Uniqueness and reconstruction formulas for phase retrieval via reference objects

with applications in coherent diffractive imaging

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SFB 755 - Nanoscale Photonic Imaging

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Motivation

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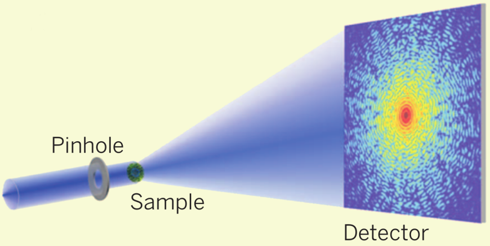

(a) Sketch of a CDI setup [Miao et al., 2015]

- Microscopic sample is illuminated by coherent X-Rays
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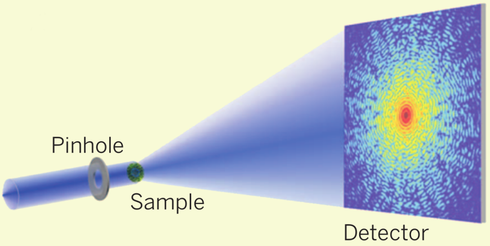

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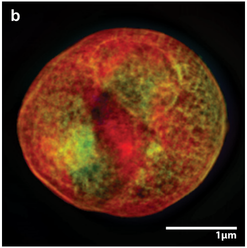

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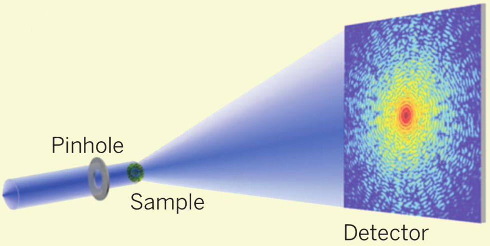

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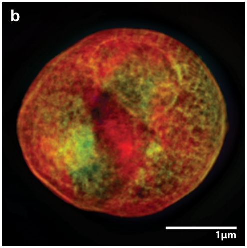

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Forward map:

$$F : f = \underbrace{-\mathrm{i}\phi - \mu}_{\substack{\textbf{Phase shifts}\\ \text{(+absorption)}}} \quad \mapsto \quad I = \Big| \underbrace{\mathcal{F}}_{\substack{\text{Fourier}\\ \text{transform}}} \underbrace{(p \cdot \exp(-\mathrm{i}\phi - \mu))}_{=f \text{ (exit wave field)}} \Big|^2$$

The Phase Retrieval Problem

Inverse Problem 1 (Phase Retrieval)

Recover $f \in A \subset \left\{h \in L^1_c(\mathbb{R}^m) : \operatorname{supp}(h) \subset \Omega\right\}$ *from* $\hat{g} := |\mathcal{F}(f)|^2$ *for some (compact) support domain* $\Omega \subset \mathbb{R}^m$*.*

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- *Non-uniqueness:*
  - In $m = 2$D: discrete problem is "almost always" unique [Barakat and Newsam, 1984]
  - *Counter-example:* for $f(x, y) = \mathbf{1}_{[0;1]^2}(x, y) \cdot \exp(x)$, IP1 has infinitely many real-valued solutions $\tilde{f} \in L^2([0, 1]^2)$.

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This talk: What if a part of the signal $f = p + h$ is known *a priori*?

Holography: Phase Retrieval with Reference Signals

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In the setting of Inverse Problem 1, let $f = p + h$ *with* $p = \delta_0$ *(Dirac-delta) and* $\operatorname{supp}(h) \subset \Omega_h \subset \mathbb{R}^m$ *with* $\operatorname{dist}(\Omega_h, 0) > \operatorname{diam}(\Omega_h)$. *Then*

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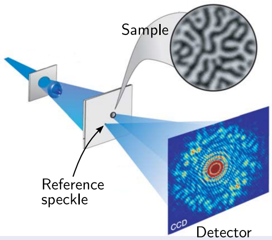

