Parameter retrieval methods in ptychography

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Abstract: We present a parameter retrieval method which combines ptychography and additional prior knowledge about the object. The proposed method is applied to two applications: (1) parameter retrieval of small particles from Fourier ptychographic dark field measurements; (2) parameter retrieval of a rectangular structure with real-space ptychography. The influence of Poisson noise is discussed in the second part of the paper. The Cramér Rao Lower Bound in both applications is computed and Monte Carlo analysis is used to verify the calculated lower bound. With the computation results we report the lower bound for various noise levels and the correlation of particles in Application 1. For Application 2 the correlation of parameters of the rectangular structure is discussed.

1. Introduction

Ptychography [1–6] is a scanning coherent diffraction imaging method for reconstructing a complex valued object function from intensity measurements recorded in the Fraunhofer or Fresnel diffraction region. In ptychography the object is partially illuminated multiple times with varying position of the illumination spot, so that the entire object is covered and adjacent illuminations partially overlap [7]. The technique provides a solution to the so-called ‘phase problem’ and is found to be very suitable for EUV [8,9] and X-ray imaging applications [10–13] due to its high fidelity and its minimum requirement on optical imaging elements. Moreover, abundant studies show that ptychography is able to provide a wide field-of-view and retrieve the illumination probe also [14,15]. During the last two decades, ptychography has been successfully demonstrated with X-ray radiation sources [11,16,17], electron beams [18] and visible light sources [19].

More recently, Fourier ptychographic microscopy [20,21] has been proposed, which can be regarded as an extension of ptychography [22]. The technique overcomes the resolution limit of conventional microscopy by enlarging the effective cut-off spatial frequency in the pupil plane. This is done by applying several plane wave illuminations to the sample. The detector is in the image conjugate to the sample plane, and each measurement corresponds to an individual incident angle of the illumination. With each tilted illumination, the diffraction pattern of the sample is shifted in the plane of the exit pupil of the lens, over the aperture used for imaging. Consecutive illumination tilts generate partially overlapping diffraction patterns within the aperture. With all of the Fourier ptychographic measurements, the spatial spectrum of the sample can be synthesized by using ptychographic algorithms while interchanging the real space and reciprocal space coordinates [23–25].

In general, the framework of real-space ptychography can be described as follows. Let \( \mathbf{r} \) and \( \mathbf{k} \) be 3D coordinates in real space and reciprocal space:

\[
\mathbf{r} = [x, y, z]^T = [r_\perp, z]^T, \quad \mathbf{k} = [k_x, k_y, k_z]^T = [k_\perp, k_z]^T.
\]  

(1)

and \( O(\mathbf{r}_\perp) \) the object transmission function. We use a laterally shifted probe, denoted by \( P(\mathbf{r}_\perp) \), to illuminate the object multiple times. For the \( j \)th illumination, the exit wave immediately
behind the object is:

$$\Psi_j(r_\perp) = P(r_\perp - R_{\perp,j}) \cdot O(r_\perp) = P_j(r_\perp) \cdot O(r_\perp),$$  \hspace{1cm} (2)

where $R_{\perp,j}$ specifies the shift of the $j$th illumination. The probe function is assumed to have a finite support with, for instance, a circular boundary:

$$P(r_\perp) = \begin{cases} P(r_\perp), & |r_\perp| \leq r_0, \\ 0, & |r_\perp| > r_0. \end{cases}$$  \hspace{1cm} (3)

For a detector located at distance $z$ in the far field, the diffraction intensity pattern $I_j(r')$ for the $j$th illumination is:

$$I_j(r'_\perp) = \left\{ \prod_j \Psi_j(r_\perp) \exp \left( \frac{-i2\pi r_\perp \cdot r'_\perp}{4z} \right) dr_\perp \right\}^2 = |\mathcal{F} (\Psi_j) (k'_\perp)|^2.$$  \hspace{1cm} (4)

where $\mathcal{F}$ is the Fourier transform operator. $r'_\perp$ is 2D coordinate in the detector plane. The relation between $r'_\perp$ and $k'_\perp$ is:

$$k'_\perp = 2\pi r'_\perp (4z)^{-1}.$$  

The task of ptychography is to find an estimate of the object which fits the given a priori knowledge, while a cost function $E$ is minimized. For the case of real-space ptychography, the a priori knowledge is the exact information of the probe function and the set of relative positions $R_j$.

The cost function $E$ is defined as the $l_2$-distance between the modulus of the far field diffraction pattern $|\mathcal{F} (\Psi_j) (k'_\perp)|$ and the square root of the measured intensity $I^m_j(k'_\perp)$:

$$E = \sum_j E_j = \sum_j \sum_{k'_\perp} \left( |\mathcal{F} (\Psi_j) (k'_\perp)| - |\sqrt{I^m_j(k'_\perp)}| \right)^2,$$  \hspace{1cm} (5)

where $N_x^{\det}$ and $N_y^{\det}$ are the number of pixels of the detector in $x$-axis and $y$-axis, respectively. One way to minimize $E$ is to use the gradient descent method. If we apply the gradient descent method to each $E_j$ sequentially, the algorithm is equivalent to the ptychography iterative engine (PIE) [5, 6]. Another popular choice is the difference map algorithm, which is formulated in terms of finding the intersection of two constraint sets [14, 26]. When the ptychographic measurements contain a relatively large amount of noise and hence the reconstruction is disrupted, one can utilize de-noising ptychographic algorithms to obtain a better image of the object. One of the most powerful and robust de-noising methods is the Maximum Likelihood estimation [23, 27–29], which requires the knowledge of the noise model.

The ptychographic measurement $I_j(k'_\perp)$ is commonly recorded by a 2D detector, e.g. a charge-coupled device (CCD). Therefore $k'_\perp$ is a discretized grid and is meshed according to the distance $z$ and the size of pixel of the detector. The retrieved object function, denoted by $\hat{O}$, is also on a discretized grid $r_\perp$. $r_\perp$ and $k'_\perp$ have the relation:

$$[\Delta x, \Delta y]^T = 2\pi \left( (N_x^{\det} \Delta k'_x)^{-1}, (N_y^{\det} \Delta k'_y)^{-1} \right)^T,$$  \hspace{1cm} (6)

where $\Delta x$ and $\Delta y$ are the spacing of a single grid cell in $x$-axis and $y$-axis, respectively, and $\Delta k'_x$ and $\Delta k'_y$ are the spacing of a grid cell in $k_x$ and $k_y$, respectively. Note that the total field-of-view (FoV) in the object plane is:

$$\text{FoV} = [N_x \Delta x, N_y \Delta y]^T,$$  \hspace{1cm} (7)

where $N_x > N_x^{\det}$ and $N_y > N_y^{\det}$ due to that ptychography is a scanning imaging technique which provides an extended FoV. In line with this extended FoV, we have the effective spacing of the grid cell in the reciprocal space:

$$[\Delta k_x, \Delta k_y]^T = \left( (N_x)^{-1} N_x^{\det} \Delta k'_x, (N_y)^{-1} N_y^{\det} \Delta k'_y \right)^T.$$  \hspace{1cm} (8)
We can see that, when the influence of noise is negligible, the relation given in Eq. (6) imposes a resolution limit to the reconstruction in ptychography. To overcome this limit, many 'superresolution' methods have been proposed [30–32]. One of the ideas lying behind these methods is to impose additional a priori knowledge about the object, e.g. analytical continuity or sparsity, to the algorithm. In this paper we show a parameter retrieval algorithm which combines ptychography and additional a priori knowledge about the object. We present this algorithm by numerically demonstrating two applications:

1. Parameter retrieval of sub-wavelength particles using Fourier ptychography with dark field measurements only. For this example the configuration is in line with the 'RapidNano' particle scanner developed by TNO [33, 34]. The particle scanner is supposed to detect nano-particles on an EUV reticle. Since only darkfield images are recorded in the scanner, the part of the spatial spectrum of the object in the neighborhood of $|k_\perp| = 0$ is lost. The missing data can in principle be filled in by analytic continuation using the fact that the object has bounded support, however, this method is highly unstable and leads in practice to incorrect reconstructions. However, as shown in Section 2, the proposed parameter retrieval algorithm is able to extract information of sub-wavelength particles from the incomplete data.

