Thesis to get the degree of a Master of Science

Title of the thesis

Subtitle

Avina Chetana Kalle

20th March 2023

Universität Hamburg
Faculty of Mathematics, Informatics and Natural Sciences
Department of Mathematics

Supervisor
Prof. Dr. Christina Brandt

Reviewers
Prof. Dr. aaa bbb
Prof. Dr. xxx yyy

Acknowledgments

...

Contents

List of Figures

Abstract

Abstract/Summary text

1. Introduction

1.1. Problem Description

1.2. Objective

1.3. Investigative Approach

This thesis will be investigating the problem using theoretical, numerical and computational methods.

Computational methods, like simulating the problem, the algorithms and displaying data, are done using the programming language Julia 1.4.2 [BEKS17] with the use of the following libraries:

1. LinearAlgebra
2. Plots [CSR+22] with the GR Plots backend.
3. FFTW [FJ05]
4. OffsetArrays [Off]
5. ColorSchemes [Col]
6. StatsBase [Sta]

The Julia scripts (.jl files) referenced in this thesis is available in the compact disc (CD) attached to the hardcopy and are uploaded to Github (https://github.com/AvinacK/MScThesis_Ptychography). They are original works of the author and the references used to write each script are mentioned in this thesis and in the scripts themselves.

1.4. Outline

2. Pre-requisite Concepts

2.1. Fourier Transformation

Define the following notations in continuous and discrete spaces:

Definition 2.1. (Fourier Transform) Consider the function $f(x) : \mathbb{R} \to \mathbb{C}$. The continuous Fourier transform (FT) of $f(x)$ is defined by

$$\begin{aligned} &\mathcal{F} : \mathbb{C} \to \mathbb{C} \\ &\mathcal{F}[f(x)] = F(\omega) = \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-i\omega x)\, dx \end{aligned} \tag{2.1}$$

Definition 2.2. (Fourier Transform) Similarly, the continuous inverse Fourier transform (IFT) of $F(x)$ is defined by

$$\begin{aligned} &\mathcal{F}^{-1} : \mathbb{C} \to \mathbb{C} \\ &\mathcal{F}^{-1}[F(x)] = f(\omega) = \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(x) \exp(i\omega x)\, d\omega \end{aligned} \tag{2.2}$$

Definition 2.3. (Discrete Fourier Transform) Consider a vector $\mathbf{z} = [z_0, z_1, ..., z_{N-1}] \in \mathbb{C}^N$. The discrete Fourier transform (DFT) of $\mathbf{z}$ is $\mathbf{Z} := [Z_0, Z_1, ..., Z_{N-1}]$ and is defined by

$$\begin{aligned} &\mathbb{F} : \mathbb{C}^N \to \mathbb{C}^N \\ &\mathbb{F}(\mathbf{z}) = \mathbf{Z}; \qquad Z_k = \textstyle\sum_{n=0}^{N-1} z_n \exp\left(-i\frac{2\pi}{N}kn\right) \end{aligned} \tag{2.3}$$

Definition 2.4. Similarly, the discrete inverse Fourier transform (DIFT) is defined as

$$\begin{aligned} &\mathbb{F}^{-1} : \mathbb{C}^N \to \mathbb{C}^N \\ &\mathbb{F}^{-1}(\mathbf{Z}) = \mathbf{z}; \qquad z_k = \tfrac{1}{N} \textstyle\sum_{n=0}^{N-1} Z_n \exp\left(i\frac{2\pi}{N}kn\right) \end{aligned} \tag{2.4}$$

	Continuous variable/ operation	Discrete equivalent
Time coordinate	$x \in \mathbb{R}$	$n\Delta x \in \mathbb{R}, n \in \mathbb{Z}$
Frequency coordinate	$\omega \in \mathbb{R}$	$m\Delta\omega \in \mathbb{R}, m \in \mathbb{Z}$
Fourier transform	$\mathcal{F}$	$\mathbb{F}$
Inverse Fourier transform	$\mathcal{F}^{-1}$	$\mathbb{F}^{-1}$

Table 2.1.: Continuous and discrete variables and operations

Remark 2.1. The discrete spacing of the real/ time space (i.e., Δx) and the discrete spacing of the reciprocal/ frequency space (i.e., $\Delta\omega$) is inversely related as follows:

$$\Delta x = \frac{1}{\Delta\omega} . \frac{2\pi}{N} \tag{2.5}$$

Proof. As a consequence of the definitions of continuous and discrete Fourier transform (2.1 and 2.3), the exponential functions must be equal:

$$\begin{aligned}
&\exp\left(-i\omega x\right) = \exp\left(im\Delta\omega \cdot n\Delta x\right) = \exp\left(-i\tfrac{2\pi}{N}mn\right) \\
&\implies im\Delta\omega \cdot n\Delta x = \tfrac{2\pi}{N}mn \\
&\therefore \Delta\omega\Delta x = \tfrac{2\pi}{N}
\end{aligned}$$

□

2.2. Some useful functions and their Fourier transforms

In the course of this project, there are some important functions that will be used.

Definition 2.5. (Lorentzian function) [Wei]: For $x \in \mathbb{R}$, the Lorentzian function is defined by

$$\begin{aligned}
L : \mathbb{R} \to \mathbb{R} \\
L(x; x_0, \Gamma) = \tfrac{1}{\pi} \tfrac{\frac{1}{2}\Gamma}{(x-x_0)^2 + \left(\frac{1}{2}\Gamma\right)}
\end{aligned} \tag{2.6}$$

