Thesis to get the degree of a Master of Science

Title of the thesis

Subtitle

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Acknowledgments

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1. Introduction

1.1. Problem Description

Nuclear Resonance Phase Spectroscopy (NRPS) is a nuclear physics technique used to study the properties of nuclei in solids and liquids. It involves the excitation of a sample with high-energy synchrotron radiation, and the measurement of the scattered radition in order to extract information about the sample.

Let $\mathcal{O}(\omega)$ be the object (or sample), the measurement (of intensity, $I(x)$) taken is defined by:

$$I(x) = \left|\mathcal{F}\left[\mathcal{O}(\omega)\right]\right|^2$$

where $\mathcal{F}$ is the fourier transformation function.

Due to problems with the uniqueness of a solution (further described in 3.2.1.2), multiple probes ($\mathcal{P}_{\tilde{m}}(\omega)$, indexed by $\tilde{m}$) are introduced and the problem becomes:

$$I_{\tilde{m}}(x) = \left|\mathcal{F}\left[\mathcal{O}(\omega) \circ \mathcal{P}_{\tilde{m}}(\omega)\right]\right|^2$$

where we need to find the complex function $\mathcal{O}(\omega)$ with known $I_{\tilde{m}}(x)$ measurements.

1.2. Investigative Approach

This thesis will be investigating the problem using theoretical, numerical and computational methods. The main steps are as follows:

1. Literature Review
2. Defining the research question
3. Mathematically formulate and analyse the question
4. Selecting numerical methods: Upon literary review, the following algorithms (or ptychographic iterative engines, PIEs) will be implemented and evaluated
   a) Gerchberg-Saxton method (1972)
   b) Rodenburg-Faulkner PIE (2004)

5. Implementing numerical methods[1]
   Computational methods, like simulating the problem, the algorithms and displaying data, are done using the programming language Julia 1.4.2 [8] with the use of the following libraries:
   a) LinearAlgebra
   b) Plots [10] with the GR Plots backend.
   c) FFTW [11]
   d) OffsetArrays [1]
   e) ColorSchemes [2]
   f) StatsBase [3]
6. Evaluate methods and results
7. Conclusion

[1]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/Avina-cK/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.

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

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

Remark 2.1. Some properties of Fourier transform are as follows:

1. Linearity:
2. Shift in domain:

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

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

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

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

	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

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

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

Remark 2.2. 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) [19]: For $x \in \mathbb{R}$, the Lorentzian function is defined by

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

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

$$\mathcal{F}\left[L\right](k) = \exp\left(-2\pi ikx_0 - \Gamma\pi\left|k\right|\right) \tag{2.7}$$

