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Phase-space analysis of transport of intensity equation under partially coherent illumination

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ABSTRACT

We introduced a generalized version of the transport of intensity equation from a partially coherent phase-space perspective that relates axial intensity derivative to the transverse divergence of the conditional frequency moment of the Wigner distribution function. This expression provides a powerful analytical tool for the study of phase retrieval and computational imaging under partially coherent illuminations. The correspondence between the Wigner distribution function and the light field in the geometric optics enables extracting phase information from the light field and vice versa for slowly varying specimen under certain simplified illumination conditions.

Keywords: transport-of-intensity equation; phase retrieval; phase space; partially coherent fields

1. INTRODUCTION

Optical phase retrieval is a central problem throughout physics and optics because phase carries important information about the object structure but cannot be directly measured. The transport of intensity equation (TIE) was originally derived by Teague [1] as a non-iterative propagation-based phase retrieval method for a completely coherent field, in which context the definition of phase is clear. However, as we know no currently physically realizable sources are intrinsically perfectly coherent, and one must consider the effect of partial coherence on phase retrieval. The fact that TIE is not restricted to the purely coherent regime but works also with a partially coherent source seems to be very well known, and a wide range of applications in x-ray diffraction, electron-beam microscopy, and quantitative optical phase microscopy have been reported [2-6]. Besides, some variants of TIE have been reported to account for the partial coherence explicitly. Streibl [7] first pointed out the validity of Teague's TIE for a non-coherent imaging system, provided that the source distribution is symmetrical about the optical axis. Paganin and Nugent [8] created a meaningful definition of phase for partially coherent fields using the concept of the Poynting vector. An alternative interpretation with generalized eikonal was described by Gureyev *et al.*, [9] based on the spectrum decomposition of a polychromatic field. Zysk *et al.* [10] further explicitly considered the spatially partial coherence with use of coherent mode decomposition, showing that the phase recovered by TIE is a weighted average of the phases of all modes. Petrucci *et al.* [11] developed a partially-coherent form of TIE allowing removal of illumination-induced phase inaccuracies.

The aim of this paper to extend the theory of phase-space optics to reinterpret TIE particularly for a partially coherent field. The mutual intensity function is conveniently replaced by the Wigner distribution function, yielding an elegant description and intuitive understanding of issues related to TIE and optical systems under partially coherent illumination. With this tool, we interpret the physical meaning of the phase recovered from the TIE, investigate the effect of partially coherent illumination and finite aperture of imaging systems on phase retrieval. The correspondence between the Wigner distribution function and the light field in the geometric optics enables extracting phase information from the light field and vice versa for slowly varying specimen under certain simplified illumination conditions.

2. THEORY

Let $U(\mathbf{x})$ be a stationary and ergodic paraxial scalar field with arbitrary spatial and temporal coherence, where $\mathbf{x}$ is the two-dimensional spatial vector. The mutual coherence function of this statistical field is defined by

$$\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_2, \tau) = \langle U(\mathbf{x}_1, t) U^*(\mathbf{x}_2, t + \tau) \rangle, \quad (1)$$

where the sharp bracket denotes an ensemble average. The temporal power spectrum of the mutual coherence function

$$\Gamma(\mathbf{x}_1, \mathbf{x}_2, \omega) = \int \hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_2, \tau) \exp(i2\pi\omega\tau) d\tau, \quad (2)$$

called the cross-spectral density, plays a central role in the classic coherence theory since it describes the ensemble-averaged correlations of a given monochromatic component (characterized by the optical frequency $\omega = c/\lambda$, where c is the speed of light and λ is the wavelength) of the whole field. Next we prefer to convert the cross-spectral density into WDF defined in 4D phase space $(\mathbf{x}, \mathbf{u})$, through a Moyal transform given as

$$W_\omega(\mathbf{x}, \mathbf{u}) = \int \Gamma\left(\mathbf{x} + \frac{\mathbf{x}'}{2}, \mathbf{x} - \frac{\mathbf{x}'}{2}, \omega\right) \exp(-i2\pi\mathbf{u}\mathbf{x}') d\mathbf{x}', \quad (3)$$

where $\mathbf{u}$ is spatial frequency vector corresponding to $\mathbf{x}$. With use of the Liouville transport equation [12], we can derive a generalized transport of intensity equation (GTIE) which is valid under partially coherent field

$$\frac{\partial I(\mathbf{x})}{\partial z} = -\nabla_{\mathbf{x}} \cdot \iint \lambda \mathbf{u} W_\omega(\mathbf{x}, \mathbf{u}) d\mathbf{u} d\omega. \quad (4)$$

