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Linear algorithms for phase retrieval in the Fresnel region. 3. Validity conditions

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ABSTRACT

We describe the relationship between different forms of linearized expressions for the spatial distribution of intensity of X-ray projection images obtained in the Fresnel region. We prove that under the natural validity conditions some of the previously published expressions can be simplified without a loss of accuracy. We also introduce modified validity conditions which are likely to be fulfilled in many relevant practical cases, and which lead to a further significant simplification of the expression for the image-plane intensity, permitting simple non-iterative linear algorithms for the phase retrieval.

1. Introduction

In recent years several results have been published [1–21] presenting various forms of linearized analytical expressions for the spatial distribution of the image-plane intensity in the case of in-line (projection) imaging (which involves free-space propagation of the transmitted wave from the exit surface of the object to the detector plane). The validity conditions under which the respective formulae can be derived have been discussed and analysed with varying degrees of rigour. No serious attempt seems to have been made so far to reconcile some of the "competing" expressions and compare theoretically their respective regions of validity. In the present paper we perform a detailed analysis of the validity conditions that were used explicitly or implicitly in previous publications and attempt to establish a definitive relationship between the respective results. We demonstrate that if the validity conditions required for their derivation are applied consistently, some of the formulae can be further simplified. The simplified expressions may also be more amenable to standard phase-retrieval approaches, where one collects one or more images in planes orthogonal to the optic axis at different object-to-detector distances, and then uses these images to retrieve the distribution of phase of the transmitted wave in the object plane.

We then suggest a modified validity condition which is likely to be fulfilled in many relevant experimental arrangements, with the new condition leading to a particularly simple linearized expression for the image-plane intensity as a function of the object-plane phase. We also demonstrate that all of the considered linearized expressions reduce to the Transport of Intensity equation (TIE) in the limit of large Fresnel numbers, and they reduce to the first Born approximation (also known in this context as the weak object or Fourier Optics approximation) in the limit of weak absorption and small phase shifts. We hope that this exposition will help to clarify the relationship between the previously published results and will establish sufficiently clear validity conditions that could be used by researchers to determine the limits of applicability of various expressions under particular experimental conditions that may be encountered in the practice of phase-contrast imaging and tomography.

Recently, the phase-retrieval method based on the assumption of homogeneity (also called monomorphicity) of the imaged sample, that was originally proposed in Ref. [8], has gained widespread acceptance and has been successfully used for a broad variety of practical imaging applications, largely due to the fact that it only requires a single in-line image to be collected in order to reconstruct both the object-plane phase and intensity distributions (the phase and the logarithm of intensity distributions are assumed to be related via a fixed proportionality constant in this method). The other two well-known cases, where a single image is sufficient for unambiguous phase retrieval, namely contact imaging (where the phase does not affect the registered intensity distribution) and pure-phase objects (that have negligible absorption),

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can be naturally considered as special cases of the homogeneous object approximation [12,14]. The practical advantages of this approach are not limited to the fact that it requires a single image for phase retrieval, instead of two or more images required in the general case, but also to a related benefit of substantial extra robustness with respect to image noise and artefacts, compared to the general in-line phase retrieval. In the present work, however, we do not analyse homogeneous versions of the phase retrieval formulae considered here, as the transition from the general to the homogeneous case has been already extensively studied elsewhere (see e.g. [8,12,14,21,22]). A reader interested in in-depth comparative analysis of most popular varieties of in-line phase-retrieval methods, with emphasis on their application in phase-contrast tomography, can be advised to consult an excellent review [23].

