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Improving the Contrast of Neutron Interferometry Phase Measurements Using Online Bayesian Markov Chain Monte Carlo Methods (Super Tentative Crappy Title)

by

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A thesis submitted in partial fulfillment for the
degree of Bachelor of Science with Honours

in the
Faculty of Science
Department of Physics

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Declaration of Authorship

I, Thomas Alexander, declare that this thesis titled, 'THESIS TITLE' and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.

- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.

- Where I have consulted the published work of others, this is always clearly attributed.

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"Such is the vastness of his genius that he can outwit even himself."

Steven Erikson

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Abstract

Faculty of Science

Department of Physics

Bachelors of Science with Honours

by Thomas Alexander

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgements and the people to thank go here, don't forget to include your project advisor...

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Abbreviations

t transmitted beam amplitude coefficient

r reflected beam amplitude coefficient

Physical Constants

$$\text{Speed of Light} \quad c \quad = \quad 2.997\ 924\ 58 \times 10^8\ \tfrac{m}{s}$$

Symbols

k	quantum wave number	m^{-1}
v	velocity	ms^{-1}
ω	angular frequency	rads^{-1}

For/Dedicated to/To my. . .

Chapter 1

Introduction

1.1 Neutron Interferometry

1.1.1 History

Interferometry has long been a powerful tool for experimental physics. Its various forms have been used in the discovery of many historically significant results such as the Michelson-Morley experiment which showed that the speed of light was independent of inertial reference frames and experimental data in support of Bell's Inequality. [1][2]

The key concept of interferometry is the superposition of waveforms upon each other in order to deduce meaningful physical properties from the resultant combination. If one considers two waves of identical frequency than the waves when superimposed will combine constructively when in phase and de-constructively when out of phase. The technique of interferometry can be applied to many different experimental systems, the requirement being that the interferometry medium be described as a wave mathematically. Such systems that have been used in the past include electromagnetic waves, water waves, electrons and neutrons. Although electrons and neutrons classically are described as point particles the development of quantum mechanics allows that all matter is actually described by a waveform and therefore interferometry techniques may be applied to the electron and neutron waveforms. This paper focuses primarily on neutron interferometry.

The first Neutron Interferometer with slow neutrons was constructed by Maier-Leibnitz and Springer in 1962 and was effectively equivalent to a double slit experiment. However, their interferometer was not effective for measuring physical properties of materials. In 1965 the perfect single-crystal interferometer was theorized by Ulrich Bonse and Michael

Hart, however it was not until 1974 that their interferometer was made functional by Helmut Raunch and his student Wolfgang Treimer. Their interferometer used a single perfect crystal in which two horizontal slices were removed from the interior to form a three-blade interferometer.[3] **INSERT FIGURE**. Using the single-crystal design researchers Colella,Overhauser and Werner to perform the famous COW experiment which measured the phase shift due to the gravitational potential difference between two neutron beams separated by a small displacement in height.[4] Further experiments made such contributions to experimental physics such as the measurement of the Aharonov-Bohm effect and the the effect of the Earth's rotation on a quantum system.[3] It was quickly realized that neutron interferometry measurements provide an incredible level of accuracy and isolation in experimental measurements. This is due to the fact that the neutron has essentially zero electric charge and therefore does not feel the Coulomb force. Therefore for the case of slow neutrons there is no need to isolate for stray electric fields.

1.1.2 Application to Quantum Information

As the neutron interferometry provides a low-noise experimental system it provides an ideal test-bench for testing certain aspects of quantum information theory. Such an example was the use of a five-blade interferometer which allowed the quantum information encoded in the neutron waveform by using additional blades to exploit the symmetry of mechanical vibrations in the interferometer and decouple these modes.[5]. This is an example of encoding the information into a decoherence-free subspace and is a technique that may be applicable in future scalable quantum computation systems. Additionally it has been shown that neutron interferometers can be used for the generation of single neutron entangled states. [6] Additionally there is interest in the quantum discord of neutron interferometry systems and there application towards non-classical discord algorithms.[7]. It is unlikely that a scalable quantum computer will be realizable with neutrons due to their low interaction with other quantum systems.