Note the only assumption employed in deriving Eq. (4) is the paraxial field to be stationary and ergodic, thus it is general enough to cover various optical fields with arbitrary spatial and temporal coherence. The spectral dependence ω can be eliminated by assuming the field to be quasi-monochromatic, and thus the GTIE for partially spatially coherent fields can be written as

$$\frac{\partial I(\mathbf{x})}{\partial z} = -\lambda \nabla_{\mathbf{x}} \cdot \int \mathbf{u} W(\mathbf{x}, \mathbf{u}) d\mathbf{u}. \quad (5)$$

In completely coherent case, the field can be fully described by the 2D complex amplitude $U(\mathbf{x}) = \sqrt{I(\mathbf{x})} \exp[i\phi(\mathbf{x})]$, where ϕ is the (conventional) phase. From the time(space)-frequency analysis perspective, the completely coherent field can be regarded as a mono-component signal, and the first conditional frequency moment of WDF (instantaneous frequency) relates to the transverse gradient of the phase of the complex field [13]:

$$\frac{\int \mathbf{u} W(\mathbf{x}, \mathbf{u}) d\mathbf{u}}{\int W(\mathbf{x}, \mathbf{u}) d\mathbf{u}} = \frac{1}{2\pi} \nabla \phi(\mathbf{x}). \quad (6)$$

Substitution of Eq. (6) into Eq. (5) leads to coherent TIE

$$\frac{\partial I(\mathbf{x})}{\partial z} = -\frac{1}{k} \nabla \cdot [I(\mathbf{x}) \nabla \phi(\mathbf{x})]. \quad (7)$$

This equation is a second-order elliptic partial differential equation, which provides a simple and deterministic method for phase retrieval from intensity measurements. Provided the intensity distribution is strictly positive, the phase can be uniquely determined (up to an arbitrary additive constant) by solving the equation with appropriate boundary conditions [14, 15]. The partially coherent field does not have a well-defined phase since the field experiences statistical fluctuations over time. However, the phase-space representation on LHS of Eq. (6) is still valid, leading to a new meaningful and more general definition of “phase”. Here we refer the new “phase” $\hat{\phi}(\mathbf{x})$ defined by Eq. (6) as the generalized phase of partially coherent fields to distinguish it from its coherent counterpart. The generalized phase behaving precisely as the conventionally defined phase and directly reduces to conventional phase when the field is fully coherent. It is seen from Eq. (6) that the generalized phase is a scalar potential whose gradient yields the conditional frequency moment of the WDF [16]. It is clear from a distribution point of view, that quantity is the average frequency at a particular location. Furthermore, the simultaneous space-frequency description of WDF closely resembles the ray

concept in geometrical optics, which conveys information about the amplitude and direction of flow of energy (Poynting vector). However, the WDF is not a rigorous probability distribution in phase space since it can take negative values. But it is rather instructive to adopt this simple interpretation as link between physical optics and geometrical optics. Furthermore, this simple interpretation provides an illuminating physical picture of beam propagation and energy transport with reasonable accuracy where the diffraction effects and the vectorial nature of the field can be safely ignored.

3. PHASE RETRIEVAL UNDER PARTIALLY COHERENT ILLUMINATION

Since the partial coherence is explicitly considered in GTIE, it can be used to analyze the phase retrieval under partially coherent illumination. It should be emphasized that the major concern in such scenario is the well-defined phase shift introduced by the specimen rather than the generalized phase of the partially coherent field itself. This leads to the nature choice of treating the contributions of the incident illumination and specimen separately by considering the transmitted field as a product of the illumination function $U_{in}(\mathbf{x})$ and the sample transmission function $T(\mathbf{x}) = \sqrt{\tau(\mathbf{x})} \exp[i\phi(\mathbf{x})]$, where $\tau(\mathbf{x})$ and $\phi(\mathbf{x})$ are the amplitude and the phase functions of the specimen. It is thus not hard to find the WDF of the resultant field just leaving the object can be represented as the object transmittance WDF $W_T(\mathbf{x}, \mathbf{u})$ windowed by the illumination WDF $W_{in}(\mathbf{x}, \mathbf{u})$

$$W_{out}(\mathbf{x}, \mathbf{u}) = \int W_T(\mathbf{x}, \mathbf{u}') W_{in}(\mathbf{x}, \mathbf{u} - \mathbf{u}') d\mathbf{u}' = W_T(\mathbf{x}, \mathbf{u}) \otimes_{\mathbf{u}} W_{in}(\mathbf{x}, \mathbf{u}), \quad (8)$$

