Simulation of Propagation of Coherent and Partially-Coherent Photon Beams Across Beamlines





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Outline

- SR Calculation Basics
- Wavefront Propagation Calculation using Fourier Optics and Compatible Methods
- Examples of Partially-Coherent SR Emission and Propagation Calculations for Beamlines in Low-Emittance Storage Rings
- Estimating Advantages of Round Beams by Simulations
- Conclusions





Emission by a Relativistic Charged Particle in Free Space: Retarded Potentials Approach

Exact expression, valid in the Near Field:

$$\mathbf{E}_{\omega} = iec^{-1}\omega \int_{-\infty}^{+\infty} [\mathbf{\beta}_{e} - [1 + ic/(\omega R)] \cdot \mathbf{n}] R^{-1} \exp[i\omega(\tau + R/c)] d\tau \qquad (\checkmark)$$

The equivalence of ($\sqrt{}$) to the well-known expression of Jackson can be shown by integration by parts

$$\mathbf{E}_{\omega} = ec^{-1} \int_{-\infty}^{+\infty} \frac{\mathbf{n} \times [(\mathbf{n} - \boldsymbol{\beta}_{e}) \times \boldsymbol{\beta}_{e}'] + cR^{-1}\gamma^{-2}(\mathbf{n} - \boldsymbol{\beta}_{e})}{R \cdot (1 - \mathbf{n} \cdot \boldsymbol{\beta}_{e})^{2}} \cdot \exp[i\omega(\tau + R/c)]d\tau$$

Emission by a Relativistic Charged Particle Efficient Computation

Exact expression obtained from Retarded Potentials:

$$\mathbf{E}_{\omega} = iec^{-1}\omega \int_{-\infty}^{+\infty} [\mathbf{\beta}_{e} - [1 + ic/(\omega R)] \cdot \mathbf{n}] R^{-1} \exp[i\omega(\tau + R/c)] d\tau$$

Phase expansion valid in the Near Field:

$$\omega \cdot (\tau + R/c) \approx \Phi_0 + \frac{\pi}{\lambda} \left[s \gamma^{-2} + \int_0^s |\boldsymbol{\beta}_{e\perp}|^2 d\tilde{s} + \frac{(x - x_e)^2 + (y - y_e)^2}{z - s} \right]$$

Particle dynamics in external magnetic field:

$$\mathbf{r}_{e} = \mathbf{r}_{e}(s, \mathbf{r}_{e0}, \boldsymbol{\beta}_{e0}); \ \boldsymbol{\beta}_{e} \approx d\mathbf{r}_{e}/ds$$

Asymptotic expansion of the radiation integral (to accelerate computation):

$$\int_{-\infty}^{+\infty} F \exp(i\Phi) ds = \int_{s_1}^{s_2} F \exp(i\Phi) ds + \int_{-\infty}^{s_1} F \exp(i\Phi) ds + \int_{s_2}^{+\infty} F \exp(i\Phi) ds$$
$$\int_{-\infty}^{s_1} F \exp(i\Phi) ds + \int_{s_2}^{+\infty} F \exp(i\Phi) ds \approx \left[\left(\frac{F}{i\Phi'} + \frac{F'\Phi' - F\Phi''}{\Phi'^3} + \dots \right) \exp(i\Phi) \right]_{s_2}^{s_1}$$

Temporally-Incoherent and Coherent Spontaneous Emission by Many Electrons

Electron Dynamics:

$$\begin{vmatrix} x_{e} \\ y_{e} \\ z_{e} \\ \beta_{xe} \\ \beta_{xe} \\ \beta_{ye} \\ \delta\gamma_{e} \end{vmatrix} = \mathbf{A}(\tau) \begin{pmatrix} x_{e0} \\ y_{e0} \\ z_{e0} \\ z_{e0} \\ x'_{e0} \\ y'_{e0} \\ \delta\gamma_{e0} \end{pmatrix} + \mathbf{B}(\tau) + \mathbf{B}(\tau)$$

