Reconstructing mode mixtures in the optical near-field

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Abstract: We propose a reconstruction scheme for hard x-ray inline holography, a variant of propagation imaging, which is compatible with imaging conditions of partial (spatial) coherence. This is a relevant extension of current full-field phase contrast imaging, which requires full coherence. By the ability to reconstruct the coherent modes of the illumination (probe), as demonstrated here, the requirements of coherence filtering could be relaxed in many experimentally relevant settings. The proposed scheme is built on the mixed-state approach introduced in [Nature, 494 (2013)], combined with multi-plane detection of extended wavefields [Opt. Commun., 199 (2011); Opt. Express, 22 (2014)]. Notably, the diversity necessary for the reconstruction is generated by acquiring measurements at different defocus positions of the detector. We show that we can recover the coherent mode structure and occupancy numbers of the partial coherent probe. Practically relevant quantities as the transversal coherence length can be computed from the reconstruction in a straightforward way.

References and links
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The coherence properties of the illumination (probe) are a fundamental prerequisite for lensless coherent imaging techniques [1, 2], both in the optical near-field and far-field. When reconstructing from measured data, the assumption in particular of a spatially fully coherent illumination is ubiquitous, even though it is clear that this condition is never (and can never be exactly) fulfilled [3]. The effects of image degradation by partial coherence have been described in many different settings [4, 5]. Measured or estimated spatial [6] or temporal [7] coherence properties have also been incorporated in the phase reconstruction process.

1. Introduction

The coherence properties of the illumination (probe) are a fundamental prerequisite for lensless coherent imaging techniques [1, 2], both in the optical near-field and far-field. When reconstructing from measured data, the assumption in particular of a spatially fully coherent illumination is ubiquitous, even though it is clear that this condition is never (and can never be exactly) fulfilled [3]. The effects of image degradation by partial coherence have been described in many different settings [4, 5]. Measured or estimated spatial [6] or temporal [7] coherence properties have also been incorporated in the phase reconstruction process.
Wavefront sensing and coherence measurements have therefore attracted significant attention in the past, especially in the x-ray regime where coherent imaging has stirred much interest as a way to circumvent the lack of suitable lenses [8–17]. The rationale for measuring coherence properties in these studies is that by experimental control of the probe, spatial coherence can be increased sufficiently high to warrant that the coherence length $\xi$ exceeds the field of view. In this way the requirements of conventional phase retrieval algorithms can be met. Recently, however, the methodology for phase retrieval has been extended by Thibault and Menzel to include the reconstruction of multiple coherent modes in the phase retrieval process [18]. Their approach follows the concept of coherent mode representation [3, 19] which has been widely used in many optical disciplines. The coherent modes are a particular example of the concept of state mixtures. Mixed states can also account for aberrations in the object (vibrations) and detection (point spread function) plane. They have demonstrated, that the inclusion of the mode reconstruction in the phase retrieval process can yield not only an enhanced reconstruction quality for objects under partial coherent imaging conditions but also a description of the partial coherent probe in terms of modes. The additional information required for the reconstruction can be generated from ptychography [20, 21], where diversity in the data is increased by scanning the object through the probe. The state mixture concept was extended and applied to different experimentally relevant configurations, for example for non-monochromatic radiation [22] or a (deliberate) smearing of the probe during on-fly-scans [23]. Further it has been shown, that the reconstruction of states can reveal more information about a specimen [24]. The symmetry of the operations in the ptychographic reconstruction algorithm can also lead to ambiguities in the reconstructed states and additional constraints are required in some cases to break these ambiguities [25].

However, the extension to the coherent imaging in the optical near-field has so far been lacking. At the same time, multi-mode reconstructions of extended wavefields are of considerable interest. Firstly, extended multi-mode reconstructions can help to understand on a fundamental level why the near-field imaging is found to be more tolerant to partial coherence than its far-field counterparts. Secondly, full-field x-ray imaging is of tremendous practical importance, in particular for larger specimen and for tomography, where scanning techniques are prohibitive. Importantly, near-field or propagation imaging is almost always known to be implemented in a partial-coherence setting, including robust exploitation of phase contrast at laboratory sources [26–29].

