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PROPAGATION OF GAUSSIAN WIGNER FUNCTION THROUGH A MATRIX-APERTURE BEAMLINE*

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Abstract

We develop a simplified beam propagation model for x-ray beamlines that includes partial coherence as well as the impact of apertures on the beam. In particular, we consider a general asymmetric Gaussian Schell model, which also corresponds to a Gaussian Wigner function. The radiation is thus represented by a 4×4 symmetric second-moment matrix. We approximate rectangular apertures by Gaussian apertures, taking care that the loss in flux is the same for the two models. The beam will thus stay Gaussian through both linear transport and passage through the apertures, allowing a self-consistent picture. We derive expressions for decrease in flux and changes in second moments upon passage through the aperture. We also derive expressions for the coherence lengths and analyze how these propagate through linear transport and Gaussian apertures. We apply our formalism to cases of low emittance light source beamlines and develop a better understanding about trade-offs between coherence length increase and flux reduction while passing through physical apertures. Our formulae are implemented in RadiaSoft's Sirepo Shadow application allowing easy use for realistic beamline models.

GAUSSIAN WIGNER FUNCTION

Transverse coherence properties of partially coherent light at a given distance from the source can be described by means of the cross-spectral density (CSD) function, $\Gamma(\mathbf{r}_1, \mathbf{r}_2; t)$ in the time domain or $\tilde{\Gamma}(\mathbf{r}_1, \mathbf{r}_2; \omega)$ in the frequency domain [1–3]. An equivalent description can be effected in terms of the Wigner function (WF), $W(\mathbf{r}, \boldsymbol{\theta})$, related to the CSD $\tilde{\Gamma}(\mathbf{r}_1, \mathbf{r}_2; \omega)$ via the Fourier transform w.r.t. the pair of variables $\mathbf{r}_1 - \mathbf{r}_2$ and $\boldsymbol{\theta}$. Thus, one can choose to track either the CSD or the corresponding WF when modeling the propagation of partially coherent x-ray light through the beamline. One useful property of the WF is that it can be used just as a regular phase space density distribution for computing the moments with respect to the phase space variables. When the dynamics in the horizontal and vertical trace spaces are decoupled, both the WF and the CSD are separable, so that one is faced with a much simpler task of tracking functions of 2D phase space variables.

In the frequently encountered case where the radiation source is adequately described by the Gaussian Schell model, the corresponding Wigner function at the source is known to be Gaussian. As such, it is fully described by specifying its covariance matrix Σ, whose elements are the second-order moments, *viz.*, $\sigma_{xx} = \langle x^2 \rangle$, etc. Specifically, denoting the the vector of the 4D phase space variables $\vec{z} \equiv (\vec{x}, \vec{\theta})^T \equiv (x, y, \theta_x, \theta_y)^T$, the normalized Gaussian WF is given by

$$W(\vec{x}, \vec{\theta}) = \frac{1}{2\pi\sqrt{\det \Sigma}} \exp\left(-\frac{1}{2}\vec{z}^T \Sigma^{-1} \vec{z}\right) . \tag{1}$$

When x and y trace spaces are decoupled, we denote the 2D phase space variables (x, θ), and write for the Σ matrix and the rms emittance ϵ

$$\Sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{x\theta} \\ \sigma_{x\theta} & \sigma_{\theta\theta} \end{pmatrix} \tag{2}$$

and

$$\epsilon = \sqrt{\sigma_{xx}\sigma_{\theta\theta} - \sigma_{x\theta}^2} = (\det \Sigma)^{1/2} , \tag{3}$$

respectively. For convenience, we also introduce the quantities α, β and γ (similar to the Twiss parameters used in accelerator physics):

$$\epsilon\beta = \sigma_{xx}, \quad \epsilon\gamma = \sigma_{\theta\theta}, \quad \epsilon\alpha = -\sigma_{x\theta}, \tag{4}$$

which are constrained by the identity

$$\beta\gamma - \alpha^2 = 1 . \tag{5}$$

The inverse of Σ is then given in the 2D phase space case by

$$\Sigma^{-1} = \frac{1}{\det \Sigma} \begin{pmatrix} \sigma_{\theta\theta} & -\sigma_{x\theta} \\ -\sigma_{x\theta} & \sigma_{xx} \end{pmatrix} = \frac{1}{\epsilon} \begin{pmatrix} \gamma & \alpha \\ \alpha & \beta \end{pmatrix} , \tag{6}$$

and for the Gaussian WF we have these parametrized expressions:

$$\begin{aligned} & 2\pi\sqrt{\det \Sigma}\, W(x, \theta) \\ &= \exp\left[-\frac{1}{2 \det \Sigma}(\sigma_{\theta\theta}x^2 - 2\sigma_{x\theta}x\theta + \sigma_{xx}\theta^2)\right] \\ &= \exp\left[-\frac{1}{2\epsilon}(\gamma x^2 + 2\alpha x\theta + \beta\theta^2)\right] . \end{aligned} \tag{7}$$