2. Parameter retrieval of rectangular objects using real-space ptychography. This example can also be applied to the metrology of EUV reticles [35, 36]. We demonstrate the proposed parameter retrieval method for this application in Section 3.

To study the influence of Poisson noise on the proposed parameter retrieval scheme, we compute the Cramér Rao Lower Bound (CRLB) and perform Monte Carlo analysis for both two applications in the second part of this paper. We derive the general form of the Fisher information matrix in Section 4. For application 1, the calculated CRLB and Monte Carlo result are shown in Section 5. For Application 2, the discussion about the correlation of the parameters of the rectangular structure can be found in Section 6.

2. Application 1: parameter retrieval of sub-wavelength particles using Fourier ptychography with dark field measurement

2.1. Description of the 'RapidNano 3' particle scanner

The 'RapidNano 3' particle scanner [33, 34] is designed to detect small dielectric particles on a flat uniform substrate. The particles are made of polystyrene latex (PSL) beads and the typical diameter of the particle is $\sim 50\,nm$. The scanner has a lower detection limit of 42 nm PSL particles, i.e. the capture rate is 95% at this size. Note that the particles on the substrate can be any material and PSL is only the calibration standard. The substrate is reflective, made of silicon, and its lateral size can be up to 6x6 inch, i.e. the size of an (EUV) mask. The illumination is a 532nm, $p$-polarized, fully coherent plane wave laser beam. The incident angle of the illumination is 60 degree, with 9 regularly distributed azimuth incident directions around 360 degree. The NA of the objective lens is 0.4, therefore the measurement is a dark field image of the sample as is illustrated in Fig. 1.

2.2. Single dipole radiation

Considering that the diameter of the detected particles is around 10 times smaller than the illumination wavelength, we begin by using dipole radiation formula to model the wavefield scattered by the particles. Suppose that there are $N$ dipoles in the plane $z = 0$, and the $i$th oscillating dipole is located at position $\mathbf{r}_i = [r_{\perp}, 0]^T$, $i = 1, 2, \cdots, N$, and is excited by an
The electric field at the exit pupil is given by:

\[ E_{\text{exit}} = A e^{i k_y r} \hat{e}_p(k_j) = A e^{i k_y r \hat{e}_p(k_j)}, \]  

(9)

where \( A \) is the illumination power. \( \hat{e}_p(k_j) \) denotes the polarization direction.

For the \( i \)th dipole with position \( r_{i,j} \), we denote the dipole moment by:

\[ p_{i,j} = 4 \pi \varepsilon_0 \alpha_i E_{\text{in},j} = 4 \pi \varepsilon_0 \alpha_i A e^{i k_y r \hat{e}_p(k_j)}, \]  

(10)

where \( \varepsilon_0 \) is the permittivity of free space and \( \alpha_i \) is the polarisability of the particle. For a dielectric sphere with diameter \( d \), the dipole moment \( p^\text{sphere}_{i,j} \) in the quasi-static approximation is given by:

\[ p^\text{sphere}_{i,j} = 4 \pi \varepsilon_0 \left( \frac{\varepsilon_r - 2}{\varepsilon_r + 1} \right) d_i^2 E_{\text{in},j}, \]  

(11)

where \( \varepsilon_r = n_{\text{PSL}}^2 \) is the relative permittivity of the dielectric. \( n_{\text{PSL}} \) is the refractive index of the small particles. Since the real part of \( n_{\text{PSL}} \) is \( \sim 10^6 \) times larger than the imaginary part, i.e. than the absorption index, we assume the \( \alpha_i \) is real valued for the rest of this paper. We see that \( \alpha_i \) is proportional to the volume of the dielectric particle.

The electric field radiating from the \( i \)th dipole due to the \( j \)th illumination is given by [37, 38]:

\[ E_{\text{scat},i,j} = \frac{k^2}{4 \pi \varepsilon_0} \leftrightarrow G (r, r_i) p_{i,j}, \]  

(12)

where \( \leftrightarrow G (r, r_i) \) is the dyadic GreenâĂŹs function:

\[ \leftrightarrow G (r, r_i) = \left( \begin{array}{c} \leftrightarrow 1 + \frac{1}{k^2 \nabla \nabla} \end{array} \right) e^{i k |r - r_i|} \frac{|r - r_i|}{|r - r_i|}, \]  

(13)

where \( \leftrightarrow 1 \) is the \( 3 \times 3 \) identity matrix. Considering that the detector of the particle scanner is insensitive to the polarization state and that the NA of the objective lens is 0.4, we ignore the effect of the polarization of the wavefield for simplicity. Hence we arrive at a scalar scattered amplitude given by:

\[ E_{\text{scat},i,j} = A k^2 \alpha_i e^{i k_y r \hat{e}_p(k_j)} G (r, r_i), \]  

(14)

where

\[ G (r, r_i) = \frac{e^{i k |r - r_i|}}{|r - r_i|}. \]  

(15)

2.3. dark field measurement from the particle scanner

By Fourier transforming Eq. (14) with respect to \( r_{\perp} \), we have:

\[ \mathcal{F} (E_{\text{scat},i,j}) (k_{\perp}, z) = A k^2 \frac{e^{i k_z |z|}}{2i k_z} \alpha_i e^{-i r_{\perp} \cdot (k_{\perp} - k_{i,j})}. \]  

(16)

\( \mathcal{F} (E_{\text{scat},i,j}) \) can be regarded as the 2D spatial spectrum of the scattered wavefield in the plane \( z \). The electric field at the exit pupil is given by:

\[ \mathcal{F} (E_{\text{scat},i,j})_{\text{exit}} (k_{\perp}, z) = I_{\text{NA}}(k_{\perp}) A k^2 \frac{e^{i k_z |z|}}{2i k_z} \alpha_i e^{-i r_{\perp} \cdot (k_{\perp} - k_{i,j})}, \]  

(17)
where $1_{\text{NA}}(\mathbf{k}_\perp)$ represents the numerical aperture of the objective lens:

$$1_{\text{NA}}(\mathbf{k}_\perp) = \begin{cases} 1, & |\mathbf{k}_\perp| \leq \text{NA}, \\ 0, & |\mathbf{k}_\perp| > \text{NA}. \end{cases} \quad (18)$$