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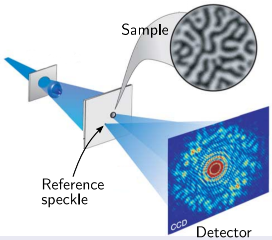

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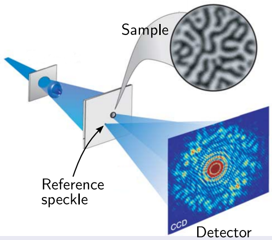
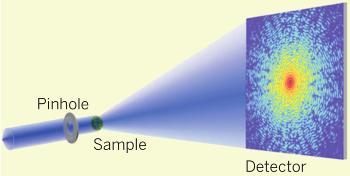


Is there a holographic principle in standard CDI?



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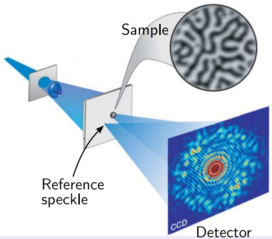

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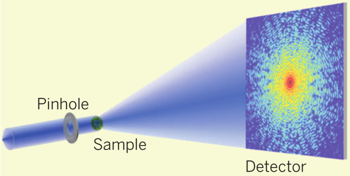
$$= \Big|\underbrace{\mathcal{F}(p)}_{\substack{\text{probing beam}\\ \text{(= reference)}}} + \mathcal{F}\big(\underbrace{p \cdot (\exp(-\mathrm{i}\phi - \mu) - 1)}_{=h \text{ (unknown object signal)}}\big)\Big|^2$$



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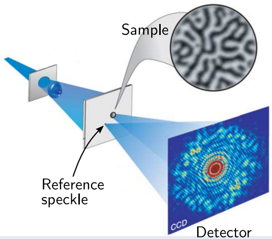

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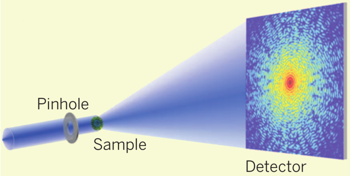
⇝ Simplest achievable setting: $p = p_0 \cdot \mathbf{1}_{\text{pinhole}}$



Basic Notions and Concepts

Abstract Setting

Definitions/Notation:

- *Convolution:* $f * g : \; x \mapsto \int_{\mathbb{R}^m} f(x-y)g(y)\,\mathrm{d}y$
- *Reflection:* $f^{-} : x \mapsto \overline{f(-x)}$
- *Hermitean and anti-hermitean parts:* $f^{\mathrm{h}} := \frac{1}{2}(f + f^{-})$, $f^{\mathrm{a}} := \frac{1}{2}(f - f^{-})$
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$$g = \mathcal{F}^{-1}\left(\left|\mathcal{F}(p+h)\right|^2 - \left|\mathcal{F}(p)\right|^2\right)$$

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Observation: Extra information $2p^{\mathrm{h}} * h^{\mathrm{h}} + 2p^{\mathrm{a}} * h^{\mathrm{a}}$ if terms are separable!

Support Theorem for Convolutions

Theorem 2 (Support of convolutions (e.g. [Hörmander, 2003]))

Let $u_1, u_2 \in L^1_c(\mathbb{R}^m)$ *be compactly supported. Then*

$$\operatorname{conv}(\operatorname{supp}(u_1 * u_2)) = \operatorname{conv}(\operatorname{supp}(u_1)) + \operatorname{conv}(\operatorname{supp}(u_2)),$$

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For $p \in L^1_c(\mathbb{R}^m)$*, let* $\Omega_p := \mathrm{conv}\,(\mathrm{supp}(p))$*,* $B := (1 + c) \cdot \Omega_p$ *for some* $c \geq 0$ *and* $M := \mathbb{R}^m \setminus B$*. Let* $h_1, h_2 \in L^1_c(\mathbb{R}^m)$ *such that*

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- $(p * \Delta h)|_M \neq 0 \rightsquigarrow$ *contradiction!* □

