Partially coherent image computation using elementary functions

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ABSTRACT
It is well-known that calculations of the propagation of partially coherent light, such as those required for the calculation of two-dimensional image intensities, involve four-dimensional functions. Recently, Wald et al [Proc SPIE, 59621G, 2005] outlined a method for reducing the four-dimensional problem to a purely two-dimensional one. Instead of an exact modal expansion of the mutual coherence function or cross-spectral density, an approximate expansion is used, into what we call elementary functions. In this paper, rules of thumb are developed for fast and efficient computation of the image intensity in a simple partially coherent lithographic imaging system.

Keywords: partial coherence, excimer, imaging

1. INTRODUCTION
It is well-known that calculations of the propagation of partially coherent light, such as those required for the calculation of two-dimensional image intensities, involve four-dimensional functions. The reason for 4D calculations is that for partially coherent light the correlation between fields at different points in space must be taken into account, so integration must be performed not just over all points of a 2D field distribution, but over all pairs of points. This presents problems in regards to speed and storage. The quantity representing the field correlations can be either the mutual coherence function (time domain) or the cross-spectral density (frequency domain), and this quantity is then propagated through the optical system. This is time-consuming. A 1000 by 1000 pixel image therefore requires one tera-word of storage, large even by modern standards. Modal expansions\(^1\) of various kinds can speed up the computation time and complexity, but still require a four-dimensional calculation to find the modes themselves.

Recently, Wald et al\(^2\) outlined a method for reducing the four-dimensional problem to a purely two-dimensional one. Instead of an exact modal expansion of the mutual coherence function or cross-spectral density, an approximate expansion is used, into what we call in this paper elementary functions (to distinguish them from true modes). The method is not mathematically exact in the way of the coherent-mode expansion, but the method is similar in that the source can be represented by the superposition of elementary functions. Certain approximations limit its application to relatively well-behaved fields, e.g. a partially coherent field from an excimer laser.

2. THEORY
The transform that forms the basis of the theoretical approach was introduced in 2005 by Wald et al.\(^2\). This transform reduces the propagation calculations from 4D to 2D. However, in order to use it numerically, it must be rewritten as a discrete sum, or an expansion rather than a transform. A sampling criterion is also developed to define how densely the basis functions need to be placed, and to show that the sampling density affects the values of the expansion coefficients.

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2.1. The continuous case

A partially coherent field can be described using the cross spectral density \( G_0(r_1, r_2) \). The intensity is \( I_0(r) = G_0(r, r) \). All quantities are implicitly assumed to depend on the frequency \( \nu \) of the light as e.g. \( G_0(r_1, r_2, \nu) \) and \( I_0(r, \nu) \).

It is assumed that we know \( G_0(r_1, r_2) \) over a plane, two-dimensional region where \( r_j = (x_j, y_j) \), and we wish to propagate it to any other region. We also need to make an important assumption: that the cross-spectral density is real in the plane where we start the propagation. This implies the beam must not be diverging or converging as this adds complex phase terms to the cross-spectral density. However this can be avoided if the diverging or converging parts are included in the propagation, and not as part of the cross-spectral density expression. The propagation is performed using

\[
G(r_1, r_2) = \int_{-\infty}^{\infty} d^2r_1' \int_{-\infty}^{\infty} d^2r_2' h^*(r_1, r_1')h(r_2, r_2')G_0(r_1', r_2'),
\]

where \( h(r, r') \) is an impulse response function and depends on the system. Introducing the transform, we assume the initial cross-spectral density may be written as

\[
G_0(r_1, r_2) = \int_{-\infty}^{\infty} d^2r \ a(r')f(r_1 - r')f(r_2 - r')
\]

where the elementary function \( f(r) \) is real and even. The expression describes a transform, and provided that the functions \( a(r') \) and \( f(r) \) exist, it is exact. We now find \( a(r') \) and \( f(r) \), in a similar way to the method introduced by Wald et al.,\(^2\) taking the Fourier transform of the cross-spectral density. This leads to the following expression

\[
\hat{f}(u) \propto \sqrt{\hat{G}_0(u-u)}
\]

where \( \hat{f}(u) \) is the two-dimensional Fourier transform of \( f(r) \). The shape of the function \( f(r) \) can be found from the inverse Fourier transform. It can then be normalized.