2. Guigay conditions and linearizability

Let an object (scatterer) be located in a vicinity of the optic axis in the half-space $z < 0$ immediately before the 'object' plane $z = 0$. We assume for simplicity that the wave incident on the sample is a plane monochromatic wave with wavelength λ and unit intensity, propagating along the optic axis z, i.e. the complex amplitude of the incident wave is $\exp(ikz)$, $k = 2\pi/\lambda$. Generalization of the following results to cases involving polychromatic and spatially partially coherent incident radiation can be carried out similarly to the way described in Ref. [14]. The scattering properties of the object are assumed to be such that the wave transmitted through the object is paraxial, i.e. all the wavefront normals in the object plane are contained in a narrow cone around the direction of the z axis. The transmitted wave propagates in the free half-space $z > 0$ until it reaches a position-sensitive detector. As the transmitted wave has been assumed to be paraxial, its evolution in the free half-space $z > 0$ can be described by the Fresnel diffraction integral [1],

$$\mathbf{Fr}\left[q,R\right](x,y) = \frac{\exp(ikR)}{i\lambda R}\iint \exp\left\{\frac{i\pi}{\lambda R}\left[\left(x-x'\right)^2+\left(y-y'\right)^2\right]\right\} \times q\left(x',y'\right)\,\mathrm{d}x'\mathrm{d}y', \tag{1}$$

where $q(x,y) \equiv a(x,y)\exp[i\varphi(x,y)]$ is the complex scalar amplitude of the wave in the object plane and R is the distance between the object and image planes. The detector is assumed to be capable of measuring the spatial distribution of intensity in the image plane,

$$I_R(x,y) = \left|\mathbf{Fr}\left[q,R\right](x,y)\right|^2. \tag{2}$$

In phase-contrast imaging and phase-contrast tomography one is often interested in finding the object-plane phase $\varphi(x,y)$ and absorption[1] $\mu(x,y) = -\ln a(x,y)$ from the measured intensity distribution in one or more image planes $z = R_m, m = 1,2,\ldots,M$. It is easy to see that Eq. (2) is non-linear with respect to the object-plane phase and amplitude, and as such is usually rather challenging to solve analytically or numerically. Therefore, it appears useful to derive linearized forms (approximations) of Eq. (2) which would be sufficiently accurate under certain well-specified conditions.

For simplicity, in what follows we mostly consider the one-dimensional situation (i.e. we omit the dependence of all functions on y). Generalizations of the derivations to the corresponding two-dimensional cases are straightforward and do not require any new insight.

The starting point for many known derivations of linear approximations to Eq. (2) is the following expression for the Fourier transform of image intensity distribution given by Guigay [2]:

$$\hat{I}_R(u) = \int \exp(i2\pi\, ux)\, q(x+\lambda Ru/2)\;\; q^*(x-\lambda Ru/2)\;\; dx, \tag{3}$$

where $\hat{f}(u) = \int \exp(i2\pi\; ux) f(x)\, dx$ denotes Fourier transform and the superscript asterisk denotes complex conjugation. Eq. (3) can be obtained directly by applying Fourier transform to the square modulus of (the one-dimensional version of) Eq. (1). The following two assumptions were effectively employed in Refs. [10,11,15] in order to linearize Eq. (3) with respect to the object-plane phase distribution:

$$\varphi(x+\lambda Ru/2) - \varphi(x-\lambda Ru/2) \;= O(\varepsilon), \tag{4}$$

$$a(x\pm\lambda Ru) - a(x) \mp \lambda Ru\;\, a'(x) = O\left(\varepsilon^2\right), \tag{5}$$

where $\varepsilon << 1$ is a small (asymptotic) parameter, superscript prime sign denotes a derivative, and $O(\varepsilon)$ and $O(\varepsilon^2)$ denote quantities that are of the order of ε and ε^2, respectively. Eq. (4) is known as Guigay's condition; it was first used in Ref. [2]. Eq. (5) represents a form of linearizability condition for the real amplitude.