By summing over all the dipoles, we find the total field in the exit pupil, which is denoted by $\Psi_j$:

$$\Psi_j(\mathbf{k}_\perp, z) = \sum_i \mathcal{F}\left( E_{\text{scat},i,j} \right)_{\text{exit}}(\mathbf{k}_\perp, z)$$

$$= 1_{\text{NA}}(\mathbf{k}_\perp)Ak^2 \frac{e^{ik_z|z|}}{2ik_z} \sum_i \alpha_i e^{-i\mathbf{r}_{\perp,i} \cdot (\mathbf{k}_\perp - \mathbf{k}_{\perp,j})}$$

$$= Q(\mathbf{k}_\perp, z) \cdot O(\mathbf{k}_\perp - \mathbf{k}_{\perp,j}), \quad (19)$$

where

$$Q(\mathbf{k}_\perp, z) = 1_{\text{NA}}(\mathbf{k}_\perp)Ak^2 \frac{e^{ik_z|z|}}{2ik_z}, \quad (20)$$

and $O(\mathbf{k}_\perp)$ is the Fourier transform of the object defined by

$$O(\mathbf{k}_\perp) = \sum_i \alpha_i e^{-i\mathbf{k}_\perp \cdot \mathbf{r}_{\perp,i}}. \quad (21)$$

Note that the object function is assumed to be independent of the angle of incidence, i.e. the only effect of the tilted illumination is the shift of the object function over the pupil plane. Finally, by inverse Fourier transforming $\Psi_j$ and taking the squared modulus, we arrive at the expression for the measured intensity in the detector plane:

$$I_j(\mathbf{r}'_\perp, z) = \left| \mathcal{F}^{-1}(\Psi_j) \right|^2(\mathbf{r}'_\perp, z)$$

$$= \left| \mathcal{F}^{-1} \left[ Q(\mathbf{k}_\perp + \mathbf{k}_{\perp,j}, z) \cdot O(\mathbf{k}_\perp) \right] \right|^2(\mathbf{r}'_\perp, z), \quad (22)$$

where $\mathbf{r}'_\perp$ is the 2D regular grid.

![Fig. 1. Graphical illustration of $O(\mathbf{k}_\perp)$. (a) the blue disk is defined by $1_{\text{NA}}(\mathbf{k}_\perp)$ and indicates information about $O$ included in the single measurement $I_j(\mathbf{r}'_\perp, z)$. (b) the retrievable part of $O$ from all given dark field measurements.](image-url)
For the configuration of the particle scanner, $|k_{\perp,l}|$ is fixed and equal to $k \sin(\frac{\pi}{2})$. The NA of the objective lens is $\sim 0.4$. Therefore, the intensity measurements do not contain any information about $O(k_l = 0)$ and its surrounding region, as shown in Fig. 1. The blue shaded area in Fig. 1(a) illustrates the information about $O(k_l)$ included in the single measurement $I_j(r_{\perp}^j, z)$, while the blue shaded area in Fig. 1(b) represents the retrievable information from all measurements. We denote this retrievable part of $O$ by $1_\Omega O(k_{\perp})$, where $\Omega$ is the blue shaded region in Fig. 1(b).

2.4. Retrieving the parameters of the particles

To retrieve $\alpha_i$ and the position $r_{\perp,l}$ of the dipoles, we first reconstruct the complex valued function $1_\Omega O(k_{\perp})$ in the pupil plane from the set of intensity measurements $I_j(r_{\perp}^j)$. This can be done by applying a ptychographic algorithm. We use $1_\Omega \hat{O}(k_{\perp})$ to denote the reconstruction obtained by the ptychographic method.

Once $1_\Omega \hat{O}(k_{\perp})$ is obtained, we apply the method of least square to estimate $\alpha_i$ and $r_{\perp,l}$ of all dipoles. The number of freedom in this problem is $N \times 3$, where $N$ is the number of dipoles within the field-of-view (FoV). Note that if $\alpha_i$ is complex valued, the number of freedom should be $N \times 4$. When $N$ is in the order of $10^3 \sim 10^4$, we have much less degrees of freedom than in the traditional Fourier ptychography problem.

Our proposed parameter retrieval algorithm is shown in the following.

1. Use a ptychographic algorithm to retrieve the complex valued wavefield $1_\Omega O(k_{\perp})$ in the pupil plane.

2. From all the dark field intensity measurements, find the lower and upper bound of $\alpha_i$ and $r_{\perp,l}$ for $i = 1, 2, \cdots, N$. These bounds are denoted by: $\alpha_i^l$, $\alpha_i^u$, $r_{\perp,l}^l$, and $r_{\perp,l}^u$.

3. Solve the following problem:

$$\arg \min_{\alpha_i,r_{\perp,l}} \left\| 1_\Omega \hat{O}(k_{\perp}) - \sum_{k_l \in \Omega} e^{-i k_l \cdot r_{\perp,l}} \right\|^2,$$

subject to $\alpha_i^l \leq \alpha_i \leq \alpha_i^u$, $i = 1, 2, \cdots, N$, $r_{\perp,l}^l \leq r_{\perp,l} \leq r_{\perp,l}^u$, $i = 1, 2, \cdots, N$, \hspace{1cm} (23)

where $\preceq$ denotes vector inequality: $r_{\perp}^l \preceq r_{\perp}^u$ means $x^l \leq x^u$ and $y^l \leq y^u$.

2.5. Simulation

To validate the proposed parameter retrieval algorithm, a preliminary simulation is reported in this section. The configuration is drawn in Fig. 2 and the parameter settings of the setup is described in Table 1. Since the NA of the imaging system is smaller than $|k_{\perp,l}|$, the measurements at the detector plane are always dark field images. We assume that the detector is insensitive to the polarization state of the wavefield.

The simulated sample consists of two dipoles. The actual scattering strength $\alpha_i$ and the position $r_{\perp,l}$ of the dipoles are listed in Table 2. Based on these given parameters, we first construct the actual complex valued function $1_\Omega O(k_{\perp})$ according to Eq. (21). The dark field intensity measurements are noise-free and computed in accordance with Eq. (22). In line with the $1^{st}$ step of the proposed method given in Section 1.4, the reconstructed object function, denoted by $1_\Omega \hat{O}(k_{\perp})$, is obtained by applying the Fourier ptychography method. We assume that the function $Q(k_{\perp, + k_{\perp,l}, z})$ is known and we ignore the polarization state. In the simulation we notice that only 9 incident plane waves cannot provide sufficient data redundancy. Instead we use 36 plane waves with regularly distributed azimuth incident directions around 360 degrees in this simulation. The actual function $O$ and the reconstructed one are shown in Fig. 3(a) and
Fig. 2. Illustration of the setup of Application 1. The incident angle of the illumination is 60 degree, with multiple azimuth incident directions around 360 degree.

| illumination | imaging system |
|--------------|----------------|
| wavelength   | NA             |
| incident angle| magnification  |
| 500 nm       | 0.4            |
| 60 degree    | 20             |

Table 1. Configuration settings in the simulation

- detector
  - pixel size: 5 µm
  - pixel number: 200 x 200
  - FoV: 50 µm
  - grid spacing in object plane: 133.3 nm

Fig. 3(b), respectively. Fig. 3(c) illustrates the illuminated area in the reciprocal space, i.e. $\sum_j I_{\Delta A}(k_\perp + k_{\perp,j})$, for 9 and 36 dark field measurements, respectively.

Fig. 3. (a) The amplitude and phase of the actual complex function $I_{O}(k_\perp)$. (b) The amplitude and phase of $I_{O}(k_\perp)$ which is reconstructed from the Fourier ptychographic algorithm. (c) Illustration of the illuminated area in the reciprocal space, i.e. $\sum_j I_{\Delta A}(k_\perp + k_{\perp,j})$, for 9 and 36 dark field measurements, respectively.