The coefficient function \( a(r') \) can be found in a similar way.

\[
\hat{a}(u) = \frac{\hat{I}_0(u)}{\hat{f}^2(u)},
\]

provided \( \hat{f}^2(u) \neq 0 \) for all values of \( u \), \( \hat{I}_0(u) \) is the Fourier transform of \( I_0(r) \), \( \hat{a}(u) \) the Fourier transform of \( a(r') \), and \( \hat{f}^2(u) \) the Fourier transform of \( f^2(r) \), the square of \( f(r) \). The coefficient function \( a(r') \) can then be found by an inverse Fourier transform. Further details of this proof can be found in.\(^3\)

To reach the results above, three assumptions were made. First, the initial cross-spectral density was assumed to be real. This puts limitations on the applicability, but could be fulfilled for most beams. Divergent or convergent beams will have complex cross-spectral densities, but can be modeled as part of the impulse response function \( h \) instead. Second, it was assumed that the elementary function \( f(x) \) is real and even. For real and even cross-spectral densities this should not cause any problems. Third, it was assumed that \( \hat{f}^2(u) \) has no zeroes. This may be the most restricting assumption, limiting the method to cross-spectral densities made up from smooth envelope functions such as Gaussians or super-Gaussians.

2.2. Discrete expansion

Instead of the exact transform in Eq. (2) we use the corresponding discrete sum, namely the expansion

\[
G_0(r_1, r_2) = \sum_n \sum_m a_{mn}f(r_1 - r_{mn})f(r_2 - r_{mn}).
\]

Here \( r_{mn} = (x_m, y_n) \) are sampled on a grid as \( x_m = m\Delta x \) and \( y_n = n\Delta y \). All other assumptions are the same as in the continuous section. The values of \( \Delta x \) and \( \Delta y \) will be found by establishing a sampling criterion. We
prove that Eq. (5) is valid by finding functions \( f(r) \) and sampling coefficients \( a_{mn} \) to fulfil the relation, in a manner resembling the continuous approach.

Assuming, as before, that \( f(r) \) is real and even, we find

\[
\hat{G}_0(u, -u) = \hat{f}^2(u) \sum_m \sum_n a_{mn} 
\]

and, provided that the sum exists, we find

\[
\hat{f}_0(u) \propto \sqrt{\hat{G}_0(u, -u)}.
\]

Thus we have found the basis functions and proved that the expansion does exist. The basis functions will not necessarily be orthogonal. In fact, with most distributions we can assume they are not. For non-orthogonal sets of basis functions, finding the expansion coefficients becomes much more difficult than for orthogonal sets of functions. We can regard Eq. (5) as an interpolation function, where the coefficients \( a_{mn} \) are some kinds of samples of the cross-spectral density. This allows us to use the sampling and interpolation theory developed for non-orthogonal basis sets,\(^4\) which can be used both to find a sampling criterion and to retrieve the values of the coefficients. Further sampling considerations will be outlined in §2.3.

### 2.3. Sampling Considerations

The traditional Shannon-Whittaker sampling criterion cannot be applied, since it implies that sinc functions of appropriate width will be used as interpolation functions. In our case the interpolating function, i.e., the elementary function, will not be a sinc function and its width will be quite different from that assumed in traditional sampling and interpolation. Sampling and interpolation can be investigated using the intensity rather than the cross-spectral density. The intensity can be written as

\[
I_0(r) = G_0(r, r) = \sum_m \sum_n a_{mn} f^2(r - r_{mn}),
\]

where \( \varphi_{mn}(\tilde{r}) = D f^2(\Delta x(\tilde{x} - m), \Delta y(\tilde{y} - n)) \) can be regarded as our basis functions.

The new coordinates \( \tilde{r} = (\tilde{x}, \tilde{y}) = (x/\Delta x, y/\Delta y) \) ensure the function is sampled at integer values, and the constant \( D \) ensures that \( \hat{\varphi}(0) = 1 \). These small changes allow us to use the three conditions for expansion as presented by Unser.\(^4\) First, the sequence of coefficients must be square-integrable, that is

\[
\|a\|^2 = \sum_m \sum_n |a_{mn}|^2
\]

must exist.

Second, the set of basis functions need to form a Riesz basis. That means the condition

\[
A \cdot \|a\|^2 \leq \left\| \sum_m \sum_n a_{mn} \varphi_{mn}(r) \right\|^2 \leq B \cdot \|a\|^2,
\]

where \( A > 0 \) and \( B < \infty \), must be fulfilled. The linear independence needs to be checked for each new set of functions.

The third condition is by far the most demanding, and is also the one that will be used to obtain a sampling criterion. It is known as the partition of unity condition:

\[
\sum_n \sum_m \varphi(\tilde{x} + m, \tilde{y} + n) = 1
\]

for all real \((\tilde{x}, \tilde{y})\). In the Fourier domain it translates as

\[
\hat{\varphi}(m, n) = \delta_m \delta_n,
\]
where the difference from Ref. [4] originates from different definitions of the Fourier transform and

$$\delta_m = \begin{cases} 1 & : m = 0, \\ 0 & : m \neq 0. \end{cases} \quad (13)$$

where $m$ is an integer. This condition affects how closely a function can be reproduced, by making the sampling step sufficiently small. This is also the most problematic condition, since our elementary functions are not likely to fulfil it exactly. So we are forced to accept an approximate version of the partition of unity condition. This removes the formal guarantee that the expansion will be accurate to a certain limit, so care must always be taken to ensure that the expansion is numerically adequate. This subject is dealt with more rigorously in a publication.3

