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Alexander H. Barnett , Charles L. Epstein , Leslie Greengard , Jeremy Magland
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Geometry of the Phase Retrieval Problem

Recovering the phase of the Fourier transform is a ubiquitous problem in imaging applications from astronomy to nanoscale X-ray diffraction imaging. Despite the efforts of a multitude of scientists, from astronomers to mathematicians, there is as yet no satisfactory theoretical or algorithmic solution to this class of problems. Written for mathematicians, physicists, and engineers working in image analysis and reconstruction, this book introduces a conceptual, geometric framework for the analysis of these problems, leading to a deeper understanding of the essential, algorithmically independent, difficulty of their solutions. Using this framework, the book studies standard algorithms and a range of theoretical issues in phase retrieval and provides several new algorithms and approaches to these problems with the potential to improve the reconstructed images. The book is lavishly illustrated with the results of numerous numerical experiments that motivate the theoretical development and place it in the context of practical applications.

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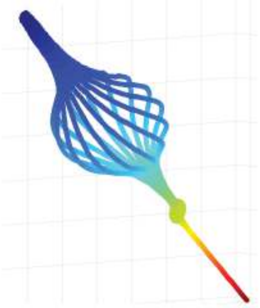

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Contents

Preface

Coherent diffraction imaging (CDI) is an experimental technique for determining the detailed structure of an object at the nanometer length scale. Coherent X-ray sources are used to illuminate the sample, and the scattered photons are captured in the far field on a detector array. In this regime, classical electromagnetic theory, in the Born approximation, shows that the measured intensity at each pixel in the detector is well approximated as the square of the modulus of the 3D Fourier transform, $|\widehat{\rho}(\boldsymbol{k})|^2$, of the X-ray scattering density, $\rho(\boldsymbol{x})$. Throughout this book we use the "mathematician's" convention for the $\boldsymbol{k}$ vector, in which exponentials take the form $e^{2\pi i\langle \boldsymbol{x},\boldsymbol{k}\rangle}$, rather than the "physicist's" convention, in which they are $e^{i\langle \boldsymbol{x},\boldsymbol{k}\rangle}$. With this convention the forward Fourier transform is defined by

$$\hat{\rho}(\boldsymbol{k}) = \mathscr{F}(\rho)(\boldsymbol{k}) \overset{d}{=} \int_{\mathbb{R}^d} \rho(\boldsymbol{x}) e^{-2\pi i\langle \boldsymbol{x},\boldsymbol{k}\rangle} d\boldsymbol{x}, \tag{1}$$

with inverse

$$\rho(\boldsymbol{x}) = \mathscr{F}^{-1}(\hat{\rho})(\boldsymbol{x}) \overset{d}{=} \int_{\mathbb{R}^d} \hat{\rho}(\boldsymbol{k}) e^{2\pi i\langle \boldsymbol{x},\boldsymbol{k}\rangle} d\boldsymbol{k}. \tag{2}$$

We assume that the illuminating light is a plane wave, $\boldsymbol{A}e^{2\pi i\langle \boldsymbol{x},\boldsymbol{p}_0\rangle}$, with wave vector $\boldsymbol{p}_0 = (0,0,p)$ in the above convention. If the detector array is oriented orthogonal to the illuminating light at a distance D downstream from the source, then the measured spatial frequency, $\boldsymbol{k}$, is related to the location of the measurement point $\boldsymbol{y} = (y_1, y_2, D)$ by the *Ewald Sphere* construction:

$$\boldsymbol{k} = p\left(\frac{\boldsymbol{y}}{\|\boldsymbol{y}\|} - (0,0,1)\right). \tag{3}$$

Here we assume that the experimental parameters are in the so-called Fraunhofer regime: D is much larger than R, the diameter of the support of ρ, and furthermore $\lambda D \gg R^2$, where $\lambda = 1/p$ is the wavelength. The maximum frequency component that is measured is determined by the frequency p, and the physical extent of the detector array. In particular, for small-angle scattering it is approximately p multiplied by the maximum scattering angle in radians.

