbunching in the first cascade only, which is characterized by a relatively small frequency multiplication factor $N < 5$. In EEHG schemes instead, the generation of coherent radiation in the soft X-ray wavelength range should be achieved with a single upshift stage using a UV (200 nm or 270 nm) laser beam. In this case the frequency multiplication factor amounts to about $N \sim 200$. Consequently, the EEHG technique is much more sensitive to laser wavefront errors. This disadvantage is actually related to the key EEHG advantage, that is to allow for high frequency multiplication numbers within a single, compact scheme.

To understand the effects of wavefront errors we shall use an analogy between time and space. This analogy suggests the possibility of simply translating the effects related to phase perturbation in time into effects related to wavefront perturbations as shown in Table 1.

We defined the ideal seed pulse as a transform-limited pulse i.e. a pulse without phase variations in time. The space-domain analog of a transform-limited pulse is a diffraction-limited beam, i.e. a beam without phase variations in space. From this definition follows that a beam can be diffraction-limited only at its waist, where it takes on the minimum possible product between size and spatial frequency bandwidth. In fact, beam propagation leads to a beam broadening and to a spatial quadratic phase chirp. Since the ideal seed laser beam is characterized by microbunching wavefront without phase variation across the electron beam, it follows that the seed laser beam must be diffraction-limited at its waist, which must be placed in the middle of the modulator undulator.

Simple physical considerations directly lead to a crude approximation for the amplification bandwidth. As already discussed in paragraph 3.2, in the time domain the amplification bandwidth is about two order of magnitudes larger than transform-limited bandwidth:

$$\tau_b \Delta\omega_a \sim 10^2 \ . \tag{30}$$

This fact has some interesting consequences. Suppose that we consider microbunching with linear phase chirp in time, which is actually equivalent to a shift of the signal frequency. In the case when the shift is smaller than the amplification bandwidth, the temporal quality and the output power of the radiation pulse are not changed. At variance, microbunching with nonlinear phase chirp leads to a spectral broadening of the output radiation and, consequently, to degradation of the temporal quality. However, in the case when the broadening is smaller than the amplification bandwidth, the output power is not suppressed. The situation is quite different when considering the spatial domain. In fact, qualitatively, the spatial frequency amplification bandwidth and the diffraction-limited bandwidth are the same, so that any shift or broadening of the spatial frequency spectrum immediately leads to input signal suppression.

Let us study the discrepancy between the direction of the electron motion and the normal to the microbunching wavefront. In the case when the discrepancy between these two directions is larger than the FEL angular amplification bandwidth the input signal is exponentially suppressed. Let us assume that the spatial profile of the microbunching is close to that of the electron beam, and is characterized by a Gaussian shape with standard deviation σ_b. The FEL angular amplification bandwidth can then be estimated as $\Delta\theta_a \sim (k\sigma_b)^{-1}$, where k is wavenumber at the target harmonic.

One can then estimate the angular spectrum of e.g. the LCLS output for the wavelength of 1.5 nm. The transverse distribution of the electron beam is described by $\sigma_b \sim 30\mu$m, and our estimations give $\Delta\theta_a \sim 8\mu$rad. The angular amplification bandwidth corresponds to the HWHM of the FEL output angular distribution. Results of numerical simulations, confirmed by experimental results, give an angular distribution of the radiation intensity with HWHM $\sim 10\mu$rad. From these numbers one can see that the above approach provides an adequate description, at least in the wavelength range around 1 nm. The value $\Delta\theta_a$ can subsequently be used to estimate the maximum angular error allowed between the normal to the laser beam wavefront (at its waist) and the direction of the electron beam motion in the modulator undulator. It follows from the previous reasoning that in the case of radiation wavelength around 1 nm we find an alignment tolerance of about 10μrad.

The wavefront tilting is a relatively simple (first order) geometrical distortion and its measure is simply an angle, which is the same for the microbunching wavefront and for the laser beam wavefront. The width of the seed laser beam at its waist can be much larger than the width of the electron beam, but the tilt is completely characterized by such angle only. There are several criteria to analyze the performance of laser system to higher order aberrations. To characterize the spatial quality of the laser beam, we will use the Strehl ratio S, usually defined [5] as:

$$S = \frac{\max[|FT\{E(x,y)\exp[i\phi(x,y)]\}|^2]}{\max[|FT[E(x,y)]|^2]} \ , \qquad (31)$$

where "FT" indicates the 2D spatial Fourier transform operation, $E(x, y)$ is the ideal wave amplitude, and $\phi(x, y)$ is the phase aberration. The Strehl ratio S becomes an important figure of merit from the viewpoint of seeding evaluation.