Uniqueness Results and Reconstruction Formulas for Hermitean Reference Objects

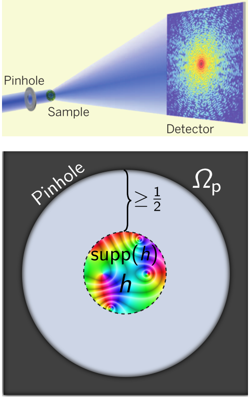
Reconstruction of Complex-valued Objects

Theorem 4 (Reconstruction of small inclusions)

Let $p \in L^1_c(\mathbb{R}^m) \setminus \{0\}$ *be known and hermitean with* $\Omega_p := \operatorname{conv}(\operatorname{supp}(p))$. *Let*

$$A := \left\{ h \in L^1_c(\mathbb{R}^m) : \operatorname{supp}(h) \subset 1/2 \cdot \Omega_p \right\}. \qquad (3.1)$$

Then any $h \in A$ *is uniquely determined by the data* $\Delta I = |\mathcal{F}(p+h)|^2 - |\mathcal{F}(p)|^2$ *up to reflection* $h \mapsto h^-$.



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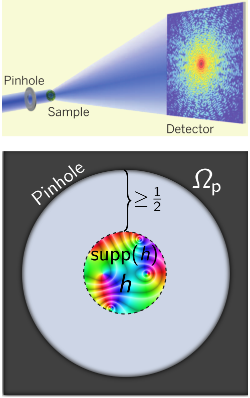
Then any $h \in A$ *is uniquely determined by the data* $\Delta I = |\mathcal{F}(p+h)|^2 - |\mathcal{F}(p)|^2$ *up to reflection* $h \mapsto h^{-}$. *Moreover,* h^{h} *and* $\pm h^{\mathrm{a}}$ *can be reconstructed via*

$$\left(2p * h^{\mathrm{h}}\right)|_{\mathbb{R}^m \setminus \Omega_p} = \mathcal{F}^{-1}(\Delta I)\,|_{\mathbb{R}^m \setminus \Omega_p} \qquad (3.2\mathrm{a})$$

$$-\mathcal{F}(h^{\mathrm{a}})^2 = \Delta I - \mathcal{F}\left(2p * h^{\mathrm{h}} + h^{\mathrm{h}} * h^{\mathrm{h}}\right) \qquad (3.2\mathrm{b})$$



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$$\left(2p * h^{\mathrm{h}}\right)|_{\mathbb{R}^m \setminus \Omega_p} = \mathcal{F}^{-1}(\Delta I)\,|_{\mathbb{R}^m \setminus \Omega_p} \qquad (3.2a)$$

$$-\mathcal{F}(h^{\mathrm{a}})^2 = \Delta I - \mathcal{F}\left(2p * h^{\mathrm{h}} + h^{\mathrm{h}} * h^{\mathrm{h}}\right) \qquad (3.2b)$$

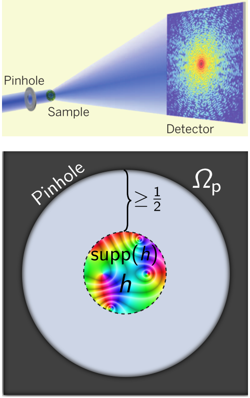

Fig.: Setting of Theorem 4

Proof:

- Since $p^{\mathrm{a}} = 0$, $p = p^{\mathrm{h}}$: $\mathcal{F}^{-1}(\Delta I) = 2p * h^{\mathrm{h}} + \underbrace{h^{\mathrm{h}} * h^{\mathrm{h}} - h^{\mathrm{a}} * h^{\mathrm{a}}}_{\operatorname{supp}() \subset 2\cdot\operatorname{conv}(\operatorname{supp}(h)) \subset \Omega_p}$.