which is a mere convolution over the spatial frequency variable $\mathbf{u}$. Equation (12) reveals that the partially coherent incident illumination blurs the object WDF along the spatial frequency dimension. By taking it into LHS of Eq. (6), it is then readily to find the generalized phase of the transmitted field $\hat{\phi}_{out}(\mathbf{x})$ should satisfy the following expression

$$\frac{\int \mathbf{u} W_{out}(\mathbf{x}, \mathbf{u}) d\mathbf{u}}{\int W_{out}(\mathbf{x}, \mathbf{u}) d\mathbf{u}} = \frac{\int \mathbf{u} W_T(\mathbf{x}, \mathbf{u}) d\mathbf{u}}{\int W_T(\mathbf{x}, \mathbf{u}) d\mathbf{u}} + \frac{\int \mathbf{u} W_{in}(\mathbf{x}, \mathbf{u}) d\mathbf{u}}{\int W_{in}(\mathbf{x}, \mathbf{u}) d\mathbf{u}}, \quad (9)$$

or equivalently,

$$\nabla_{\mathbf{x}} \hat{\phi}_{out}(\mathbf{x}) = \nabla_{\mathbf{x}} [\hat{\phi}_{in}(\mathbf{x}) + \phi(\mathbf{x})]. \quad (10)$$

This representation shows the generalized phase accrues upon propagation through the object, behaving precisely as would the conventionally defined phase. In general, the determination of object phase requires two independent measurements, performed respectively with and without the presence of the specimen. The sample-free measurement is used to characterize the incident beam $\hat{\phi}_{in}(\mathbf{x})$ and is subsequently subtracted from the total generalized phase $\hat{\phi}_{out}(\mathbf{x})$ to get the net phase introduced by the object only. However, if the illumination is chosen judiciously to directly nullify $\hat{\phi}_{in}(\mathbf{x})$,

$$\int \mathbf{u} W_{in}(\mathbf{x}, \mathbf{u}) d\mathbf{u} = 0. \quad (11)$$

The total generalized phase $\hat{\phi}_{out}(\mathbf{x})$ directly gives $\phi(\mathbf{x})$ and one single measurement is sufficient to recover the object phase even though the illumination is not fully coherent. For purely coherent illumination, Eq. (11) simply means the incident illumination is an on-axis plane wave. For the illumination created by an incoherent extended source, the condition Eq. (11) means the primary source distribution must be symmetrical about the optical axis.

4. SHACK HARTMANN SENSOR AND LIGHT FIELD IMAGING

For completely coherent fields, the phase-space representation is highly redundant because the complex field is defined only over the 2D plane $\mathbf{x}$. The 2D intensity and the reconstructed phase distribution gives total knowledge about the complex field so that the behavior of the field can be perfectly predicted. Such complete knowledge permits a variety forms of coherent optical imaging systems such as the Zernike phase contrast and the differential interference contrast imaging to be computationally emulated without resort to actual optical hardware [5, 17]. If the phase varies slowly such that the approximations $\phi(\mathbf{x} + \mathbf{x}/2) - \phi(\mathbf{x} - \mathbf{x}/2) \approx \mathbf{x} \cdot \nabla \phi(\mathbf{x})$ is valid, the phase space redundancy becomes more apparent since the signal occupies only a single slice in phase space

$$W(\mathbf{x}, \mathbf{u}) = I(\mathbf{x}) \delta\left[\mathbf{u} - \frac{1}{2\pi} \nabla \phi(\mathbf{x})\right]. \quad (12)$$

The form of WDF given above now is a true energy probability distribution in phase-space, telling us the geometric ray or energy flow at single position travels only along single direction described by the phase normal. This is an advantageous feature to allow phase measurement simply by measuring the directions of the rays, using the Shack-Hartmann sensor [18].

Fig. 1 Principle of the Shack-Hartmann sensor and Light field Imaging. (a) Shack-Hartmann sensor. (b) Light field Imaging.

The Shack-Hartmann sensor is an array of lenslets, each of which brings the incident field to a focus. When normally incident plane waves are shone onto the sensor, each lenslet brings the light to a focus at the center of its associated detector. If an aberrated wave is incident onto the sensor, then the location of each spot will be displaced by a vector proportional to the average phase gradient $\nabla\phi(\mathbf{x})$ over the lenslet. This displacement may be sensed by, for example, a quadrant detector. The resulting signals should be integrated to create an estimate of the phase distribution. Though its conceptual simplicity, the disadvantage of the Shack-Hartmann sensor is obvious: the spatial resolution over the wavefront is limited by the size and number of the lenslets.