In Fig. 4(a) we show the incoherent sum of all 36 simulated noise-free intensity measurements, i.e. $\sum_j I_j(r'_0)$, and in Fig. 4(b) we present the squared amplitude of the scattered field from the
The incoherent sum of all 36 dark field measurements, i.e. \( \sum_j I_j(r'_\perp) \). (b) The amplitude of scattering wavefield at plane \( z \to 0 \), i.e. \( |\mathcal{F}^{-1}(\Omega\hat{O})(r_\perp)|^2 \), which is reconstructed with the Fourier ptychography method. The inserted graphs correspond to the dipole \( i = 1 \).

Sample at plane \( z \to 0 \), i.e. \( |\mathcal{F}^{-1}(\Omega\hat{O})(r_\perp)|^2 \). For Application 1 the spacing of grid \( r'_\perp \) and \( r'_{\perp,i} \) fulfills:

\[
[\Delta x, \Delta y]^T = \left[(N_x)^{-1}N_{\text{det}}x', (N_y)^{-1}N_{\text{det}}y' \right]^T,
\]

which can be derived from Eq. (8) by interchanging the real space and reciprocal space coordinates. The inserted graphs in Fig. 4 correspond to the dipole of \( i = 1 \). In line with Table 1, every dark field measurement is a 200 \( \times \) 200 array of with a 250\( \text{nm} \) pixel size. The reconstructed scattered field shown in Fig. 4(b) only contains information of \( k_\perp \in \Omega \). The side-lobe appears in the neighborhood of the particles in Fig. 4(b) is due to the fact that the reconstruction is convoluted by \( \mathcal{F}^{-1}(\Omega\hat{O})(r_\perp) \). Without knowing the wavefield at \( k_\perp = 0 \) and its surrounding region or without considering any prior information about the sample, the reconstructed scattering field cannot provide a unique physical solution.

Once \( \Omega\hat{O}(k_\perp) \) is obtained, we retrieve \( \alpha_i \) and \( r_{\perp,i} \) by minimizing the least square function given in Eq. (23). This is done by using the ‘fmincon’ solver in MATLAB. To facilitate the solver to find the global minimum, a proper starting search point and a set of bounds for \( \alpha_i \) and \( r_{\perp,i} \) are needed. From Fig. 4 we see that one can deduce a guess about the scattering strength and the position of the dipoles from the dark field measurements. Based on the guess we can obtain the starting point and the bounds. The accuracy of the guess of the position is limited by the pixel size of the detector. In the simulation we use a random number generator to create a starting search point which is close to the actual parameters. The starting point of all parameters are shown in Table 2. The retrieved parameters are listed in the most right column of the same table.

| \( \alpha_1/(\lambda^3) \) | actual value | initial guess | retrieved value |
|--------------------------|--------------|---------------|-----------------|
| \( \alpha_2/(\lambda^3) \) | 1.000 \( \times \) 10\(^{-3} \) | 1.195 \( \times \) 10\(^{-3} \) | 1.000 \( \times \) 10\(^{-3} \) |
| \( x_1 \) | \(-8.333 \text{ \( \mu m \)} \) | \(-8.349 \text{ \( \mu m \)} \) | \(-8.333 \text{ \( \mu m \)} \) |
| \( y_1 \) | \(0.000 \text{ \( \mu m \)} \) | \(0.113 \text{ \( \mu m \)} \) | \(0.000 \text{ \( \mu m \)} \) |
| \( \alpha_2/(\lambda^3) \) | 0.512 \( \times \) 10\(^{-3} \) | 0.329 \( \times \) 10\(^{-3} \) | 0.512 \( \times \) 10\(^{-3} \) |
| \( x_2 \) | 8.356 \( \mu m \) | 8.327 \( \mu m \) | 8.356 \( \mu m \) |
| \( y_2 \) | 0.088 \( \mu m \) | \(-0.029 \text{ \( \mu m \)} \) | 0.088 \( \mu m \) |
3. Application 2: parameter retrieval of a rectangular object using real-space ptychography

3.1. Single object embedded in constant surrounding

Now we consider a real-space ptychography setup as shown in Fig. 5. The object can be written in the following form:

\[ O(\mathbf{r}_\perp)(A_1, \phi_1, a_1, b_1, \mathbf{r}_{\perp,1}) = 1 + \left(A_1 e^{i\phi_1} - 1\right) \Pi_{a_1, b_1}(\mathbf{r}_\perp - \mathbf{r}_{\perp,1}) \]

where \( C_1 \) is a complex valued coefficient and \( \Pi_{a_1, b_1}(\mathbf{r}_\perp - \mathbf{r}_{\perp,1}) \) is the 2D rectangular function defined by parameters:

\[ \Pi_{a_1, b_1}(\mathbf{r}_\perp - \mathbf{r}_{\perp,1}) = \Pi_{a_1}(x - x_1) \Pi_{b_1}(y - y_1) = \begin{cases} 0, & |x - x_1| > \frac{a_1}{2} \text{ or } |y - y_1| > \frac{b_1}{2}, \\ 1, & |x - x_1| < \frac{a_1}{2} \text{ and } |y - y_1| < \frac{b_1}{2}. \end{cases} \]  

(26)

where we leave the values of the function at \( x = x_1 \pm \frac{a_1}{2} \) and \( y = y_1 \pm \frac{b_1}{2} \) be undefined because these values cannot be retrieved under the thin object approximation.

We aim to retrieve the parameters:

\[ \Theta = [A_1, \phi_1, a_1, b_1, \mathbf{r}_{\perp,1}]^T, \text{ where: } A_1 \in (0, 1], \; a_1 > 0, \; b_1 > 0. \]  

(27)

The diffracted wavefield in the far field for the \( j \)th illumination is:

\[ \mathcal{F} \{ \Psi_j(\mathbf{k}_\perp') \} = \mathcal{F} \{ P_j(\mathbf{k}_\perp) \} + \mathcal{F} \{ P_j(\mathbf{k}_\perp') \} \ast \left[ C_1 a_1 b_1 \sin \left( \frac{a_1 k_x}{2} \left( \frac{b_1 k_y}{2} \right) \right) e^{i\mathbf{k}' \cdot \mathbf{r}_{\perp,1}} \right]. \]

(28)

where \( \ast \) denotes convolution.

3.2. Retrieving the parameter of the rectangle

We can see in Eq. (28) that, when we have the exact knowledge of the probe, the diffraction pattern is a function of the of the rectangular. This fact offers us the chance to retrieve these parameters from the measurements \( I_j(\mathbf{k}_\perp') \) for all \( j \). In this section we propose and validate a feasible method to retrieve the parameter from ptychographic measurement.
The first step of the proposed method is to reconstruct the object function in real space, denoted by: \( \hat{O}(a_1, x_1) \), from \( I_j(k_{1j}') \) for all \( j \). This can be done by applying the PIE [4,5] algorithm or other ptychography algorithms [14,29,39,40]. Note that the discretization of \( r_\perp \) and \( k_{1j}' \) follows Eq. (6). For noisy measurement, one may use the Maximum Likelihood estimator (MLE) if one can find a dominant noise model [27,28]. For the case of Poisson noise, we can apply gradient descent methods [41,42] to minimize the likelihood function \( L \) given by Eq. (S7) in the Supplementary.