As long as the WF stays Gaussian, its evolution is fully captured by tracking its moments through the second order (*i.e.*, tracking the elements of the 4×4 coupled Σ matrix or a pair of or 2×2 matrices in the uncoupled case). This closely parallels tracking the moments of the phase space distribution function in the particle beam dynamics setting. If the dynamics of the space space variables over a section of the beamline are linear and described by a transport matrix

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M, such that $\vec{z} = M\vec{z}(0)$, then the concurrent evolution of the Σ matrix is given by

$$\Sigma = M\Sigma(0)M^T, \tag{8}$$

and the Gaussian WF remains Gaussian. Matrix elements are known for most common optical beamline elements with the exception of apertures.

A Gaussian radiation WF does not remain Gaussian after passing through a hard-edge aperture. However, as we show below, it is possible to construct an effective Gaussian aperture such that the WF after the aperture is Gaussian and matches the FWHM size in phase space of the physical (non-Gaussian) WF. This allows one to model the propagation of an x-ray beam through a beamline (represented as a sequence of appropriate transfer matrices separated by apertures) by tracking only the covariance matrix Σ of the approximating Gaussian WF and keeping track of the flux loss due to the apertures.

PROPAGATION OF A GAUSSIAN WF THROUGH AN APERTURE (2D PHASE SPACE)

The flux loss for a straight-hard-edge aperture extending in x from $-a_h$ to a_h is found by purely geometric considerations. If the intensity distribution I_i immediately before the aperture is given by

$$I_i = I_0 \frac{1}{\sqrt{2\pi}\sigma_x} \exp\left(-\frac{(x-\mu)^2}{2\sigma_x^2}\right), \tag{9}$$

the ratio of the flux F_f immediately after the aperture to the flux F_i before the aperture will be

$$F_f/F_i = \frac{1}{2}\left[\mathrm{erf}\left(\frac{a_h+\mu}{\sqrt{2}\sigma_x}\right) + \mathrm{erf}\left(\frac{a_h-\mu}{\sqrt{2}\sigma_x}\right)\right]. \tag{10}$$

The corresponding result for a rectangular aperture in two spatial dimensions is, of course, a product of the 1D results in x and y.

The radiation WF after the aperture is computed by performing a convolution of the WF of the incident radiation with the "Wigner function" of the aperture, convolving in the angle variable θ only. In terms of the aperture transfer function $t(x;a)$ for the E-field of the radiation wavefront,

$$\vec{E}_f(x) = t(x,a)\vec{E}_i(x), \tag{11}$$

the aperture "Wigner function" is formally defined in the same way as the radiation WF is defined from the electric field of a coherent wavefront:

$$W_a(x,\theta) = \frac{1}{\lambda}\int_{\infty}^{\infty} t^*(x-\xi/2;a)t(x+\xi/2;a)e^{-i2\pi\theta\xi/\lambda}d\xi. \tag{12}$$

Unlike the WF for the radiation field, the aperture "Wigner function" is not normalized to unity.

For a hard-edge aperture the transfer function is a unit-height top-hat function $\Pi_{a_h}(x)$, and the WF for a matched incoming Gaussian radiation beam at some distance L_d after the aperture works out to [2]

$$\begin{aligned} W(x,\theta;a_h,L_d) &= \frac{1}{(2\pi)^{3/2}}\frac{1}{\sigma_x\sigma_\theta}\exp\left(-\frac{(x-\theta L_d)^2}{2\sigma_x^2} - \frac{\theta^2}{2\sigma_\theta^2}\right) \\ &\times \Pi_{a_h}(x-\theta L_d) \\ &\times Re\left[\mathrm{erf}\left(\frac{4\pi\sigma_\theta(a_h-|x-\theta L_d|)}{\sqrt{2}\lambda} + i\frac{\theta}{\sqrt{2}\sigma_\theta}\right)\right]. \end{aligned} \tag{13}$$

