

Thesis to get the degree of a Master of Science

Title of the thesis

Subtitle

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Acknowledgments

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Abstract

Abstract/Summary text

1. Introduction

1.1. Problem Description

1.2. Objective

1.3. Investigative Approach

1.4. Outline

2. Pre-requisite Concepts

2.1. Fourier Transformation

Definition 2.1. (Fourier Transform) Consider a vector $\mathbf{z} = [z_0, z_1, \dots, z_{N-1}] \in \mathbb{C}^N$. The discrete Fourier Transform (FT) of \mathbf{z} is $\mathbf{Z} := [Z_0, Z_1, \dots, Z_{N-1}]$ and is defined by

$$\begin{aligned} \mathcal{F} : \mathbb{C}^N &\rightarrow \mathbb{C}^N \\ \mathcal{F}(\mathbf{z}) = \mathbf{Z}; \quad Z_k &= \sum_{n=0}^{N-1} z_n \exp\left(-i\frac{2\pi}{N}kn\right) \end{aligned} \tag{2.1}$$

Definition 2.2. Similarly, the inverse Fourier Transform (IFT) is defined as

$$\begin{aligned} \mathcal{F}^{-1} : \mathbb{C}^N &\rightarrow \mathbb{C}^N \\ \mathcal{F}^{-1}(\mathbf{Z}) = \mathbf{z}; \quad z_k &= \frac{1}{N} \sum_{n=0}^{N-1} Z_n \exp\left(i\frac{2\pi}{N}kn\right) \end{aligned} \tag{2.2}$$

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

$$\begin{aligned} L : \mathbb{R} &\rightarrow \mathbb{R} \\ L(x) &= \frac{1}{\pi} \frac{\frac{1}{2}\Gamma}{(x-x_0)^2 + \left(\frac{1}{2}\Gamma\right)} \end{aligned} \tag{2.3}$$

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

$$\mathcal{F}[L](k) = \exp(-2\pi i k x_0 - \Gamma \pi |k|) \tag{2.4}$$

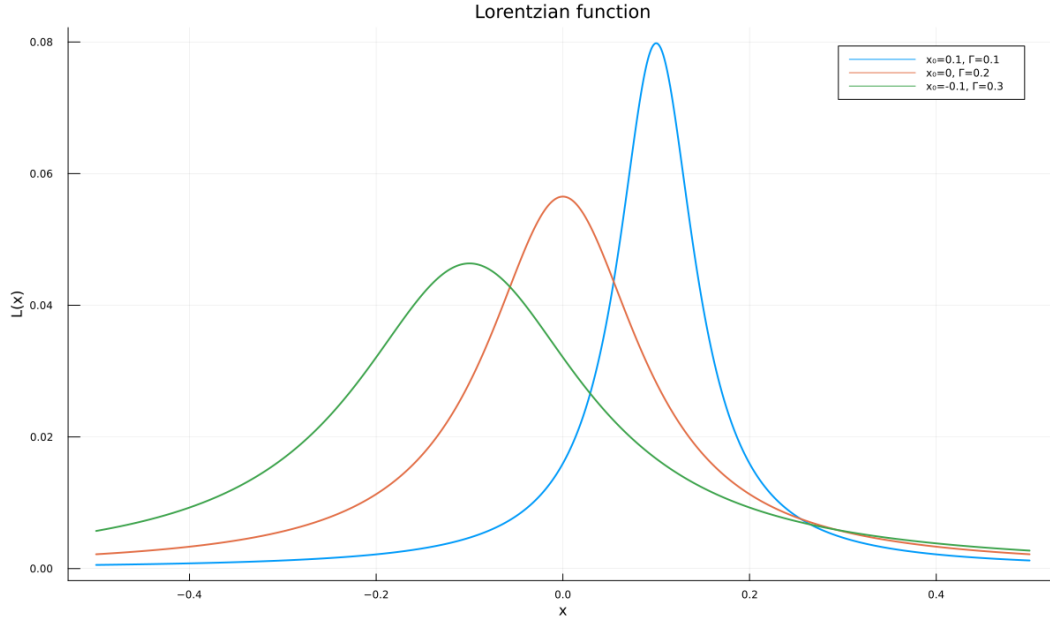


Figure 2.1.: Lorentzian function

Definition 2.4. (Gaussian function) [Wik22]: For $x \in \mathbb{R}$, the Gaussian function is defined by

$$G : \mathbb{R} \rightarrow \mathbb{R}$$

$$G(x) = a \exp\left(-\frac{(x-b)^2}{2c^2}\right) \quad (2.5)$$

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

$$\mathcal{F}[G](k) = ac\sqrt{2\pi} \exp\left(-2\pi^2 k^2 c^2\right) \quad (2.6)$$