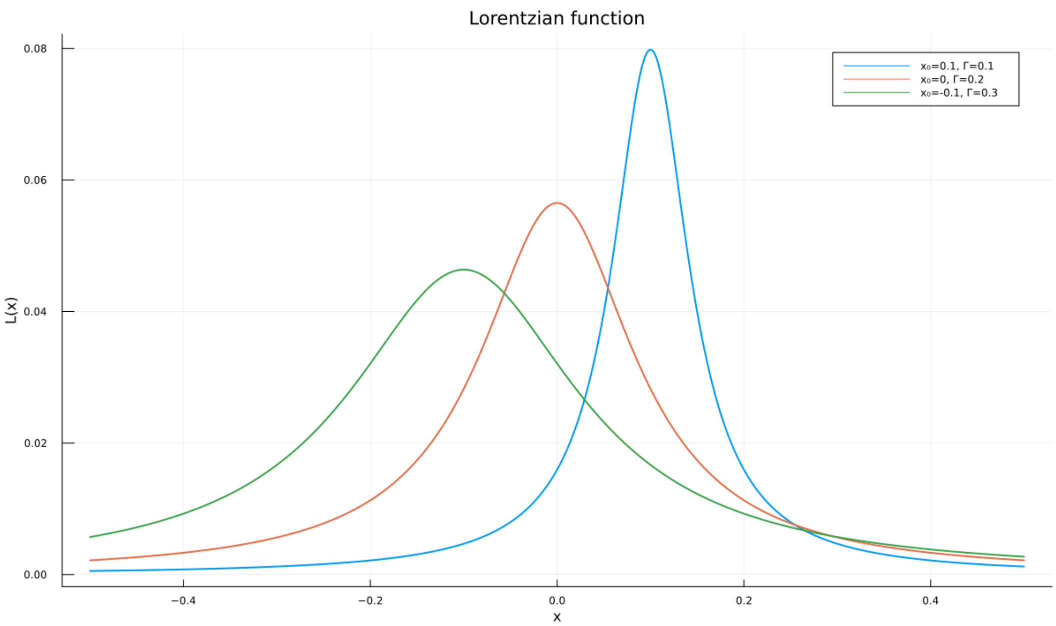


Figure 2.1.: Lorentzian function

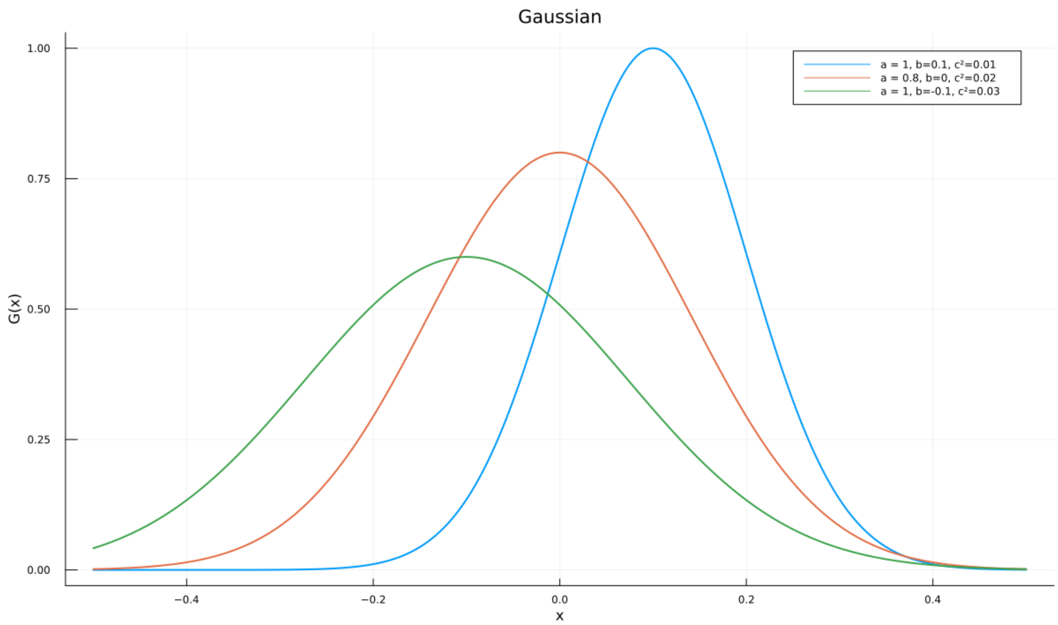


Figure 2.2.: Gaussian function

where $x_0 \in \mathbb{R}$ is the centre and $\Gamma \in \mathbb{R}^+$ is a parameter specifying the width of the function. It is normalized such that $\int_{-\infty}^{\infty} L(x) = 1$. Figure 2.1 shows the Gaussian function.

The Fourier transform of the Lorentzian function is

$$\mathcal{F}\left[L\right](k) = \exp\left(-2\pi i k x_0 - \Gamma\pi\left|k\right|\right) \tag{2.7}$$

Definition 2.6. (Gaussian function) [Wik22]: For $x \in \mathbb{R}$, the Gaussian function is defined by

$$\begin{aligned} G &: \mathbb{R} \to \mathbb{R} \\ G(x) &= a\exp\left(-\frac{(x-b)^2}{2c^2}\right) \end{aligned} \tag{2.8}$$

where $a \in \mathbb{R}^+$ is the height of the peak, $b \in \mathbb{R}$ is the centre of the peak and $c \in \mathbb{R}^+$ specifies the width of the curve. Figure 2.2 shows the Gaussian function.

The Fourier transform of a simple Gaussian function $G_s(x) = a\exp\left(-\frac{x^2}{2c^2}\right)$ is

$$\mathcal{F}\left[G\right](k) = ac\sqrt{2\pi}\exp\left(-2\pi^2k^2c^2\right) \tag{2.9}$$

Definition 2.7. (Step function) For $x \in \mathbb{R}$, $a_i \in \mathbb{R}$and $A_i$are disjoint intervals, the step function is defined by

$$\begin{aligned} &S : \mathbb{R} \to \mathbb{R} \\ &S(x) = \textstyle\sum_i a_i\chi_{A_i}(x)\,; \quad \chi_{A_i}(x) = \begin{cases} 1 & x \in A \\ 0 & x \notin A \end{cases} \end{aligned} \tag{2.10}$$

Definition 2.8. Schur (or Hadamard) product [Mil07]: Let $M_{m \times n}$ be the set of matrices of dimension $m \times n$. For $A, B \in M_{m \times n}$, the Schur product $A \circ B$ is defined to be:

$$\begin{aligned} \circ : M_{m \times n} &\to M_{m \times n} \\ (A \circ B)_{ij} = (B \circ A)_{ij} &= (A)_{ij} (B)_{ij} \end{aligned} \tag{2.11}$$

Equivalently, this function can be called an element-wise function of multiplication.

3. Nuclear Phase Retrival Spectroscopy

3.1. Experimental Set-up

A schematic of the Nuclear Phase Retrieval Spectroscopy (NPRS) is shown in Figure 3.1. A synchrotron source emits synchrotron radiation (SR). SR has high spectral brightness and can be easily focus on to small objects (at the micrometre scale). [BG19]

This radiation is initially scattered by the probe (which may be of known properties) and then scattered by the target/ object. The scattered light's intensity is, then, measured by the detector.

The probe is shifted forwards and backwards to create multiple detected data. It is important to know that the probe is shifted in such a way that there are overlaps in each dataset. These data and the mathematical model are used to retrieval the complex energy response of the sample.