Reconstruction of Complex-valued Objects

Theorem 4 (Reconstruction of small inclusions)

Let $p \in L^1_c(\mathbb{R}^m) \setminus \{0\}$ *be known and hermitean with* $\Omega_p := \operatorname{conv}(\operatorname{supp}(p))$. *Let*

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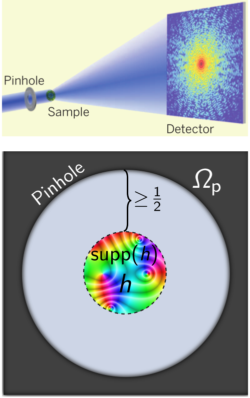

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- Corollary 3: $\mathcal{F}^{-1}(\Delta I)\,|_{\mathbb{R}^m \setminus \Omega_p} = \left(2p * h^{\mathrm{h}}\right)|_{\mathbb{R}^m \setminus \Omega_p}$ uniquely determines h^{h}

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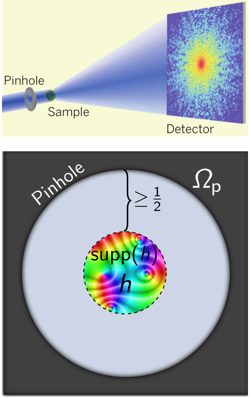

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- The *sign retrieval problem* (3.2b) is uniquely solvable up to "±" □

Reconstruction of Weak Phase Objects

Theorem 5 (Reconstruction of weak phase objects)

Let $p \in L^1_{\mathrm{c}}(\mathbb{R}^m) \setminus \{0\}$ *be known, hermitean and real-valued with* $\Omega_p := \operatorname{conv}(\operatorname{supp}(p))$. *Let*

$$A := \left\{ \mathrm{i}\phi : \phi \in L^1_{\mathrm{c}}(\mathbb{R}^m) \text{ real-valued}, \operatorname{supp}(\phi) \subset \Omega_p \right\}. \tag{3.3}$$

Then any $h \in A$ *is uniquely determined by the data* $\Delta I = |\mathcal{F}(p+h)|^2 - |\mathcal{F}(p)|^2$ *up to reflection* $h \mapsto h^{-}$. *Moreover,* h^{h} *and* $\pm h^{\mathrm{a}}$ *can be reconstructed via*

$$2p * h^{\mathrm{h}} = \mathrm{i}\Im\left(\mathcal{F}^{-1}(\Delta I)\right) \tag{3.4a}$$

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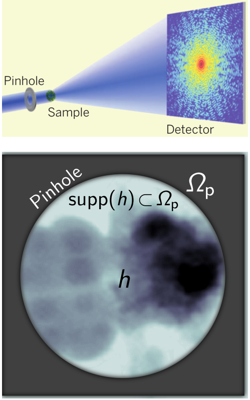

Fig.: Setting of Theorem 5

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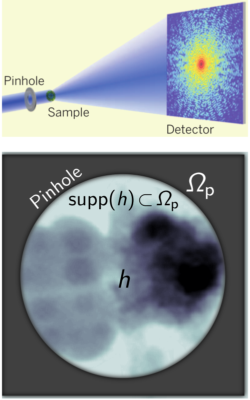

Fig.: Setting of Theorem 5

Proof:

- We have $\mathcal{F}^{-1}(\Delta I) = 2p * h^{\mathrm{h}} + h^{\mathrm{h}} * h^{\mathrm{h}} - h^{\mathrm{a}} * h^{\mathrm{a}}$
- $2p * h^{\mathrm{h}}$ is *purely imaginary* and $h^{\mathrm{h}} * h^{\mathrm{h}} - h^{\mathrm{a}} * h^{\mathrm{a}}$ is *real-valued* □

Simple Objects

X-ray CDI-contrast: $h \propto \exp\Big(-\mathrm{i} \underbrace{\phi}_{\text{phase shifts}} - \underbrace{\mu}_{\text{attenuation}} \Big) - 1.$

Definition 6 (Simple Objects)

We call a class of functions $A \subset L^1_{\mathrm{c}}(\mathbb{R}^m)$ *simple* if for any $h \in A$ and any $\Omega \subset \mathbb{R}^m$, the anti-Hermitean part $h^{\mathrm{a}}|_\Omega$ is uniquely determined by $h^{\mathrm{h}}|_\Omega$.