In this work we show by numerical simulations, that the extraction of coherent modes can be also applied to reconstruct the extended probe as it is used in x-ray propagation imaging or inline x-ray holography. To this extent we present an algorithm based on multiple magnitude projections (MMP) [30] generalized to mixed states, i.e. partial coherence. We have previously used MMP for probe characterization [31, 32] under the assumption of full coherence. We denote its multi-modal generalisation by mmMMP. In both the MMP and mmMMP schemes, the detector is moved to different longitudinal distances (propagation distances). This movement changes the Fresnel number of the probe with respect to some reference plane (e.g. the first measurement or the focal plane) and introduces diversity in the measurements, which is required for a reliable reconstruction. Note that in general, mmMMP will require more detection planes than MMP to compensate for the information loss inflicted by partial coherence. We show that mmMMP algorithm is capable of recovering the coherent modes with their accompanying occupation and the degree of coherence of the ensemble of modes.

Sec. 2 describes the setup for data generation after a short recapitulation of coherence properties primarily for the sake of notational clarity. Section 3 details the algorithm and numerical implementation. The results of the numerical experiment are shown in Sec. 4 before the paper closes in Sec. 5 with a summary and outlook.
2. Simulation model

The basis for the physical model of partially coherent image formation is the representation of the probe’s wavefield as a superposition of uncorrelated but coherent modes $\Psi_m \in \mathbb{C} [3, 19, 33]$ i.e the coherent mode expansion with $m \in \{1 \ldots M\}$ denoting the mode index and $\Psi_m$ satisfying orthogonality

$$\langle \Psi_m, \Psi_n \rangle = \delta_{nm}, \quad (1)$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product. The $\Psi_m$ are propagated individually through free space by use of the Fresnel propagator $D_{\Psi}$ and interact separately with optics or objects. Non-linear extensions of the model are beyond the scope of this paper and typically not relevant to x-ray imaging. In the detection plane, the intensities are computed for each mode

$$I_m = |D_{\Psi}(\Psi_m)|^2, \quad (2)$$

and their incoherent superposition is taken to be the measurement $I$

$$I = \sum_m \lambda_m I_m, \quad (3)$$

where $\lambda_m$ denotes the occupation number of $\Psi_m$, i.e the intensity for the mode. Equation (1) to Eq. (3) are sufficient to setup a straightforward numerical implementation for the propagation of a partially coherent probe. In order to determine the spatial coherence properties from the coherent mode expansion, we have to introduce auxiliary variables. We assume stationary and monochromatized undulator radiation, so that the equal-time coherence function or mutual intensity can be used

$$J_m(\hat{r}_1, \hat{r}_2) = \Psi_m^*(\hat{r}_1)\Psi_m(\hat{r}_2). \quad (4)$$

$J_m$ has to be calculated for each mode $\Psi_m$ with $\hat{r}_{1/2}$ points in the plane of $\Psi_m$. The collective $J(\hat{r}_1, \hat{r}_2)$ of the ensemble of modes is obtained by summing $J(\hat{r}_1, \hat{r}_2) = \sum_m J_m(\hat{r}_1, \hat{r}_2)$. Normalization yields the complex degree of coherence

$$j(\hat{r}_1, \hat{r}_2) = \frac{J(\hat{r}_1, \hat{r}_2)}{\sqrt{J(\hat{r}_1, \hat{r}_1)J(\hat{r}_2, \hat{r}_2)}}. \quad (5)$$

Note, that this quantity is 4-dimensional. By assuming translational invariance and isotropy of the coherence properties we reduce the $(\hat{r}_1, \hat{r}_2)$ dependence to a distance $d = \sqrt{||\hat{r}_1 - \hat{r}_2||^2}$ dependence. Using this simplification $j(d)$ is depictable in a $||j(d)||$ vs $d$ plot, cf. Fig. 4. The spatial coherence length $\xi$ is defined as the crossing point of $||j(d)||$ with a given threshold value, in this work $0.5$.