Definition 2.5. 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:

$$\circ : M_{m \times n} \rightarrow M_{m \times n}$$

$$(A \circ B)_{ij} = (B \circ A)_{ij} = (A)_{ij} (B)_{ij} \quad (2.7)$$

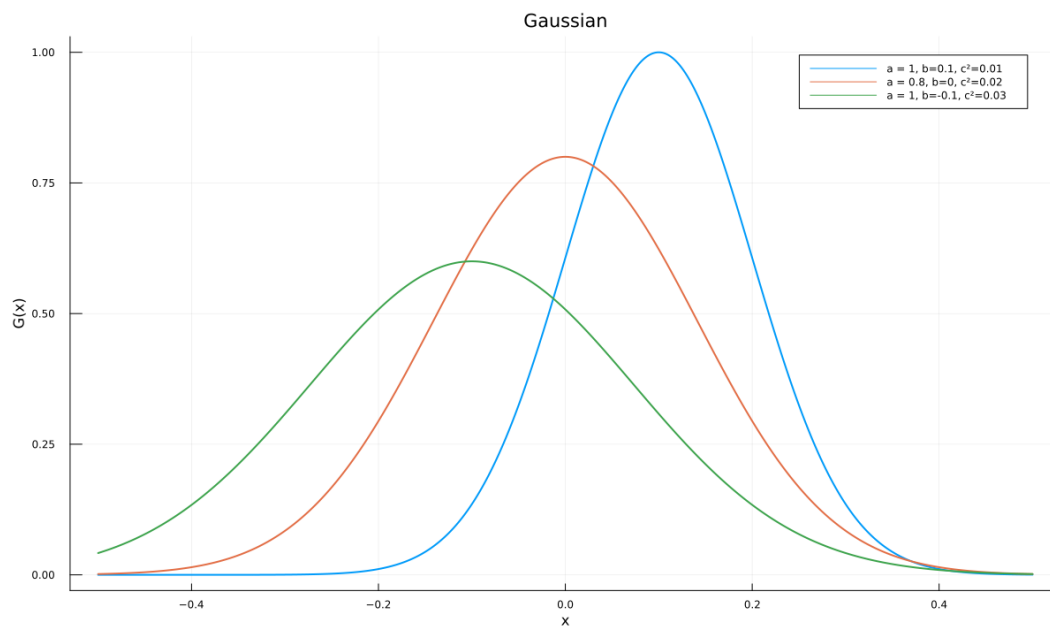


Figure 2.2.: Gaussian function

3. Nuclear Phase Retrieval Spectroscopy

3.1. Experimental Set-up

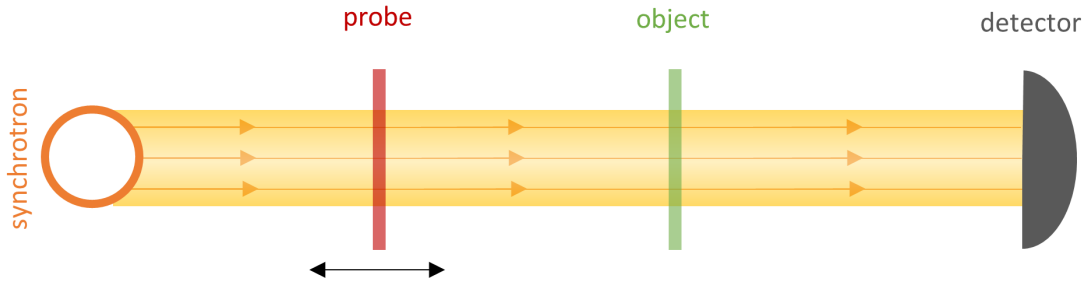


Figure 3.1.: Schematic of the Nuclear Phase Retrieval Spectroscopy set-up

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

2. Response function of the object : $\mathcal{O}(\omega)$. Discretized, this is the vector

$$\mathbf{O} = (\mathcal{O}(-\omega_{max}), \mathcal{O}(-\omega_{max} - \Delta\omega), \dots, \mathcal{O}(\omega), \mathcal{O}(\Delta\omega), \dots, \mathcal{O}(\omega_{max}))$$

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

$$\mathbf{P} = (\mathcal{P}(-\omega_{max} + m\Delta\omega), \dots, \mathcal{P}(\omega + m\Delta\omega), \mathcal{P}(\Delta\omega + m\Delta\omega), \dots, \mathcal{P}(\omega_{max} + m\Delta\omega))$$

4. Measured intensities : $I_m(t)$

A. Appendix

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