Once the minimum of the likelihood function is found, we can compute the Fourier transform of the reconstructed object, denoted by \( \mathcal{F}(\hat{O})(k_{\perp}) \). The spacing of grid \( r_\perp \) and \( k_{\perp} \) is given in Eq. (8). The parameter of the rectangular can be retrieved by minimizing a cost function \( G \) defined by:

\[
G = \left\| \mathcal{F} \left( \hat{O} \right) - C_1 a_1 b_1 \text{sinc} \left( \frac{a_1 k_x}{2}, \frac{b_1 k_y}{2} \right) e^{i k_{\perp} r_\perp} \right\|^2,
\]

where \( \| \cdot \|^2 \) denotes the \( l_2 \) norm. To give an example about the relation between \( G \) and the rectangular parameters, we show in Fig. 7 the value of \( G \) as a function of \( a_1 \) and \( x_1 \). The configuration parameter of Fig. 7 will be given later in Section 4.2. It is seen that \( G \) is convex in the neighborhood of the actual \( a_1 \) and \( x_1 \), which offers us the chance to retrieve the parameter by minimizing \( G \). In order to find the minimum of \( G \), it will be beneficial to start the algorithm from a point closed to the actual parameter. This starting point can be determined from \( \hat{O}(r) \).

In summary, our proposed method includes the following steps:

(1) Use ptychographic algorithm to retrieve the complex valued wavefield \( \hat{O}(r_\perp) \).

(2) Find the lower and upper bound \( \Theta \) from \( \hat{O}(r_\perp) \). \( \Theta \) is the parameter vector defined by Eq. (27). These bounds are denoted by: \( \Theta_l \) and \( \Theta_u \).

(3) Solve the following problem:

\[
\arg \min_{\Theta} G, \quad \text{subject to } \Theta_l \leq \Theta \leq \Theta_u.
\]

3.3. Simulation

To validate our proposed method, a preliminary simulation is shown. We consider the setup as shown in Fig. 5. Details of the configuration are shown in Table 3. The Fresnel number of this configuration is 0.0014. According to Eq. (28), we first generate the complex value wavefield in Fourier space \( \mathcal{F}(\Psi_j')(k_{1j}') \) based on the given probe and object. The Fourier transform of the object function \( \mathcal{F}(\hat{O})(k_{\perp}) \) is illustrated in Fig. 6(a). The object consists of one rectangular and its actual parameters can be found in Table 4. Fig. 6(b) shows the normalized amplitude and the phase of the probe. In this simulation we assume the probe is known and the ptychographic measurement is noise-free. In Fig. 6(c) we illustrate the Fourier transform of the reconstructed object function \( \mathcal{F}(\hat{O})(k_{\perp}) \). The inverse Fourier transform of \( \mathcal{F}(\hat{O})(k_{\perp}) \) is illustrated in Fig. 6(d).

After we obtained \( \mathcal{F}(\hat{O})(k) \), we can retrieve the parameters of the rectangular by solving optimization problem in Eq. (30). In Fig. 7 we demonstrate the evaluation of the cost function \( \mathcal{E} \) with respect to \( a_1 \) and \( x_1 \), which are the width and position of the rectangular in \( x \)-axis. The orange arrow in both plots point to the actual value of \( a_1 \) and \( x_1 \). We see in Fig. 7 that it is possible to accurately retrieve the value of \( a_1 \) and \( x_1 \) by minimizing \( \mathcal{E} \). To compute the solution of the problem in Eq. (30), we again implemented the 'fmincon' solver in MATLAB. The actual value of the parameters, the starting search point and the retrieved results are presented in Table 4. We can see that the proposed method can successfully retrieve the rectangular parameters.
Table 3. The characteristic parameters of the configuration in the simulation

|       | probe   | grid size | grid spacing | wavelength | scanning grid | overlap ratio | radius of circular support |
|-------|---------|-----------|--------------|------------|---------------|-----------------|-----------------------------|
|       | 60 × 60 | 30 nm     | 30 nm        | 5 × 5      | 75%           | 0.45 µm        |                             |
| object| grid size | 90 × 90   | 30 nm        | detector   | pixel number  | pixel size     | propagation distance       |
|       | 60 × 60 | 50 µm     | 1.88 cm      |            |               |                 |                             |

![Fig. 6](image)

Fig. 6. (a) The simulated object in Fourier space. The object has one rectangular which is embedded in constant surrounding. (b) The normalized amplitude and the phase of the probe, which is known in the simulation. (c) The retrieved object function in Fourier space from ptychographic measurement. (d) The inverse Fourier transform of \( F(\hat{O})(k_\perp) \).

![Fig. 7](image)

Fig. 7. The evaluation of \( E \) with respect to \( a_1 \) and \( x_1 \). The value of \( E \) is normalized to its maximum in both plots. The orange arrow points to the actual value of \( a_1 \) and \( x_1 \) in this simulation.

4. The CRLB analysis of the parameter retrieval scheme for Poisson noise

In estimation theory, the Cramér Rao Lower Bound (CRLB) gives a lower bound on the variance of any unbiased estimator for a parameter that is to be estimated. The estimators that can reach the lower bound are called the minimum variance unbiased estimators. Minimum variance unbiased estimators are often not available [43, 44]. To find the CRLB, one needs to compute the Fisher information matrix which is the expectation of the second order derivative of the
Table 4. Retrieved parameters of one rectangular

|         | \(a_1/\lambda\) | \(b_1/\lambda\) | \(x_1/\lambda\) | \(y_1/\lambda\) | \(A_1\) | \(\phi_1\) |
|---------|-----------------|-----------------|-----------------|-----------------|--------|----------|
| initial guess | 11.00 | 28.00 | 4.00 | 3.00 | 0.73 | 3.17 |
| actual value | 11.46 | 25.99 | 5.71 | 1.42 | 0.70 | 3.14 |
| retrieved value | 11.46 | 25.99 | 5.71 | 1.42 | 0.70 | 3.14 |

likelihood function. Detailed description about CRLB, Fisher information matrix and Maximum Likelihood Estimation is given in Section 1.A of Supplementary.

In this paper we study the CRLB for Poisson distributed photon counting noise, which is the most dominant source of noise which occurs even under the best experimental conditions [27,28]. The expectation of the second order derivative of the Poisson likelihood function can be found in Section 1.B of Supplementary.

5. The CRLB analysis of Application 1

5.1. The Fisher information matrix for retrieval a single dipole

Now we calculate the Fisher matrix for the \(i\)th dipole. According to Eq. (23), the parameters we aim to estimate are:

\[
\Theta = [\theta_1, \theta_2, \ldots, \theta_N]^T = [\alpha_1, x_1, y_1, \alpha_2, x_2, y_2, \ldots, \alpha_N, x_N, y_N]^T.
\]