The Gaussian aperture is defined by a single parameter a_g. With $t(x;a) = \exp(-x^2/2a_g^2)$, the "Wigner function" for a Gaussian aperture is given by

$$W_a(x,\theta) = \frac{2\sqrt{\pi}a_g}{\lambda}\exp\left(-\frac{x^2}{a_g^2}\right)\exp\left(-\frac{\theta^2}{(\lambda/2\pi a_g)^2}\right), \tag{14}$$

where λ is the radiation wavelength, and the radiation WF out of the aperture is

$$\begin{aligned} W_f(x,\theta) \propto \exp\Bigg[-\frac{1}{2}\Bigg(\left(\frac{2}{a^2} + \frac{1}{2\sigma_{xx}} + \frac{\sigma_{x\theta}^2}{\sigma_{\theta,f}^2\sigma_{xx}^2}\right)x^2 \\ -\frac{2\sigma_{x\theta}}{\sigma_{\theta,f}^2\sigma_{xx}}x\theta + \frac{1}{\sigma_{\theta,f}^2}\theta^2\Bigg)\Bigg], \end{aligned} \tag{15}$$

where we used a shorthand

$$\sigma_{\theta,f}^2 = \frac{\epsilon}{\beta} + \frac{\lambda^2}{8\pi^2a^2} = \frac{\det\Sigma}{\sigma_{xx}} + \frac{\lambda^2}{8\pi^2a^2}. \tag{16}$$

The elements of the Σ matrix after the aperture, denoted by the subscript *"f"*, in terms of the parameter a of the Gaussian aperture and the elements of the Σ matrix before the aperture, are therefore given by

$$\sigma_{xx,f} = \frac{a^2\sigma_{xx}}{a^2+2\sigma_{xx}}, \tag{17}$$

$$\sigma_{x\theta,f} = \frac{a^2\sigma_{x\theta}}{a^2+2\sigma_{xx}}, \tag{18}$$

and

$$\sigma_{\theta\theta,f} = \sigma_{\theta\theta} - \frac{2\sigma_{x\theta}^2}{a^2+2\sigma_{xx}} + \frac{\lambda^2}{8\pi^2a^2}. \tag{19}$$

Emittance after the Gaussian aperture is related to that before the aperture as

$$\epsilon_f^2 - \left(\frac{\lambda}{4\pi}\right)^2 = \left[\epsilon^2 - \left(\frac{\lambda}{4\pi}\right)^2\right]\frac{a^2/2}{\sigma_{xx}+a^2/2}, \tag{20}$$

whence it is also clear that

$$\lim_{a\to 0}\epsilon_f = \frac{\lambda}{4\pi}. \tag{21}$$

This means the radiation becomes fully coherent in the limit of infinitely small aperture size. (Of course, the trade-off is that the transmitted flux is approaching zero in this limit.)

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CROSS-SPECTRAL DENSITY AND COHERENCE LENGTH

The cross-spectral density is related to the WF via

$$\tilde{\Gamma}(x_1, x_2) = \int W\left(\frac{x_1 + x_2}{2}, \theta\right) e^{i2\pi(x_1 - x_2)\theta/\lambda} d\theta \ . \qquad (22)$$

The transverse coherence length ξ can be computed from the spectral degree of coherence $\mu(x_1, x_2)$, defined as

$$\mu(x_1, x_2) = \frac{\tilde{\Gamma}(x_1, x_2)}{\sqrt{\tilde{\Gamma}(x_1, x_1)}\sqrt{\tilde{\Gamma}(x_2, x_2)}} \ . \qquad (23)$$

For a Gaussian WF, we find that

$$\mu(x_1, x_2) = \exp\left[-i\frac{\pi\alpha}{\lambda\beta}(x_1 + x_2)(x_1 - x_2) - \frac{(x_1 - x_2)^2}{2}\left(\frac{-1}{4\sigma_{xx}} + \frac{4\pi^2}{\lambda^2}\frac{\epsilon^2}{\sigma_{xx}}\right)\right] \propto \exp\left[-\frac{(x_1 - x_2)^2}{2\xi^2}\right] \ . \qquad (24)$$

Using the results for the elements of the Σ matrix before and after the Gaussian aperture, one finds that $\xi_f = \xi$, *i.e.*, the transverse coherence length does not change. However, the rms transverse beam size becomes smaller, so the ratio ξ/σ_x becomes larger and by this measure the beam becomes more coherent.

