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ROSA: RECONSTRUCTION OF SPECTROGRAM AUTOCORRELATION FOR SELF-AMPLIFIED SPONTANEOUS EMISSION FREE-ELECTRON LASERS

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Abstract

X-ray Free Electron Lasers (FELs) have opened new avenues in photon science, providing coherent x-ray radiation pulses orders of magnitude brighter and shorter than previously possible. The emerging concept of "beam by design" in FEL accelerator physics aims for accurate manipulation of the electron beam to tailor spectral and temporal properties of radiation for specific experimental purposes, such as x-ray pump/x-ray probe and multiple wavelength experiments. A cost-efficient method to extract information on longitudinal Wigner distribution function of emitted FEL pulses is proposed. It requires only an ensemble of measured FEL spectra.

INTRODUCTION

There has been a rapid growth both in the number of scientific users and in the diversity of new science enabled by Free-Electron laser sources. This growth is possible due to the continuously improving capabilities of FEL facilities. One promising avenue which opens the way to new experiments is is the tuning of spectral and temporal properties of radiation for specific experimental purposes, e.g., generating wide bandwidth [1–3], narrow-bandwidth [4] or extremely short [5,6] radiation pulses. Some information about duration of the typical radiation pulse, hence the length of an electron beam lasing window, can be extracted from radiation spectra of FEL operating in Self-Amplified Spontaneous Emission (SASE) mode. Taking advantage of the radiation statistical properties [7] and assuming a particular temporal profile, spectral correlation analysis gives an estimate of the average duration of the SASE FEL pulse [8,9]. The close relation between electron phase space and radiation characteristics must be taken into account while trying to performing radiation pulse diagnostics. For example, a chirp in the electron beam energy yields a chirp in radiation frequency [10], it affects the range of spectral coherence [11], and hence the spectrum-based estimation of the SASE pulse duration. We present a fast and efficient method to provide feedback on the temporal and spectral properties of FEL radiation: measurement of the autocorrelation of an ensemble-averaged pulse Wigner distribution. We study an ensemble-averaged Wigner distribution of SASE FEL pulses and its temporal autocorrelation. We discuss how to calculate it based on measured SASE spectra and what information such reconstruction reveals. We also present results of numerical simulations performed with the code GENESIS [12] and compare calculated Wigner distribution with evaluated reconstructions. It relies entirely on spectrometry of the generated pulses and does not require additional equipment.

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THEORY

Consider a scalar field $E(t)$ in the time domain and slowly varying field amplitude $\widetilde{E}(\omega) = \bar{E}(\omega)\exp(-i\omega_c z/c)$ of its Fourier transform $\bar{E}(\omega)$, where ω_c is a carrier frequency and z is the direction of propagation.

Measurable single-shot radiation spectra are proportional to the square-modulus of the single-shot scalar field[1]

$$\widetilde{I}(\omega) \equiv \widetilde{E}(\omega)\widetilde{E}^*(\omega)\ . \tag{1}$$

The statistical autocorrelation function of the field $E(t)$ in the time and frequency domains can then be defined as

$$\Gamma(t,\Delta t) = \left\langle E\left(t-\frac{\Delta t}{2}\right)E^*\left(t+\frac{\Delta t}{2}\right)\right\rangle\ ,$$
$$\widetilde{\Gamma}(\omega,\Delta\omega) = \left\langle \widetilde{E}\left(\omega-\frac{\Delta\omega}{2}\right)\widetilde{E}^*\left(\omega+\frac{\Delta\omega}{2}\right)\right\rangle\ , \tag{2}$$

where angle brackets $\langle\rangle$ denote ensemble average. Note that the autocorrelation function depends on both time t and time separation Δt, allowing to describe non-stationary radiation fields. The intensity autocorrelation function is, instead

$$\Gamma_I(t,\Delta t) = \left\langle I\left(t-\frac{\Delta t}{2}\right)I\left(t+\frac{\Delta t}{2}\right)\right\rangle\ ,$$
$$\widetilde{\Gamma}_I(\omega,\Delta\omega) = \left\langle \widetilde{I}\left(\omega-\frac{\Delta\omega}{2}\right)\widetilde{I}\left(\omega+\frac{\Delta\omega}{2}\right)\right\rangle\ . \tag{3}$$