We consider that we aim to retrieve the parameters of the \(i\)th dipole while assuming that the parameters of all other dipoles are known. To find the Fisher matrix, we need to calculate the derivative of \(I_j\) with respect to the parameters of dipole \(i\). The derivatives of \(I_j\) are given in Section 1.C of Supplementary. For Application 1, we have the Fisher matrix with elements:

\[
I_F^{\text{dip}} = \begin{bmatrix} I_{F,\alpha_i,\alpha_i} & I_{F,\alpha_i,\alpha_j} \\ I_{F,\alpha_j,\alpha_i} & I_{F,\alpha_j,\alpha_j} \end{bmatrix},
\]

where:

\[
I_{F,\alpha_i,\alpha_i}^{\text{dip}} = \frac{2}{\hbar\omega} \sum_{r_{i,j}} \left| F^{-1}(\psi_{i,j}) \right|^2 \frac{\partial}{\partial \alpha_i^2} + \Re \left( F^{-1}(\psi_j)^\ast \left[ F^{-1}(\psi_{i,j}) \right]^2 \right),
\]

\[
I_{F,\alpha_i,\alpha_j}^{\text{dip}} = \frac{2}{\hbar\omega} \sum_{r_{i,j}} \left| \nabla_{r_{i,j}} F^{-1}(\psi_{i,j}) \right|^2 + \Re \left( F^{-1}(\psi_j)^\ast \nabla_{r_{i,j}} F^{-1}(\psi_{i,j}) \right). \]

It is of interest to first study the diagonal terms in \(I_F\). For instance, suppose that we have exact knowledge about the dipole’s position and illumination power, then \((I_{F,\alpha_i,\alpha_i}^{\text{dip}})^{-1}\) is the CRLB of \(\alpha_i\) for any unbiased estimator. When only one dipole exists in the sample, the diagonal terms in \(I_F^{\text{dip}}\) can be re-written as:

\[
I_{F,\alpha_i,\alpha_i}^{\text{dip}} = \frac{4}{\hbar\omega} \sum_{r_{i,j}} \left| F^{-1}\left[ Q(k_\perp + k_{\perp,j}, z)e^{-ik_\perp r_{i,j}} \right] \right|^2,
\]

\[
I_{F,r_{i,j},r_{i,j}}^{\text{dip}} = \frac{4 |C|^2}{\hbar\omega} \sum_{r_{i,j}} \left| \frac{J_2(kN|\mathbf{r}'_\perp - \mathbf{r}_{\perp,i}|)}{|\mathbf{r}'_\perp - \mathbf{r}_{\perp,i}|^2} \right|^2.
\]
where $C$ is the complex valued constant:

$$C = \alpha_i A e^{i k z |z|^2}.$$

(37)

In Eq. (36) we used the following relation [45]:

$$\frac{d}{dx} \left( J_1(x) \right) = -\frac{J_2(x)}{x},$$

(38)

where $J_1$ and $J_2$ are the Bessel function of the first kind of order 1 and 2, respectively.

We can see in Eq. (35) that the CRLB of $\alpha_i$ is inversely proportional to the total illumination power $A^2$. Therefore, it is needed to enhance the illumination power to determine the value of $\alpha_i$ for smaller particles. However, when the illumination power is enhanced too much, one may reach a saturation point limited due to the dynamic range of the detector. Taking dark field images of the sample, as shown in Fig. (3), can avoid this limit. Furthermore, we observe that $I_{dip \perp i}$ does not only depend on the values of $A$ and $\alpha_i$, but also on the NA. Therefore, to decrease the CRLB of $r_{\perp i}$, one can increase the illumination power or the value of $\alpha_i$, or one can enlarge NA, or enhance both. It is interesting that $I_{dip \perp i}$ is not a function of $z$ nor of $k_{\perp i}$, which indicate that neither de-focusing nor adjusting the illumination’s incident angle can lead to any change of the CRLB of $r_{\perp i}$ for the case of a single particle.

When more than one particle are on the planer surface, we have to calculate the Fisher information by Eq. (33) and Eq. (34). We see from these equations that there is a correlation between the particles. Suppose there are two particles, then the CRLB of one of the particles is a function of the parameters of the other particle, as follows from the second term on the right-hand side of Eq. (33) and Eq. (34). A more detailed study of the cross-correlation is presented in the next section.

5.2. The CRLB of the dipole

We study the CRLB of the dipole strength and the position of the dipole along the $x$-axis. We follow the configuration as described in Fig. (3) and Table. 1. We first investigate the variance and the squared bias of parameters, $\alpha_1$ and $x_1$, of the dipole $i = 1$. To find the variance and bias for various noise levels, we define the illumination power by counting the time-averaged number of photons scattered by the dipole $i = 1$, which is given by:

$$P_{N_{dip}} = \left| \int \frac{F^{-1}}{\int_\Omega} \left( A k^2 e^{ikz|z|} \alpha_i e^{-i r_{\perp 1} \cdot k_i} \right) \right|^2_{i=1}.$$  

(39)

The variance and bias are obtained from Monte Carlo simulations. We generated 1000 Fourier ptychographic dark field data-sets for $P_{N_{dip}} = 10^4, 10^6, 10^8$. The parameters are reconstructed from the data-sets by applying the parameter retrieval algorithm described in Section 2.4. The variance and squared bias for $P_{N_{dip}} = 10^4, 10^6, 10^8$, are shown in Table. 5.

When $P_{N_{dip}} = 10^4$, we see that the variance of $x_1$ obtained from the retrieval method is 10 times larger than the squared bias. This variance-bias-ratio becomes higher when $P_{N_{dip}}$ is increased. This observation means that the retrieval method of $x_1$ is asymptotically unbiased when $P_{N_{dip}} > 10^4$. These variances are illustrated in Fig. 8, together with the computed CRLB. It is shown that the variance of the retrieval of $x_1$ is indeed bounded by the CRLB when $P_{N_{dip}} > 10^4$. The value of the bound is inversely proportional to the value of $P_{N_{dip}}$.

However, Table. 5 also shows that the variance of $\alpha_1$ obtained from the algorithm is much smaller than the squared bias when $P_{N_{dip}} < 10^6$, and indeed the retrieval algorithm of $\alpha_1$ is not unbiased as long as $P_{N_{dip}} < 10^8$ for the current setup. Therefore, the variance of the retrieved $\alpha_i$
Table 5. The variance and squared bias of $\alpha_i$ and $x_i$ of the dipole of $i = 1$ for different $PN_{\text{dip}}$, obtained from Monte Carlo result.

| $PN_{\text{dip}}$ | $10^4$   | $10^6$   | $10^8$   |
|-------------------|----------|----------|----------|
| $\text{Var} \left[ \alpha_{i=1} / (\lambda^3) \right]$ | $3.14 \times 10^{-12}$ | $2.54 \times 10^{-14}$ | $2.62 \times 10^{-16}$ |
| $\text{Bias} \left[ \alpha_{i=1} / (\lambda^3) \right]^2$ | $3.22 \times 10^{-10}$ | $1.03 \times 10^{-13}$ | $1.26 \times 10^{-17}$ |
| $\text{Var} \left[ x_{i=1} / \lambda \right]$ | $4.54 \times 10^{-6}$ | $4.28 \times 10^{-8}$ | $4.23 \times 10^{-10}$ |
| $\text{Bias} \left[ x_{i=1} / \lambda \right]^2$ | $4.32 \times 10^{-7}$ | $4.03 \times 10^{-11}$ | $1.89 \times 10^{-13}$ |

may not be bounded by the CRLB when $PN_{\text{dip}} < 10^8$. On the other hand, we can see in Eq. (14) that the accuracy of the reconstruction of $\alpha_i$ is not only influenced by the Poisson noise, but also by the the fluctuation of the illumination power $A$. That is, the uncertainty about the exact value of $A$ will lead to uncertainty of the retrieval of $\alpha_1$. Therefore, it is more difficult to determine $\alpha_1$ than the position with the current scheme.