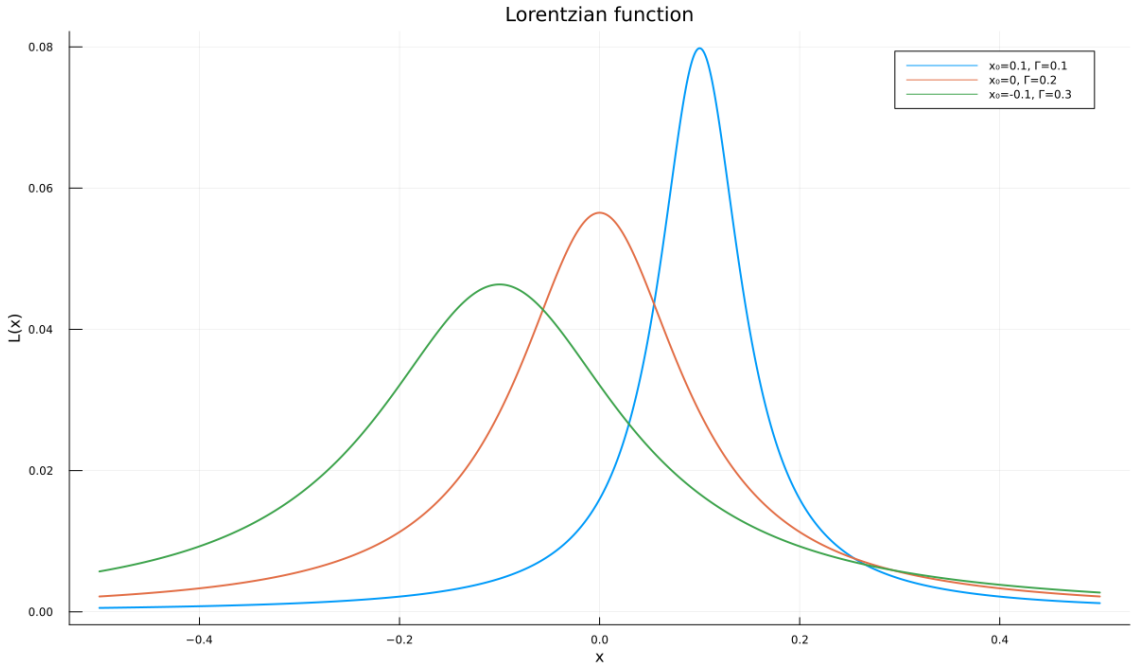


Figure 2.1.: Lorentzian function

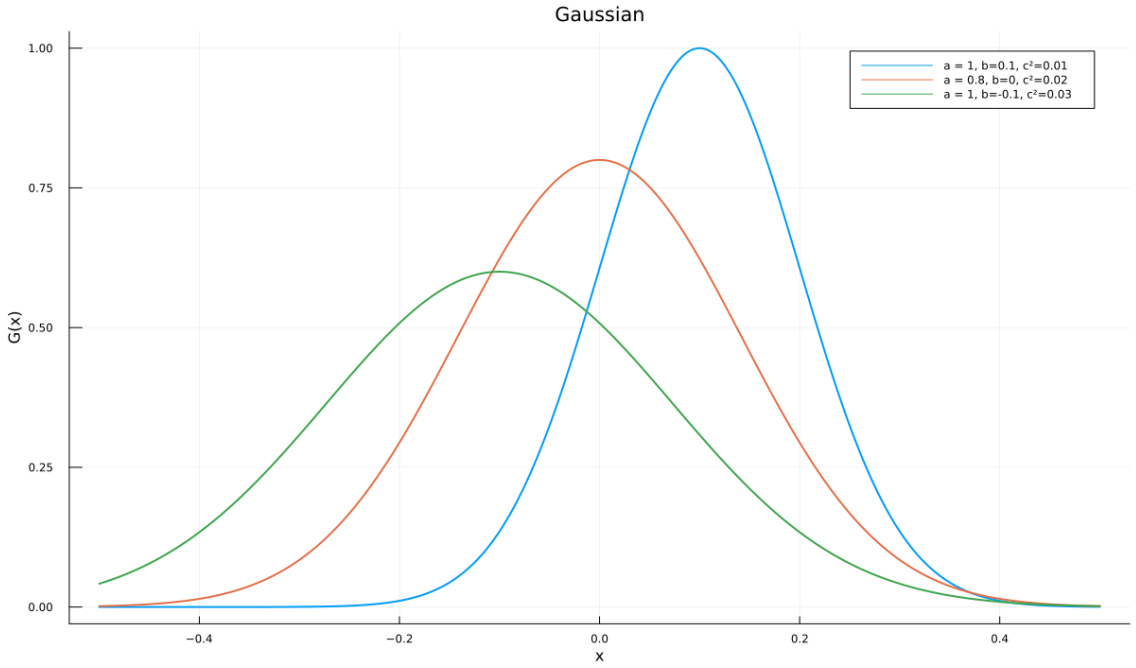


Figure 2.2.: Gaussian function

Definition 2.6. (Gaussian function) [20]: For $x \in \mathbb{R}$, the Gaussian function is defined by

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

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

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

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 [14]: 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:

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

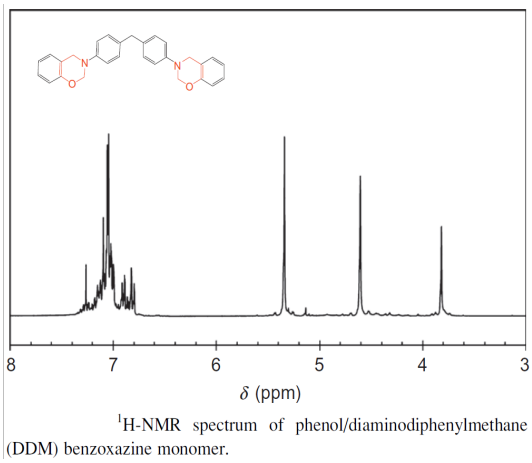
Equivalently, this function can be called an element-wise function of multiplication.

3. Nuclear Phase Retrival Spectroscopy

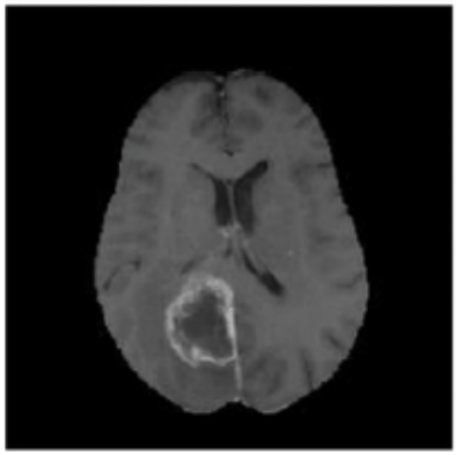
Nuclear Phase Retrieval Spectroscopy (NPRS) is a method used to measure the phase of a nuclear magnetic resonance (NMR) signal. While measuring signal in NMR spectroscopy, the phase is generally lost; but using NPRS, one can recover the lost data.

NMR spectroscopy is widely used to study the structure and properties of molecules. It is used in a variety of applications including chemical analysis [17], biomolecular structure determination [13], and medical imaging [6].

In chemistry and biochemistry, NPRS is used to study the structure (Figure 3.1a), dynamics and interactions between those of small molecules, polymers, and macromolecules such as proteins and nucleic acids. In medical imaging, it is used to study tissues and organs. A well known example of this is magnetic resonance imaging (MRI) which is used to diagnose and monitor medical conditions like tumors (an MRI scan of a brain with a tumor is shown in Figure 3.1b) and neural disorders.



(a) NMR spectrum from chemistry [5]



(b) MRI scan [7]

Figure 3.1.: Examples of NPRS

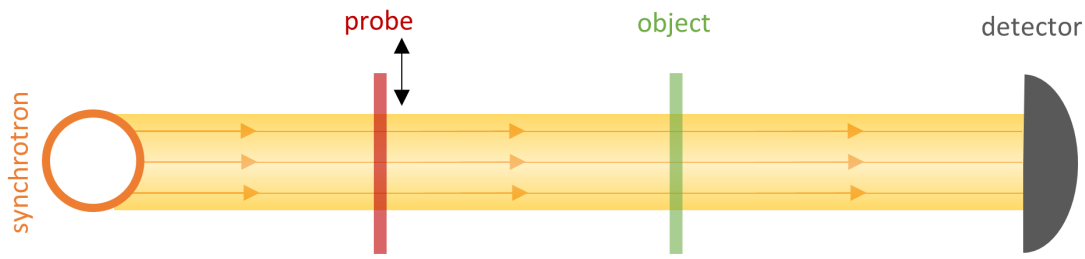


Figure 3.2.: Schematic of the Nuclear Phase Retrival Spectroscopy set-up

3.1. Experimental Set-up

A schematic of NPRS is shown in Figure 3.2. The experimental setup for NPRS typically consists of the following:

1. Radiation source: 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). [9] SR is produced to interact with the probe and sample.
2. Probe and object: This radiation is initially scattered by the probe and then scattered by the target/ object.
3. Detector: The scattered light's intensity is measured by the detector.
4. Data acquisition and analysis: A data acquisition system is used to collect and store the detector's data. Data analysis software is used to process the data and retrieve the phase information of the nuclear scattering signals.

In a typical set-up, there is no probe. In this case, a probe (which may be of known properties) is used to combat possible issues with the uniquesses of retreived phase (discussed further in Section 3.2.1.2). 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. This is described in 4. These data and the mathematical model(s) are used to retrieval the complex energy response (more specifically, its phase) of the sample.