The Wigner distribution

$$\mathcal{W}(t,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d(\Delta t)\Gamma(t,\Delta t)\exp(i\omega\Delta t)$$
$$= \int_{-\infty}^{\infty} d(\Delta\omega)\widetilde{\Gamma}(\omega,\Delta\omega)\exp(-i\Delta\omega t) \tag{4}$$

is commonly used to describe properties of FEL radiation [13–17].

Spectrogram of a signal is a two-dimensional convolution of Wigner distribution of that signal with Wigner distribution of the spectrogram window function:

[1] considering cross section perpendicular to the direction of propagation

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$$S_f(t,\omega) = \mathcal{W}_f(t,\omega) * * \mathcal{W}_h(-t,\omega)\ . \tag{5}$$

RECONSTRUCTION ALGORITHM

The algorithm of reconstruction of the spectrogram autocorrelation consists of the following conceptual steps.

First, sufficiently large (around thousand events) statistics of single shot SASE FEL spectra, in the form of Eq. (1) is acquired. Here we assume that only SASE-related fluctuations are present. Otherwise, the measured data should be filtered since they are prone to additional jitter, unrelated to the SASE process.

Second, we calculate the quantity

$$Q(\omega,\Delta\omega) \equiv \left|\widetilde{\Gamma}(\omega,\Delta\omega)\right|^2 = \left\langle \widetilde{I}\left(\omega-\frac{\Delta\omega}{2}\right)\widetilde{I}\left(\omega+\frac{\Delta\omega}{2}\right)\right\rangle - \left\langle \widetilde{I}\left(\omega-\frac{\Delta\omega}{2}\right)\right\rangle\left\langle \widetilde{I}\left(\omega+\frac{\Delta\omega}{2}\right)\right\rangle\ . \tag{6}$$

Finally, third, an inverse Fourier transform yields the reconstruction function $R(t,\omega)$:

$$R(t,\omega) = \int_{-\infty}^{\infty} d(\Delta\omega) Q(\omega,\Delta\omega)\exp(-i\Delta\omega t)\ . \tag{7}$$

It can be shown that $R(t,\omega)$ is the frequency-wise temporal autocorrelation of the Wigner distribution and can be directly calculated based on measured spectra of SASE FEL radiation

$$R(t,\omega) = \mathcal{A}\left[\mathcal{W}(t,\omega)\right] = \int_{-\infty}^{\infty} d\tau \mathcal{W}(\tau,\omega)\mathcal{W}(t+\tau,\omega)\ . \tag{8}$$

NUMERICAL SIMULATIONS AND DISCUSSION

In order to illustrate reconstruction capabilities, we simulated several ensembles of FEL spectra with the FEL code GENESIS [12] and analysed them with the OCELOT package [18].

If no energy chirp is present in the electron beam, the undulator resonance condition is constant along the beam and the generated radiation pulse has no frequency chirp (Figure 1). In this special case the Wigner distribution, and hence the reconstruction, are factorisable and the total pulse length can be estimated: the autocorrelation of the flat-top power profile with length Δs would yield an autocorrelation result with triangular shape and full width at half maximum (FWHM) equal to $\Delta s/2$. In the case of a Gaussian radiation pulse with FWHM Δs, the FWHM size of its autocorrelation will be $\sqrt{2}\Delta s$.

