Generalized Eikonal of Partially Coherent Beams and Its Use in Quantitative Imaging

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The generalized eikonal of a partially coherent paraxial wave is introduced via a differential equation describing the evolution of the time-averaged intensity. The theoretical formalism provides an analytical tool for the study of partially coherent imaging systems. It also makes possible quantitative phase retrieval and compositional mapping of weakly absorbing samples using phase-contrast imaging with broadband polychromatic radiation of known spectral distribution. An experimental demonstration is presented of the quantitative reconstruction of the projected thickness of a sample, given a phase-contrast image obtained using a polychromatic microfocus x-ray source.

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Phase contrast is a valuable tool for imaging transparent samples with electrons, x rays, and other forms of radiation and matter waves [1–3]. While most forms of phase contrast are used in a qualitative fashion, quantitative phase imaging is being actively developed for the needs of nondestructive testing and structural analysis [4–8]. Quantitative phase-contrast imaging is closely related to the problem of phase retrieval [9]. A difficulty in extending the existing theories of phase-contrast imaging from coherent to partially coherent waves arises from the fact that the notion of phase in the latter case is nontrivial, as each coherent component of the wave may have a different direction of propagation and, hence, a different wave front and phase. It has been suggested that, at least in the paraxial case, an average phase can be associated with the average direction of propagation (or energy flow) of a partially coherent beam [8,10,11]. Following this general approach, we show in the present paper that, under broad conditions, the eikonal (optical path) of a partially coherent beam can be defined as a function of the transverse redistribution of the time-averaged intensity of the beam on propagation. We also demonstrate that such an eikonal can be naturally expressed in terms of the monochromatic components of the beam. The new formalism allows simple solutions for some practical direct and inverse imaging problems, including that of quantitative sample reconstruction using polychromatic phase-contrast images [12,13].

Let $U(\mathbf{r};t)$, $\mathbf{r}=(x,y,z)$, be the complex scalar amplitude of a stationary and ergodic beam (paraxial wave) in an arbitrary state of partial coherence, propagating along optic axis z. We introduce a quantity $z+\psi_z(x,y)$, which we call the "generalized eikonal" of the partially coherent beam $U(\mathbf{r};t)$, which by definition satisfies an equation similar to the monochromatic transport of intensity equation (TIE) [2],

$$-\nabla_\perp\cdot[I_z(x,y)\nabla_\perp\psi_z(x,y)]=\partial_z I_z(x,y), \tag{1}$$

where $I_z(x,y)\equiv\lim_{T\to\infty}(2T)^{-1}\int_{-T}^{T}|U(\mathbf{r};t)|^2\,dt$ is the time-averaged intensity of the beam and $\nabla_\perp\equiv(\partial_x,\partial_y)$. If $I_z(x,y)$ does not have zeros in a given area of the transverse plane z, Eq. (1) can be uniquely solved for the unknown function $\psi_z(x,y)$ satisfying appropriate boundary conditions. Thus, Eq. (1) indeed provides a constructive definition for the generalized eikonal. Using the notion of the generalized eikonal and arbitrarily choosing a wavelength $\bar\lambda$, we can define the corresponding "generalized" or "average" phase $\bar k z+\bar\varphi_z(x,y;\bar\lambda)\equiv\bar k[z+\psi_z(x,y)]$, $\bar k=2\pi/\bar\lambda$, of the partially coherent beam $U(\mathbf{r};t)$. As the definition of average phase inevitably depends on the choice of some average wavelength, the notion of generalized eikonal appears to be more fundamental in this context.

In order to clarify the physical nature of the generalized eikonal, we consider the monochromatic decomposition of a partially coherent beam via the (generalized) Fourier transform over the frequencies, $U(\mathbf{r};t)=\int U(\mathbf{r};\nu)\exp(i2\pi\nu t)\,d\nu$, where $\nu=c/\lambda$ is the frequency of a given monochromatic component, c is the speed of light, and $U(\mathbf{r};\nu)=0$ for $\nu<0$ [1]. Note that the spectrum $U(\mathbf{r};\nu)$ contains complete information about the stationary and ergodic beam $U(\mathbf{r};t)$, including all of its spatial coherence properties. As every monochromatic component of the beam, $U(\mathbf{r};\nu)\exp(i2\pi\nu t)$, is perfectly coherent, it satisfies the paraxial equation, $(2ik\partial_z+\nabla_\perp^2)U(\mathbf{r};\nu)=0$. As a consequence, the spectral density $S_z(x,y;\lambda)$ satisfies the TIE [11],