3.2. Mathematical Formulation

Let us define the following notations:

1. Energy range:

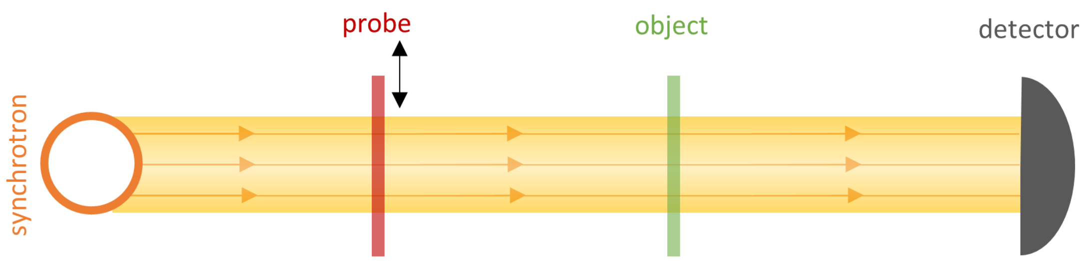


Figure 3.1.: Schematic of the Nuclear Phase Retrival Spectroscopy set-up

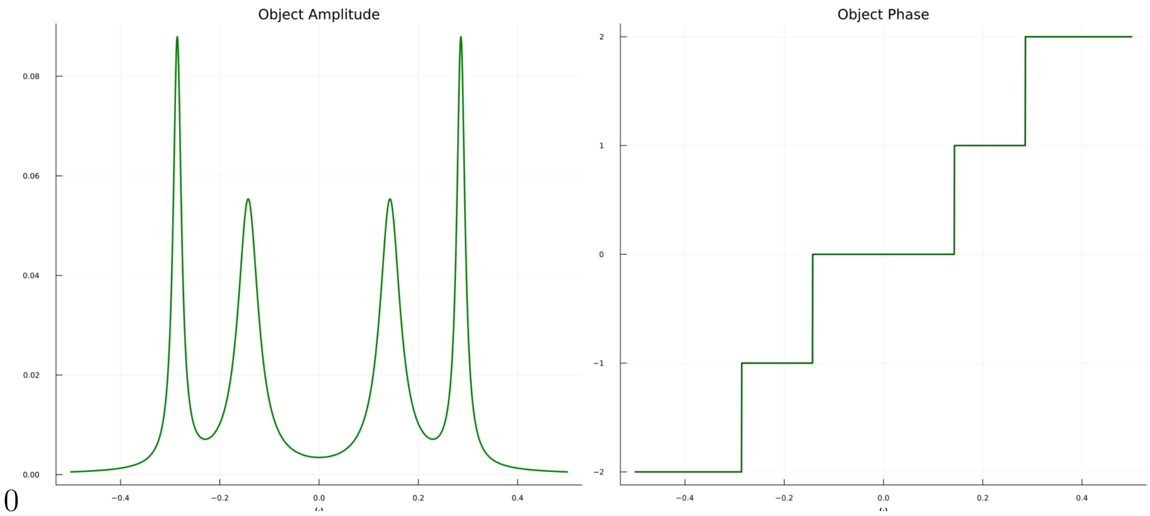


Figure 3.2.: Response function of the object

   a) The energy range is an interval of the real line. The response function of the object and probe is defined on it.

   b) Discretize the energy (frequency) range as $\boldsymbol{\omega} = [-M\omega, M\omega] \subset \mathbb{R}$ with a step-size of $\Delta\omega \in \mathbb{R}$ and $2M + 1$ is the number of elements in the range. Each element is denoted by ω_j where $j \in [1, 2M + 1] \subset \mathbb{Z}^+$.

2. Time range:

   a) Like the energy range, the time range is also an interval of the real line. The fourier transform of functions are defined on it.

   b) Discretize the time (space) range as $\mathbf{x} = [-N\Delta x, N\Delta x] \subset \mathbb{R}$ with a step-size of $\Delta x \in \mathbb{R}$ whose value is given by Equation 2.5 and $2N + 1$ is the number of elements in the range.
   Each element is denoted by x_j where $j \in [1, 2N + 1] \subset \mathbb{Z}^+$.

3. Response function of the object: $\mathcal{O}(\omega)$.

   a) In general, the response function of the object is a function that is defined on the energy range and has complex (with phase $\theta_{\mathcal{O}}$) or real values.

$$\begin{aligned} &\mathcal{O} : \mathbb{R} \to \mathbb{C} \\ &\omega \to \mathcal{O}(\omega); \quad \mathcal{O}(\omega) = |\mathcal{O}(\omega)| \exp\left(i\theta_{\mathcal{O}}\left(\omega\right)\right) \end{aligned} \tag{3.1}$$

   b) In NPRS, the response function of the sample can be constrained by the following:

      i. Defined on a finite (energy) domain: $[-M\omega, M\omega] \subset \mathbb{R}$. This is due to the finite nature of the experimental object.

$$\mathcal{O}(\omega) = 0, \quad \text{for} \omega \notin [-M\omega, M\omega]$$

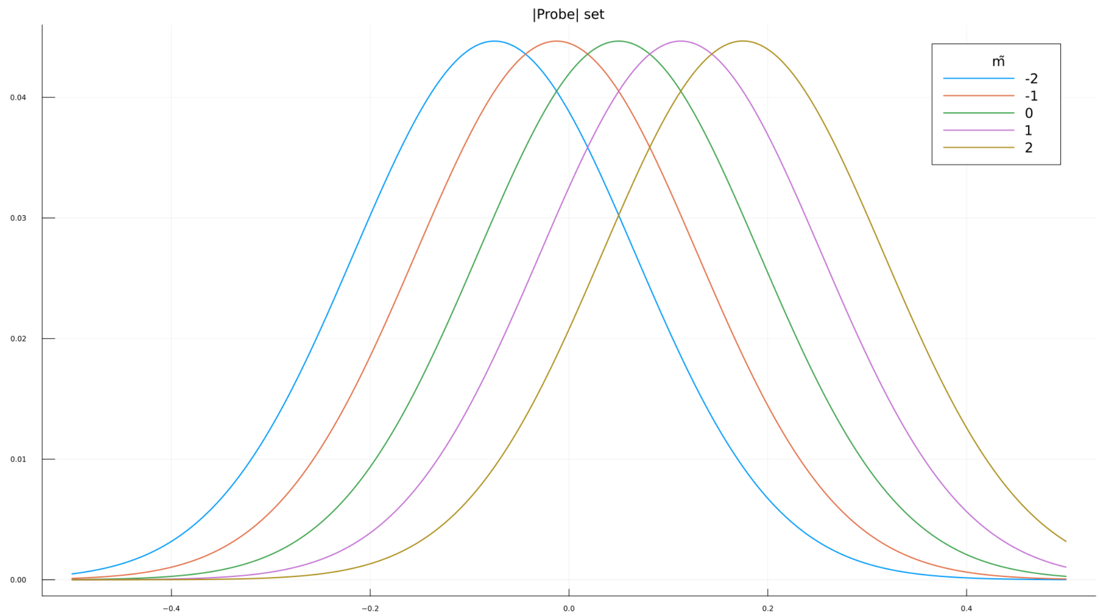


Figure 3.3.: Example of (the amplitude of the) probe set

ii. $\mathcal{O}(\omega)$ is bounded.