PROPAGATION THROUGH A GAUSSIAN APERTURE (4D PHASE SPACE)

When the horizontal and vertical dimensions are coupled and the aperture's "Wigner function" is known, a convolution-in-$\boldsymbol{\theta}$ procedure that parallels the one used for the 2D phase space is used to calculate analytically the WF after the aperture. For a Gaussian aperture, the convolution of two Gaussians results in a WF that is Gaussian. Writing the *inverse* of the covariance matrix Σ^{-1} as an arrangement of four 2×2 blocks A, B, C, and D,

$$\Sigma^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \ , \qquad (25)$$

and making use of the symmetry properties of Σ, we find the corresponding 2×2 blocks A_f, B_f, C_f, and D_f of the inverse covariance matrix after the aperture:

$$A_f = A + A_A - BD^{-1}C + BD^{-1}(D^{-1} + D_A^{-1})^{-1}D^{-1}C \ , \qquad (26)$$

$$B_f = BD^{-1}(D^{-1} + D_A^{-1})^{-1} \ , \qquad (27)$$

$$C_f = (D^{-1} + D_A^{-1})^{-1}D^{-1}C = B_f^T \ , \qquad (28)$$

and

$$D_f = (D^{-1} + D_A^{-1})^{-1} \ , \qquad (29)$$

where, in terms of the parameters a_x and a_y specifying the Gaussian aperture in the x and y directions,

$$A_A = \begin{pmatrix} 2/a_x^2 & 0 \\ 0 & 2/a_y^2 \end{pmatrix} \qquad (30)$$

and

$$D_A^{-1} = \frac{\lambda^2}{8\pi^2}\begin{pmatrix} 1/a_x^2 & 0 \\ 0 & 1/a_y^2 \end{pmatrix} \ . \qquad (31)$$

The covariance matrix Σ_f after the aperture is then computed via a numerical inversion procedure.

These formulae are being implemented to include apertures in the beam statistics report produced by the Sirepo web interface for the SHADOW code [4, 5].

HARD-EDGE APERTURE AND EFFECTIVE GAUSSIAN APERTURE

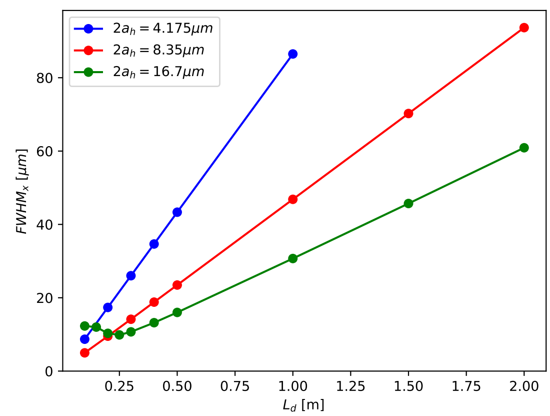

Figure 1: $FWHM_x$ as a function of distance from the aperture for a physical (Lorentzian) beam, for 3 values of the hard-edge aperture size $2a_h$.

A key question is how to relate the parameter(s) a_g of the effective Gaussian aperture to the size $2a_h$ of the physical hard-edge aperture. Here we briefly outline the general approach, leaving details to a separate publication. The approach is to match the FWHM sizes (in phase space) of the physical and approximating Gaussian beams in the post-aperture drift, sufficiently far from the aperture. The transverse size of the Gaussian beam is known to grow asymptotically linearly with distance L from the aperture at large L: $FWHM_x \approx 2.355\sigma_\theta L$, with $\sigma_\theta = const$ in free space. The projections of an initially-Gaussian WF on x and on θ after a hard-edge aperture we found to be approximately Lorentzian at distances of practical interest from the aperture, with the same asymptotically linear growth law for the transverse beam size, $FWHM_x \approx FWHM_\theta L$, as illustrated in Fig. 1. (The example shown in the figure is for $\lambda = 3.98 \times 10^{-10}$ m, $\epsilon = 5\lambda/4\pi = 1.58 \times 10^{-10}$ μm.) This allows us to match the size of the approximating Gaussian beam to that of the physical beam and use Eq. 19 to compute the requisite parameter of the Gaussian aperture,

$$a_g = \frac{\lambda}{4\pi}\sqrt{\frac{2}{\sigma_{\theta\theta,f} - \sigma_{\theta\theta}}} \qquad (32)$$

(assuming here an incident Gaussian WF with $\sigma_{x\theta} = 0$).

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