Coherence transport through imperfect x-ray optical systems

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Abstract: The latest generation of synchrotron sources, so-called third generation sources, are able to produce copious amounts of coherent radiation. However it has become evident that the experimental systems that have been developed are unable to fully utilize the coherent flux. This has led to a perception that coherence is lost while the radiation is transported down the beamline. However it is well established that the degree of coherence must be preserved, or increased, by an experimental system, and so this apparent "decoherence" must have its origin in the nature of the measurement process. In this paper we use phase space methods to present an argument that the loss of useful coherent flux can be attributed to unresolved speckle in the x-ray beam.

OCIS codes: (340.6720) Synchrotron radiation; (030.1670) Coherence; (030.1640) Coherent optical effects

References and links

1. A. Snigirev, I Snigereva, V.Kohn, S.Kuznetsov, I Schelokov, "On the possibilities of x-ray phase contrast microimaging by coherent high-energy synchrotron radiation," Rev. Sci. Instrum. **66**, 5846-5492 (1995).
2. K.A. Nugent, T.E.Gureyev, D.F. Cookson, D.Paganin and Z.Barnea, "Quantitative phase imaging using hard x-rays", Phy. Rev. Letts. **77**, 2961-2964 (1996)
3. P. Cloetens, M. Pateyron-Salome, J.Y.Buffiere, G.Peix, J.Baruchel, F.Peyrin and M.Sclenker, "Observation of microstructure and damage in materials by phase sensitive radiography and tomography," J. Appl. Phys. **81**, 5878-5886 (1997)
4. S.W.Wilkins, T.E.Gureyev, D.Gao, A.Pogany and A.W.Stevenson, "Phase-contrast imaging using polychromatic hard x-rays," Nature **384**, 335-338 (1996)
5. V.E.Coslett and W.C.Nixon., *X-ray microscopy*, (Cambridge University Press, Cambridge, 1960)
6. M. Sutton, S.G.J. Mochrie, T. Greytak, S.E. Nagler, L.E. Berman, G.A. Held and G.B. Stephenson "Observation Of Speckle By Diffraction With Coherent X-Rays," Nature **352**, 608-610 (1991)
7. I.A.Vartanyants and I.K.Robinson, "Origins of decoherence in coherent X-ray diffraction experiments," Opt. Commun. **222**, 29-50 (2003).
8. D. Paterson, B.E. Allman , P.J. McMahon, J.J.A. Lin, N. Moldovan, K.A. Nugent, I. McNulty, C.T. Chantler, C.C. Retsch, T.H.K. Irving and D.C. Mancini, "Spatial coherence measurement of X-ray undulator radiation," Opt. Commun. 195 (1-4): 79-84 (2001)
9. M.Born and E.Wolf, *Principles of Optics*, 6th edition, (Pergamon, Oxford, 1980).
10. A. Walther, "Radiometry and Coherence," J. Opt. Soc. Am. **58**, 1256 (1968)
11. M.J. Bastiaans, "Application Of The Wigner Distribution Function To Partially Coherent-Light," J. Opt. Soc. Am. A **3**, 1227-1238 (1986)
12. L.Mandel and E.Wolf, *Optical Coherence and Quantum Optics*, (Cambridge University Press, Cambridge, 1995)

Introduction

The establishment of third-generation x-ray sources is leading to the development of coherent x-ray optics as an independent area of investigation. However it is being reported that the benefit of the high coherence of the beams is not being transferred to the experimental station and the beam is said to be losing its coherence. This observation contradicts well-established laws of physics, such as Liouville's theorem, and so must have its origins in the practicalities

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of the measurement process. The aim of this paper is to explore the source of this apparent "decoherence".

One of the striking developments arising from third-generation synchrotrons is that of phase contrast imaging. As third-generation sources came on line, intensity contrast arising from quite moderate window imperfections became very obvious [1]. It was quickly realized that the higher coherence of the radiation was such that refractive effects were easily visible. This observation has subsequently been used to perform quantitative x-ray phase contrast imaging [2] as well as phase tomography [3]. Moreover, it was also realized that this effect can be seen in laboratory sources [4], and that phase contrast effects had been seen in laboratory radiographs, but not understood, for many years [5].