When the energy chirp in the electron beam, in terms of the relative difference of electron energy in the head and

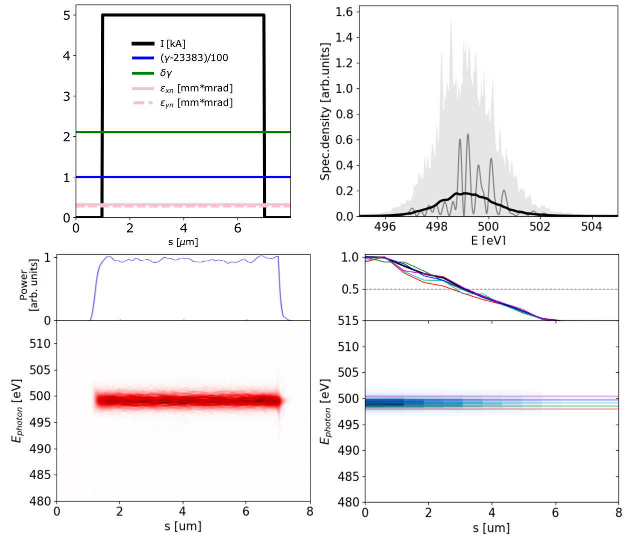

Figure 1: A 6 µm-long flattop model electron beam without energy chirp, see top left plot, used to generate SASE radiation. It is dumped during the exponential growth for 500 statistically independent events. SASE spectra are presented on the top right plot. The ensemble-averaged Wigner distribution of the SASE radiation is presented on the bottom left plot. Hereafter the diverging colormap of a Wigner distribution is normalized to its maximum absolute value, while its zero value is depicted with a white color.The spectrogram autocorrelation reconstruction $R(s,\hbar\omega/e)$ is presented on the bottom right plot. $s = -ct$ is the coordinate along the radiation propagation direction.

tail, exceeds the FEL efficiency parameter $\Delta\gamma/\gamma \gtrsim \rho$, a frequency chirp along the SASE pulse can be observed. As a consequence, it will yield a broader spectrum (which is the integral of the Wigner distribution over time) and typically a shorter pulse length at all photon energies [10] (horizontal line-offs of the Wigner distribution), as presented on Figure 2. These effects are also reflected in the spectral correlation functions, and, if not accounted for, an underestimation of the total pulse duration will take place. Our reconstruction cannot provide information on the group delay of different photon energies, as this information is lost with radiation phases.

In general, the electron beam formation system may yield a highly non-linear energy chirp, as illustrated on Figure 3 (top left plot). If the relative peak-to-valley energy difference in the electron beam is comparable or larger than a Pierce parameter ρ, the electron beam energy chirp will be imprinted into the SASE radiation spectrogram as a radiation frequency chirp. In the given example two distinct pulses of 501 eV photon energy, separated by about 6 µm, are visible on the radiation spectrogram. The separation of these "double pulses" grows with the photon energy, following the separation of the electron beam slices with an equal Lorenz factor γ. Such photon-energy-dependent separation can be straightforwardly observed in the reconstruction function.

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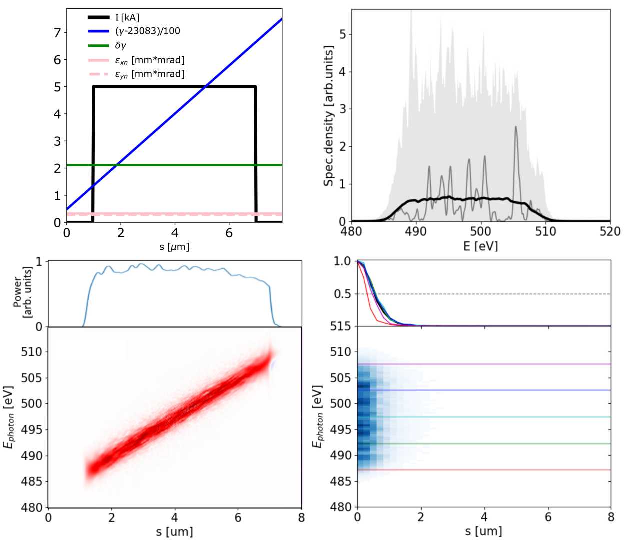

Figure 2: A 6 µm-long flattop model electron beam with linear energy chirp, see top left plot, used to generate SASE radiation. It is dumped during the exponential growth for 500 statistically independent events. Subplots and notations identical to those on Figure 1.