![Fig. 8](image.png)

Fig. 8. (a) The computed CRLB and variance of $x_1$ of the dipole $i = 1$ for various $PN_{\text{dip}}$. (b) The computed CRLB and variance of $x_1$ for various values of $\alpha_2$, for the case of $PN_{\text{dip}} = 10^8$. The blue line of both plots are the computed CRLB and the red crosses show the variance obtained from Monte Carlo experiment.

5.3. The correlation between two dipoles

As has been noted in Section 5.1, when there are two particles on the surface, varying the parameters of one particle can lead to a change of the CRLB of the another particle. To verify this correlation between the particles, we calculated the CRLB of $x_1$ with various values of $\alpha_2$. The value of $PN_{\text{dip}}$ is chosen to be $10^8$ because the retrieval algorithm is asymptotically unbiased for this noise level, as has been shown in Section 5.2. The computed CRLB is validated by using Monte Carlo simulations, as illustrated in Fig. 8(b).

It is seen in Fig. 8(b) that one can lower the CRLB of $x_1$ obtained from the algorithm by enhancing the scattering power of the dipole $i = 2$. This observation can be understood by studying the property of the Poisson distribution. The signal-to-noise ratio (SNR) of Poisson noise is equal to $\sqrt{n(r_{\perp}')}$, where $n(r_{\perp}')$ is the number of photons detected by the pixel at $r_{\perp}'$. When the scattering power of particle $i = 1$ is fixed, $n(r_{\perp}')$ is increased by enhancing the scattering power of the other particle, and therefore the signal-to-noise ratio of the system is increased. Note that second order scattering is neglected in the current model, i.e. we ignore the scattered wavefield from the first particle which is excited by the second one because the particles are sparsely distributed on the sample.
6. The CRLB analysis of Application 2

6.1. Fisher information matrix for single rectangular object

For Application 2, the parameter vector we want to retrieve is:

$$\Theta = [\theta_1, \theta_2, \cdots]^T = [A_1, \phi_1, a_1, b_1, r_{\perp, 1}]^T.$$  

(40)

To find the Fisher information matrix, we start from the expectation of the second order perturbation of $L_P$:

$$E \left( \delta^2 L_P \right)(\Theta)(\delta \Theta, \delta \tilde{\Theta}) = \frac{2}{\hbar \omega} \sum_{\mathbf{k}_{1, j}} R \left[ F \left( P_j \delta O(\Theta)(\delta \Theta) \right) F^\dagger \left( P_j \delta O(\Theta)(\delta \tilde{\Theta}) \right) \right]$$

$$+ \frac{2}{\hbar \omega} \sum_{\mathbf{k}_{1, j}} R \left[ F \left( \Psi_j \right) F^\dagger \left( \Psi_j \right)^* \right] F \left( P_j \delta O(\Theta)(\delta \Theta) \right) F^\dagger \left( P_j \delta O(\Theta)(\delta \tilde{\Theta}) \right)^*.$$  

(41)

which is derived from Eq. (S11) in Supplementary. The function $O$ is defined in Eq. (25). $\delta O$ is the derivative of $O$ w.r.t. $\Theta$. $\delta \Theta$ and $\delta \tilde{\Theta}$ are small perturbations of the parameters of the rectangle. The explicit expression of $\delta O$, $\delta \Theta$ and $\delta \tilde{\Theta}$ are given in Section I.D of Supplementary.

By using Eq. (41), Eq. (S2) and Eq. (S23) in the Supplementary, we obtain the diagonal elements of the Fisher matrix:

$$I_{F,A_1,A_1}^\text{rect} = \frac{2}{\hbar \omega} \sum_{r, j} \left| P_j \Pi_{a_1, b_1, r_1} \right|^2 + \frac{2}{\hbar \omega} \sum_{r, j} R \left[ F^{-1} \left( \frac{F \left( \Psi_j \right)}{F \left( \Psi_j \right)^*} \right) e^{-2i\phi_1} \left[ \left( P_j \Pi_{a_1, b_1, r_1} \right)^* \right] \right]^2.$$  

(42)

$$I_{F,\phi_1}^\text{rect} = A_1^2 I_{F,A_1,A_1}.$$  

(43)

$$I_{F,a_1}^\text{rect} = \frac{1}{2\hbar \omega} \sum_{y, j} \left| C_1 \Pi_{b_1, y_1} \right|^2 \left[ \left| P_j \right|^2 (x_1 + \frac{a_1}{2}, y) + \left| P_j \right|^2 (x_1 - \frac{a_1}{2}, y) \right]$$

$$+ \frac{1}{2\hbar \omega} \sum_{y, j} R \left[ \left( C_1^* \Pi_{b_1, y_1} \right)^2 F^{-1} \left( \frac{F \left( \Psi_j \right)}{F \left( \Psi_j \right)^*} \right) \left( P_j \right)^2 (x_1 + \frac{a_1}{2}, y) \right]$$

$$+ \frac{1}{2\hbar \omega} \sum_{y, j} R \left[ \left( C_1^* \Pi_{b_1, y_1} \right)^2 F^{-1} \left( \frac{F \left( \Psi_j \right)}{F \left( \Psi_j \right)^*} \right) \left( P_j \right)^2 (x_1 - \frac{a_1}{2}, y) \right]$$

$$+ \frac{1}{\hbar \omega} \sum_{y, j} R \left[ \left( C_1^* \Pi_{b_1, y_1} \right)^2 F^{-1} \left( \frac{F \left( \Psi_j \right)}{F \left( \Psi_j \right)^*} \right) (2x_1, y) P_j^* (x_1 + \frac{a_1}{2}, y) P_j (x_1 - \frac{a_1}{2}, y) \right].$$  

(44)
can be obtained by taking the above equation and interchanging \( x \) with \( y \) and \( a_1 \) with \( b_1 \).

\[
I_{rect}^{F, y|b_1} = \frac{2}{\hbar \omega} \sum_{y,j} |c_1 \Pi_{b_1,y}|^2 \left[ |P_j|^2 (x_1 + \frac{a_1}{2}, y) + |P_j|^2 (x_1 - \frac{a_1}{2}, y) \right] \\
+ \frac{2}{\hbar \omega} \sum_{y,j} \Re \left[ \left( c_1 \Pi_{b_1,y} \right)^2 \mathcal{F}^{-1} \left( \frac{\mathcal{F} \left( \Psi_j \right)}{\mathcal{F} \left( \Psi_j \right)} \right) (2x_1 + a_1, y) \left( P_j^* \right)^2 (x_1 + \frac{a_1}{2}, y) \right] \\
+ \frac{2}{\hbar \omega} \sum_{y,j} \Re \left[ \left( c_1 \Pi_{b_1,y} \right)^2 \mathcal{F}^{-1} \left( \frac{\mathcal{F} \left( \Psi_j \right)}{\mathcal{F} \left( \Psi_j \right)} \right) (2x_1 - a_1, y) \left( P_j^* \right)^2 (x_1 - \frac{a_1}{2}, y) \right] \\
- \frac{4}{\hbar \omega} \sum_{y,j} \Re \left[ \left( c_1 \Pi_{b_1,y} \right)^2 \mathcal{F}^{-1} \left( \frac{\mathcal{F} \left( \Psi_j \right)}{\mathcal{F} \left( \Psi_j \right)} \right) (2x_1, y) P_j^* (x_1 + \frac{a_1}{2}, y) P_j^* (x_1 - \frac{a_1}{2}, y) \right].
\]

(45)

\[
I_{rect}^{F, x|a_1} \text{ can be obtained by taking the above equation and interchanging } x \text{ with } y \text{ and } a_1 \text{ with } b_1.
\]

We again focus on the diagonal elements of the Fisher matrix. Referring to the first term on the right-hand side of Eq. (42) and Eq. (43), we can immediately see that the CRLB of \( A_1 \) and \( \phi_1 \) is partially determined by the illumination power. Similarly, in Eq. (44) and Eq. (45) we see that the CRLB of \( a_1 \) and \( x_1 \) is partially determined by the illumination power at \( x_1 \pm \frac{a_1}{2} \), which is the edge of the rectangular. We can also notice in Eq. (43) that the CRLB of \( \phi_1 \) is inversely proportional to \( A_1^2 \). This observation means that one can retrieve \( \phi_1 \) more accurately by increasing the transmission of the rectangular, assuming that the estimator is unbiased.