Speckle is the intensity manifestation of small phase effects after the light has propagated some distance from a random surface. It might be argued that the phase contrast used in imaging is the early manifestation of the development of speckle. Given this, speckle is likely to be a major contribution to the experimental measurement. Although x-ray speckle methods are being actively researched [6], the effect

of speckle has not been extensively discussed in the context of direct x-ray imaging. In this paper we argue that one such effect is the apparent loss of coherence by light traveling through the optics in a beamline.

The problem of "decoherence" has been discussed in a very recent paper [7] where it is argued that the presence of high spatial frequency imperfections in elements such as beryllium windows contributes a low coherence component into the radiation field. In this paper we discuss coherent optics in terms of the phase space density, or generalized radiance, to sharpen this argument into one that states that the finite resolution of the experimental system performs a *de facto* spatial ensemble average that therefore appears to the experimentalist as a loss of coherence. Paterson et al [8], in their investigation of the coherence of an undulator beam, report an observation of distorted fringes that could be interpreted as a loss of coherence in some experiments. They argue that this effect is visible due to the very low effective numerical aperture of their experimental arrangement. This paper provides a more general theoretical context for that observation and further develops their argument that this is the source of "decoherence".

The paper begins with a brief discussion of the phase-space formulation of partially coherent optics. We then introduce an appropriate general form describing the light from a synchrotron source and use this to produce a generic model of an experiment with which to discuss the effect of imperfect optical systems on quasi-monochromatic radiation.

The phase space formulation for optics

A fully coherent beam is characterized by its phase and amplitude. In general, radiation fields are not fully coherent and require a more refined description. Most commonly, a partially coherent field is described using the correlations in the field via the Mutual Coherence Function [9]:

$$\Gamma(\vec{r}_1,\vec{r}_2,\tau)=\left\langle E(\vec{r}_1,t)E^*(\vec{r}_2,t+\tau)\right\rangle , \tag{1}$$

where $E(\vec{r},t)$ represents the fluctuating electric field strength of the light and <> represents a time average. In this work, we limit our discussion to the quasi-monochromatic form of Eq (1), the Mutual Optical Intensity, $J(\vec{r}_1,\vec{r}_2)$, and its related functions [9].

We use the coordinate transformation:

$$\vec{r}\equiv(\vec{r}_1+\vec{r}_2)/2\,; \qquad \vec{q}\equiv\vec{r}_1-\vec{r}_2\,, \tag{2}$$

and adopt the paraxial approximation, which is well-satisfied by a synchrotron beamline, to write the quasi-monochromatic generalized radiance (GR) [10]:

$$B(\vec{r},\vec{u})=\int J(\vec{r}+\vec{q}/2\,,\vec{r}-\vec{q}/2)e^{2\pi i\vec{u}\bullet\vec{q}/\lambda}d\vec{q}\,, \tag{3}$$

where λ is the wavelength. In the context of quantum mechanics, this expression is termed the Wigner distribution and it is the joint probability distribution for position and momentum. It is

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also the Liouville invariant for the x-ray beam and so describes its phase-space distribution. The more coherent the light field, the more localized is this quantity. The optical properties of the GR have been extensively discussed elsewhere [11]. In particular, propagation over a distance z_0 is particularly simple in this formalism, and is described by

$$B_{z=z_0}(\vec{r},\vec{u}) = B_{z=0}(\vec{r} - z_0\vec{u},\vec{u}). \tag{4}$$

If the wave encounters a complex transmission function $T(\vec{r})$, then we define what we will term the phase-space response function for the aperture [11]

$$G(\vec{r},\vec{u}) \equiv \int T(\vec{r}+\vec{q}/2)T^*(\vec{r}-\vec{q}/2)e^{2\pi i\vec{u}\bullet\vec{q}/\lambda}d\vec{q}\ , \tag{5}$$

and the diffracted GR is described by:

$$B_{diff}(\vec{r},\vec{u}) = \int B(\vec{r},\vec{u}')G(\vec{r},\vec{u}-\vec{u}')d\vec{u}'. \tag{6}$$