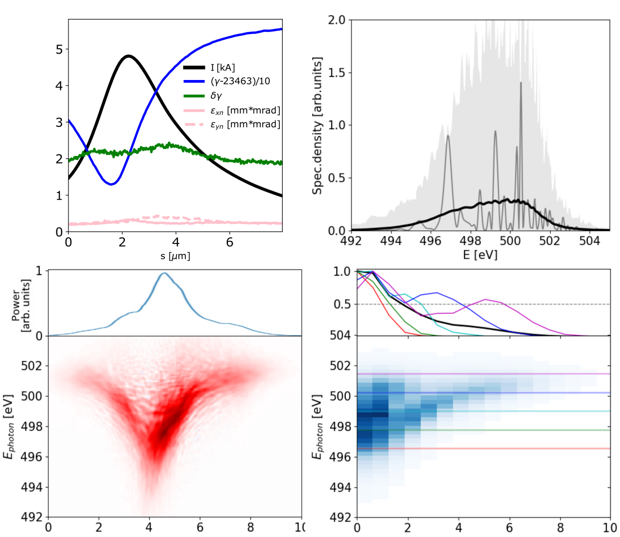

Figure 3: The European XFEL 100 pC electron beam with a non-linear energy chirp produces SASE radiation with different durations at different photon energies. Note the bifurcation in Wigner distribution above 499 eV. Analysis based on 1000 simulated SASE spectra. Subplots and notations identical to those on Figure 1.

CONCLUSION

In this work we show that based on the measureable second order spectral correlation function it is possible to calculate an autocorrelation of the ensemble-averaged Wigner distribution of the radiation. The latter, upon noise filtering via binning, is close in terms of its properties to the well-known spectrogram distribution. Therefore, we call the proposed method ROSA: Reconstruction of Spectrogram Autocorrelation.

It constitutes an extended method to study the time-frequency distribution of X-ray SASE FEL radiation. The method does not require any hardware aside for a high-resolution single-shot spectrometer, which is typically available at XFEL facilities.

The proposed method allows one to characterize the pulse length and approximate temporal shape individually for any photon energy present in the radiation. For instance, it indicates the presence of two temporally separated FEL pulses with overlapping photon energies and provides information about their duration and temporal separation. Comparison of the apriori known Wigner distributions with calculated ROSA distributions for simulation results shows that ROSA distributions provide extensive information about the pulse structure.

The method relies upon the fact that FEL pulses are short, narrow-bandwidth, and follow Gaussian statistics, at least up saturation. Also, it is statistical in nature and relies upon the assumption that FEL hardware provides a reproducible electron beam along the stable orbit. Otherwise, discrimination of outlier events should take place.

In comparison with the conventional method of fitting the second-order spectral correlation function with a theoretical form-factor [8, 9], the proposed method does not require an initial assumption on the power profile of the SASE pulse. On the contrary: it yields additional information about the time domain of the SASE radiation. We suggest that in many cases, the analysis of a radiation Wigner distribution employing its temporal autocorrelation may be more straightforward and less misleading than fitting, especially when no information about the electron beam longitudinal phase space is available. We expect ROSA to be a valuable tool for XFEL operation and "beam-by-design" applications.

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REFERENCES

[1] S. Serkez, V. Kocharyan, E. Saldin, I. Zagorodnov, G. Geloni, O. Yefanov, "Extension of SASE Bandwidth up to 2% as a Way to Increase Number of Indexed Images for Protein Struc-

ture Determination by Femtosecond X-Ray Nanocrystallography at the European XFEL", 2013. arxiv:1306.4830v1

[2] I. Zagorodnov, G. Feng and T. Limberg, "Corrugated structure insertion for extending the SASE bandwidth up to 3% at the European XFEL", *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 837, pp. 69–79, 2016. doi:10.1016/j.nima.2016.09.001

[3] E. Prat, M. Calvi and S. Reiche, "Generation of ultra-large-bandwidth X-ray free-electron-laser pulses with a transverse-gradient undulator", *J. Synchrotron Radiat.*, vol. 23, no. 4, pp. 874-879, 2016. doi:10.1107/S1600577516007177

[4] S. Reiche, "Overview of Seeding Methods for FELs", in *Proc. IPAC'13*, Shanghai, China, May 2013, paper WEZB102, pp. 2063–2067.