$$\mathcal{O}(\omega) < \infty$$

c) In this thesis, we shall aim to use the following functions:

$$\begin{aligned} |\mathcal{O}(\omega)| = & \quad \sum_i L\left(x; x_i, \Gamma_i\right) \\ \theta_{\mathcal{O}}\left(\omega\right) = & \quad \sum_i a_i \chi_{A_i}\left(x\right) \end{aligned} \tag{3.2}$$

The modulus part is a sum of Lorentzian functions (as given by Equation 2.6) and the phase is a step function (as given by Equation 2.10). The above equation is illustrated in Figure 3.2.

d) Discretized, this is the vector

$$\boldsymbol{O}\left(\boldsymbol{\omega}\right) = (\mathcal{O}(-\omega_{max}), \mathcal{O}(-\omega_{max} - \Delta\omega), ..., \mathcal{O}(\omega), \mathcal{O}(\Delta\omega), ..., \mathcal{O}(\omega_{max})) \tag{3.3}$$

4. Response function of the probe: $\mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega)$.
Here, $\tilde{m} \in [-\tilde{m}_{max}, \tilde{m}_{max}] \subset \mathbb{Z}$ represents the shift in the probe to create multiple data intensities.

   a) In general, the response function of the phase is a function that is defined on the energy range and has complex (with phase $\theta_{\mathcal{P}}$) or real values.

$$\mathcal{P} : \mathbb{R} \to \mathbb{C}$$
$$\omega \to \mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega); \quad \mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega) = |\mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega)| \exp\left(i\theta_{\mathcal{P}}\left(\omega + \tilde{m}\Delta\omega\right)\right)$$

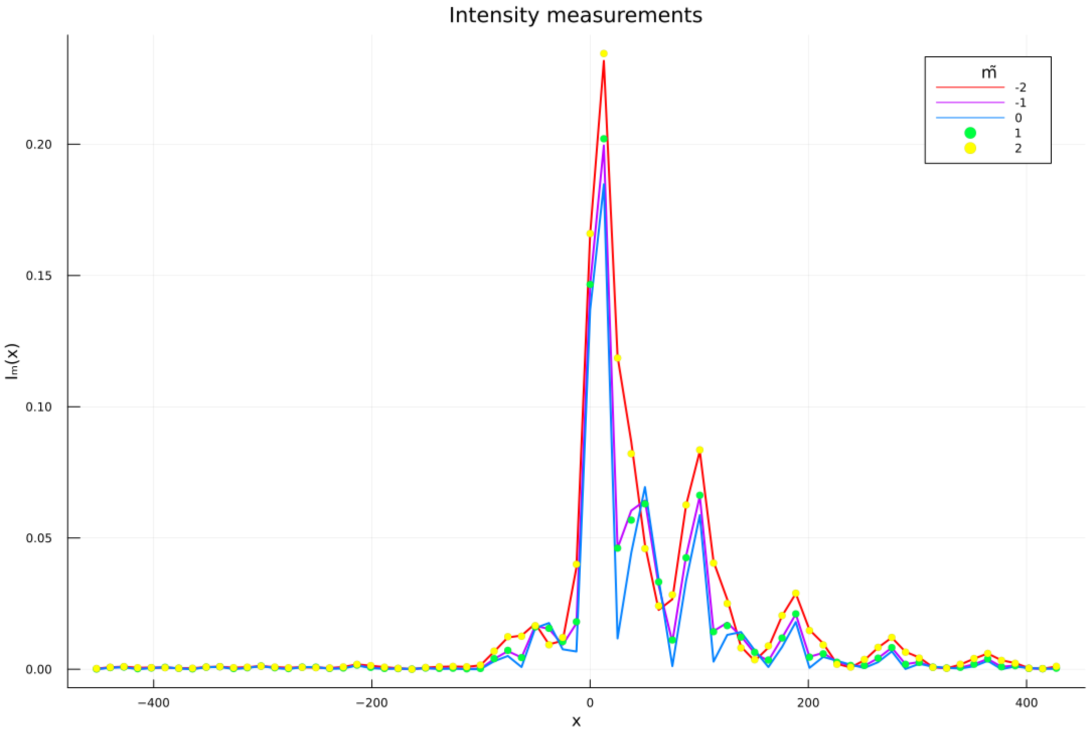


Figure 3.4.: Intensity measurements

$$ \tag{3.4}$$

An example of such a function is illustrated in Figure 3.3.

b) Similar to the case of the object, the following constraints are made on the probe function:

i. Defined on a finite (energy) domain: $[-M\omega, M\omega] \subset \mathbb{R}$.

$$\mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega) = 0, \quad \text{for}(\omega + \tilde{m}\Delta\omega) \notin [-M\omega, M\omega]$$

ii. $\mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega)$ is bounded.

iii. $\mathcal{P}_{\tilde{m}}(\omega + \tilde{m}\Delta\omega)$ is non-negative.

c) Discretized, this is the vector

$$\boldsymbol{P}_{\tilde{m}} = \left(\mathcal{P}\left(\left(\tilde{m} - M\right)\Delta\omega\right), ..., \mathcal{P}\left(\tilde{m}\Delta\omega\right), ..., \mathcal{P}\left(\left(m + M\right)\Delta\omega\right)\right) \tag{3.5}$$

5. Measured intensities : $I_{\tilde{m}}\left(x\right)$ is a sequence of $\tilde{m}$ measurements

a) The function that defines the measured intensity for a particular $\tilde{m}$ is as follows:

$$\begin{gathered} I : \left(\mathcal{O}, \mathcal{P}_{\tilde{m}}\right) \to \mathbb{R} \\ I_{\tilde{m}}(x) = \left|\mathcal{F}\left[\mathcal{O}\left(\omega\right) \circ \mathcal{P}_{\tilde{m}}\left(\omega\right)\right]\right|^2 \end{gathered} \tag{3.6}$$

b) Discretized, this can be written as:

$$\begin{aligned} &\boldsymbol{I} : (\boldsymbol{O}, \boldsymbol{P}_{\tilde{m}}) \rightarrow \mathbb{R}^{2N+1} \\ &\boldsymbol{I}_{\tilde{m}}(\mathbf{x}) = \left|\mathbb{F}\left[\boldsymbol{O} \circ \boldsymbol{P}_{\tilde{m}}\right]\right|^2 \end{aligned} \tag{3.7}$$