3.2. Mathematical Formulation

Let us define the following notations:

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

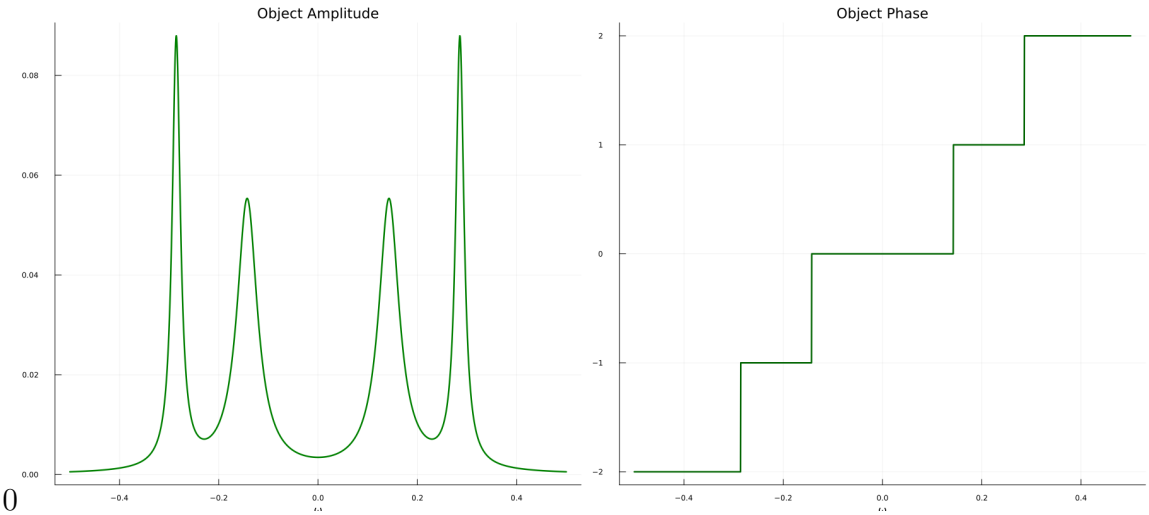


Figure 3.3.: Response function of the object

b) Discretize the energy (frequency) range as $\boldsymbol{\omega} = [-M\Delta\omega, M\Delta\omega] \subset \mathbb{R}$ 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.

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

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

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

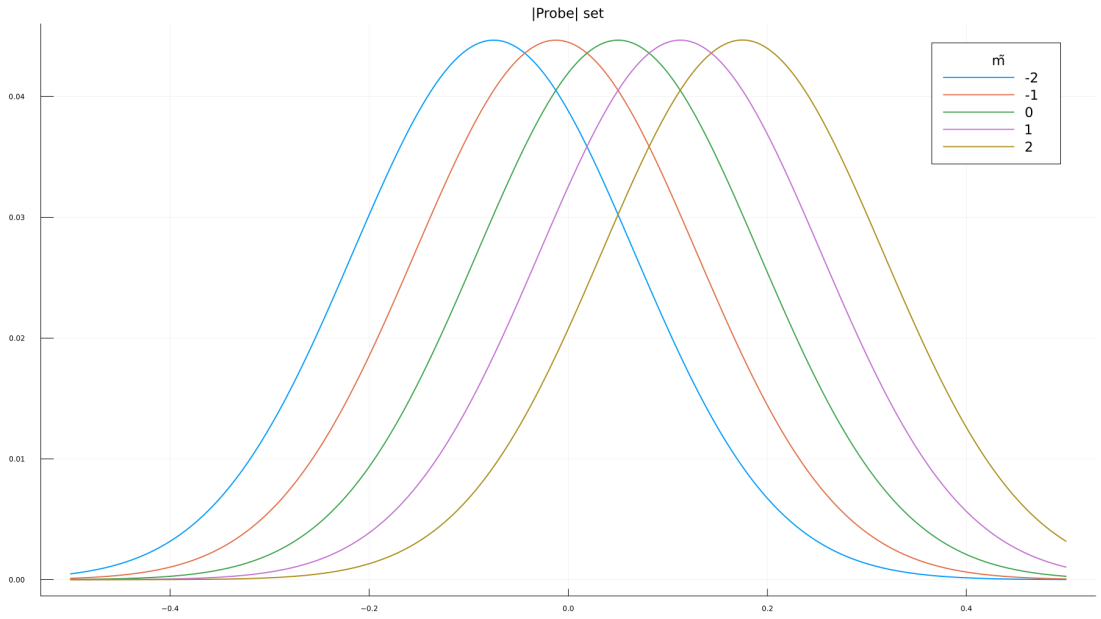


Figure 3.4.: Example of (the amplitude of the) probe set

iii. Symmetry is not guaranteed in NPRS. However, in the above example, the function is even (i.e., $\mathcal{O}(-\omega) = \mathcal{O}(\omega)$ for $\omega \geq 0$).

iv. Sectionally continuous.

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

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

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 3.3.

d) Discretized, this is the vector

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

4. Response function of the probe: $\mathcal{P}_{\tilde{m}}(\omega)$.
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.

$$\begin{aligned} &\mathcal{P} : \mathbb{R} \to \mathbb{C} \\ &\omega \to \mathcal{P}_{\tilde{m}}(\omega); \quad \mathcal{P}_{\tilde{m}}(\omega) = |\mathcal{P}_{\tilde{m}}(\omega)| \exp\left(i\theta_{\mathcal{P}_{\tilde{m}}}(\omega)\right) \end{aligned} \tag{3.4}$$

An example of such a function is illustrated in Figure 3.4.

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

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

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

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

$$\mathcal{P}_{\tilde{m}}(\omega) < \infty \quad \forall\omega \in \mathbb{R}$$

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

$$\mathcal{P}_{\tilde{m}}(\omega) \geq 0 \quad \forall\omega \in \mathbb{R}$$

iv. Each consecutive probe (with respect to $\tilde{m}$) has an overlap.

$$\forall\tilde{m}, P_{\tilde{m}}(\omega) \cap P_{\tilde{m}\pm1}(\omega) \neq \emptyset$$

c) Discretized, this is the vector

$$\boldsymbol{P}_{\tilde{m}} = (\mathcal{P}_{\tilde{m}}(-\omega_{max}), ..., \mathcal{P}_{\tilde{m}}(-\Delta\omega), \mathcal{P}_{\tilde{m}}(\omega), \mathcal{P}_{\tilde{m}}(\Delta\omega), ..., \mathcal{P}_{\tilde{m}}(\omega_{max})) \tag{3.5}$$

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

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

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

b) Discretized, this can be written as:

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

An example of this intensity measurements is illustrated in Figure 3.5.

c) The measured intensities have the following properties:

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

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

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

$$I_{\tilde{m}}(x) < \infty \quad \forall x \in \mathbb{R}$$

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

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

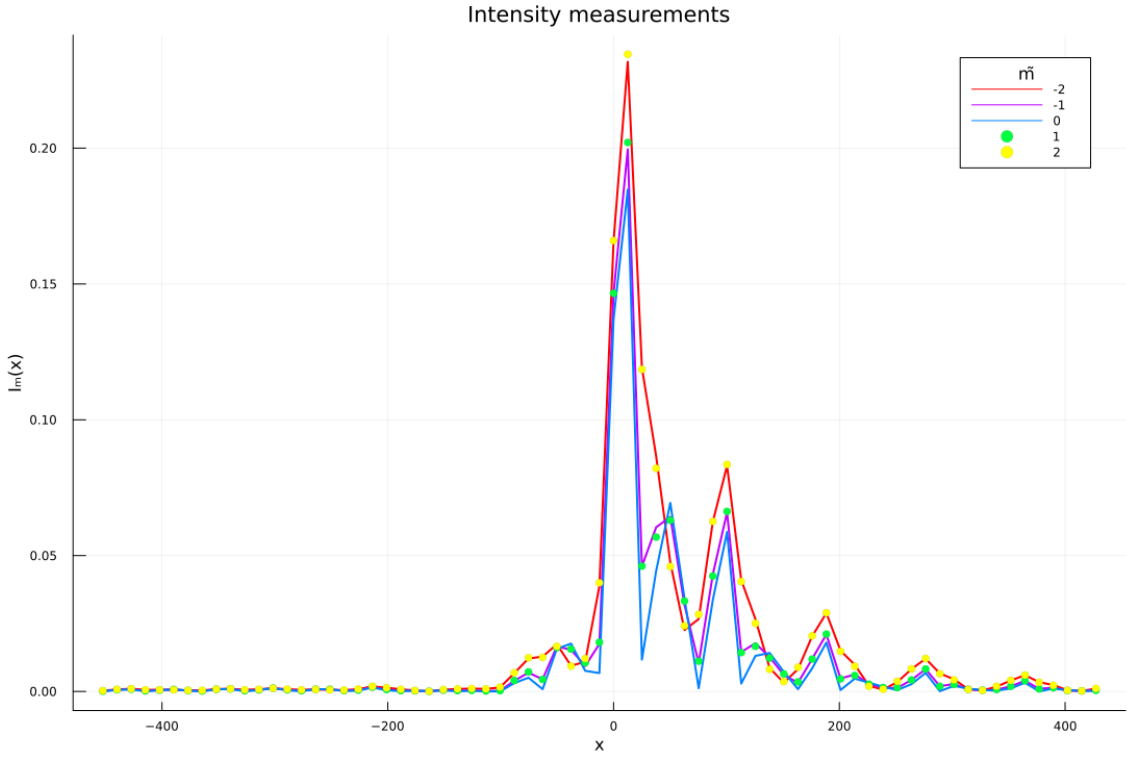


Figure 3.5.: Intensity measurements

3.2.1. Mathematical Analysis of the Problem

3.2.1.1. Linearity

Definition 3.1. Linear Transformation (or mapping) [4]: Let V, W be vector spaces defined over a scalar field $\mathbb{S}$. A function $T : V \to W$ is called a linear transformation (or mapping) if, $\forall p \in \mathbb{S}$ and $\forall y, z \in V$, the following conditions are true

1. $T(y+z) = T(y) + T(z)$
2. $T(a \cdot y) = a \cdot T(y)$

Example. Consider the vector spaces of complex numbers, $\mathbb{C}$ with elements $y \in \mathbb{R}$. Take a function $T : \mathbb{C} \to \mathbb{C}$ defined such that $T(z) = z^2$.

Take two elements, $y = 2 + 4i$ and $z = 5 + 2i \in \mathbb{C}$.

$$
\begin{array}{lrcl}
1. & T(y+z) & ; & T(y) + T(z) \\
\implies & T(2+4i+5+2i) & ; & T(2+4i) + T(5+2i) \\
\implies & (5+6i)^2 & ; & (2+4i)^2 + (5+2i)^2 \\
\implies & -11+60i & \neq & 9+36i
\end{array}
$$

$\therefore T(z) = z^2$ is non-linear.

Using the above example, without loss of generality, it can also be (trivially) proved that the intensity function (given by Equation 3.6) is non-linear.

3.2.1.2. 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?

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

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

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

□

Example. Assume that there exists two functions $f_1(\omega)$ and $f_2(\omega)$ such that $|\mathcal{F}[f_1(\omega)]|^2 = |\mathcal{F}[f_2(\omega)]|^2 = 1$.
Consider $f_1(\omega) = \sqrt{2\pi}\delta(\omega - 1)$ and $f_2(\omega) = \sqrt{2\pi}\delta(\omega)$, where $\delta(\omega)$ is the dirac delta function [18].

$$\begin{aligned}
&g_1(x) = \mathcal{F}[f_1(\omega)] = \exp(ix) && \text{and} && g_2(x) = \mathcal{F}[f_2(\omega)] = 1 \\
&\implies |g_1(x)|^2 = |\cos(x) + i \cdot \sin(x)|^2 = 1 && \text{and} && \implies |g_1(x)|^2 = |1|^2 = 1 \\
&\implies |g_1(x)|^2 = |g_1(x)|^2 \\
&\therefore |\mathcal{F}[f_1(\omega)]|^2 = |\mathcal{F}[f_2(\omega)]|^2 \not\Rightarrow f_1(\omega) = f_2(\omega)
\end{aligned}$$

To combat the problem, the shifting probe is used in the hope of reaching a unique solution from multiple readings. A question of whether the solution to this problem can be explored in the future.

3.2.2. 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 3.6). This is, theoretically, wrong; however, for the sake of practical knowledge, we shall implement this method.