$$-\nabla_\perp\cdot[S_z(x,y;\lambda)\nabla_\perp\psi_z(x,y;\lambda)]=\partial_z S_z(x,y;\lambda), \tag{2}$$

where $\psi_z(x,y;\lambda)\equiv\varphi_z(x,y;c/\nu)/k\equiv[\arg U(\mathbf{r};\nu)]/k-z$ is the eikonal of the monochromatic component, and its spectral density $S_z(x,y;\lambda)\equiv S_z(x,y;c/\nu)\equiv\tilde S_z(x,y;\nu)$ is defined as the Fourier transform of the temporal coherence function, $\Gamma(\mathbf{r},\mathbf{r};\tau)$, with respect to the time delay τ [1]. The time-averaged intensity of a partially coherent beam coincides with the integral of the spectral density over all frequencies, $I_z(x, y) = \Gamma(\mathbf{r}, \mathbf{r}; 0) = \int S_z(x, y; c/\nu)\, d\nu$. Hence, we can integrate Eq. (2) over all frequencies and use Eq. (1) to obtain

$$\nabla_\perp \cdot [I_z(x, y)\nabla_\perp \psi_z(x, y)] = \nabla_\perp \cdot \left[\int S_z(x, y; c/\nu)\nabla_\perp \psi_z(x, y; c/\nu)\, d\nu\right]. \quad (3)$$

Equation (3) describes the relationship of the generalized eikonal, $\psi_z(x, y)$, to the spectral density and the eikonals of the monochromatic components of the beam. In the case of a beam with a spectral density distribution that is slowly varying with respect to spatial coordinates (x, y), in a given transverse plane z, a solution to Eq. (3) can be obtained by neglecting the transverse derivatives of the intensity and the spectral density [11],

$$\psi_z(x, y) = \int S_z(x, y; c/\nu)\psi_z(x, y; c/\nu)\, d\nu / I_z(x, y). \quad (4)$$

In this approximation, the generalized eikonal of a given partially coherent beam is equal to a weighted average of the optical paths of its monochromatic components, with weights proportional to the spectral density at each wavelength.

The above notion of the generalized eikonal of a partially coherent beam is related to the average local Poynting vector introduced in [10]. Indeed, at every wavelength λ the transverse component of the Poynting vector of a paraxial field is $\mathbf{P}_\perp(\mathbf{r}; \lambda) = (c/\lambda^2)S_z(x, y; \lambda) \times \nabla_\perp \psi_z(x, y; \lambda)$. Using the identity $|d\nu| = (c/\lambda^2)|d\lambda|$, and defining the transverse component of the Poynting vector of partially coherent beam $U(\mathbf{r}; t)$ as $\mathbf{P}_\perp(\mathbf{r}) \equiv I_z(x, y) \times \nabla_\perp \psi_z(x, y)$, we obtain from Eq. (3) that $\mathbf{P}_\perp(\mathbf{r}) = \int \mathbf{P}_\perp(\mathbf{r}; \lambda)\, d\lambda$. The corresponding physical picture implies that the normals to the wave front $z + \psi_z(x, y) = \text{const}$ defined by the generalized eikonal represent average directions for the rays corresponding to the individual monochromatic components. Note that this approach is formally different from the one adopted in [10] where the Poynting-vector averaging was performed over the time variable. As we demonstrate below, the use of the monochromatic decomposition, Eq. (3), may be more convenient than time averaging for the solution of certain practical problems.