1.1.3 Application to Quantum Fundamentals

Neutron interferometry has played a large role in experimentally gathering information on the fundamental behaviour of quantum systems. Such as the Aharonov-Bohm effect, the effect of gravity,quantum discord and verifying Bell's Inequality. [3][4][7][2]. More recently researchers at the Institute for Quantum Computing are designing an experimental neutron interferometer that is equivalent to a triple-slit experiment in the search

for third order interference effects that are theoretically non-existent but if found may be evidence of new quantum theories.[8]

1.1.4   National Institute of Standards and Technology

The majority of the work presented in this thesis applies directly to the neutron interferometry setup at the National Institute of Standards and Technology in Gaithersburg, MD. The neutrons are produced at the NIST Research Reactor and extracted via a dual-crystal parallel-tracking monochromator with energy of $4 - 20meV$. They are fed along wave-guides to the isolated interferometry setup. NIST has three,four and five blade perfect single-crystal interferometry assemblies although we focus on solely the three blade assembly. Neutron detection is provided by ^3He detectors or by high resolution position-sensitive detectors.[9][10] **INSERT FIGURES**.

1.2   Bayesian Markov Chain Monte Carlo Methods

Chapter 2

Theory

2.1 Neutrons

2.1.1 Particle Description of Neutrons

The neutron is a subatomic hadron particle that is present in the nucleus of every atom except ^1H. The neutron is composed of two down quarks and a single up quarks. This composition gives a neutral electric charge for the neutron making it an ideal candidate for sensitive experiments, however the downside is that neutrons are much more difficult to manipulate. The neutron is also therefore a fermion and by the Pauli exclusion principle only a single neutron is allowed in each quantum state. The free neutron is unstable and undergoes beta decay with a lifetime of just $881.5 \pm 1.5s$. The neutron has a rest mass of approximately $939.56 Mev$. Free neutrons are produced using either neutral fission or fusion although in practical experiments fission is almost always used. At the NIST Research Reactor free neutrons are produced from the fission of ^{235}U.

2.1.2 Thermal Neutrons

Neutron interferometry utilizes thermal neutrons which are free neutrons that follow a Boltzmann distribution. The neutrons at NIST are found in the kinetic energy range of 4-20meV around room temperature of $T = 293.15K$. This gives gives neutron velocities of $875 - 1956 \frac{m}{s}$ which gives $v << c$ and therefore relativistic affects do not play a role. Therefore thermal neutrons are in near thermal equilibrium with their surroundings. Neutrons are decelerated to a thermal state in the reactor by collisions with neutron moderators in the reactor. From de Broglie relations the wavelength of thermal neutrons is approximately $\lambda = \frac{h}{p} = 2.0$-$4.5\mathring{A}$. After being emitted form the NIST reactor the

neutrons follow a wave-guide and using a wave splitter are sent into individual labs. As the strongest known phase space density of a neutron source is around 10^-14 it can be safely assumed that the probability of two neutrons interacting inside the wave-guide or interferometer is sufficiently low that it can be disregarded and therefore detected neutrons have no correlation between each-other.

2.2   Neutron Interferometry

The Neutron interferometer is similar to other forms of interferometry in which an incoming wave is split and than allowed to interfere at a later point which allows the two wave paths to be compared. The modern day neutron interferometer is functionally equivalent to an optical Mach-Zender (MZ) interferometer.