An example of this intensity measurements is illustrated in Figure 3.4.

c) The measured intensities have the following properties:

i. Since it involves a fourier transformation, the domain is the time range: $\mathbf{x} = [-N\Delta x, N\Delta x] \ni x$.

$$I_{\tilde{m}}(x) = 0, \quad \text{for} x \notin \mathbf{x}$$

ii. $I_{\tilde{m}}(x)$ is bounded. ($\because$ $\mathcal{O}$ and $\mathcal{P}_{\tilde{m}}$are bounded, and $\mathcal{F}$ is a bounded function)

$$I_{\tilde{m}}(x) < \infty$$

iii. $I_{\tilde{m}}(x)$ is non-negative. ($\because |\quad|^2 \geq 0$)

$$I_{\tilde{m}}(x) \geq 0 \quad \forall x \in \mathbb{R}$$

3.2.1. Naïve Reconstruction

A very naïve reconstruction (NR) of this problem is to take the square root, "ignore" the absolute value function, inverse fourier transform and then divide by the probe function (described in Figure 3.5). This is, theoretically, wrong; however, for the sake of practical knowledge, we shall implement this method.

The results of this "algorithm" is shown in Figure 3.5. As one can see, both graphs show an incredible deviation from the expected function.

The next natural step to try is to take the average of all the obtained objects. The results are as follows:

3.2.2. Uniqueness of solution

As seen from Equation 3.6, the measurable quantity is the intensity, from which we would like to find the object. For a particular intensity, is the object function unique?

Let us take a much simpler case: Given two complex signals $f_1(x)$ and $f_2(x)$ such that $|\mathcal{F}[f_1(x)]|^2 = |\mathcal{F}[f_2(x)]|^2$, is $f_1(x) = f_2(x)$? Unfortunately, not.

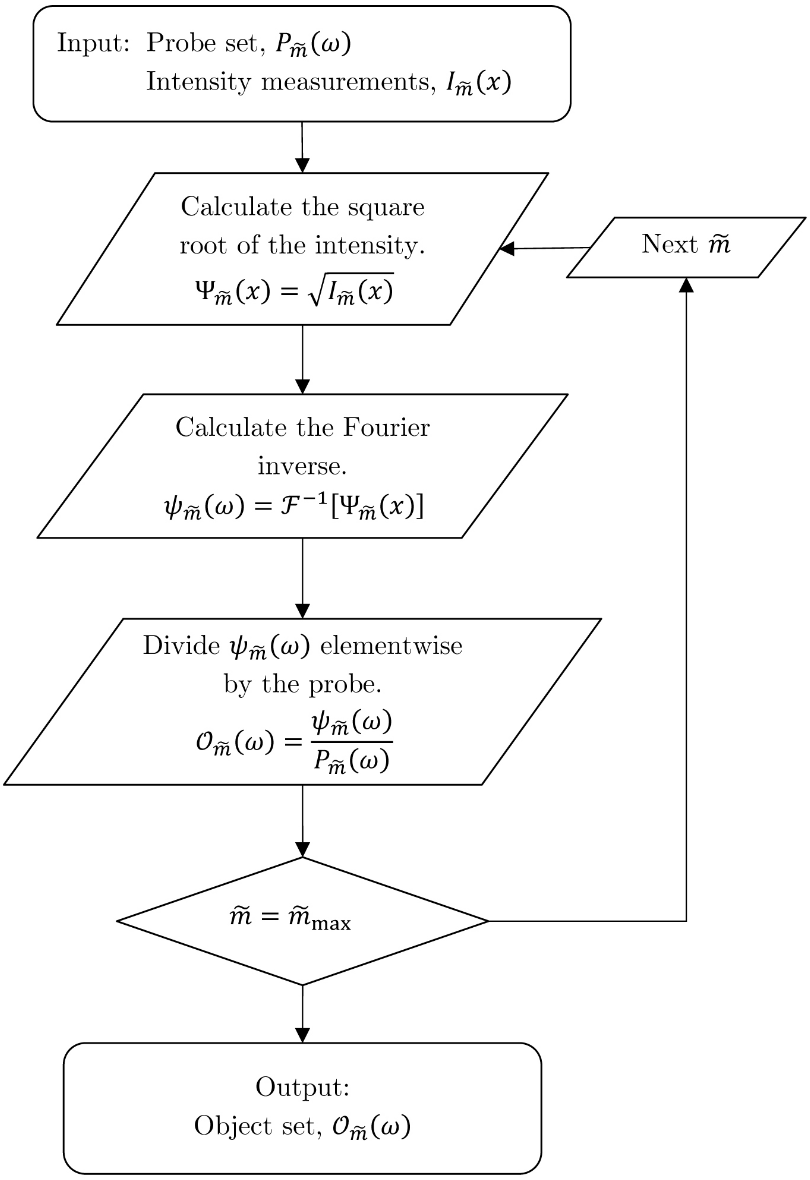
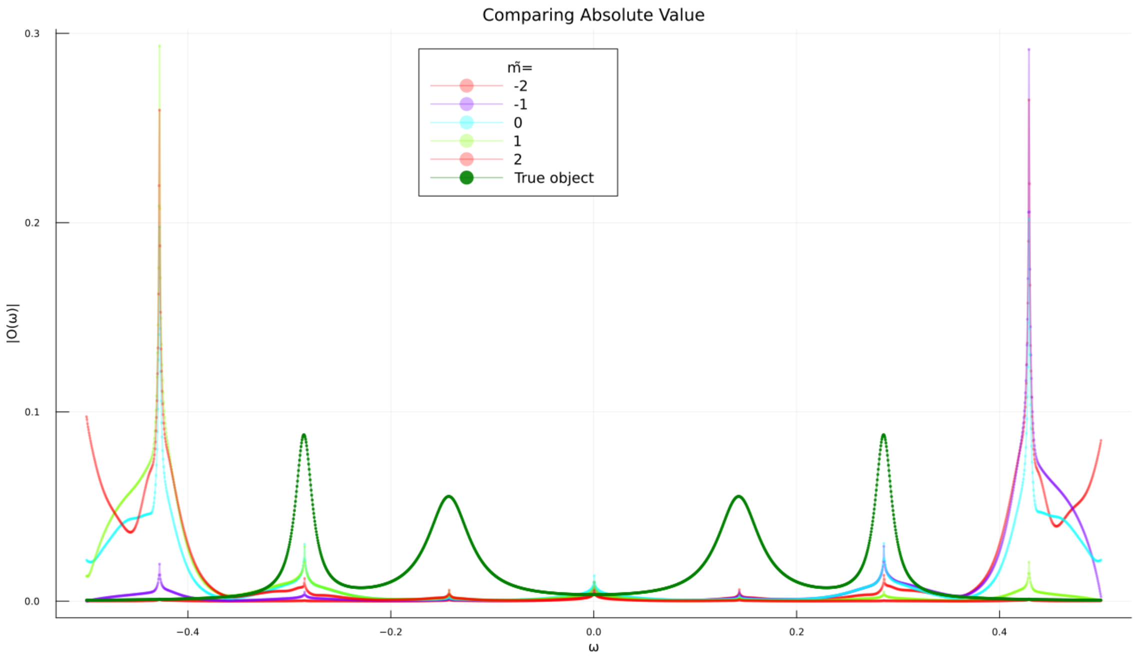
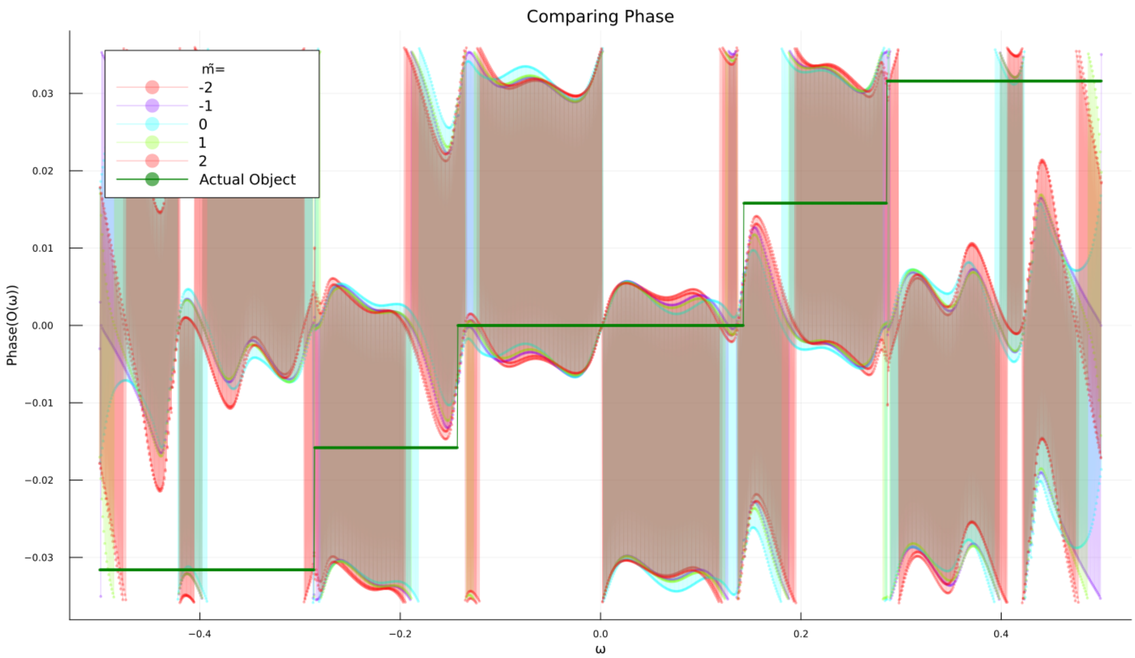