The effect of diffraction, then, is to re-distribute the momentum in the beam. If an aperture may be factored into two functions with phase space response functions $G_1(\vec{r},\vec{u})$ and $G_2(\vec{r},\vec{u})$, then the total response function may be expressed as a convolution:

$$G(\vec{r},\vec{u}) = \int G_1(\vec{r},\vec{u}')G_2(\vec{r},\vec{u}-\vec{u}')d\vec{u}'. \tag{7}$$

The Gaussian-Schell model for coherence

The source distribution in a synchrotron storage ring is often modeled as having a Gaussian spatial distribution and a Gaussian beam divergence. These properties are emulated using the Gaussian-Schell model [12] for the coherence function, which can be written:

$$J(\vec{r}_1,\vec{r}_2) = I_0\ exp\left[-\left(x^2/w_x^2 + y^2/w_y^2\right)\right]exp\left[-\left(q_x^2/4\sigma_x^2 + q_y^2/4\sigma_y^2\right)\right], \tag{8}$$

where $\vec{r} \equiv (x,y)$ and $\vec{q} \equiv (q_x,q_y)$. The Gaussian-Schell model has the particular property that its GR also has a very simple form:

$$B(\vec{r},\vec{u}) = 4\pi\sigma_x\sigma_y I_0\ exp\left[-\left\{x^2/w_x^2 + y^2/w_y^2\right\}\right]exp\left[-\left(\pi^2/\lambda^2\right)\left\{\sigma_x^2u_x^2 + \sigma_y^2u_y^2\right\}\right]. \tag{9}$$

where w_x and w_y are the widths of the beam in the *x* and *y* directions respectively and σ_x and σ_y are the corresponding characteristic spatial coherence lengths. Equation (9) may be factorized into x and y dependent components. In the remainder of this paper, we will restrict our attention to only the *x*-component and we will set $I_0 = 1$.

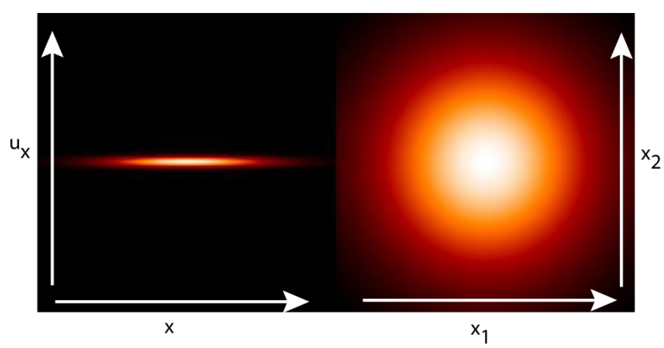

Fig. 1. (344KB) Left hand panel shows the Generalized Radiance as a function of position *x* and u_x. The panel on the right shows the absolute value of the Mutual Optical Intensity as a function of x_1 and x_2. The movie shows the relationship between these two representations as the coherence changes.

The relationship between the mutual optical intensity and the generalized radiance for a Gaussian-Schell source is demonstrated in figure 1 which shows the variation of both the coherence function and the generalized radiance as a function of the coherence parameter,

σ_x. It can be seen that as the distribution in momentum increases, the correlation function narrows.

A model experimental set-up

Generalized radiance of the field

We suppose that the x-ray beam is transported from the source to the experimental hutch via a series of optical components. We will model the optical properties of the experimental system as contained in a complex exit pupil, $P(x)$, located a distance z_1 from a source with phase-space distribution $B_{source}(x,u_x)$. The optical system will, in general, not be perfect and we introduce a phase changing plane at the exit pupil which will encapsulate the effects of optical imperfections such as wave aberrations and surface roughness in the optical system. In this model, then, the generalized radiance at the exit pupil is

$$B_{exit}(x,u_x) = \int B_{source}(x - z_1 u'_x, u'_x) G_{exp}(x, u'_x - u_x) du'_x \,, \tag{10}$$

where

$$G_{exp}(x,u_x) = \int G_{ideal}(x,u'_x) G_{error}(x, u_x - u'_x) du'_x \,; \tag{11}$$