2.2.1   Mach-Zehnder Interferometer

The MZ utilizes a half-mirror to split the incoming electromagnetic wave and the resultant two beam paths are refocused on a second beam-splitter. The two interfered waveforms exit the second beam-splitter and are incident on two detectors that can be visualized as Detector 1 & 2 in fig(2.1),
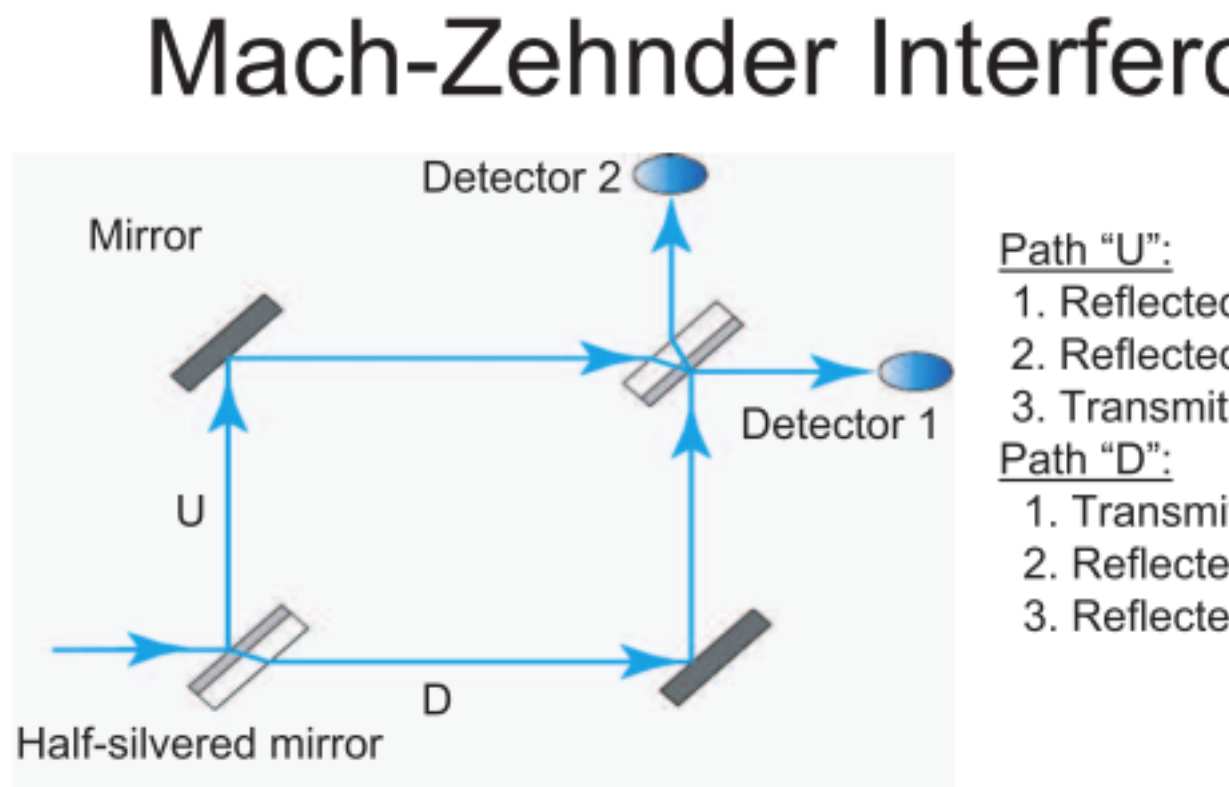

FIGURE 2.1: The Mach-Zehnder interferometer

As reflection results in a phase shift of π and assuming transmission through the half-mirrors results in a phase shift of δ we easily calculate the phase differences of the two paths at the two detectors. At detector 1 and path U there is a total of two reflections and a single transmission which results in a phase shift of $2\pi + \delta$. Similarly for path D the phase shift is also $2\pi + \delta$. therefore at detector 1 there is constructive interference. At detector 2 path U has a phase of $2\pi + 2\delta$ and path D has a phase of $\pi + 2\delta$. Therefore at detector 2 there is destructive interference.[11]

2.2.2 Bragg Scattering

In neutron interferometry the crystal planes of the interferometer blades act as diffraction gratings. Incident waves that satisfy the Bragg condition 2.1 are coherently scattered.

$$n\lambda = 2dsin(\theta_b) \tag{2.1}$$

Where n is a positive integer, d is the distance between the atomic planes of the crystal lattice and θ_b is the angle between the incident beam and the atomic plane of the crystal. The amplitudes of the transmitted and the reflected beams are given by the coefficients t (transmitted) and r reflected.[11]

2.2.3 Quantum Scattering Theory

Starting with the assumption the Hamiltonian has the form of

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V} \quad \mathcal{H}_0 = \frac{\mathbf{p}^2}{2m} \tag{2.2}$$

The presence of the potential $\mathcal{V}$ causes the solution to be different than the free particle state

$$\mathcal{H}_0 \left| \Phi \right\rangle = E \left| Phi \right\rangle$$

Therefore we are looking for solutions to the Schrdinger equation of the form

$$\mathcal{H}_0 + \mathcal{V} \left| \Psi \right\rangle = E \left| \Psi \right\rangle \tag{2.3}$$

A valid solution should have that $\left| \Psi \right\rangle \to \left| \Phi \right\rangle$ as $\mathcal{V} \to 0$. A solution that satisfies these requirements is known as the Lippmann-Schwinger equation.

$$\left| \Psi^{\pm} \right\rangle = \left| \Phi \right\rangle + \frac{1}{E - \mathcal{H}_0 \pm i\epsilon} \mathcal{V} \left| \Psi^{\pm} \right\rangle \tag{2.4}$$