Spectral Photon Flux per unit Surface emitted by the whole Electron Beam:

$$\frac{dN_{ph}}{dtdS(d\omega/\omega)} = \frac{c^{2}\alpha I}{4\pi^{2}e^{3}} \langle |\mathbf{E}_{\omega}|^{2} \rangle$$

$$(|\mathbf{E}_{\omega}|^{2}) = \int |\mathbf{E}_{\omega0}(\mathbf{r}; x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0})|^{2} f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dz_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0} + (N_{e} - 1) |\int \mathbf{E}_{\omega0}(\mathbf{r}; x_{e0}, y_{e0}, z_{e0}, x'_{e0}, \delta\gamma_{e0}) f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, \delta\gamma_{e0}) dx_{e0} dy_{e0} dz_{e0} dx'_{e0} dy'_{e0} d\delta\gamma_{e0}|^{2}$$

$$(Coherent SR)$$
Common Approximation for CSR: "Thin" Electron Beam: $\langle |\mathbf{E}_{\omega}|^{2} \rangle_{CSR} \approx N_{e} |\int_{-\infty}^{\infty} \tilde{f}(z_{e0}) \exp(ikz_{e0}) dz_{e0} |^{2} |\mathbf{E}_{\omega 1}|^{2}$
For Gaussian Longitudinal Bunch Profile: $\langle |\mathbf{E}_{\omega}|^{2} \rangle_{CSR} \approx N_{e} \exp(-k^{2}\sigma_{b}^{2}) |\mathbf{E}_{\omega 1}|^{2}$

If $f(x_{e0}, y_{e0}, z_{e0}, x'_{e0}, y'_{e0}, \delta\gamma_{e0})$ is Gaussian, 6-fold integration over electron phase space can be done analytically for the (Mutual) Intensity of Incoherent SR and for the Electric Field of CSR

Wavefront Propagation in the Case of Full Transverse Coherence

Kirchhoff Integral Theorem applied to Spontaneous Emission by One Electron



$$\mathbf{E}_{\omega 2 \perp}(P_2) \approx \frac{k^2 e}{4\pi} \int_{-\infty}^{+\infty} d\tau \iint_{\Box} \frac{\mathbf{\beta}_{e \perp} - \mathbf{n}_{\perp}}{RS} \exp[ik(c\tau + R + S)] \cdot (\mathbf{l} \cdot \mathbf{n}_{p_e p_1} + \mathbf{l} \cdot \mathbf{n}_{p_1 p_2}) d\Sigma$$

Valid at large observation angles; Is applicable to complicated cases of diffraction inside vacuum chamber

Huygens-Fresnel Principle
$$\mathbf{E}_{\omega 2\perp}(P_2) \approx \frac{k}{4\pi i} \iint_A \mathbf{E}_{\omega 1\perp}(P_1) \frac{\exp(ikS)}{S} (\mathbf{l} \cdot \mathbf{\tilde{n}} + \mathbf{l} \cdot \mathbf{n}_{p_1 p_2}) d\Sigma$$

Fourier Optics

Free Space: (between parallel planes perpendicular to optical axis)

"Thin" Optical Element:

"Thick" Optical Element: (propagation from transverse plane before the element to a transverse plane just after it)

$$\mathbf{E}_{\omega^{2\perp}}(x_2, y_2) \approx \frac{k}{2\pi i L} \iint \mathbf{E}_{\omega^{1\perp}}(x_1, y_1) \exp[ik[L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}] dx_1 dy_1$$

Assumption of small angles

$$\mathbf{E}_{\omega 2 \perp}(x, y) \approx \mathbf{T}(x, y, \omega) \, \mathbf{E}_{\omega 1 \perp}(x, y)$$

$$\mathbf{E}_{\omega 2 \perp}(x_2, y_2) \approx \mathbf{G}(x_2, y_2, \omega) \exp[ik\Lambda(x_2, y_2, k)] \mathbf{E}_{\omega 1 \perp}(x_1(x_2, y_2), y_1(x_2, y_2))$$

"Economic" and Numerically Stable Version of the Free-Space Fourier-Optics Propagator

Huygens-Fresnel Principle:

(paraxial approximation)

$$\mathbf{E}_{\omega 2 \perp}(x_2, y_2) \approx \frac{k}{2\pi i L} \iint \mathbf{E}_{\omega 1 \perp}(x_1, y_1) \exp[ik[L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}] dx_1 dy_1$$

Analytical Treatment of Quadratic Phase Term:

Before Propagation:

$$\mathbf{E}_{\omega 1 \perp}(x_1, y_1) = \mathbf{F}_{\omega 1}(x_1, y_1) \exp\left[ik \frac{(x_1 - x_0)^2}{2R_x} + ik \frac{(y_1 - y_0)^2}{2R_y}\right]$$

After Propagation:

$$\begin{split} \mathbf{E}_{\omega 2 \perp}(x_{2}, y_{2}) &\approx \frac{k}{2\pi i L} \exp(ikL) \iint_{\Sigma} \mathbf{F}_{\omega 1}(x_{1}, y_{1}) \exp\left[ik \frac{(x_{1} - x_{0})^{2}}{2R_{x}} + ik \frac{(y_{1} - y_{0})^{2}}{2R_{y}} + ik \frac{(x_{2} - x_{1})^{2} + (y_{2} - y_{1})^{2}}{2L}\right] dx_{1} dy_{1} \\ &= \frac{k}{2\pi i L} \exp\left[ikL + ik \frac{(x_{2} - x_{0})^{2}}{2(R_{x} + L)} + ik \frac{(y_{2} - y_{0})^{2}}{2(R_{y} + L)}\right] \times \\ &\times \iint_{\Sigma} \mathbf{F}_{\omega 1}(x_{1}, y_{1}) \exp\left[ik \frac{R_{x} + L}{2R_{x}L} \left(x_{1} - \frac{R_{x}x_{2} + Lx_{0}}{R_{x} + L}\right)^{2} + ik \frac{R_{y} + L}{2R_{y}L} \left(y_{1} - \frac{R_{y}y_{2} + Ly_{0}}{R_{y} + L}\right)^{2}\right] dx_{1} dy_{1} \\ &= \mathbf{F}_{\omega 2}(x_{2}, y_{2}) \exp\left[ik \frac{(x_{2} - x_{0})^{2}}{2(R_{x} + L)} + ik \frac{(y_{2} - y_{0})^{2}}{2(R_{y} + L)}\right] \end{split}$$

An Approach to High-Accuracy Partially-Coherent Emission and Wavefront Propagation Simulations

Averaging (over phase-space volume occupied by e-beam) of the intensity (or "mutual" intensity, or mathem. brightness) obtained from electric field emitted by an electron and propagated through an optical system:

$$\begin{split} I_{\omega}(x,y) &= \int I_{\omega 1}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) f(x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) dx_{e} dy_{e} dz_{e} dx'_{e} dy'_{e} d\delta\gamma_{e} \\ I_{\omega 1}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) &= \left| \mathbf{E}_{\omega 1 \perp}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \right|^{2} \\ M_{\omega 1}(x,y,\tilde{x},\tilde{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) &= \mathbf{E}_{\omega 1 \perp}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \mathbf{E}_{\omega 1 \perp}^{*}(\tilde{x},\tilde{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \\ B_{\omega 1}(x,y,\theta_{x},\theta_{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \sim \mathbf{E}_{\omega 1 \perp}(x,y;x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \int \mathbf{E}_{\omega 1 \perp}^{*}(\tilde{x},\tilde{y};x_{e},y_{e},z_{e},x'_{e},y'_{e},\delta\gamma_{e}) \exp\left[i\frac{\partial}{\partial}(\theta_{x}\tilde{x}+\theta_{y}\tilde{y})\right] d\tilde{x}d\tilde{y} \end{split}$$

This method is general and accurate. For the most part, it is already implemented in SRW code. However, it can be **CPU-intensive**, requiring **parallel calculations** on a multi-core server or a small cluster. Several approaches are considered for increasing the efficiency, including use of low-discrepancy sequences (collaboration with R. Lindberg, K.-J. Kim, X. Shi, ANL), "improved Monte-Carlo" type techniques, as well as "coherent mode decomposition".

NOTE: the **smaller** the **e-beam emittance** (the higher the radiation coherence) – the **faster** is the **convergence** of simulations with this general method.

NOTE: **convolution** can be valid in some cases, such as pure projection geometry, focusing by a thin lens, diffraction at one slit, etc.

$$I_{\omega}(x, y) \approx \int \widetilde{I}_{\omega 1}(x - \widetilde{x}_{e}, y - \widetilde{y}_{e}) \widetilde{f}(\widetilde{x}_{e}, \widetilde{y}_{e}) d\widetilde{x}_{e} d\widetilde{y}_{e}$$

If convolution is valid, the **calculations can be accelerated** dramatically. The validity of the convolution relation can be easily verified numerically.