and

$$G_{ideal}(x,u_x) \equiv \int P(z + q_x/2) P^*(z - q_x/2) e^{2\pi i u_x q_x/\lambda} dq_x \,, \tag{12}$$

which is the phase space response function for the ideal optical system; and

$$G_{error}(x,u_x) \equiv \int e^{i[\Phi(x+q_x/2) - \Phi(x-q_x/2)]} e^{2\pi i u_x q_x/\lambda} dq_x \,, \tag{13}$$

which is the phase-space response function for the screen containing random phase errors, $\Phi(x)$, that describe the system imperfections. The field at the detection plane a distance z_2 from the pupil is therefore

$$B_{det}(x,u_x) = B_{exit}(x - z_2 u_x, u_x) \,. \tag{14}$$

The central tenet of this paper is that the way that the field is detected is critical to the apparent coherence and so we now pay some attention to the partially coherent detection process.

The partially coherent detection process

We regard the detection process as one in which the field is apertured by the sensitive area of the detector and the resulting field is spatially integrated over the detector area. The effect of an aperture is described by Eqs. (5) & (6). In the context of detection, then, we must form the phase space response function for a detector aperture located at x_0, $G_{det}(x_0,u_x)$. The field immediately after the detector aperture is therefore given by:

$$B_{meas}(x_0,u_x) = \int B_{det}(x,u'_x) G_{det}(x - x_0, u_x - u'_x) du_x dx \,. \tag{15}$$

The response of a detector located at x_0 is the spatial integration of this field over the response of a detector centered on that point. Equation (15) demonstrates reciprocity in the detection process, which is to say that the sensitivity of the detector aperture is identical to its diffraction pattern. In this letter, we argue that the aperture of most detectors is large compared to the diffraction limit of the observed field. In this spirit, then, we will assume that the detector is sufficiently large that we may ignore its diffractive effects (i.e. it is equally sensitive to all incident wave vectors). Given Eq. (6), negligible diffraction implies that

$$G_{det}(x,u_x) \approx D(x)\delta(u_x) \,, \tag{16}$$

where $D(x)$ is the detector intensity transmission function and we assume $\int_{-\infty}^{+\infty} D(x) dx = 1$.

This will be an excellent approximation in most x-ray optical cases. Given Eq. (16), we find

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$$B_{meas}(x_0,u_x) \approx \int B_{det}(x,u_x) D(x-x_0) dx . \quad (17)$$

Using Eqs. (10), (14) and (17) gives

$$B_{meas}(x_0,u_x) \approx \int\int B_{source}(x-(z_1+z_z)u'_x, u'_x) G_{exp}(x-z_2u_x, u'_x-u_x) du'_x \times D(x-z_2u_x-x_0) dx . \quad (18)$$

In order to assess the impact of the detector, let us suppose that it is designed to be matched to the experimental measurement and so, in the absence of the random phase errors, has a negligible effect on the experimental output, which means that the integral over *x* need only be considered over the response function for the phase error term:

$$B_{meas}(x_0,u_x) \approx \int B_{source}(x_0-(z_1+z_2)u'_x, u'_x) \int G_{ideal}(x_0-z_2u_x, u'_x-u''_x) du'_x \times \int G_{error}(x-z_2u_x, u''_x) D(x-z_2u_x-x_0) dx du''_x . \quad (19)$$

In what follows, we use this expression to ask what the effect is of the finite detector on the apparent coherence.

An effective coherence function

Let us assume that the phase effects are small so we can Taylor expand the exponential term in Eq. (13) to obtain

$$G_{error}(x,u_x) \approx \delta(u_x) + i\int \Delta\Phi(x,q_x) e^{2\pi i u_x q_x/\lambda} dq_x , \quad (20)$$

where $\Delta\Phi(x,q_x) = \Phi(x+q_x/2) - \Phi(x-q_x/2)$ is a quantity closely related to the structure function of the random process [6].