Figure 3.5.: Naïve Reconstruction

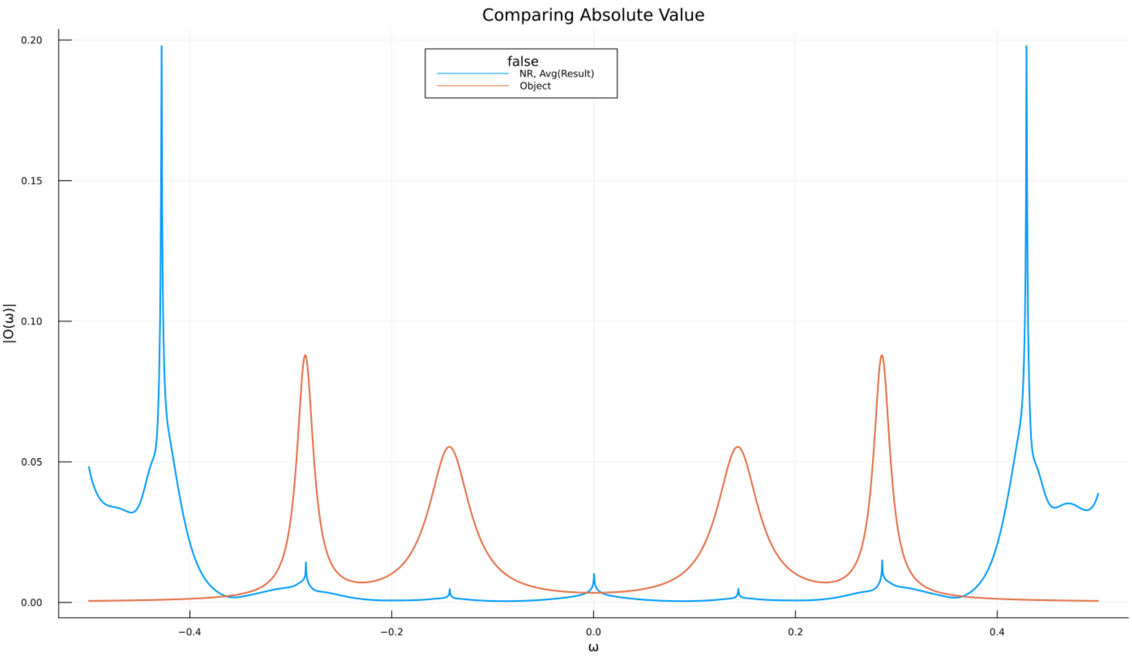


(a) NR: Comparing absolute value of result(s)