Let us consider the practical situation in which both laser and electron beams are characterized by a Gaussian shape, and in which the width of the laser beam at its waist is much larger than the width of the electron beam. With this assumption, within the electron beam, at the laser beam waist in the plane $z = 0$ we have asymptotically $E(x, y, 0) = \mathrm{const} \cdot \exp[i\phi(x, y)]$, where $E(x, y, 0)$ is the wave amplitude, and $\phi(x, y)$ describes phase aberrations. For our purposes it is interesting to consider the Gaussian-weighted Strehl ratio S

$$S = \left|\left\langle \exp[i\phi(x,y)]\right\rangle\right|^2 \ , \qquad (32)$$

where

$$\left\langle \exp[i\phi(x,y)]\right\rangle = (2\pi\sigma_p^2)^{-1} \int dxdy \exp\left[-\frac{x^2+y^2}{2\sigma_p^2}\right] \exp[i\phi(x,y)] \ . \qquad (33)$$

Here σ_p is a Gaussian parameter of the same order of magnitude of the rms width of the electron beam, σ_b. If the phase is sufficiently small to accurately replace $\exp[i\phi]$ with $1 + i\phi - \phi^2/2$, one obtains

$$S = 1 - \sigma_\phi^2 \ , \qquad (34)$$

where

[5] With this definition, the Strehl ratio is related to the transverse M^2 parameter by $S = 1/M^2$

$$\sigma_\phi^2 =< \phi^2 > - < \phi >^2 \tag{35}$$

is the variance of the phase aberration weighted across a Gaussian-amplitude pupil. To be more specific, we define the average of $\phi(x, y)$ across the pupil as

$$< \phi >= (2\pi\sigma_p^2)^{-1} \int dxdy \exp\left[-\frac{x^2 + y^2}{2\sigma_p^2}\right] \phi(x, y) , \tag{36}$$

and, likewise, the average of the square of $\phi(x, y)$ as

$$< \phi^2 >= (2\pi\sigma_p^2)^{-1} \int dxdy \exp\left[-\frac{x^2 + y^2)}{2\sigma_p^2}\right] \phi^2 . \tag{37}$$

It follows that if the root-mean-square variations of the wavefront are of the order of a tenth of the wavelength only, we obtain a Strehl ratio of 0.6.

Let us now discuss the spatial quality of the microbunching wavefront. The interesting value to know for EEHG operation is the input coupling factor between the microbunching and the ground eigenmode of the FEL amplifier. Let us consider the amplitude of the electron density modulation at the carrier frequency $\omega_0 = (m - 1)\omega_l$:

$$\rho(x, y, t) = a(x, y, t) \exp[i(m - 1)\omega_l t] . \tag{38}$$

In ideal case, the electron density modulation exhibits a plane wavefront and a Gaussian shape across the electron beam:

$$a(x, y, t) = a_0(t) \exp\left[-\frac{x^2 + y^2}{2\sigma_b^2}\right] . \tag{39}$$

In such ideal case, the input coupling factor is therefore

$$C = \int dxdy \exp\left[-\frac{x^2 + y^2}{2\sigma_b^2}\right] \Psi(x, y) , \tag{40}$$

where $\Psi(x, y)$ is the field distribution of the ground eigenmode. In the high gain linear regime, the FEL output radiation power scales as

$$W_{\mathrm{output}} \sim |C|^2 . \tag{41}$$

In the case of a non-ideal microbunching wavefront, expressions for $a(x, y, t)$ and for the input coupling factor respectively transform to:

$$a(x, y, t) = a_0(t) \exp[i\phi_m(x, y)] \exp\left[-\frac{x^2 + y^2}{2\sigma_b^2}\right] , \tag{42}$$

and

$$C = \int dxdy\, a(x, y, t)\Psi(x, y) , \tag{43}$$

where $\phi_m(x, y)$ is the microbunching phase aberration. The ratio of the output power for the case including microbunching wavefront errors to the output power for the case of a plane microbunching wavefront is a simple and convenient measure of the departure from the ideal situation. In our case this ratio is simply

$$\frac{W_{\mathrm{nonideal}}}{W_{\mathrm{ideal}}} = \frac{|C_{\mathrm{nonideal}}|^2}{|C_{\mathrm{ideal}}|^2} . \tag{44}$$