Here the energy E was made slightly complex with the addition of $\pm\epsilon$ to deal with the singular nature of the operator $1/(E - \mathcal{H}_0)$. It can easily be seen that the application of the operator $E - \mathcal{H}_0$ reduces (2.4) to the desired solution (2.3) when neglecting the imaginary component. By taking the Lipmann-Schwinger equation to the position basis explicitly it can be represented as

$$\langle \boldsymbol{x} \mid \Psi^{\pm} \rangle = \langle \boldsymbol{x} \mid \Phi \rangle - \frac{2m}{\hbar^2} \int d^3 x' \frac{e^{\pm ik\left|\boldsymbol{x} - \boldsymbol{x}'\right|}}{4\pi \left|\boldsymbol{x} - \boldsymbol{x}'\right|} \left\langle \boldsymbol{x}' \mid \mathcal{V} \mid \Psi^{\pm} \right\rangle \tag{2.5}$$

As our scattering potentials are a function of position only the assumption can be made that the potential is *local* such that it is diagonal in the position representation. Specifically the potential satisfies the requirement that

$$\langle \boldsymbol{x}' |\mathcal{V}| \boldsymbol{x}'' \rangle = \mathcal{V}(\boldsymbol{x}')\delta^{(3)}(\boldsymbol{x}' - \boldsymbol{x}'') \tag{2.6}$$

Utilizing this potential we obtain

$$\langle \boldsymbol{x} \mid \mathcal{V} \mid \Psi^{\pm} \rangle = \int d^3 x'' \langle \boldsymbol{x}' |\mathcal{V}| \boldsymbol{x}'' \rangle \langle \boldsymbol{x}'' | \Psi^{\pm} \rangle = \mathcal{V}(\boldsymbol{x}') \langle \boldsymbol{x}' | \Psi^{\pm} \rangle \tag{2.7}$$

With this result the Lippmann-Schwinger equation can be reduced to

$$\langle \boldsymbol{x} \mid \Psi^{\pm} \rangle = \langle \boldsymbol{x} \mid \Phi \rangle - \frac{2m}{\hbar^2} \int d^3 x' \frac{e^{\pm ik\left|\boldsymbol{x} - \boldsymbol{x}'\right|}}{4\pi \left|\boldsymbol{x} - \boldsymbol{x}'\right|} \mathcal{V}(\boldsymbol{x}') \left\langle \boldsymbol{x}' \mid \Psi^{\pm} \right\rangle \tag{2.8}$$

Given that we are concerned with studying finite range scatters and that any observations that will be made will be made outside the range of the potential due to the macroscopic nature of neutron detectors the assumption can be made that $|\boldsymbol{x}| >> \left|\boldsymbol{x}'\right|$.
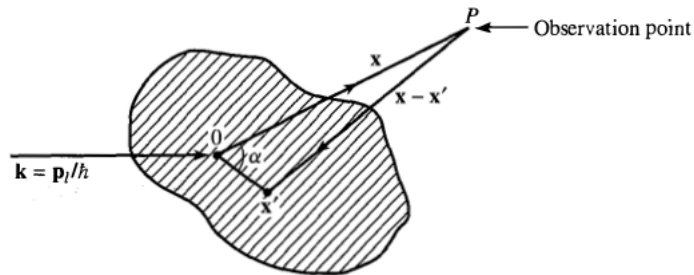

FIGURE 2.2: The finite range scattering potential. Any observations via detectors will be outside the range of the potential and therefore approximations can be made when evaluating (2.8).

Keeping in mind this result we can define

$$r = |\boldsymbol{x}|$$

$$r^{'} = \left|\boldsymbol{x}^{'}\right|$$

$$\alpha = \angle(\boldsymbol{x}, \boldsymbol{x}^{'})$$

$$\hat{\boldsymbol{r}} \equiv \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$$

$$\left|\boldsymbol{x} - \boldsymbol{x}^{'}\right| \approx r - \hat{\boldsymbol{r}} \cdot \boldsymbol{x}^{'} \tag{2.9}$$

$$\boldsymbol{k}^{'} \equiv k\hat{\boldsymbol{r}} \tag{2.10}$$

Utilizing equations (2.9,2.10)

$$e^{\pm ik\left|\boldsymbol{x} - \boldsymbol{x}^{'}\right|} \approx e^{\pm ikr}e^{\mp i\boldsymbol{k}^{'} \cdot \boldsymbol{x}^{'}} \tag{2.11}$$