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Classes of Simple Objects:

- *Weak homogeneous objects:* For $a, b \in \mathbb{R} \setminus \{0\}$ fixed, let $A = \Big\{(a + \mathrm{i}b)\phi : \phi \in L^1_c(\mathbb{R}^m) \text{ real-valued}\Big\}$. Then

$$h^{\mathrm{a}}(x) = \frac{a}{b}\mathfrak{I}(h^{\mathrm{h}}(x)) + \frac{\mathrm{i}b}{a}\mathfrak{R}(h^{\mathrm{h}}(x)) \quad \text{a.e. for all} \quad h \in A$$

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$$h^a(x) = \frac{a}{b}\Im(h^h(x)) + \frac{\mathrm{i}b}{a}\Re(h^h(x)) \qquad \text{a.e. for all} \qquad h \in A$$

- *Pure phase objects:* For fixed sign "±", let $A = \Big\{\exp(\pm\,\mathrm{i}\phi) - 1 : \phi \in L^1_c(\mathbb{R}^m) \text{ real-valued, } 0 \le \phi < \frac{\pi}{2} \text{ a.e.}\Big\}$. Then

$$h^a(x) = \pm\,\mathrm{i}\frac{h^h(x) + 1}{|h^h(x) + 1|} \cdot (1 - |h^h(x) + 1|^2)^{\frac{1}{2}} \qquad \text{a.e. for all} \qquad h \in A$$

Reconstruction of Simple Objects

Theorem 7 (Reconstruction of simple objects)

Let $p \in L^1_c(\mathbb{R}^m) \setminus \{0\}$ *be known and hermitean with* $\Omega_p := \operatorname{conv}(\operatorname{supp}(p))$. *For some* $\varepsilon > 0$, *let*

$$A \subset \left\{ h \in L^1_c(\mathbb{R}^m) : \operatorname{supp}(h) \subset (1-\varepsilon) \cdot \Omega_p \right\}. \qquad (3.5)$$

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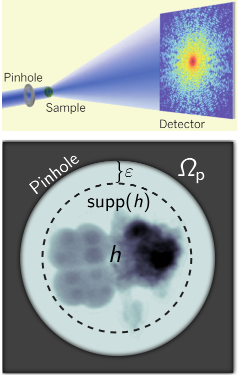

Fig.: Setting of Theorem 7

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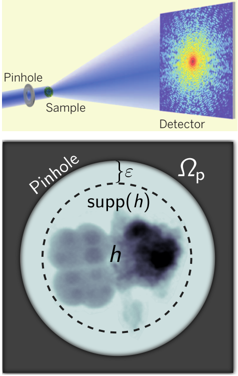
$$\begin{aligned}
&\text{Intialize:} && k = 0,\ h_0 = 0 \\
&\text{Iterate:} && g_k = \left(\mathcal{F}^{-1}(\Delta I) - h_k * h_k^{-}\right)|_{M_k} \\
& && \text{Solve } (2p * h^{\mathrm{h}}_{k+1})|_{M_k} = g_k \\
& && h_{k+1} = \left(h^{\mathrm{h}}_{k+1} + h^{\mathrm{a}}(h^{\mathrm{h}}_{k+1})\right)|_{\Omega_k} \\
& && k \leftarrow k+1
\end{aligned}$$