It is interesting that \( I_{rect}^{F, x|a_1} \) and \( I_{rect}^{F, x|a_1} \) are functions of \( \Pi_{b_1,y} \). This fact means that enlarging the width of the rectangular in the \( y \)-direction will decrease the CRLB of \( a_1 \) and \( x_1 \), which are parameters along the \( x \)-axis. This correlation between \( b_1 \) and the CRLB of \( a_1 \) and \( x_1 \) is demonstrated in the next subsection. The computed CRLB is validated by Monte Carlo simulations.

### 6.2. The CRLB of the width and the position of the rectangle

Now we consider the configuration of Section 3. As described in Section 5.2, we need to provide a measure of the noise level in terms of photon counting. For Application 2, we define the illumination power by means of the total photon number counting over the cross section of the probe:

\[
\text{PN}_\text{rect} = \sum_{r_x} \frac{\|P(r_x)\|^2}{\hbar \omega},
\]

(46)

where the probe \( P(r_x) \) is shown in Fig. 6(b).

Here we study the influence of the width of the rectangular in the \( y \)-direction on the variance of retrieved width and position along the \( x \)-axis. The computed CRLB of \( a_1 \) and \( x_1 \) are shown in Fig. 9, for various values of \( b_1 \). The value of \( \text{PN}_\text{rect} \) is chosen to be \( 10^8 \). To validate the computation of the CRLB, the result of Monte Carlo Monte simulations is shown in Fig. 9 also. To obtain the variance, 1000 ptychographic data-sets are created in the Monte Carlo analysis. The data-sets are post-processed by using the parameter retrieval algorithm given in Section 3.2. The exact value of the variance and the squared bias of the parameters for the case of \( b_1/\lambda = 1, 5, 15 \), are listed in Table. 6.

We see in Fig. 9(a) and Fig. 9(b) that when \( \text{PN}_\text{rect} = 10^8 \) the CRLB of \( a_1/\lambda \) and \( x_1/\lambda \) are in the order of \( 10^{-6} \), which indicates that the resolution of the current parameter retrieval scheme is not limited by the grid discretization in real space. The Monte Carlo result confirm this
Fig. 9. The CRLB and variance of $a_1$, $x_1$, $b_1$ and $y_1$ of the rectangle, for various of $b_1$. The $PN_{rect}$ of this figure is $10^8$. The blue line is the computed CRLB and the red crosses show the variance obtained from Monte Carlo simulations.

Table 6. The variance and squared bias of $a_1$ and $x_1$ of the rectangle, obtained from Monte Carlo result for $PN_{rect} = 10^8$.

| $b_1/\lambda$ | 1         | 5         | 15        |
|---------------|-----------|-----------|-----------|
| $\text{Var}(a_1/\lambda)$ | $3.576 \times 10^{-7}$ | $1.455 \times 10^{-7}$ | $9.017 \times 10^{-8}$ |
| $\text{Bias}(a_1/\lambda)^2$ | $7.825 \times 10^{-10}$ | $4.254 \times 10^{-10}$ | $8.386 \times 10^{-11}$ |
| $\text{Var}(x_1/\lambda)$ | $9.057 \times 10^{-8}$ | $2.527 \times 10^{-8}$ | $1.824 \times 10^{-11}$ |
| $\text{Bias}(x_1/\lambda)^2$ | $6.423 \times 10^{-12}$ | $6.879 \times 10^{-11}$ | $4.947 \times 10^{-11}$ |

conclusion. Moreover, the squared bias of $a_1/\lambda$ and $x_1/\lambda$ is around $10^3$ times smaller that the variance, which means the algorithm is asymptotically unbiased when $PN_{rect} = 10^8$, and hence the variance obtained by the algorithm should be bounded by the CRLB. The CRLB of both $a_1/\lambda$ and $x_1/\lambda$ decrease when the value of $b_1$ is increased. This result agrees with Eq. (44) and Eq. (45). The CRLB of $a_1/\lambda$ and $x_1/\lambda$ in Fig. 9 decreases rapidly when $b_1/\lambda < 5$. The reason is that the sensitivity of the retrieval of the parameters is determined by the number of photons which encodes the information about the parameters. That is, There are more photons which contain the information about $a_1$ and $x_1$ when $b_1$ is larger. On the other hand, we can see that the CRLB of $b_1/\lambda$ and $y_1/\lambda$ do not vary too much when the value of $b_1/\lambda$ is sufficiently small. When $b_1/\lambda > 40$, the the CRLB of $b_1/\lambda$ and $y_1/\lambda$ start to increase as the value of $b_1/\lambda$ is enlarged. This is because the boundary of the rectangle in $y$-axis fall to the outside of the illuminated area of the object, which is not a desired situation since $b_1/\lambda$ and $y_1/\lambda$ are needed to be retrieved also. Therefore, for the current configuration, the optimal chosen range of the value of $b_1/\lambda$ is $(5, 40)$.

7. Conclusion

To summary, a parameter retrieval method is demonstrated in this paper. The idea of the method is to use available $a$ priori information about the object in the general ptychography framework. Two applications of the method are studied in the paper. In Application 1 we explored how to retrieve the parameters of small particles from Fourier ptychographic dark field measurements. The simulation result shows that, when sufficient prior knowledge about the sample is provided, the parameter of particles can be uniquely determined from dark field measurement only. In
Application 2 the retrieval of the parameters of a rectangle embedded in constant surrounding was studied.

The influence of Poisson noise on the parameter retrieval method is discussed in the second part of the paper. The CRLB of the parameters are theoretically derived and numerically computed from the Fisher information matrix for both applications. Monte Carlo analysis is used to validate the computed CRLB. The CRLB, variance and bias of the retrieved parameters in Application 1 were determined for various photon counts. It was found that the uncertainty of the parameter retrieval is inversely proportional to the photon counts, and potentially is not limited by the sizes of individual cells of the discretized meshgrid in the object space. The calculated CRLB shows the correlation between the particles. We proved that the CRLB of the position of one particle is influenced by the scattering power of the other particle. This conclusion is confirmed by the Monte Carlo result. The correlation of parameters in Application 2 is also inferred from the computed CRLB. The influence of the width of the rectangle in the y-direction on the CRLB of the parameters along the x-axis is investigated by analyzing the CRLB and Monte Carlo result. For the same number of photons in the illuminating probe, the uncertainty of the parameters along the x-axis can be reduced by enlarging the width in the y-direction.

See Supplement 1 for supporting content.

Funding

H2020 Marie Skłodowska-Curie Actions (675745).

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