Figure 1 shows a sketch of the setting for the case of 3 modes, represented by the iconic images of a 1,2 and 3. Following the MMP scheme, we need to generate $I$ for different propagation distances, or corresponding Fresnel numbers $F_{nk}$, where the index $k \in \{1 \ldots K\}$ is used to enumerate the $K$ measurements $I_k$. Figure 2(a) shows the input images which are processed to yield the orthogonal modes (b) for the numerical experiment. For each complex-valued input two images represented by $N_x \times N_y$ matrices are chosen. One is interpreted as phase $\phi \in [-0.4, 0.4]\text{rad}$ the other as amplitude $A \in [0.8, 1.2]\text{arb.u.}$ and then combined according to $A \cdot \exp(i\phi)$. Next, the inputs are reinterpreted as column vectors of a matrix $\mathbf{A} \in \mathbb{C}^{(N_x \times N_y) \times (M+1)}$, which is then fed into a $QR$-factorization. The $QR$-factorization is a method from linear algebra to compute the factorization $\mathbf{A} = \mathbf{Q} \cdot \mathbf{R}$, where $Q \in \mathbb{C}^{(N_x \times N_y) \times (M+1)}$ is a unitary matrix and $R \in \mathbb{C}^{(M+1) \times (M+1)}$ is a upper triangular matrix. The column vectors of the resulting $Q$ are reshaped to obtain $M + 1$ matrices of size $N_x \times N_y$ representing the orthogonal modes used for subsequent simulation of the measurements. The $QR$-factorization can be computed by different algorithms e.g. Gram-Schmidt process, Householder reflections or Givens rotations [34]. Since the $QR$-factorization
makes the $\Psi_m$ orthogonal with respect to the preceding mode, an additional mode has to be generated for initialization of the process, which does not contribute of the ensemble of modes used in the numerical experiment in Sec. 4. Thus, all subsequent $QR$-factorizations during the reconstruction operate only on the $M$ propagation modes, which still form a orthogonal basis.

The next step is to choose occupation numbers $\lambda_m$ for the respective $\Psi_m$. For the example shown here, we choose $\lambda_0 = 4 \cdot 10^6 [0.5, 0.3, 0.2]$. Next, the modes are propagated Eq. (2) and summed up Eq. (3) to yield $I_k$. As a final step of data generation noise can be applied. The set of $I_k$ is then be used as input for the reconstruction algorithm presented in the next section.

3. Algorithm

Given the measurements $I_k$ (intensity only), we aim to reconstruct the ensemble of modes $\hat{\Psi}$ with $M$ modes $\Psi_m$ with the respective occupation $\lambda_m$. This is an example of the classical phase problem, however, now in the setting of partial coherence. We solve this problem via the use of iterative projection algorithms [35, 36]. These algorithms are quite versatile, since the problem specific part is coded only in the projectors and the applicability is not limited to any specific assumptions as for single-step solutions cf. [37]. We here use the Relaxed Averaged Alternating Reflections (RAAR)-algorithm [38] with adapted projections. A new iterate is given by the RAAR-algorithm:

$$
\hat{\Psi}_{n+1} = \frac{\beta_n}{2} \left( R_S(R_I(\hat{\Psi}_n)) + \hat{\Psi}_n \right) + (1 - \beta_n) P_I(\hat{\Psi}_n),
$$

where $R_S/I(\hat{\Psi}) = 2P_S/I(\hat{\Psi}) - \hat{\Psi}$ denotes a (mirror) reflection by a given constraint set and $n$ the iteration index. Operations acting on $\hat{\Psi}$ have to be read in a per-mode manner. The parameter $\beta_n$ controls the relaxation. For the present problem we found that a fixed $\beta_n = 0.99$ is best suited.
a) Input Images for Orthogonalization

```
Amplitude (a.u.)  Phase (rad)
```

b) Unitary modes

```
\Psi_1  \Psi_2  \Psi_3
```

Fig. 2. Generation of coherent modes. Test images (a) were taken and interpreted as amplitudes and phases of the coherent modes. Using these modes as input for a QR-factorization, suitable, i.e. orthogonal, modes (b) are obtained for propagation and data generation, following the scheme introduced in Fig. 1. The modes are scaled according to their occupation number.
to assure stability of the reconstruction process. The projection on the measurements \( P_f \) is a nested operation. The operation is carried out independently for each mode and measurement. The information from the overall \( K \) measurements for one mode is merged by taking the average over the projected wave fields. This has the advantage, that all \( I_k \) constraints are 'equally well' satisfied whereas in a sequential projection the last constraint projected on is always preferred, in terms of a error metric. As a drawback we note that this parallel projection can diminish the speed of convergence. The single projection of \( \Psi_m \) on measurement \( K \) is given by \( P_{I_k} (\Psi_m) = D_{-F_{rk}} (A_{I_k} \left[ D_{F_{rk}} (\Psi_m) \right]) \), (7)

