Extracting coherent modes from partially coherent wavefields

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A method for numerically recovering the coherent modes and their occupancies from a known mutual optical intensity function is described. As an example, the technique is applied to previously published experimental data from an x-ray undulator source. The data are found to be described by three coherent modes, and the functional forms and relative occupancies of these modes are recovered. © 2009 Optical Society of America

Coherent methods in x-ray physics are emerging rapidly and are being particularly driven by the development of x-ray free-electron lasers. Of particular interest is the development of coherent imaging methods [1], based on iterative reconstruction techniques [2] and oversampling of the data [3], which have been applied to a number of scientific problems including the high-resolution examination of the structure and properties of nanocrystals [4,5], nanofoams [6], integrated circuits [7], x-ray optics [8], and biological cells [9–11].

While a prime interest is the application of these imaging methods to single molecules [12], major potential scientific applications will nonetheless use third-generation synchrotron sources [4,6,7]. However, it is well established that the output from third-generation sources are not fully coherent [13,14], and the four-dimensional coherence function has now been measured in some detail [15]. It is also now established theoretically [16] and experimentally [17] that less than perfect coherence can have a detrimental effect on the ability to recover images from diffraction data.

The incorporation of temporal coherence into coherent diffractive imaging has recently been demonstrated using high-harmonic-generation light sources [18]. This method treated the incident light as a set of mutually incoherent spectral modes for forward propagation and then propagated a single mode back to the image plane so as to impose the support constraint. The aim of the present letter is to demonstrate that it is possible to identify analogous coherent modes for nonperfect spatial coherence.

The coherent-mode formulation by Wolf [19] provides an elegant representation of a partially coherent wavefield in a computationally convenient form. In this Letter, we restrict our attention to a partially coherent, quasi-monochromatic wavefield that is known to be constrained by a closed boundary defining a simple aperture. In the aperture plane, we write the mutual optical intensity (MOI), \( J(r_1,r_2) \), as a coherent-mode expansion of the form

\[
J(r_1,r_2) = \sum_n \eta_n \psi_n^*(r_1) \psi_n(r_2). \tag{1}
\]

The mode parameters, \( \eta_n \), are necessarily nonnegative and, consequently, may be interpreted as modal occupancy numbers. The summation over the modal index, \( n \), runs over the elements of a complete, orthonormal set of modes, \( \{\psi_n(r)\} \), so that

\[
\int \psi_m^*(r) \psi_n(r) d\mathbf{r} = \delta_{mn}, \tag{2}
\]

where \( \delta_{mn} \) is the Kronecker delta. The assumption that the wave field is bounded by an aperture further enables us to impose the condition that for all \( n \), \( \psi_n(r) = 0 \) wherever \( r \) refers to a point outside the aperture.

Any arbitrary basis set, \( \{\chi_k(r)\} \), that is complete on the two-dimensional domain defined by the aperture may be used to construct an expansion of the modes in the form

\[
\psi_n(r) = \sum_k c_{nk} \chi_k(r). \tag{3}
\]

If we multiply both sides of Eq. (1) by an arbitrary mode, \( \psi_l(r_1) \), integrate with respect to \( r_1 \), and invoke the orthonormality condition, Eq. (2), then we obtain an integral equation,

\[
\int \psi_l(r_1) J(r_1,r_2) d\mathbf{r}_1 = \eta_l \psi_l(r_2), \tag{4}
\]

for the modes. Substitution of Eq. (3) into Eq. (4) results in a generalized matrix eigenvalue equation of the form \( H \mathbf{C} = \eta \mathbf{S} \mathbf{C} \) with matrix elements defined by

\[
H_{pq} = \int \chi_p^*(r_1) J(r_1,r_2) \chi_q(r_2) d\mathbf{r}_1 d\mathbf{r}_2, \tag{5}
\]
For a given set \( \{ \chi_k(\mathbf{r}) \} \) and function \( J(\mathbf{r}_1, \mathbf{r}_2) \), these matrix elements are readily evaluated by numerical quadrature. \( \mathbf{C} \), being the matrix of eigenvectors, contains the expansion coefficients of the coherent modes over the basis \( \{ \chi_k(\mathbf{r}) \} \), and the corresponding diagonal element of \( \eta \) contains the modal occupancy \( \eta_n \) as an eigenvalue. The solution of generalized matrix eigenvalue equations of this type is readily achieved using standard methods of computational linear algebra provided that \( S \) is positive definite and nonsingular; in practice, this influences the selection of the auxiliary basis, \( \chi_k(\mathbf{r}) \). The most elementary choice of basis consists of a regular, rectilinear array of orthonormal, two-dimensional step functions of the form