We now consider possible application of the introduced generalized eikonal for solution of "direct" and "inverse" imaging problems. We consider a simple direct problem first. Suppose that we know the time-averaged intensity and generalized eikonal of a partially coherent beam $U(\mathbf{r}; t)$ on a single plane z orthogonal to the optic axis. We would like to calculate the distribution of the time-averaged intensity on other planes by some form of propagation from the plane z. Using the stationary phase formula (e.g., as in [14]), it is possible to show that if the paraxial geometric optics approximation holds for the monochromatic components of the beam, then Eq. (2) can be "extended," i.e.,

$$S_{z+\Delta z}(x, y; \lambda) = S_z(x, y; \lambda) - \Delta z \nabla_\perp \cdot [S_z(x, y; \lambda)\nabla_\perp \psi_z(x, y; \lambda)], \quad (5)$$

where the distance Δz between the planes z and $z + \Delta z$ can be arbitrarily large as long as there are no focal points between them. Integrating Eq. (5) over all frequencies as above and taking Eq. (3) into account, we obtain the following extended version of Eq. (1),

$$I_{z+\Delta z}(x, y) = I_z(x, y) - \Delta z \nabla_\perp \cdot [I_z(x, y)\nabla_\perp \psi_z(x, y)]. \quad (6)$$

Equation (6) shows that under the specified conditions the time-averaged intensity in the plane $z + \Delta z$ can be obtained by propagating from a fixed plane z just as in the monochromatic case. This formalism allows considerably more efficient solution of the direct problem compared to the more straightforward approach where the propagated intensity of the polychromatic beam would be calculated by propagating coherent components separately before evaluating and summing up the intensities.

Proceeding to inverse imaging problems, we would like to find out what quantitative information about an object (scatterer) can be obtained if the generalized eikonal of the scattered beam is recovered, e.g., using Eq. (1), from measurements of the time-averaged intensity. We consider a model of a sample consisting of J different materials with known refractive indices $n_j(\lambda) = 1 - \delta_j(\lambda) - i\beta_j(\lambda)$, $j = 1, 2, \ldots, J$. The sample is located in the half-space $z < 0$ immediately before the object plane, $z = 0$, and is illuminated by a partially coherent beam. We assume for the sake of simplicity that the projection approximation is valid for the object, i.e.,

$$\ln S_0(x, y; \lambda) = \ln S_{\text{in}}(x, y; \lambda) - (4\pi/\lambda) \sum_{j=1}^{J} \beta_j(\lambda) T_j(x, y), \quad (7a)$$

$$\psi_0(x, y; \lambda) = \psi_{\text{in}}(x, y; \lambda) - \sum_{j=1}^{J} \delta_j(\lambda) T_j(x, y), \quad (7b)$$

where $T_j(x, y)$, $j = 1, 2, \ldots, J$, are the unknown projected thicknesses of the component materials along the lines parallel to the optic axis z, and $S_{\text{in}}(x, y; \lambda)$ and $\psi_{\text{in}}(x, y; \lambda)$ are the spectral density and eikonal of the monochromatic components of the incident wave. If the transmitted spectral density can be measured at several individual wavelengths (using monochromatic radiation at different wavelengths or an energy resolving detector), then Eqs. (7a) and (7b) can be used separately or in combination to find the unknown thicknesses $T_j(x, y)$ (see, e.g., [15,16]). The problem becomes more complicated when only the time-averaged intensity of the polychromatic beam is measurable.

The use of phase contrast for structural analysis is of great value when the absorption contrast is too weak or when the transmitted intensity has to be measured at some distance from the object (e.g., in point-projection imaging) and Fresnel diffraction effects cannot be neglected. It follows from Eq. (7a) that the expression for the transmitted time-averaged intensity is generally nonlinear, but becomes linear with respect to thicknesses $T_j(x, y)$ in the case of weak absorption,

$$I_0(x, y) = I_{\mathrm{in}}(x, y) - 4\pi \sum_{j=1}^{J} T_j(x, y) \times \int S_{\mathrm{in}}(x, y; c/\nu)\beta_j(c/\nu)(\nu/c)\, d\nu, \quad (8)$$

when $\exp[-(4\pi/\lambda)\sum_{j=1}^{J}\beta_j(\lambda)T_j(x, y)] \cong 1 - (4\pi/\lambda) \times \sum_{j=1}^{J}\beta_j(\lambda)T_j(x, y)$. The expression for the generalized eikonal is also linear in this case, as implied by Eqs. (4) and (7b),

$$\psi_0(x, y) = \tilde{\psi}_{\mathrm{in}}(x, y) - \sum_{j=1}^{J} T_j(x, y) \times \int S_{\mathrm{in}}(x, y; c/\nu)\delta_j(c/\nu)\, d\nu/I_{\mathrm{in}}(x, y), \quad (9)$$