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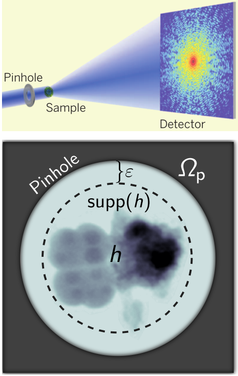
```

(with $M_k = \mathbb{R}^m \setminus (1+c_k) \cdot \Omega_p$, $\Omega_k := (1-\varepsilon)\Omega_p \setminus d_k \cdot \Omega_p$, $c_k = \max\{0, 1-(k+2)\varepsilon\}$ *and* $d_k = \max\{0, 1-(k+1)\varepsilon\}$.*)*



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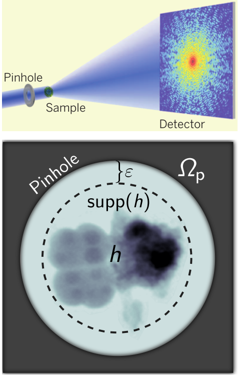


Fig.: Setting of Theorem 7

Remark:

Linear inversions + nonlinear data updates

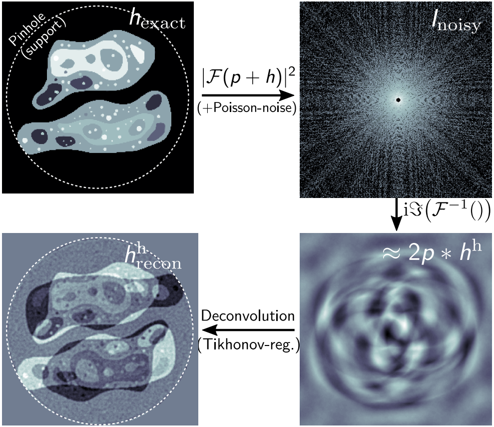
⇝ *Newton algorithm*

Numerical Examples and Conclusions

Proof-of-principle: Simulation of Weak Phase Object

Simulation:

- Circular probe $p = \mathbf{1}_{\text{circle}}$ (= reference signal)
- Weak phase object $h = p \cdot (\exp(-\mathrm{i}\phi) - 1)$ with $\phi \in [0; 0.3]$
- $I_{\text{noisy}} = |\mathcal{F}(p + h)|^2$ + Poisson noise
- Reconstruct $h^{\text{h}} \approx -\mathrm{i}\phi^{\text{a}}$ via linear deconvolution (cf. Theorem 5)



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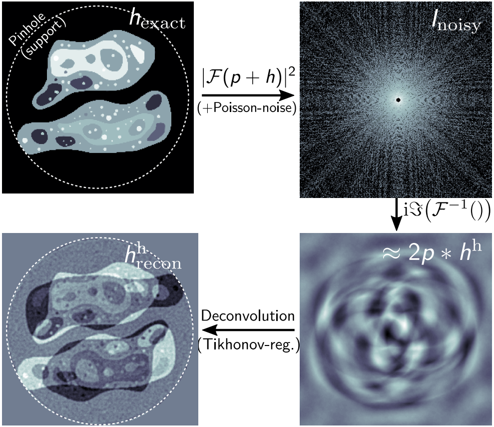


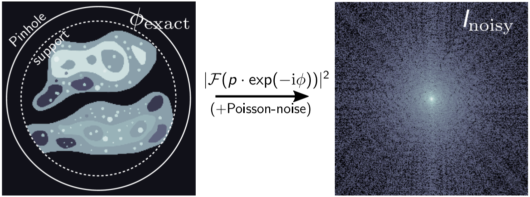
Observations:

- Stable and linear reconstruction of hermitean part h^{h}
- Remaining *nonlinear* reconstruction of h^{a} still challenging

Proof-of-principle: Simulation of Strong Phase Object

Simulation:

- Circular probe $p = \mathbf{1}_{\text{circle}}$ (= reference signal)
- Strong phase object $h = p \cdot (\exp(-\mathrm{i}\phi) - 1)$ with $\phi \in [0; 1]$ with smaller support than p
- $I_{\text{noisy}} = F(\phi) := |\mathcal{F}(p \cdot \exp(-\mathrm{i}\phi))|^2$ + Poisson noise



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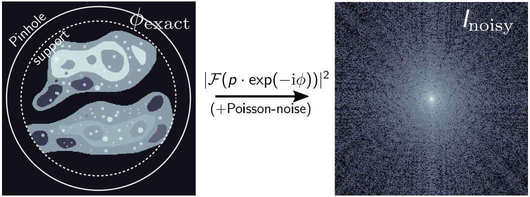
- Reconstruction by regularized Newton-method ($\rightsquigarrow$ Theorem 7)