where \( A_{I_k} \) is the adaptation of amplitudes, given by \( A_{I_k} (\bullet) = \sqrt{I_{k,m}} \cdot \sqrt{I_k} \cdot \exp (i \arg (\bullet)) \), (8)

where \( I_{k,m} = \left| D_{F_{rk}} (\Psi_m) \right|^2 \) denotes the intensity for a given \( \Psi_m \) in the measurement plane \( k \), cf. Eq. (2). The whole adaptation has to be read as a per pixel operation. The propagation to the measurement plane is performed by the Fresnel propagator \( D_{Fr} \), for a given Fresnel number \( Fr \) with respect to one pixel, \( D_{Fr_k} (\bullet) = \mathcal{F}^{-1} \left[ \mathcal{F} [\bullet] \exp \left( (-i\pi)/(2 Fr_k) (k_x^2 + k_y^2) \right) \right] \), (9)

where \( k_x \) and \( k_y \) are spatial frequencies in Fourier space. Thus \( P_f (\vec{\Psi}_n) \) is finally given as:

\[
P_f (\vec{\Psi}_n) = \begin{cases}
P_{I_k} (\Psi_1) \\
\vdots \\
\frac{1}{K} \sum_{k=1}^{K} P_{I_k} (\Psi_M)
\end{cases}
\]

The operator \( P_S \) is used to enforce the orthogonality constraint on \( \vec{\Psi} \) in the reference plane. For this purpose, a QR factorization is applied (MATLAB's implementation) with the modes given as column vectors in \( Q \) and the occupation numbers \( \lambda_m \) given as the diagonal elements of \( R \)

\[
P_S (\vec{\Psi}_n) = QR (\vec{\Psi}_n).
\]

Finally, the updated \( \vec{\Psi} \) are extracted from \( Q \) by reshaping the respective column \( m \) of \( Q \) back to the \( N_x \times N_y \) array and subsequent multiplication with the corresponding \( m \)-th entry of \( R \).

The algorithm was implemented in MATLAB, making use of the parallel computing toolbox and complemented with specialized CUDA (Compute Unified Device Architecture) kernels [39] running on the graphics processing unit for the calculation of the Fresnel propagator and \( j(\vec{r}_1, \vec{r}_2) \). The implementation of mmMMP and the simulation described in the next section are available online in Code 1 [40].

4. Numerical experiment

The setup for the numerical experiment has been guided by the experimental results [13] obtained for the instrument [41] operated by our group at P10/PETRA III (DESY). In these previous results, a number of 3 coherent modes was found for the nano-focused undulator radiation of this instrument. This in line with earlier work on a dedicated high-coherence beamline [11]. For the numerical experiment, \( M = 3 \) modes are prepared and reconstruction is performed based on a set of \( K = 10 \) measurements with Fresnel numbers tabulated in Tab. 1. The orthogonal modes are shown in Fig. 2(b). The occupation numbers \( \lambda_m^0 \) and all other experimental parameters are also tabulated in Tab. 1. As initialization for \( \vec{\Psi} \) we have generated 3 random modes...
orthogonalized by $QR$-factorization and scaled by an initial guess for the mode occupation $\lambda_m$. Figure 3 presents the results of the reconstruction after 30000 iterations with (a) showing the 3 recovered modes. Visual inspection by comparing the reconstructions to Fig. 2 demonstrates the successful reconstruction. Out of the three modes, $\Psi_1$ is recovered best, due to the fact that it has the largest occupation number. $\Psi_2$ and $\Psi_3$ also show a convincing recovery. However, some larger regions still exhibit a phase offset with respect to original. In Fig. 3(b) the evolution of the reconstructed occupation number $\lambda_m/\lambda^0_m$, normalized to the true value, is plotted as a function of iteration number. The plot shows only a slow convergence for $\lambda_m$. Interestingly, the modes $\vec{\Psi}$ are faster recovered than their occupation numbers. The plot shows some characteristics which we found to be typical when testing different parameters (different $M$, $K$ or $\lambda^0_m$). At the beginning $\Psi_1$ absorbs much of overall intensity and only following further iterations the intensity is distributed among the $\Psi_m$ in a non-monotonous reconstruction trajectory, see also App. D. Figure 3(c) shows the per pixel error of the reconstruction with respect to the (simulated) measurements, calculated from

$$\Delta_k = \sum_{\text{all pixels}} \left| \sum_m I_{k,m} - I_k \right|^2 / N.$$  (12)