where the term $\tilde{\psi}_{\mathrm{in}}(x, y)$ is a constant when the phase of the incident beam is uniform in x and y. Note that Eq. (9) establishes a quantitative relationship between the refractive index of a sample and the properties of the eikonal or phase of a transmitted partially coherent wave. Assuming that the incident beam is uniform in x and y, combine Eqs. (8) and (9) with Eq. (1) at $z = 0$ and neglect the gradient of $I_0(x, y)$ (using the weak absorption assumption), to obtain the following for sufficiently small z:

$$1 - I_z^i(x, y)/I_{\mathrm{in}}^i \cong \sum_{j=1}^{J}(\mu_j^i - z\delta_j^i\nabla_\perp^2)T_j(x, y), \quad (10)$$

where index i corresponds to different incident spectra $S_{\mathrm{in}}^i(\lambda)$, $i = 1, 2, \ldots, I$, $\mu_j^i = 4\pi \int S_{\mathrm{in}}^i(c/\nu) \times \beta_j(c/\nu)(\nu/c)\, d\nu/I_{\mathrm{in}}^i$ and $\delta_j^i = \int S_{\mathrm{in}}^i(c/\nu)\delta_j(c/\nu)\, d\nu/I_{\mathrm{in}}^i$. In the case of monochromatic radiation and a weakly absorbing object consisting of a single material ($J = 1$), Eq. (10) follows from the result obtained earlier in [17]. The system of linear partial differential equations (10) with different incident spectra $S_{\mathrm{in}}^i(\lambda)$, $i = 1, 2, \ldots, I$, can be solved with respect to the unknown projected thicknesses $T_j(x, y)$, $j = 1, 2, \ldots, J$, e.g., using Fourier transformation, provided the matrix $\boldsymbol{\chi}(\zeta) = \boldsymbol{\mu} + z\zeta^2\boldsymbol{\delta}$ is nondegenerate, where $\boldsymbol{\mu} \equiv \{\mu_j^i\}$, $\boldsymbol{\delta} \equiv \{\delta_j^i\}$, and ζ^2 corresponds to the Fourier-space representation of the operator $(-\nabla_\perp^2)$. Equation (10) can be applied for nondestructive structural analysis (including computed tomography) of weakly absorbing samples for which conventional methods based on absorption contrast do not work. The essential advantage brought by the introduction of the generalized eikonal is in the possibility to use broadband polychromatic radiation with known spectral distributions, to perform quantitative analysis using phase-contrast images.

In order to verify the method for quantitative imaging based on Eq. (10), we collected a polychromatic point-projection x-ray image of a sample consisting of several latex spheres with diameters of approximately 5.3 and 9.0 μm (see Fig. 1). The image clearly displays phase-contrast effects in the form of Fresnel fringes near the edges of the spheres. The image was obtained using an scanning-electron-microscopy–based x-ray ultramicroscope described in [16]. An Ag foil target and an accelerating voltage of 10 kV were used. The x-ray spectrum of the imaging system, $S_{\mathrm{in}}(c/\nu)$, was measured directly by using the detector in a photon-counting mode [16] (Fig. 2). The total spectrum consisted of characteristic Ag Lα lines and a broad Bremsstrahlung. Spatial resolution of Fig. 1 was mainly limited by the source size and polychromaticity to $\sim$0.5 μm. The complex refractive index of latex in the range 0.1–1 keV was calculated [18] and used in conjunction with the spectrum to evaluate the values of μ_1^1 and δ_1^1 as required by Eq. (10), with $I = J = 1$. We used the intensity measured in the background (object-free) part of the image to estimate the incident intensity in Eq. (10). We then solved Eq. (10) using a computer program based on the fast Fourier transform. The reconstructed two-dimensional distribution of

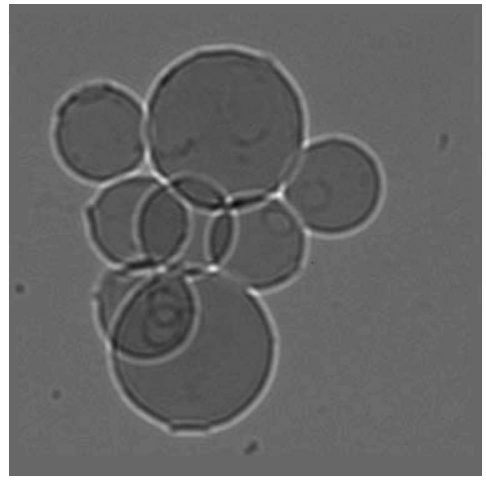

FIG. 1. Experimental point-projection image of a cluster of 5.3 and 9.0 μm latex spheres collected using a polychromatic microfocus x-ray source.