For partially coherent field (include the condition of the totally incoherent fields), the 4D WDF is generally non-redundant. From the geometrical optics perspective, the geometric ray at single position does not travel only in one direction; instead, it fans out to make a 2D distribution, which account for the higher dimensionality of the partially coherent field. The light field camera, as a counterpart of the Shack-Hartmann sensor in computer graphics community, allows joint measurement of the spatial and directional distribution of light [19]. The “light field” is a term commonly used in the computer graphics literature to represent a collection of light rays in geometric optics. It is parameterized by a four-variable function $L(\mathbf{x}, \boldsymbol{\theta})$, taking into account both the geometrical position of the rays $\mathbf{x}$ and also their directions $\boldsymbol{\theta}$. It approaches the WDF at geometric optics limit [20]. Light field imaging enables us to apply ray-tracing techniques to compute synthetic photographs, change the focus and perspective view flexibly. However, it requires elaborate optical setups and significantly sacrifices spatial resolution (traded for angular information) as compared to conventional imaging technique.

5. PHASE AND LIGHT FIELD

Transport of intensity equation provides a simple and deterministic way to recover phase from a set of defocused images. However, acquiring the through-focus image stack is usually time-consuming, as the sample stage or camera has to be moved between image captures. Though several configurations have been developed to eliminate the mechanical motion [5, 6], light field imaging enables a totally new way to collect the entire image stack in single capture, as the intensity images at an arbitrary focal plane can be computationally reconstructed from the raw light field image. This undoubtedly suggests one viable way to convert the light field to the phase.

It would be more interesting to consider this problem from a different perspective: Eq. (6) suggests that the generalized phase is a scalar potential whose gradient yields the conditional frequency moment of the WDF. Under geometric optics approximation $L(\mathbf{x}, \boldsymbol{\theta}) \approx W(\mathbf{x}, \lambda \mathbf{u})$, Eq. (6) becomes

$$\frac{\int \boldsymbol{\theta} L(\mathbf{x}, \boldsymbol{\theta}) d\boldsymbol{\theta}}{\int L(\mathbf{x}, \boldsymbol{\theta}) d\boldsymbol{\theta}} = \frac{1}{2\pi} \nabla \phi(\mathbf{x}). \quad (13)$$

It is clear from the above definition that the quantity on the LHS is the centroid of the light field - the average direction of light at one given position, suggesting that the phase gradient can be easily recovered by a simple centroid detection scheme applied to the raw light field image. This is similar with the standard procedure in the Shack-Hartmann method. Compared to the first method, which first reconstructs the through-focus stack, then solves the TIE explicitly; the second method, which employs the definition of the generalized phase here, is inherently much easier and straightforward.

It is quite understandable that the phase can be recovered from the light field since the 4D light field is inherently in a higher dimensionality which totally cover the 2-D phase information. But it would be quite interesting to consider whether the inverse of this process can be realized: with the knowledge of phase, is it possible to recover the whole light field? Apparently, the answer should be NO for the general cases. However, under certain conditions, we can indeed covert the phase to the light field. Besides the trivial case when the field is purely coherent, let us consider that the sample is illuminated by a spatial stationary illumination that is generally true for the experimental arrangements in optical microscopy [12]. The fully spatially incoherent primary source (usually at the condenser aperture plane for an optical microscope) featured by the intensity distribution $|P_c(\mathbf{x})|^2$ and the positional cross-spectral density $\Gamma(\mathbf{x} + \mathbf{x}'/2, \mathbf{x} - \mathbf{x}'/2) = |P_c(\mathbf{x})|^2 \delta(\mathbf{x}')$ produces the illumination WDF $W_{in}(\mathbf{x}, \mathbf{u})$ at the far-zone

$$W_{in}(\mathbf{x}, \mathbf{u}) = |P_c(\mathbf{u})|^2. \quad (14)$$

Equation (14) is in fact an expression of the Van Cittert-Zernike theorem. If the phase varies slowly such that the approximations $\phi(\mathbf{x} + \mathbf{x}/2) - \phi(\mathbf{x} - \mathbf{x}/2) \approx \mathbf{x} \cdot \nabla \phi(\mathbf{x})$, the resultant field just leaving the object can be represented as

$$L(\mathbf{x}, \boldsymbol{\theta}) = cI(\mathbf{x}) \left| P_c \left[\boldsymbol{\theta} - \frac{1}{k} \nabla_{\mathbf{x}} \phi(\mathbf{x}) \right] \right|^2, \quad (15)$$

where c is a constant ensuring $I(\mathbf{x}) = \int L(\mathbf{x}, \boldsymbol{\theta}) d\boldsymbol{\theta}$. Note the last step we used the approximation $L(\mathbf{x}, \boldsymbol{\theta}) \approx W(\mathbf{x}, \lambda \mathbf{u})$. Equation (15) represents exactly the geometric optical behavior of the specimen: for each incident ray, it leaves the specimen from the same position but its direction is shifted as a function of the phase gradient of the object. The specimen, can be regarded as a spread-less system, does not change the angular distribution of the incident field, which is fully determined by the source intensity distribution. Thus, with the knowledge of the source intensity distribution and the phase of the object $\phi(\mathbf{x})$ (can be retrieved from TIE with only 2 images), the 4D light-field can be fully characterized.