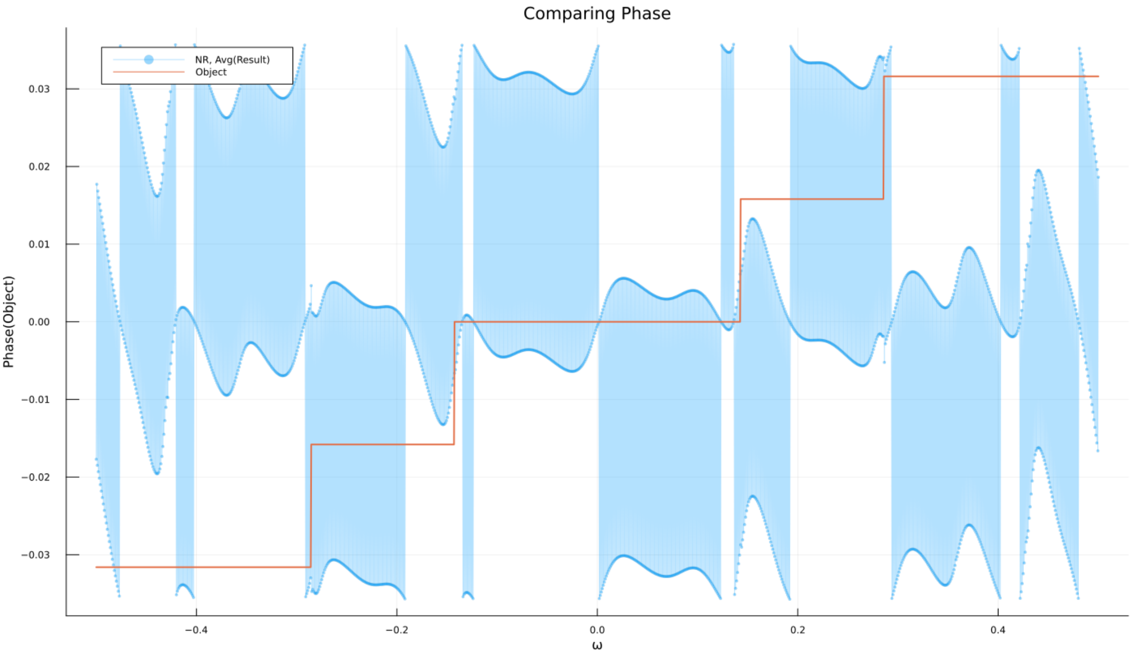


(b) NR: Comparing phase result(s)

Figure 3.6.: Naïve reconstruction of the object



(a) NR: Comparing absolute value of average result and true object



(b) NR: Comparing phase of average result and true object

Figure 3.7.: Average of naïve reconstruction

Proof. Let $\mathcal{F}\left[f_1\left(x\right)\right] = g_1\left(\omega\right)$ and $\mathcal{F}\left[f_2\left(x\right)\right] = g_2\left(\omega\right)$

$$\begin{aligned}
&\implies |g_1(\omega)|^2 = |g_2(\omega)|^2 \\
&\implies |g_1(\omega)| = |g_2(\omega)| \\
&\implies g_1\left(\omega\right) = g_2\left(\omega\right)\exp\left(i \cdot \varphi(\omega)\right) \quad \text{where} \varphi : \omega \to \varphi(\omega) \in \mathbb{R} \\
&\implies f_1\left(x\right) \neq f_2\left(x\right)
\end{aligned}$$

□

To combat the problem, the shifting probe is used in the hope of reaching a unique solution from multiple readings.

3.3. Ptychographic Iterative Engines

Ptychographic iterative engines (PIEs) are algorithms that use an initial object guess, the measured intensities and an iterative update function to calculate the unknown object's phase and modulus.

3.3.1. Rodenburg-Faulkner PIE

One of the PIEs that shall be explored in this thesis was described by Rodenburg and Faulkner, in 2004.[RF04] It is described by the following algorithm:

1. Create an initial object function (which is guessed): $O_{g,n}(\omega)$ where g represents that it is guessed and n represents the iteration number. This function should satisfy all the conditions mentioned in 3b.

2. Take the probe at a shift $\tilde{m}$,$\left(P\left(\omega + \tilde{m}\Delta\omega\right)\right)$, and multiple it with the guessed object to create:

$$\psi_{g,n}\left(\omega, \tilde{m}\right) = O_{g,n}(\omega) \circ P\left(\omega + \tilde{m}\Delta\omega\right) \tag{3.8}$$

3. Fourier transform the above function $\psi_{g,n}$ to find the function in the time domain: $\Psi_{g,n}\left(x, \tilde{m}\right)$. This can also be rewritten in terms of its amplitude $\left(\left|\Psi_{g,n}\left(x, \tilde{m}\right)\right|\right)$ and phase $\left(\theta_{g,n}\left(x, \tilde{m}\right)\right)$.

$$\Psi_{g,n}\left(x, \tilde{m}\right) = \mathcal{F}\left[\psi_{g,n}(\omega, \tilde{m})\right] = \left|\Psi_{g,n}\left(x, \tilde{m}\right)\right| \exp\left(i\theta_{g,n}\left(x, \tilde{m}\right)\right) \tag{3.9}$$

4. Replace the modulus of the above function with the corresponding known value (from the intensity measurements, $I_{\tilde{m}}(x) = \left|\Psi_{k,n}\left(x, \tilde{m}\right)\right|^2$).

$$\Psi_{k,n}\left(x, \tilde{m}\right) = \left|\Psi_{k,n}\left(x, \tilde{m}\right)\right| \exp\left(i\theta_{g,n}\left(x, \tilde{m}\right)\right) \tag{3.10}$$

5. Inverse fourier transfrom the above back to the energy space to create a new guessed version.

$$\psi_{k,n}\left(\omega,\tilde{m}\right)=\mathcal{F}^{-1}\left[\Psi_{k,n}\left(x,\tilde{m}\right)\right] \tag{3.11}$$

6. Using an update function, calculate the new guessed object function, where $\alpha(>0)\in\mathbb{R}$ and $\beta(>0)\in\mathbb{R}$ are chosen parameters.

$$\begin{aligned}O_{g,n+1}(\omega)=O_{g,n}(\omega)+\frac{|P\left(\omega+\tilde{m}\Delta\omega\right)|}{|P_{max}\left(\omega+\tilde{m}\Delta\omega\right)|}\frac{P^{*}\left(\omega+\tilde{m}\Delta\omega\right)}{\left(|P\left(\omega+\tilde{m}\Delta\omega\right)|^{2}+\alpha\right)}\\ \times\beta\left(\psi_{k,n}\left(\omega,\tilde{m}\right)-\psi_{g,n}\left(\omega,\tilde{m}\right)\right)\end{aligned} \tag{3.12}$$

The paramater α ensures that $\left(|P\left(\omega+\tilde{m}\Delta\omega\right)|^{2}+\alpha\right)>0$.