The solid lines show the mean of $\Delta_k$ for the 10 measurement planes of the multi modal reconstruction (blue) presented here and a single mode reconstruction (red) assuming full coherence using the unmodified MMP scheme. The dashed lines show the bounds of $\Delta_k$ over all measurement planes. After 30000 iterations, the multi-mode reconstruction correctly taking into account partial coherence shows a residuum which is more than two orders of magnitude smaller than the reconstruction based on the (wrongful) assumption of full coherence, which is ubiquitous in x-ray propagation imaging.

With the reconstructed $\bar{\Psi}$ at hand, we can then calculate the equal-time complex degree of coherence $j$ as shown in Fig. 4 using Eq. (5). Figure 4 compares $\|j(d)\|$ for input modes (blue) and the reconstructed modes (red). An important quantity for coherent imaging experiments is the (transversal) coherence length $\xi$. It can be defined via the intersection of $\|j(d)\|$ with a given value, here 0.5 (yellow).

The appendix provides additional parameter variations, i.e. addressing the influence of noise as well as a reduced input data set, to test the stability of the mmMMP algorithm. For the noisy simulations in App. A we chose a mean photon fluence per pixel $\mu$ with $\mu = \{1000, 100, 10\}$ but otherwise unchanged parameters (Tab. 1). The $I_k$ have been scaled accordingly, then the pixel values have been used as input for a Poissonian noise generator. Even for low fluences down to $\mu = 10$, we observe a satisfactory recovery of $\Psi_1$ and $\Psi_2$, see Fig. 6. This surprising noise tolerance can be explained based on the fact that 10 measurements are used and that the images are highly sampled. Appendix B presents reconstruction results for a reduced input data set. Not surprisingly, more diverse input data leads to a better reconstruction quality and faster convergence of the algorithm, see Fig. 7 for an exemplary reconstruction. The simulations show that for a reliable reconstruction of 3 modes $K > 6$ is necessary. In both scenarios we note that a considerable higher number of iterations is needed to recover the ensemble of modes. The reconstruction scheme seems to be more stable against noisy data than for reducing the input data set. Appendix C surveys the influence of $M$ on the reconstruction quality. We note an improvement of the reconstruction until the correct $M$ is reached. Increasing $M$ further does not improve or worsen the reconstruction. Appendix D shows the influence of the starting guess $\lambda_m$ on the reconstruction. The different reconstruction trajectories show differences in convergence speed. A desired error level can be reached in this (ideal) setup by investing more iterations.
Fig. 3. Results of the mmMMP reconstruction. (a) The set of reconstructed modes in phase and amplitude. (b) The convergence graph for the occupation numbers $\lambda_m$. The convergence is shown relatively to the current occupation in an iteration with respect to the prescribed occupation $\lambda_m^0$. (c) Comparison of the error evolution $\Delta_k$ of the mean over all measurement planes Eq. (12) for a single mode reconstruction (red) and multi mode reconstruction (blue). Dashed lines indicate the bounds of the standard deviation over all measurement planes.
Table 1. Summary of the parameters for the numerical experiment.

<table>
<thead>
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<th>Value</th>
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<td>Occupation $\lambda_m^0$</td>
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<tr>
<td>Initial guess for occupation</td>
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<tr>
<td>Iterations</td>
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</table>

Fig. 4. Comparison of the degree of coherence $||f(d)||$ for the reconstructed modes (red) and input modes (blue).

5. Summary and outlook

We have presented an extended multi plane reconstruction scheme for near-field x-ray holography under conditions of partial coherence. We carried out numerical experiments primarily on noiseless and noisy data.