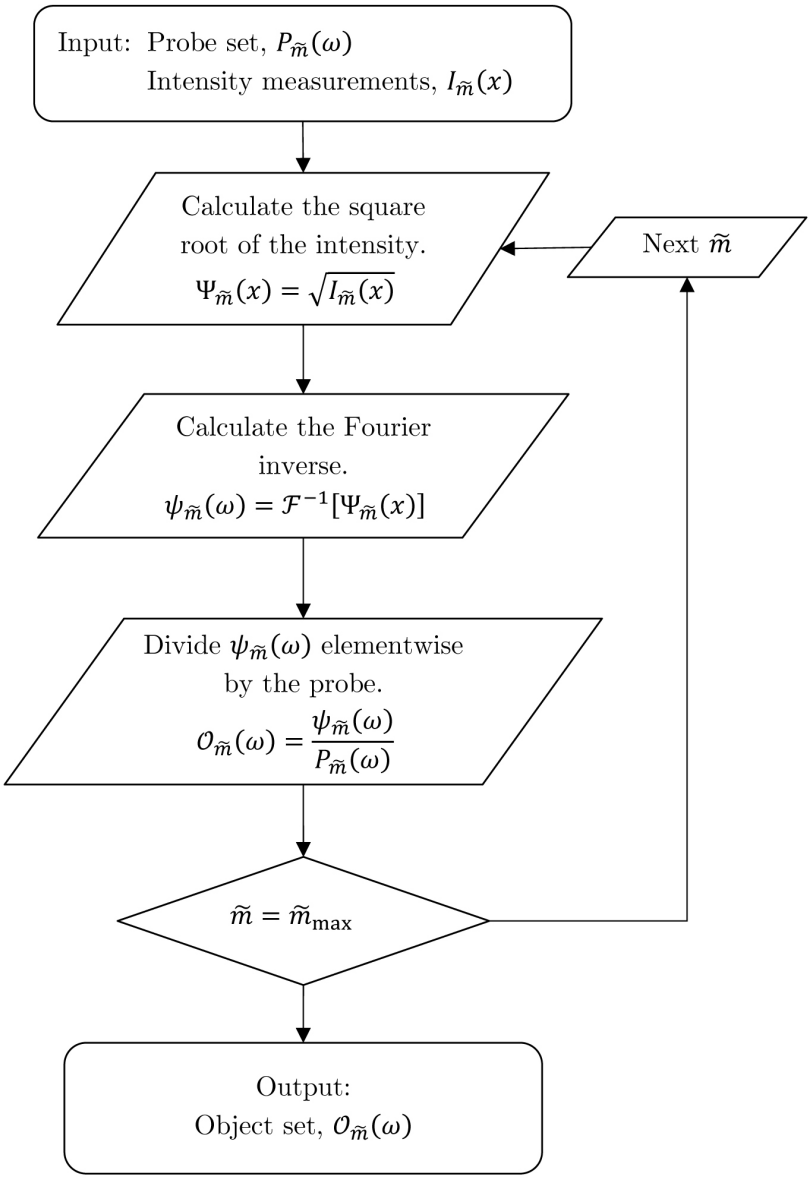
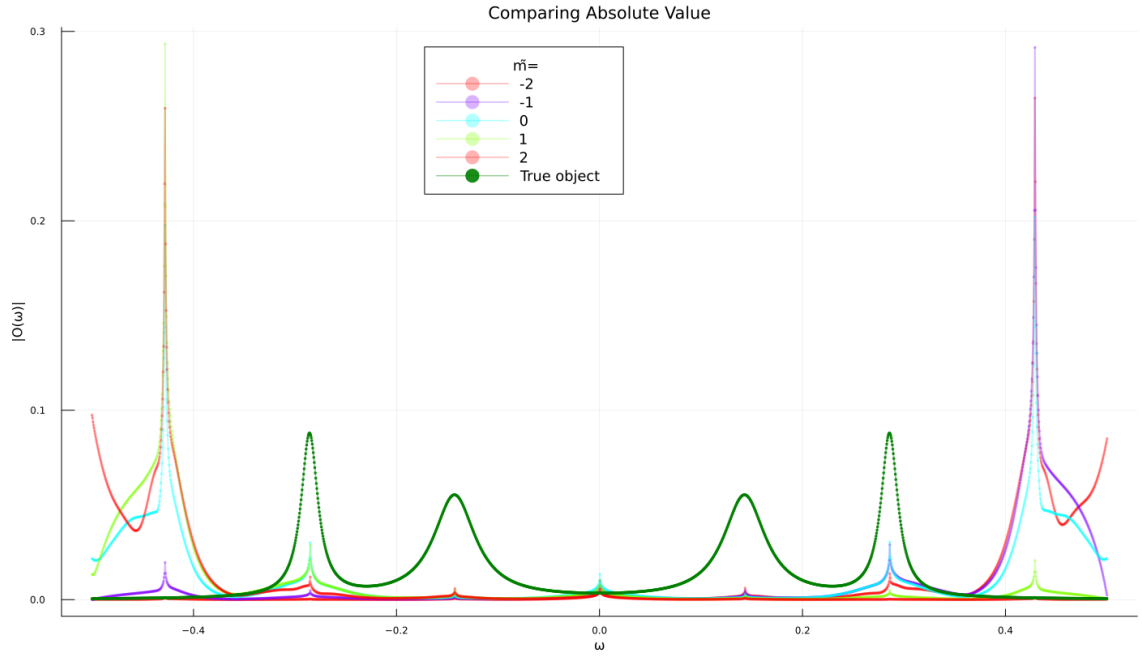
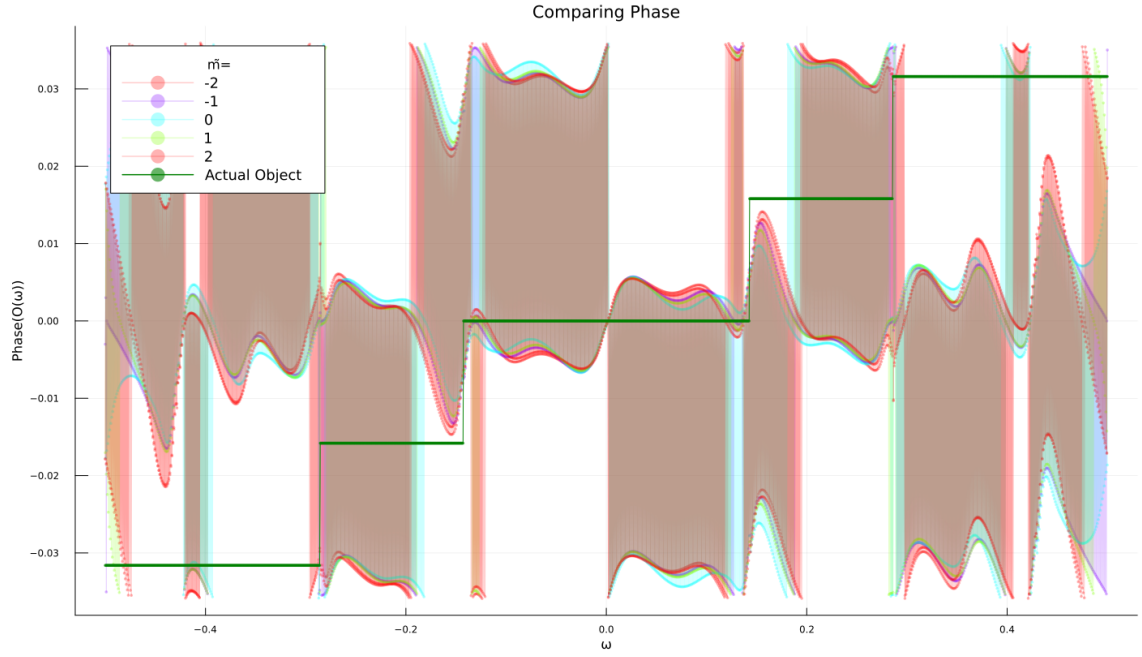