In the small-angle limit, the Ewald sphere degenerates to a plane, and the 2D measurements lie on a 2D plane in $\boldsymbol{k}$-space, and thus, one has a 2D image reconstruction problem. Its solution is the x_3-axis projection of the 3D density function $\rho(\boldsymbol{x})$,

$$P[\rho](x_1, x_2) = \int_{-\infty}^{\infty} \rho(x_1, x_2, x_3) dx_3. \tag{4}$$

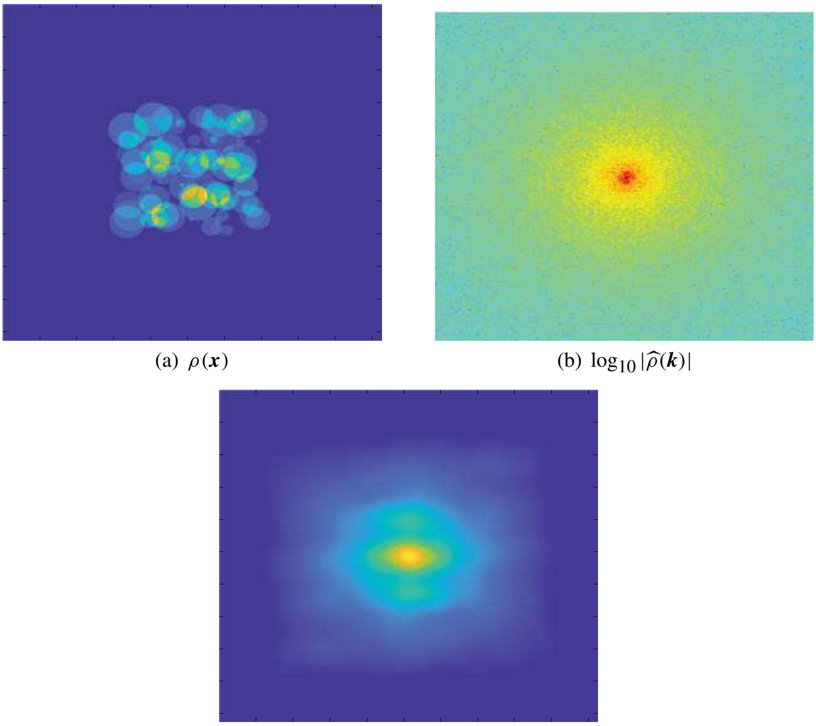
By rotating the object, in increments, about the x_1-axis, taking 2D measurements at each rotation angle, one may obtain samples of $|\rho(\boldsymbol{k})|^2$ thoughout a 3D volume. With this data one can then solve a phase retrieval problem to reconstruct the full 3D "image," $\rho(\boldsymbol{x})$. Since both $d = 2$ and $d = 3$ are of interest, d being the spatial dimension of the reconstruction, for much of the theory in this book, d is left general.

CDI is referred to as a "lensless" imaging modality, as there are no focusing optics involved. The full set of measurements is usually called a *diffraction pattern*. We assume that it is measured on (or interpolated to) a regular grid. Figures 1[a,b] show a synthetic 2D object of the sort used for numerical experiments in this book, and the diffraction pattern it would generate in the far field. The recent book, *X-Ray Microscopy* by Chris Jacobsen (Jacobsen 2019), is an excellent reference for the physics that underlie these imaging modalities and the techniques used to reconstruct images.

The measurement of $|\hat{\rho}(\boldsymbol{k})|^2$ allows for a direct reconstruction of a (band-limited) version of the autocorrelation function

$$\rho \star \rho(\boldsymbol{x}) = \int_{\mathbb{R}^3} \rho(\boldsymbol{y} + \boldsymbol{x}) \overline{\rho(\boldsymbol{y})} d\boldsymbol{y}, \tag{5}$$

as $\mathscr{F}(\rho \star \rho)(\boldsymbol{k}) = |\widehat{\rho}(\boldsymbol{k})|^2$. An example of an autocorrelation function is shown in Figure 1[c]. To reconstruct ρ itself, the phase of $\widehat{\rho}(\boldsymbol{k})$ must be "retrieved." *In principle*, this is usually possible for a compactly supported object, provided that $|\widehat{\rho}(\boldsymbol{k})|^2$ is sampled on a sufficiently fine grid relative to the size of the support of $\rho(\boldsymbol{x})$. As a practical matter, this has proved very difficult to do. The book that follows discusses the reasons that underlie this difficulty, which are largely geometric, and considers approaches to circumventing these problems. The research described herein is an unusual combination of pure mathematics and computer experimentation, without which the pure mathematics would not have been possible to do.



(a) $\rho(\boldsymbol{x})$ (b) $\log_{10}|\widehat{\rho}(\boldsymbol{k})|$ (c) $\rho \star \rho(\boldsymbol{x})$

Figure 1 A synthetic object, the (false-colored) diffraction pattern it produces, and its autocorrelation function.

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