Our results show that reconstruction of the coherent near-field modes is possible and that quantities as the coherence length and occupation numbers can be faithfully reconstructed, given sufficient longitudinal diversity of the measurements, i.e. a sufficient number of detection planes. Furthermore, our results clearly demonstrate the increased reconstruction quality which can be obtained when data recorded under condition of partial coherence is also reconstructed in a multi-modal approach, instead of the assumption of a single mode. While near-field imaging is known to be more tolerant towards partial coherence than its far-field counterpart, the present work shows that it is still important to go beyond the idealized assumption of full coherence. In the present work, we have also tested how the reconstruction quality decreases when the number of measurements $K$ is decreased. Of course, the number of measurements planes scales with the number of modes. In fact, it can be expected that $K > 2 \times M$. In our numerical experiments for $M = 3$, we found indeed that $K = 8$ still resulted in good reconstructions, however, requiring a larger number of iterations (cf. App. B).

Following this work, two next steps suggest themselves: First, the new algorithms and approach should be tested experimentally. Second, probe reconstruction as presented here should be extended to full reconstruction of object and probe, as it has already been shown for the far-field.
Appendix A: Mode reconstructions from noisy measurements

Reconstruction was tested under the influence of noise for photon fluences of $\mu = \{10, 100, 1000\}$ photons per pixel, again using modes shown in Fig. 2. The measurements $I_k$ were generated for the set of Fresnel numbers $F_{\text{Fr}}$ (cf. Tab. 1) as detailed in the manuscript (cf. Sec. 2). The $I_k$ were then rescaled according to $\mu$ and used as input for MATLAB’s imnoise-function. Figure 5 shows an example for these measurements. The set of resulting noisy $I_k$ was then used as input for mmMMP.

Figure 6 shows the obtained mode reconstructions from these input data. The reconstructed modes presented in (a) show good recovery for $\Psi_1$ but significant deviations for $\Psi_2$ and $\Psi_3$. For high fluence $\mu = 1000$, the reconstruction error $\Delta$ shown in (b) exhibits a similar functional form as for the noiseless case in the main text, but it does not quite reach the same error level (after 30000 iterations). The reconstruction for $\mu = 10$ seems to stagnate, even if we let it run over a considerable amount of more iterations (95000 iterations). Nevertheless, the reconstruction result shown in (c) after 95000 iterations for $\Psi_3$ (left) compares surprisingly well with the original $\Psi_3$ (right).

Appendix B: Mode reconstructions from a reduced data set

Next, the influence of a reduced data set was studied, to this end the number of measurements $K$ was reduced. The mode reconstruction was carried out on noiseless measurements simulated from the modes shown in Fig. 2. Starting from the initial set of $F_{\text{Fr}}$ (Tab. 1), tailing $F_r$ have been removed until the new $K$ is reached. The simulated cases $K = 6$ and $K = 8$ are presented in Fig. 7. The reconstructed modes after 50000 iterations are shown in (a), the left half for $K = 6$ and the right half for $K = 8$, respectively. While the reconstructed amplitude and phase for $\Psi_1$ is acceptable for $K = 6$, the other modes are not reconstructed. In the corners of $\Psi_2$ and $\Psi_3$ some details of a window appear, but the majority of the mode is noise. Increasing the iteration number, in this case to $n = 550000$, did not improve the mode reconstruction significantly. Contrarily, for $K = 8$ we still observe good recovery for $\Psi_2$, but $\Psi_3$ also shows noise artifacts in the middle of the image. Letting the algorithm run for more iterations in this setting (270000 iterations) yielded a reconstruction of similar quality as the one in main text.
Fig. 6. Results obtained from noisy data. (a) Reconstructed modes in phase and amplitude. The left half shows the reconstruction for $\mu = 10$ and the right for $\mu = 1000$. The amplitudes have been normalized by the mean value for the side-by-side plot. (b) Error $\Delta$ as a function of iteration $n$, for both photon numbers. Dashed lines indicate the bounds of the standard deviation over all measurement planes. (c) Reconstruction of $\Psi_3$ for $\mu = 10$ after 95000 iterations (left) compared to the input mode (right), cf. Fig. 2 of the main manuscript.
Fig. 7. Results obtained from the reduced input data set. (a) Reconstructed modes in phase and amplitude after 50000 iterations. The left half shows the reconstruction for $K = 6$ and the right for $K = 8$. (b) Error evolution for both $K$ as function of iteration number. Dashed lines indicate the bounds of the standard deviation over all measurement planes. (c) Reconstruction of $\Psi_3$ for $K = 8$ after 270000 iterations (left) compared to the input mode (right), cf. Fig. 2.
Appendix C: Influence of the choice of \( M \) for reconstruction