The action of the detector response function is to perform a spatial average over the random phase variation. Let us assume that the random phase variation is statistically stationary and that its scale is sufficiently small that the detection process forms a *de facto* ensemble average. We can then write:

$$\langle \Delta\Phi(q_x) \rangle = \int \Delta\Phi(x,q_x) D(x-x_0) dx ; \quad (21)$$

and define

$$S(u_x) \equiv i\int \langle \Delta\Phi(q_x) \rangle e^{2\pi i u_x q_x/\lambda} dq_x . \quad (22)$$

Equations (20) and (22) simply describe an additive term to the system phase space response function which implies that we obtain the following expression for the generalized radiance in the measurement plane:

$$B_{meas}(x,u_x) = B_{ideal}(x,u_x) + \int B_{ideal}(x,u_x-u'_x) S(u'_x) du'_x , \quad (23)$$

where $B_{ideal}(x,u_x)$ is the generalized radiance in the case of a perfect experiment. The detected phase space distribution of the radiation is the expected value plus an additional term that is, in a sense, smeared out (which is to say that the coherence appears reduced) by the averaging effect the detector and so appears as a lower coherence component. This appearance is purely a result of the combined effect of the random phase errors and the finite resolution of the detector. Transforming back to write the results in terms of the measured mutual optical intensity, we find

$$J_{meas}(x_1,x_2) = J_{ideal}(x_1,x_2)(1 + i\langle \Delta\Phi(x_1-x_2) \rangle) . \quad (24)$$

which describes the expected coherence function plus a term modulated by the *de facto* ensemble average performed by the detector. This is at least qualitatively similar to the conclusions of reference 7, but isolates the source of this term.

Gaussian Schell model source simulations

The effect of finite spatial resolution was simulated for a Gaussian-Schell source. The source was assumed to have a wavelength of 1nm and was passed through a random phase screen with a standard deviation of 0.5 radians, which is to say an effective surface smoothness of less than one wavelength. The detection process was modeled using the approach described here and the detector resolution was varied from 0.2 microns up to 18.6 μm. Figure 2 and the

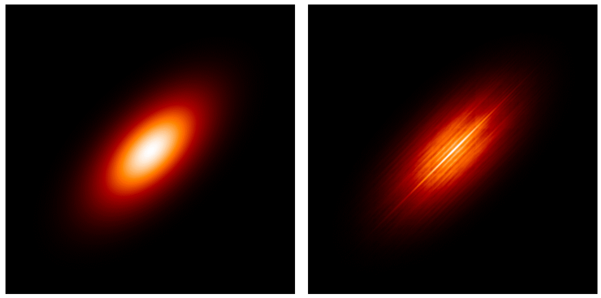

Fig. 2. (550KB) Gaussian-Schell model coherence functions for 1nm x-rays after having passed through a random Gaussian phase screen with a characteristic spatial frequency of 1 μm^{-1} and a standard deviation of 0.5 radians. The beam width w_x is 39.9 μm and σ_x is 10.0 μm. The image sizes are 120 μm × 120 μm. (a) The result obtained for a system with perfect resolution. (b) The apparent coherence function when the experimental system has finite spatial resolution of 18.6 μm. The bright streak diagonally across the screen corresponds to an apparent low coherence component.

associated movie shows the absolute value of $J_{det}(x_1, x_2)$ as a function of detector resolution. The apparent loss of coherence is clearly seen, and disappears when the resolution of the detector is very high.

Summary

Optical speckle is ubiquitous in coherent optics in the visible region and there is no physical reason why this will not also be the case for coherent x-ray optics. However, where the spatial scale of the speckle is typically comparable to the spatial resolution in optical experiments – which explains why speckle is always obvious – the same is not necessarily the case in x-ray optics.

Coherence cannot be destroyed. Indeed, an experimental system will generally select out a subset of phase space which acts to *increase* the coherence at the measurement plane. The observed decoherence reported at synchrotron sources must therefore be a result of features in the radiation field that cannot be resolved by the experimental system. This paper has formed a theoretical description of the measurement process in phase space. We have modeled the imperfections of the optical system via the introduction of an imaginary phase screen in the exit pupil of the optical system. One might imagine that the random phase gradients act as small prisms that have the effect of moving parts of the detected field in random directions. This effect is identical to that which produces the phase contrast structure in images [1]. However in the situation considered here, the spatial scale is too small to be resolved, but has the effect of emulating a loss of coherence in the field.

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