$$\phi_{k+1} = \operatorname*{argmin}_{\phi} \|F(\phi_k) + F[\phi_k](\phi - \phi_k) - I_{\text{noisy}}\|^2 + \beta\|\phi - \phi_k\|_{L^2}^2 + \alpha\|\phi\|_{L^2}^2$$



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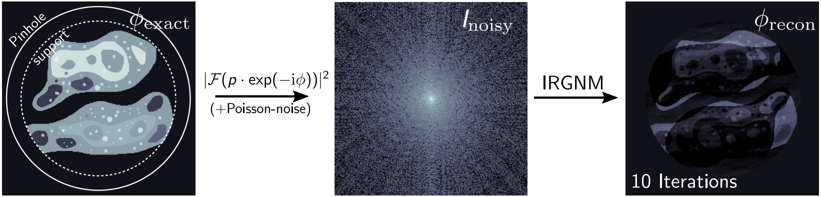

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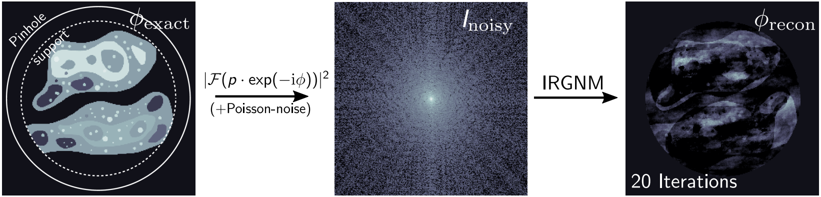

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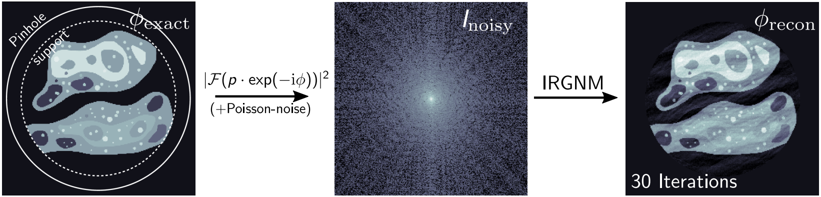

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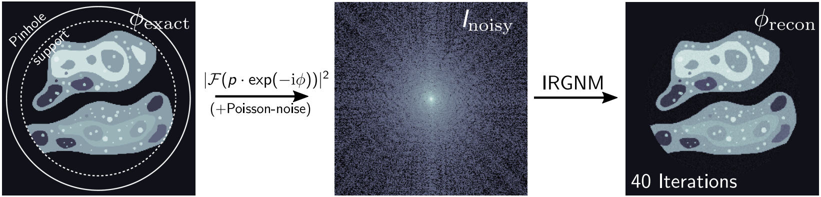

Observation: Feasible reconstruction as found in [Hohage and Werner, 2013]

Conclusions

Summary:

- CDI enables nanoscale X-ray imaging but requires phase retrieval
- Image reconstruction suffers from non-uniqueness + non-convexity
- ✓ Proved uniqueness and reconstruction formulas in the presence of a suitable reference signal $\rightsquigarrow$ *holographic approach*
- ✓ ... *deterministic*, dimension-indepedent uniqueness without restrictive structural assumptions on the object
- ✓ Main tool/reasoning: support arguments
- ✓ *Numerically*: stable recovery in experimentally relevant settings

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- CDI enables nanoscale X-ray imaging but requires phase retrieval
- Image reconstruction suffers from non-uniqueness + non-convexity

✓ Proved uniqueness and reconstruction formulas in the presence of a suitable reference signal $\rightsquigarrow$ *holographic approach*

✓ ... *deterministic*, dimension-indepedent uniqueness without restrictive structural assumptions on the object

✓ Main tool/reasoning: support arguments

✓ *Numerically*: stable recovery in experimentally relevant settings

Future Work:

- Extend to more general (*non-Hermitean*) reference signals
- Apply holographic approach to other experimental settings

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