The number of reconstructed modes \( M \) is an important parameter for physical interpretation of data. Here we have complemented the results of Fig. 3(c) with a variation of the number of modes \( M \) for multiple runs on the same (simulated) data set. Again the parameters listed in Tab. 1 have been used, no noise has been added to \( I_k \). The results are shown in Fig. 8, again we use \( \Delta_k \) according to Eq. (12) to monitor the error. The presentation of results follows Fig. 3(c), see the main text. The results show the better description of the \( I_k \) by increasing \( M \). For \( M = \{1, 2\} \) we note stagnation of the error, the \( M = 2 \) curves shows already that the stagnation is reached later and that the data is better described. For \( M = \{3, 4\} \) we see no stagnation of the error. The \( M = 4 \) curves shows no better description of the data. From these results it is possible to deduce \( M = 3 \), also for experimental data where \( M \) is not known beforehand.

Appendix D: Influence of the initial guess of \( \lambda_m \) for reconstruction

Besides \( M \) and the initialization of \( \Psi_m \), i.e. orthogonal and random, a starting guess for \( \lambda_m \) has to be chosen. Here we have tested the stability of the algorithm with regard to different choices of the starting initialization of \( \lambda_m \). In the first case all \( \Psi_m \) have the same occupation \( \lambda_m \) i.e. \( \lambda_m = \frac{1}{M} \cdot \text{number of photons} \). The results for this equal occupation reconstruction are shown in Fig. 9, the structure follows Fig. 3.

Figure 10(a) shows the trajectories of the relative occupation \( \lambda_m / \lambda^0_m \) for randomly chosen starting guess of \( \lambda_m \). The numbers in the legend for each panel denote the \( \lambda_m \). The normalized occupation of the searched ensemble of modes is \( \lambda^0 = \{0.5, 0.3, 0.2\} \).

The reconstruction with equal occupation as starting guess reproduces the reconstruction shown in Fig. 3. Further we have tested randomly chosen initializations. Here we have chosen random initializations for \( \lambda_m \) for the setting of \( M = 3 \) as described in the main text. The \( \lambda_m \) have been chosen as follows:
- Generate \( M \) random numbers \( \Lambda_m \).
- Sort \( \Lambda_m \) in descending order.
- generate the normalized occupation \( \hat{\lambda}_m = \frac{\Lambda_m}{\sum_{m=1}^{M} \Lambda_m} \).
- Calculate \( \lambda_m = \hat{\lambda}_m \cdot \text{number of photons} \).

Fig. 9. Results of the equal occupation reconstruction. (a) The set of reconstructed modes in phase and amplitude. (b) The convergence graph for the occupation numbers \( \lambda_m \). The convergence is shown relatively to the current occupation in an iteration with respect to the prescribed occupation \( \lambda^0_m \). (c) Comparison of the error evolution \( \Delta_k \) of the mean over all measurement planes Eq. (12) for a single mode reconstruction (red) and multi mode reconstruction (blue). Dashed lines indicate the bounds of the standard deviation over all measurement planes.

The ensemble of realizations shows that the algorithm is stable against variations in the start-ing guess of \( \lambda_m \). (b) shows a longer run for the realization \( \lambda m = \{0.487, 0.291, 0.222\} \). After 30000 iterations this reconstruction has not yet shown satisf actory recovery of the occupation numbers. Running more iterations, overall 100000, has finally yielded a good recovery of the occupation. The true occupation can be recovered, in unfavorable cases at the expanse of more iterations.
Fig. 10. Trajectories for the realizations of $\lambda_m$. The individual trajectories (a) of the relative occupation $\lambda_m / \lambda_m^0$ for overall 12 realizations are shown, using the parameters listed in Tab. 1. The realization with $\hat{\lambda}_m = \{0.487, 0.291, 0.222\}$ showing not satisfactory convergence after 30000 iterations, has been iterated 70000 iterations more (b).
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