[5] A. Zholents, "Electron-Beam-Based Sources of Ultrashort X-ray Pulses ", *Rev. Accel Sci. Technol.*, vol. 03, no. 1, pp. 237–259, 2010. doi:10.1142/S1793626810000415

[6] S. Serkez et al., "Overview of options for generating high-brightness attosecond x-ray pulses at free-electron lasers and applications at the European XFEL", *J. Opt.*, vol. 20, no. 2, p. 024005, 2018. doi:10.1088/2040-8986/aa9f4f

[7] E. L. Saldin, E. A. Schneidmiller and M. V. Yurkov, "Statistical properties of radiation from VUV and X-ray free electron laser ", *Opt. Commun.*, vol. 148, pp. 383-403, 1998. doi:10.1016/S0030-4018(97)00670-6

[8] A. A. Lutman, Y. Ding, Y. Feng, Z. Huang, M. Messerschmidt, J. Wu and J. Krzywinski, "Femtosecond x-ray free electron laser pulse duration measurement from spectral correlation function ", *Phys. Rev. Spec. Top. Accel Beams*, vol. 15, no. 3, p. 030705, 2012. doi:10.1103/PhysRevSTAB.15.030705

[9] Y. Inubushi *et al.*, "Determination of the Pulse Duration of an X-Ray Free Electron Laser Using Highly Resolved Single-Shot Spectra ", *Phys. Rev. Lett.*, vol. 109, no. 14, p. 144801, 2012. doi:10.1103/PhysRevLett.109.144801

[10] S. Krinsky, Z. Huang, "Frequency chirped self-amplified spontaneous-emission free-electron lasers ", *Phys. Rev. Spec. Top. Accel Beams*, vol. 6, no. 5, pp. 11-–17, 2003. doi:10.1103/PhysRevSTAB.6.050702

[11] O. Y. Gorobtsov *et al.*, "Diffraction based Hanbury Brown and Twiss interferometry at a hard x-ray free-electron laser", *Sci. Rep.*, vol. 8, no. 1, p. 2219, 2018. doi:10.1038/s41598-018-19793-1

[12] S. Reiche, Genesis 1.3 manual, 2004. http://genesis.web.psi.ch/download/documentation/genesis_manual.pdf

[13] J. Wu *et al.*, "Interplay of the chirps and chirped pulse compression in a high-gain seeded free-electron laser ", *J. Opt. Soc. Am. B: Opt. Phys.*, vol. 24, no. 3, p. 484, 2007. doi:10.1364/JOSAB.24.000484

[14] E. Allaria *et al.*, "The FERMI@Elettra free-electron-laser source for coherent x-ray physics: photon properties, beam transport system and applications", *New J. Phys.*, vol. 12, no. 7, p. 075002, 2010. doi:10.1088/1367-2630/12/7/075002

[15] G. Marcus, G. Penn, A. Zholents, "Free-Electron Laser Design for Four-Wave Mixing Experiments with Soft-X-Ray Pulses", *Phys. Rev. Lett.*, vol. 113, no. 2, p. 024801, 2014. 10.1103/PhysRevLett.113.024801

[16] S. Huang, Y. Ding, Z. Huang, G. Marcus, "Generation of subterawatt-attosecond pulses in a soft x-ray free-electron laser ", *Phys. Rev. Accel. Beams*, vol. 19, no. 8, p. 080702, 2016. doi:10.1103/PhysRevAccelBeams.19.080702

[17] S. Serkez, "Self-Seeding XFELs: Operation Principle and Challenges ", *Synchrotron Radiation News*, vol. 29, no. 3, pp. 10–14, 2016. doi:10.1080/08940886.2016.1174037

[18] OCELOT: a versatile computational tool for light sources, 2016–present. https://github.com/ocelot-collab/ocelot