Figure 3.6.: Naïve Reconstruction



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

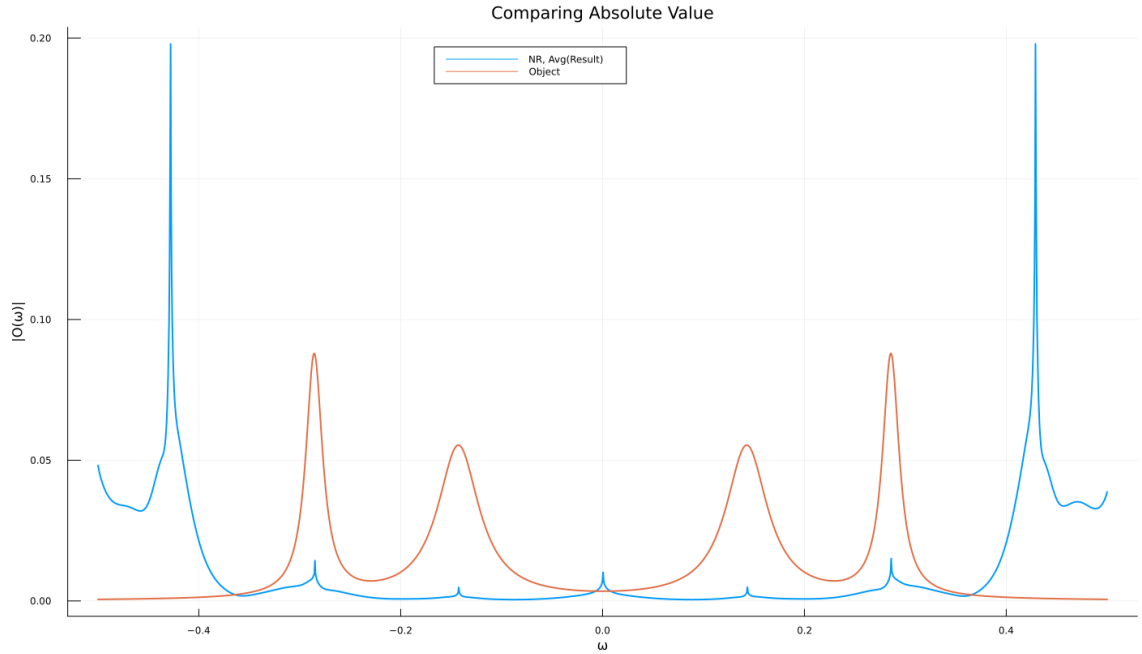


(b) NR: Comparing phase result(s)

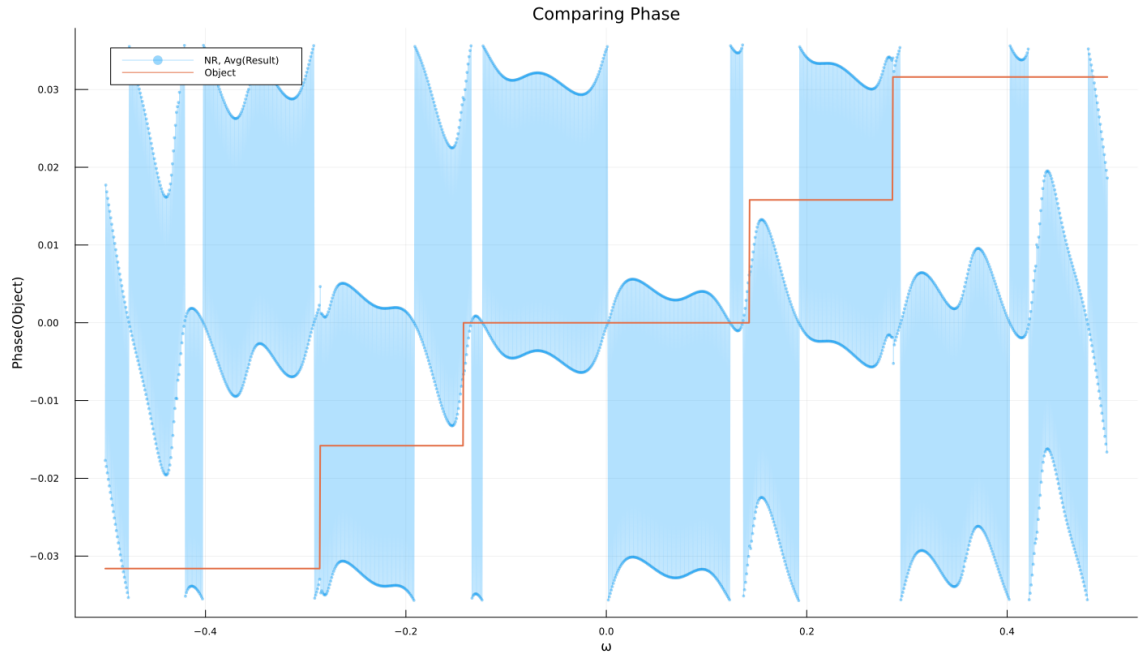
Figure 3.7.: Naïve reconstruction of the object

The results of this "algorithm" is shown in Figure 3.7. 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 shown in Figure 3.8:



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



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

Figure 3.8.: Average of naïve reconstruction

4. Ptychographic Iterative Engines

Ptychographic iterative engines (PIEs) are algorithms that are used to reconstruct high-resolution images from low-resolution measurements. The basic principle is to use an iterative algorithm that starts with a initial guess of the object and then use the measured data to improve this guess by adjusting parameters untill a certain error is minimized.