6. EFFECT OF FINITE APERTURE OF IMAGING SYSTEM

Another important assumption made in TIE is perfect imaging which is not fulfilled in a practical imaging system, such as a microscope. In fact, what we measure is the phase of the field in the image plane, which is not exactly the phase of the object itself, especially when the pupil of the imaging system is insufficient to transmit all spatial frequencies of interest in the object. In this case, understanding and quantifying the effect of the imaging system appears particularly important. Consider a practical imaging system with a finite aperture, the CSD in the image plane can be written as

$$\Gamma_{image}(\mathbf{x}_1, \mathbf{x}_2) = \Gamma_{out}(\mathbf{x}_1, \mathbf{x}_2) \otimes_{\mathbf{x}_1, \mathbf{x}_2} h(\mathbf{x}_1, \mathbf{x}_2), \quad (16)$$

with the mutual point spread function (PSF) $h(\mathbf{x}_1, \mathbf{x}_2)$ defined as $h(\mathbf{x}_1, \mathbf{x}_2) = h(\mathbf{x}_1)h^*(\mathbf{x}_2)$, where $h(\mathbf{x})$ is the coherent PSF of the imaging system. With the convolution theorem, the corresponding WDF of the wave field in the image plane can be written as

$$W_{image}(\mathbf{x}, \mathbf{u}) = W_T(\mathbf{x}, \mathbf{u}) \otimes_{\mathbf{u}} W_{in}(\mathbf{x}, \mathbf{u}) \otimes_{\mathbf{x}} W_{psf}(\mathbf{x}, \mathbf{u}). \quad (17)$$

It is seen that the effect of the imaging system is equivalent to convolving the WDF of imaging PSF over the spatial variable $\mathbf{x}$. More importantly, $W_{psf}(\mathbf{x}, \mathbf{u})$ is zero when $\mathbf{u}$ falls outside of the pupil (in most cases the pupil function is equal to a circ-function, i.e., $P(\mathbf{u})=1, |\mathbf{u}| \leq u_{NA}$ and $P(\mathbf{u})=0, |\mathbf{u}| > u_{NA}$), which means all WDF components outside the pupil will be dumped by the imaging system. Since TIE retrieves the conditional frequency moment of the WDF as the phase gradient, the reconstructed phase in the image plane is not the true phase of the object in general (except for the case of perfect imaging when the $W_{psf}(\mathbf{x}, \mathbf{u})$ reduces to $\delta(\mathbf{x})$ and $P(\mathbf{u})=1$ for all $\mathbf{u}$). Due to the bilinear nature of image formation in partially coherent systems, such kind of phase discrepancy is difficult to analyze or compensated directly. However, if we consider a slowly varying specimen under spatially stationary illumination, Eq. (17) can be further simplified as:

$$W_{\text{image}}(\mathbf{x}, \mathbf{u}) \approx cI(\mathbf{x}) \left| P_c \left[\mathbf{u} - \frac{1}{2\pi} \nabla_{\mathbf{x}} \phi(\mathbf{x}) \right] \right|^2 |P(\mathbf{u})|^2, \quad (18)$$

Thus, the reconstructed gradient of the generalized phase in the image plane is the frequency centroid of the overlapping area of the shifted primary source and the pupil function. Without considering the effect of the imaging system, the phase gradient is just the centroid of the shifted primary source. As long as the source distribution is symmetric with respect to the optical axis, the phase can be accurately retrieved, regardless of the source size (spatial coherence of the illumination). However, in a practical imaging system, it is necessary to give a higher importance to the illumination coherence, because the size of the light source has a significant influence on the imaging. Though decreasing the source size does help improve the phase retrieval accuracy (better linear transfer for lower phase gradient), it will compromise the resolution limit. Furthermore, a certain degree of illumination coherence is necessary. For incoherent imaging (the source size is larger than the pupil) the real frequency centroid corresponding to the object phase gradient can never be correctly identified by the TIE due to the apodization effects of the pupil function. For partially coherent imaging (the source size smaller than the pupil), the imaging system induced phase distortion still exists, but can be further compensated. However, this point is beyond the scope of our current work and subject to further exploration.

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