7. Measure the sum squared error (SSE) and check if it adequately small (i.e., if it is smaller than a certain ϵ).

$$\mathrm{SSE}=\frac{\left(|\Psi_{k,n}\left(x,\tilde{m}\right)|^{2}-|\Psi_{g,n}\left(x,\tilde{m}\right)|^{2}\right)^{2}}{2N+1} \tag{3.13}$$

8. If the SSE is not small enough, repeat the steps 2 to 7 until it is.

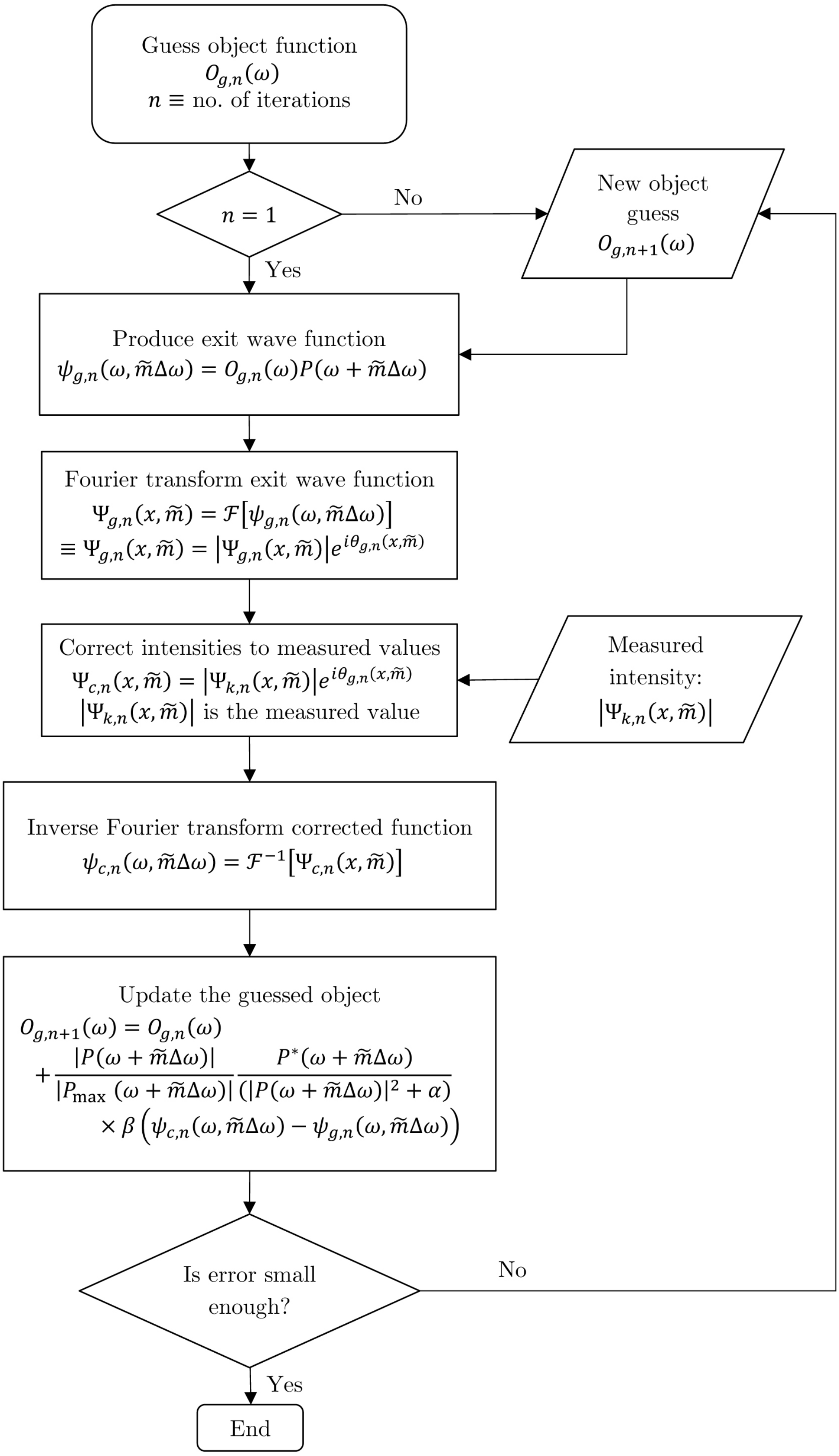


Figure 3.8.: Rodenburg-Faulkner Ptychographic Iterative Engine

A. Appendix

A.1. Notations

$\mathbb{C}$	Complex number
F	Fourier transform (continuous)
$\mathbb{F}$	Fourier transform (discrete)
$\omega \in \mathbb{R}$	Frequency coordinate (continuous)
$m\Delta\omega \in \mathbb{R}$ $m \in \mathbb{Z}$	Frequency coordinate (continuous)
G	Gaussian function
$\mathcal{F}^{-1}$	Inverse Fourier transform (continuous)
$\mathbb{F}^{-1}$	Inverse Fourier transform (discrete)
L	Lorentzian function
NPRS	Nuclear Phase Retrieval Spectroscopy
$\mathbb{R}$	Real number
$\mathcal{O}(\omega)$	Response function of the object
$\circ$	Schur product
SR	Synchrotron radiation
$x \in \mathbb{R}$	Time coordinate (continuous)
$n\Delta x \in \mathbb{R}$ $n \in \mathbb{Z}$	Time coordinate (discrete)

Bibliography

[BEKS17] Jeff Bezanson, Alan Edelman, Stefan Karpinski, and Viral B Shah. Julia: A fresh approach to numerical computing. *SIAM review*, 59(1): 65–98, 2017, https://doi.org/10.1137/141000671.

[BG19] Amardeep Bharti and Navdeep Goyal. Fundamental of synchrotron radiations. In Daisy Joseph, editor, *Synchrotron Radiation*, chapter 2. IntechOpen, Rijeka, 2019.

[Col]

[CSR+22] Simon Christ, Daniel Schwabeneder, Christopher Rackauckas, Michael Krabbe Borregaard, and Thomas Breloff. Plots.jl – a user extendable plotting api for the julia programming language, 2022.

[FJ05] Matteo Frigo and Steven G. Johnson. The design and implementation of FFTW3. *Proceedings of the IEEE*, 93(2): 216–231, 2005. Special issue on “Program Generation, Optimization, and Platform Adaptation”.

[Mil07] Million, Elizabeth. The hadamard product, 2007.

[Off]

[RF04] J. M. Rodenburg and H. M. L. Faulkner. A phase retrieval algorithm for shifting illumination. *Applied Physics Letters*, 85(20): 4795–4797, 2004, https://doi.org/10.1063/1.1823034.

[Sta]

[Wei] Eric W. Weisstein. Lorentzian function. Visited on 20/10/2022.

[Wik22] Wikipedia contributors. Gaussian function — Wikipedia, the free encyclopedia, 2022. [Online; accessed 20-October-2022].