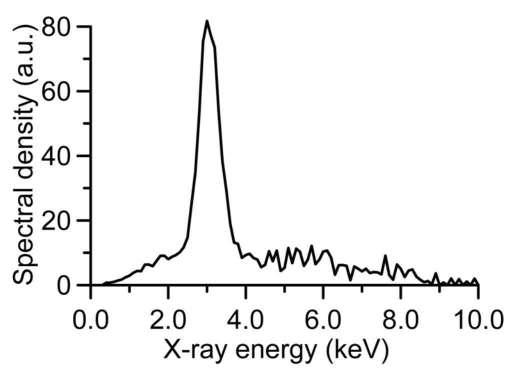

FIG. 2. Measured x-ray spectrum of the imaging system.

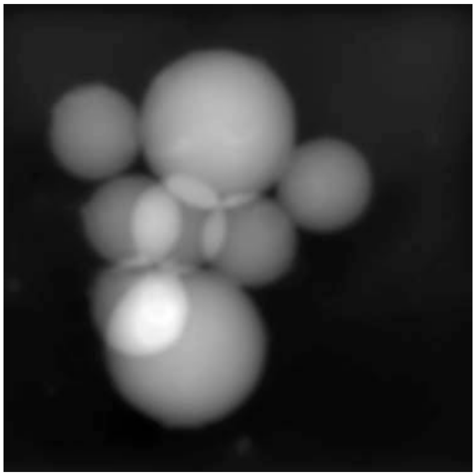

FIG. 3. Reconstructed distribution of the projected thickness of latex in the sample obtained from the image in Fig. 1.

the projected thickness of latex in the sample, $T_1(x, y)$, as presented in Fig. 3, clearly displays the expected shape of individual spheres with a correct compensation for the diffraction effects observable in Fig. 1. Figure 4 shows a horizontal cross section through the centers of the two top spheres in Fig. 3, revealing a maximum reconstructed thickness of $\sim 8.0\ \mu$m for the larger sphere and $\sim 5.3\ \mu$m for the smaller one. Spatial resolution of the reconstructed image was estimated to be $\sim 0.7\ \mu$m. While the reconstructed projected thickness for the smaller sphere is in very good agreement with that known *a priori*, the $\sim 10\%$ discrepancy in the reconstructed maximum projected thickness of the larger sphere can be attributed to the "flattening" of the sphere at the point of contact with the substrate which has been observed in these specimens. Note that an attempt to treat the image in Fig. 1 as a quasimonochromatic one, with a wavelength corresponding to the maximum of the spectral density (at ~ 3 keV), led to a much less accurate reconstruction than that demonstrated above (see Fig. 4); the estimated maximum projected thickness was $\sim 14.0\ \mu$m for the larger spheres and $\sim 8.7\ \mu$m for the smaller ones. Note also that the presence of propagation-induced phase contrast in the current image is an inevitable consequence of the point-projection imaging geometry that was adopted to obtain a magnified image without x-ray optical elements.

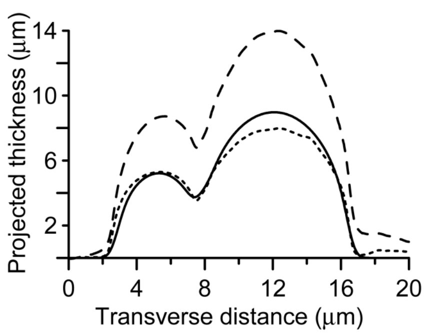

FIG. 4. Horizontal cross section through the top two spheres in the reconstructed image in Fig. 3 (short-dashed line), the same cross section for an image obtained with a conventional monochromatic reconstruction at $E = 3$ keV (long-dashed line), and a corresponding simulated projected thickness for 5.3 and 9.0 μm spheres convolved with a Gaussian distribution with standard deviation equal to 0.35 μm (solid line).

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