4.1. Gerchberg-Saxton method

One of the earliest reconstruction methods for phase retrieval was described by R. W. Gerchberg and W. O. Saxton in 1972 [12]. This algorithm was devised for a different and perhaps, simpler problem: reconstructing the phase of an object from one intensity measurement and one measurement of the object's magnitude.

Known measurements:

1. Object's magnitude measurement: $|\mathcal{O}(\omega)|$
2. Intensity measurement: $I(x) = |\mathcal{F}[\mathcal{O}(\omega)]|^2$

The algorithm is as follows (and illustrated in Figure 4.1):

1. Create an initial object function (which is guessed), $\mathcal{O}_{g,n}(\omega)$
2. Fourier transform the guessed object.

$$\begin{gathered}\Psi_{g,n}(x) = \mathcal{F}[\mathcal{O}_{g,n}(\omega)] \\ \equiv \Psi_{g,n}(x) = |\Psi_{g,n}(x)| \exp(i\Theta_{g,n}(x))\end{gathered}$$

3. Replace the modulus of the above function with the corresponding known value (from the intensity measurement).

$$\Psi_{c,n}(x) = \sqrt{I(x)} \exp(i\Theta_{g,n}(x))$$

4. Inverse Fourier transform the new function.

$$\begin{gathered}\psi_{g,n}(\omega) = \mathcal{F}^{-1}[\Psi_{g,n}(x)] \\ \equiv \psi_{g,n}(\omega) = |\psi_{g,n}(\omega)| \exp(i\theta_{g,n}(\omega))\end{gathered}$$

5. Replace the modulus of the above function with the corresponding known value (from the object's magnitude measurement).

$$\psi_{g,n}(\omega) = |\mathcal{O}(\omega)| \exp(i\theta_{g,n}(\omega))$$

6. Measure the sum squared error (SSE) and check if it adequately small (i.e., if it is smaller than a certain $\epsilon(\geq 0) \in \mathbb{R}$). Two errors can be calculated:
   a) In the object domain,

$$\mathrm{SSE}_{\mathcal{O}}(|\mathcal{O}(\omega)|, \mathcal{O}_{g,n}(\omega)) = \sum_{\omega} [|\mathcal{O}(\omega)| - |\mathcal{O}_{g,n}(\omega)|]^2$$

   b) In the Fourier domain,

$$\mathrm{SSE}_{\mathcal{F}}(\Psi_{g,n}(x), I(x)) = \frac{1}{\sqrt{N}} \sum_{x} \left[|\Psi_{g,n}(x)| - \left| \sqrt{I(x)} \right| \right]^2$$

It has been proved [15] that this algorithm will result in one of the two situations:

1. It will converge to a unique solution or
2. it will enter a loop between two or more points while maintaining a non-decreasing error.

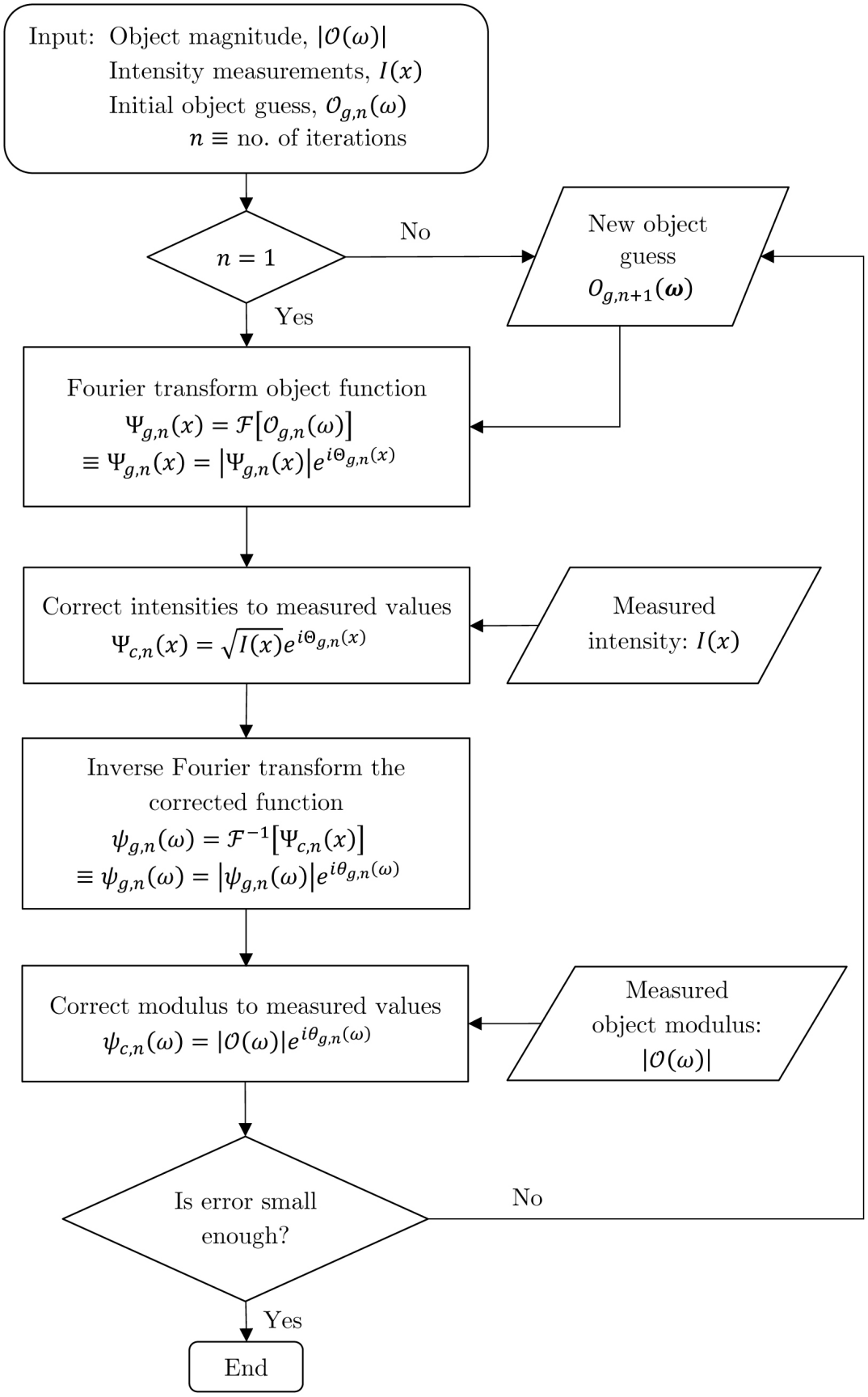


Figure 4.1.: Gerchberg-Saxton Method

4.2. Rodenburg-Faulkner PIE

One of the PIEs that shall be explored in this thesis was described by Rodenburg and Faulkner, in 2004.[16] 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 $\tilde{m}$,$(P_{\tilde{m}}(\omega))$, and multiple it with the guessed object to create:

$$\psi_{g,n}(\omega, \tilde{m}) = O_{g,n}(\omega) \circ P_{\tilde{m}}(\omega) \tag{4.1}$$