\[
\chi_k(\mathbf{r}) = \begin{cases} 
1 & x_k - h/2 \leq x \leq x_k + h/2 \\
\frac{1}{h^2} & y_k - h/2 \leq y \leq y_k + h/2, \\
0, & \text{otherwise}
\end{cases}
\]

where \( h \) is the grid spacing in each linear dimension, \( \mathbf{r}_k = (x_k, y_k) \) denotes the centroid of \( \chi_k(\mathbf{r}) \), and \( \mathbf{r} = (x, y) \). The basis possesses the property that \( S_{pq} = \delta_{pq} \) and becomes complete in the asymptotic limit \( h \to 0 \), facilitating the study of the convergence characteristic of finite expansions of the general form defined in Eq. (3).

To confirm that our numerical implementation is correct, we constructed a Gaussian Schell model MOI, extracted the modes their occupancies, and compared the results with the analytical solution by Starikov and Wolf [20]. We found agreement on both the form of the modes and the occupancies to within the numerical precision of the calculation. The first three modes are shown in Fig. 1, where they have been labeled according to a pair of numbers—the first of which represents the mode order in the \( x \) direction and the second the order in the \( y \) direction.

As an example of the approach, we apply it to the extraction of coherent modes from a previously measured MOI function. Phase-space tomography [21] has been used to measure the four-dimensional mutual optical intensity function of a quasi-monochromatic beam of 2.1 keV photons [15] emerging from the 2-ID-B undulator beamline at the Advanced Photon Source [22]. The MOI was recovered under the assumption that the field could be described as a separable function such that \( J(\mathbf{r}_1, \mathbf{r}_2) = J_x(x_1, x_2)J_y(y_1, y_2) \) and was measured for two levels of spatial coherence. The \( x \) component of the lower-coherence data set, \( J_x(x_1, x_2) \), is shown in Fig. 2(a). A full description of these data and the conditions under which they were obtained and analyzed is given in [15], and we refer the reader to that paper for more details.

These data were analyzed using the methods described here so as to determine the number, form, and occupancy of the coherent modes. In both cases, we find significant occupancy in only three modes, with the other modes being consistent with reproducing known artifacts in the reconstructed MOI. We determined the level of numerical error by quantifying.

![Fig. 1](image1.png)

Fig. 1. (Color online) Coherent modes extracted from a partially coherent Gaussian Schell-model beam. (a) (0,0) mode, (b) (1,0) mode, (c) (0,1) mode. These have a form entirely consistent with the analytical results in [19].

![Fig. 2](image2.png)

Fig. 2. (Color online) \( x \) component \( J_x(x_1, x_2) \) of the experimentally determined MOI. The full details concerning this data can be found in [15], and we refer the reader to that paper for detailed information. (a) Original MOI from [15], (b) MOI reconstructed using only three modes. Note the reduction of structure outside the aperture in (b).
the inconsistencies in the original data and by noting the magnitude of unphysical features such as modes with negative occupancies; the largest unphysical mode had an occupancy of 1.5% of the total energy. The reconstruction of the data using only the three physically meaningful modes is shown in Fig. 2(b). Figure 3 shows the individual modes for the low-coherence set of experimental data; we note that the modal forms for the high-coherence data are essentially identical, with there being only a change in the occupancy of the modes. Only the real part of the modes is shown, as the imaginary parts have negligible amplitude. We attribute the modal amplitudes outside the aperture to the presence of residual artifacts in the reconstructed MOI.

Our results show that the field with the higher coherence has $(91±2)%$ of the energy in the primary $(0,0)$ mode, with approximately $(4±2)%$ of the energy in the $(1,0)$ mode and $(5±2)%$ in the $(0,1)$ mode. The field with lower spatial coherence in the horizontal direction displayed an occupancy of $(84±2)%$ of the total in the $(0,0)$ mode, $(11±2)%$ in the $(1,0)$ mode, and $(5±2)%$ in the $(0,1)$ mode; as the experiment did not change the coherence in the vertical direction, we expect this last figure to be unchanged when compared with the high coherence case.

In conclusion, we have presented a method for the extraction of the coherent modes in a partially coherent wavefield from a measurement of the mutual optical intensity. As an example of the method, it was applied to the field emerging from an x-ray undulator source.

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