"Synchrotron Radiation Workshop" – Physical Optics Code for SR Emission and Propagation Calulations

First work on Wavefront Propagation applied to SR beamlines (PHASE code): J. Bahrdt, Appl. Opt. 36 (19) 4367 (1997)

- First official version of SRW was developed at ESRF in 1997-98 (written in C++, interfaced to IGOR Pro); compiled versions are distributed from: http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/SRW
- SRW was released to Open Source in 2012 under BSD type license.



The main Open Source repository, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub: <u>https://github.com/ochubar/SRW</u>

- SRW for Python (2.7.x and 3.x, 32- and 64-bit) cross-platform versions were released in 2012
- SRW development is partially supported by US DOE SBIR Program (BNL acts as subcontractor of RadiaSoft LLC, headed by D. Bruhwiler) Aradiasoft
- SRW under Sirepo web interface is available since 2015: <u>https://beta.sirepo.com/light#/home</u>

Single-Electron (Fully Transversely-Coherent) UR Intensity Distributions, "in Far Field" and "at Source"



Calculated UR Intensity Distributions from Finite-Emittance Electron Beam, "in Far Field" and "at Source"



NSLS-II Hard X-Ray Nanoprobe (HXN) Beamline Optical Layout and Wavefront Propagation Simulations





SSA located at 94 m, Nanofocusing Optics at 109 m from Undulator

Final Focal Spot Size and Flux vs Secondary Source Aperture Size (HXN, NSLS-II)



Secondary Source Aperture located at 94 m from Undulator Spot Size and Flux calculated for Nanofocusing Optics simulated by Ideal Lens with F = 18.14 mm, D = 150 µm located at 15 m from Secondary Source (109 m from Undulator)

NSLS-II Coherent Hard X-Ray (CHX) Beamline Optical Layout and Wavefront Propagation Simulations



Tracking Intensity and Degree of Transverse Coherence at Sample (CHX @ NSLS-II)



Towards Simulation of Complete Experiments (CHX @ NSLS-II)

Diffraction / Scattering from Test Sample 5000 "Silica Spheres", d ≈ 200 nm

Partially-coherent simulations allow for identifying best conditions (/ beamline settings) for XPCS and many other types of experiments.



Sample simulation data from A.Fluerasu

Angular distribution of scattered X-rays at E=10 keV, ΔS_{1x} = 44 µm, ΔS_{1y} = 1 mm



Attempting to Obtain Equal Horizontal and Vertical Spot Sizes and Coherence Lengths at CHX Sample (I)

Intensity Distributions Degree of Transv. Coherence Cuts vs Horizontal and Vertical Positions

Currently Attainable (at $\varepsilon_x = 0.9$ nm, $\beta_x = 2$ m, $\varepsilon_y = 8$ pm, $\beta_y = 1$ m)



Would be Attainable with a "Round E-Beam" (at $\varepsilon_x = \varepsilon_y = 85$ pm, $\beta_x = \beta_y = 2$ m)



Attempting to Obtain Equal Horizontal and Vertical Spot Sizes and Coherence Lengths at CHX Sample (II)

Intensity Distributions Degree of Transv. Coherence Cuts vs Horizontal and Vertical Positions

Currently Attainable (at $\varepsilon_x = 0.9$ nm, $\beta_x = 2$ m, $\varepsilon_y = 8$ pm, $\beta_y = 1$ m)



0

-10

-20 -

-30um -20

-30µm

<u>= 3.2x10¹³ ph/s/.1%bw</u>

0

Horizontal Position

10

20

30

-10



Conclusions

- High accuracy partially-coherent SR emission and propagation calculations for light sources are possible and (more-or-less) feasible with SRW code. Many applications are possible, including simulation of performances of IDs, X-ray optics in beamlines, and in some cases entire user experiments.
- Creating "round" electron beams in new low-emittance storage rings looks attractive for cases when round radiation spots at sample are required. This can result in gain in brightness and coherent flux and facilitates manipulations with / conditioning of X-ray beam. However, "matching" of single-electron UR angular divergences and source sizes with those of e-beam is important. Any particular case can be studied using partially-coherent simulations.





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