3. EXAMPLE: PARTIALLY COHERENT FIELDS

We present an example of a partially coherent field, similar to that of excimer lasers operating at 193nm or 248nm. To illustrate this type of source we consider the special case of a Gaussian Schell-model beam. The cross-spectral density is given by

$$G_0(x_1, x_2) = A \exp \left( \frac{x_1^2}{\sigma_1^2} \right) \exp \left( \frac{x_2^2}{\sigma_2^2} \right) \exp \left[ \frac{(x_1 - x_2)^2}{\sigma_g^2} \right] \quad (14)$$

where $\sigma_1$ represents the width of the intensity distribution and $\sigma_g$ the width of the coherence distribution. We calculate an expression for the elementary function using the method outlined in §2.1 and §2.2.

$$f(x) = \frac{1}{(\sigma_1 \sigma_g^2)^{1/2}} \left( \frac{\sigma_1^2 + \sigma_g^2}{\pi} \right)^{1/4} \exp \left[ -\frac{1}{2} x^2 \left( \frac{1}{\sigma_1^2} + \frac{4}{\sigma_g^2} \right) \right] \quad (15)$$

The elementary function has a Gaussian distribution, and its width depends on both $\sigma_1$ (the width of the intensity distribution) and $\sigma_g$ (the width of the coherence distribution). For example, if $\sigma_g \gg \sigma_1$ the light is nearly coherent, and the elementary function will be proportional to the field distribution $\sqrt{I_0(x)}$. This implies only one such function is required to represent the field. On the other hand, if $\sigma_g \ll \sigma_1$ the light is nearly incoherent, and the elementary function will become very narrow and resemble a delta function. Very small $\Delta x$ is then required. Continuing the analysis to find the coefficients $a_m$, we find

$$a_m = \Delta x A \sigma_1 \sqrt{\pi} \int_{-\Delta x}^{1/2 \Delta x} du \exp \left( -\pi^2 u^2 \frac{4 \sigma_1^4}{4 \sigma_1^4 + \sigma_g^2} \right) \exp (2 \pi i m \Delta xu) \quad (16)$$

Using the sampling criterion outlined in §2.3, the sampling distance $\Delta x$ is given by

$$\Delta x = \frac{\pi \sigma_1 \sigma_g}{\sqrt{(\pi \ln c)(\sigma_1^2 + 4 \sigma_g^2)}}. \quad (17)$$

Common practice when handling a Gaussian distribution $\exp(-x^2/\sigma^2)$ is often to consider values over a width of $6\sigma$, i.e. for $|x| \leq 3\sigma$, while values for larger $|x|$ are considered to be zero. This would correspond to using $c = \exp(-9) \approx 1.23 \cdot 10^{-4}$.

Fig 1 shows the intensity and its reconstruction (broad lines) for Gaussian Schell-model beams of different degrees of coherence, along with the scaled and shifted squares of the elementary functions (narrow lines). Adding those together gives the reconstruction. The intensity distribution is the same for all beams, with $\sigma_f = 0.01m$, while the coherence varies from high to low. As $\sigma_g$ decreases, the number of functions required to represent the source increases. For (a) $\sigma_g = 1m$, only 1 function is required, (b) $\sigma_g = 0.1m$, 5 functions required, (c) $\sigma_g = 0.01m$, 13 functions required and (d) $\sigma_g = 0.001m$ requires 115 functions. Depending on the width of the object to
Figure 1. Intensity and reconstructed intensity for Gaussian Schell-model beams of different degrees of coherence be imaged compared to the beam dimension, reducing the number of functions could still produce an accurate result.

The right hand columns of Figure 1 show the reconstruction of the cross-spectral density. Part (e) shows the reconstruction of the cross-spectral density for the parameters in (b), and (f) shows the reconstruction of the cross-spectral density for the parameters in (c).

Some numerical simulations using this method are presented in a separate publication.\textsuperscript{5}

4. CONCLUSION

The elementary function method for the propagation of partially coherent light has been outlined. This approach reduces the propagation of partially coherent light through an imaging system to a series of 2D calculations, thus reducing complexity and demands on time and memory. A sampling criterion was established for this method, based on the partition of unity condition. We presented an example of a Gaussian Schell-model beam with coherent and partially coherent cases which showed the change in sampling distance with coherence width. Applications of the elementary function method include modelling the cross-spectral density as it propagates through a lithographic system, incorporating the effects of beam homogenization optics on the coherence of the field and analysis of degradation of image quality through-focus in the image plane.

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