Comparing Eqs. (4) and (5), it can be deduced that the limits imposed by these validity conditions on the approximations that can be derived on their basis, are generally more restrictive with respect to the allowed variation of the absorption, than with respect to the refraction (i.e. phase shifts). Therefore, it may not be possible to describe X-ray imaging of samples containing strongly absorbing materials using the theories that rely on the validity of Eqs. (4) and (5), unless the distribution of strong absorbers in the samples is very uniform and slowly varying. On the mathematical side, it can be noticed in the derivations below, that, in the expressions describing free-space propagation of the image intensity, the phase shifts at different spatial points of the object plane are subtracted, allowing large shifts to cancel each other, while the absorption contributions add up, and do not allow for such beneficial cancellations. It will be also shown below (in Section 4) that conditions on the amplitude $a(x)$, similar to Eq. (4), can be imposed in order to derive a convenient linearized expression for the in-line image intensity, but that condition has to be of the higher order, namely $O(\varepsilon^2)$, i.e. more restrictive, compared to the condition of the order $O(\varepsilon)$ for the phase in Eq. (4).

Although it was not specified explicitly in Refs. [10,11,15], one can verify that for the validity of the subsequent results it is sufficient to require that Eqs. (4)–(5) hold for all x, such that $|x| < X_{\max} + \lambda R u_{\max}$, where $q(x) \equiv 1$ for $|x| \geq X_{\max}$,[2] and for all u, such that $|u| \leq u_{\max}$; here $u_{\max} \equiv \min\left\{2U_{\max}, u_{sys}\right\}$, where $U_{\max}$ is the radius of the minimal circle enclosing the support of $\hat{q}(u)$ and u_{sys} is the cut-off frequency of the imaging system (determined by its spatial resolution) (see e.g. [14,16,20]).[3] The reason for the existence of a particular upper limit on the required range of spatial frequencies in Eqs. (4)–(5) can be easier appreciated from the following alternative form of Eq. (3) which can be obtained by expressing $q(x)$ and $q^*(x)$ in Eq. (3) via their Fourier transforms:

$$\hat{I}_R(u) = \int \exp(-i2\pi\,\lambda RuU)\,\hat{q}(U+u/2)\;\;\hat{q}^*(U-u/2)\;\; dU. \tag{6}$$

It is obvious from Eq. (6) that if $|u| > 2U_{\max}$, then, for any U either $\hat{q}(U+u/2) = 0$ or $\hat{q}^*(U-u/2) = 0$, and so $\hat{I}_R(u) = 0$.

It can be easily shown that when $u_{\max} = \infty$, then Eq. (4) implies that $\varphi(x) = C + \Delta\varphi(x)$, where C is a constant and $\Delta\varphi(x) = O(\varepsilon)$ for all x (if $q(x) \equiv 1$ for $|x| \geq X_{\max}$, then $C = 0$).

Eq. (4) is used to approximate Eq. (3) with the help of the identity $\exp(\varepsilon) = 1 + \varepsilon + O\left(\varepsilon^2\right)$ applied to the phase:

$$\begin{aligned}\hat{I}_R(u) &= \int \exp(i2\pi\, ux)\, a(x+\lambda Ru/2)\;\; a(x-\lambda Ru/2) \\ &\quad\times \left[1 + i\varphi(x+\lambda Ru/2) - i\varphi(x-\lambda Ru/2)\right]\; dx + O\left(\varepsilon^2\right) \\ &= \hat{I}_R^{(0)}(u) + \hat{I}_R^{(+)}(u) + \hat{I}_R^{(-)}(u) + O\left(\varepsilon^2\right),\end{aligned} \tag{7}$$

[1] It could be more appropriate to call this quantity "attenuation", rather than "absorption", as it usually also includes various scattering processes that lead to the reduction in the number of transmitted X-ray photons reaching the detector. We will use below the two terms interchangeably.

[2] This setup corresponds to a finite object surrounded by completely transparent media; a complementary configuration, where the object is placed inside a finite aperture in an opaque screen, can be considered similarly.

[3] Strictly speaking, in the considered situation $q(x)$ cannot be band-limited, so formally $U_{\max} = \infty$, and one should use the "essential support" [24] of $\hat{q}(u)$ in place of its true support. Note however that u_{sys} is always finite, as the spatial resolution of an imaging system cannot be infinitely fine.