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

$$\Psi_{g,n}(x, \tilde{m}) = \mathcal{F}[\psi_{g,n}(\omega, \tilde{m})] = |\Psi_{g,n}(x, \tilde{m})| \exp(i\theta_{g,n}(x, \tilde{m})) \tag{4.2}$$

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

$$\Psi_{k,n}(x, \tilde{m}) = |\Psi_{k,n}(x, \tilde{m})| \exp(i\theta_{g,n}(x, \tilde{m})) \tag{4.3}$$

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

$$\psi_{k,n}(\omega, \tilde{m}) = \mathcal{F}^{-1}[\Psi_{k,n}(x, \tilde{m})] \tag{4.4}$$

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.

$$O_{g,n+1}(\omega) = O_{g,n}(\omega) + \frac{|P_{\tilde{m}}(\omega)|}{|\max(P_{\tilde{m}}(\omega))|} \frac{P^*_{\tilde{m}}(\omega)}{\left(|P_{\tilde{m}}(\omega)|^2 + \alpha\right)} \times \beta(\psi_{k,n}(\omega, \tilde{m}) - \psi_{g,n}(\omega, \tilde{m})) \tag{4.5}$$

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

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

$$\text{SSE} = \frac{\left(|\Psi_{k,n}(x, \tilde{m})|^2 - |\Psi_{g,n}(x, \tilde{m})|^2\right)^2}{2N + 1} \tag{4.6}$$

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

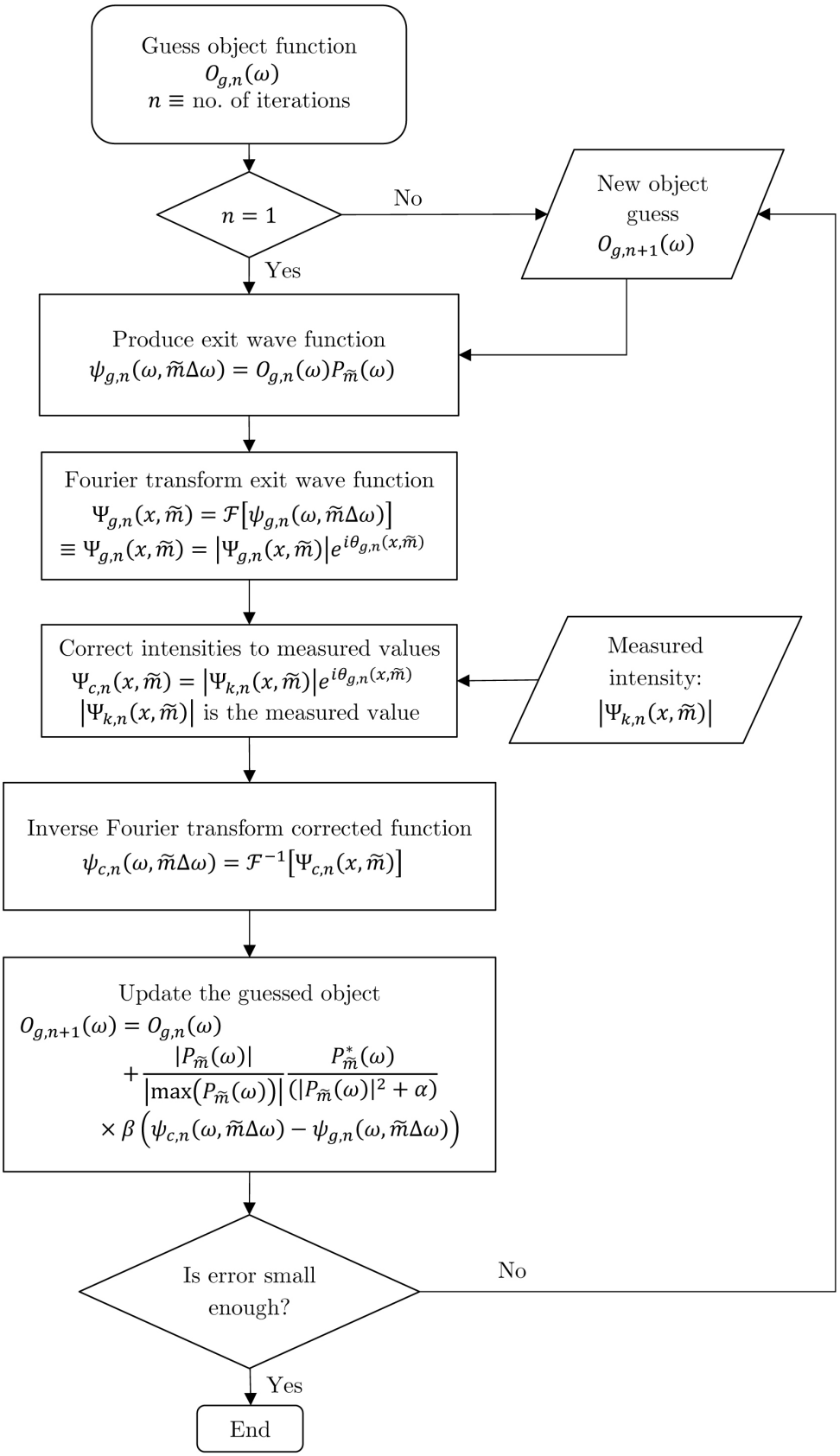


Figure 4.2.: Rodenburg-Faulkner Ptychographic Iterative Engine

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)

A.2. Code

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