Various approximations can be invoked. One of the simplest is to use the following expression for the ground FEL eigenfunction

$$\Psi(x, y) \sim \exp\left[-\frac{x^2 + y^2}{2\sigma_b^2}\right] . \tag{45}$$

With this approximation it can be shown that

$$\frac{|C_{\mathrm{nonideal}}|^2}{|C_{\mathrm{ideal}}|^2} = 1 - \sigma_\phi^2 , \tag{46}$$

where σ_ϕ^2 is the variance of the microbunching phase aberration across the Gaussian-weighted pupil with

$$\sigma_p = \frac{\sigma_b}{\sqrt{2}} . \tag{47}$$

If we now look at the ratio of the power values at the FEL exit with microbunch wavefront distortions and without distortions, we see that such ratio corresponds to the already introduced laser Strehl ratio, Eq. 34. More in general, we have the same definition given in Eq. (32), where the phase

ϕ under the integral is now defined as the phase on the microbunching wavefront ϕ_m.

Finally, we calculate the relation between the phase distortions of the laser beam and the phase distortions of the microbunching. We have concluded from our theoretical analysis in Section 2, that if the wavefront of the seed laser beam in the waist plane exhibits errors, the errors of the microbunching wavefront are multiplied by the frequency multiplication factor N. Therefore we have

$$(\sigma_\phi)_{\mathrm{laser}} = \frac{1}{N}(\sigma_\phi)_{\mathrm{microbunch}} \,, \tag{48}$$

which yields

$$1 - S_{\mathrm{laser}} = \frac{1}{N^2}[1 - S_{\mathrm{microbunch}}] \,. \tag{49}$$

For EEHG schemes, $[1 - S_{\mathrm{microbunch}}]$ must be kept below 0.4, corresponding to microbunching wavefront distortions of $\lambda/10$. This corresponds to a UV laser Strehl ratio $S_{\mathrm{laser}} > 0.99999$ at the target wavelength of 1 nm.

In order to experimentally investigate the effects of laser wavefront errors on the FEL amplification process, one should perform direct measurements of the laser beam wavefront using, for example, a Hartmann sensor. Usually, measurements of the spatial quality of the output laser beam with a Hartmann sensor give the near-field wavefront characteristics. The knowledge of the spatial phase and amplitude in a particular plane opens the possibility of calculating, by Fresnel propagation, the phase and amplitude in any other plane for a freely propagating laser beam, and in particular allows to recover results in the middle plane of the modulator undulator. Applying the definition of the Gaussian-weighted Strehl ratio in Eq. (32) with $\sigma_p = \sigma_b/\sqrt{2}$ leads to the value which needs to be compared with constraint

$$1 - S < \frac{0.4}{N^2} \,. \tag{50}$$

The arguments discussed above seem to be strong enough to suggest that EEHG FEL schemes for reaching frequency multiplication factor of N will not work when the difference of the above-defined laser Strehl ratio from the unity does not satisfy the inequality in (50). This conclusion for the spatial domain contrasts with that in the time domain, where the phase distortions lead to spectral broadening but do not have an impact on the FEL output power.

5 Conclusions

It is very desirable to have a way to model the performance of EEHG FEL with high frequency multiplication factor. Such modeling would naturally start with the Ti:Sa laser system. Calculations would involve the knowledge of the temporal and spatial properties of the Ti:Sa laser source itself together with laser field propagation through the optical components used in the EEHG beamline. Most of our calculations are, in principle, straightforward applications of conventional laser optics and general theory of frequency multiplier chains. Our paper provides physical understanding of the laser seeding setup and we expect it to be useful for practical estimations, especially at the design stage of the experiment. Detailed EEHG mechanism is so complicated that we cannot accurately determine the EEHG output by analytical methods. However, a definite relation between quality of the input signal and EEHG FEL output can be worked out without any knowledge about the EEHG internal machinery.

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