For the distant r at the observation point it is a useful approximation to say that

$$\frac{1}{\left|\boldsymbol{x} - \boldsymbol{x}^{'}\right|} \approx \frac{1}{r} \tag{2.12}$$

Now replacing our incident generic wave with an incident plane wave $|\Phi\rangle \to |\boldsymbol{p}\rangle$ and using $\boldsymbol{k} \equiv \boldsymbol{p_i}/\hbar$ To remove the $\hbar$'s from the expression. We obtain for the first term in (2.8)

$$\langle \boldsymbol{x} \,|\, \boldsymbol{k}\rangle = \int d^3k^{'} \left\langle \boldsymbol{x} \,\middle|\, \boldsymbol{k}^{'} \right\rangle \left\langle \boldsymbol{k}^{'} \,\middle|\, \boldsymbol{k} \right\rangle = \int d^3k^{'} \left\langle \boldsymbol{x} \,\middle|\, \boldsymbol{k}^{'} \right\rangle \delta^{(3)}(\boldsymbol{k}^{'} - \boldsymbol{k}) = \frac{e^{i\boldsymbol{k} \cdot \boldsymbol{x}}}{(2\pi)^{\frac{3}{2}}} \tag{2.13}$$

Using this result in (2.8) gives an expression for the scattered wave function at a relatively distant observation point for the positive Lippmann-Schwinger wavefunction.

$$\left\langle \boldsymbol{x} \,\middle|\, \Psi^{+} \right\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\boldsymbol{k} \cdot \boldsymbol{x}} + \frac{e^{ikr}}{r}f(\boldsymbol{k}^{'}, \boldsymbol{k}) \right) \tag{2.14}$$

$$f(\boldsymbol{k}^{'}, \boldsymbol{k}) = -m\left(\frac{2\pi}{h}\right)^2 \left\langle \boldsymbol{k}^{'} \,\middle|\, \mathcal{V} \,\middle|\, \Psi^{+} \right\rangle \tag{2.15}$$

It is very easy to see that the result wavefunction is a combination of the original incident plane-wave and an outgoing spherical wave with an amplitude described by (2.15). An obvious issue is that here scattering has only been treated for an incident plane-wave which is not a normalizable wavefunction. In reality to describe discrete particles such

as neutrons wave packet solutions are used to describe the incident particles. However, provided the size of the wave packet is much larger than the range of the finite potential $\mathcal{V}$ it is sufficient to treat an incident packet as a plane-wave.

2.2.4 Differential Cross-Section

The scattering cross section is an important parameter for experimental scattering physics. It relates the number of particles scattering into the solid angle $d\Omega$ per unit time to the number of incident particles into an infinitesimal element $d\sigma$ of area per unit time. We search for a relation between $d\Omega$ and $d\sigma$ which we term the differential cross section given by $d\sigma/d\Omega$. Evidently the probability of an incident particle being within
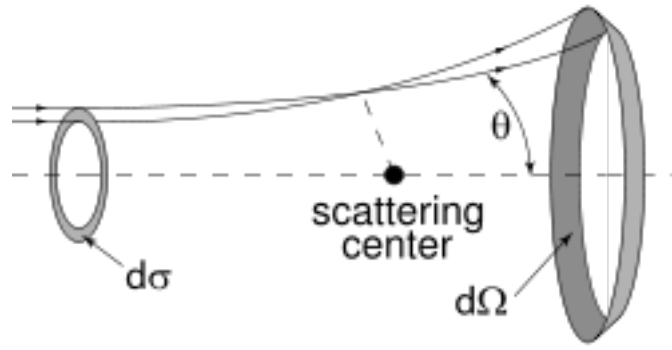

FIGURE 2.3: The differential cross section is the relationship between incident particles travelling through area $d\sigma$ to scattered particles crossing through the solid angle $d\Omega$

an area $d\sigma$ in time dt while travelling with velocity v is just

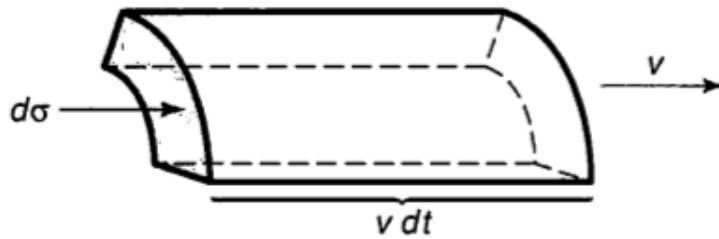$$dP = |\Psi_i|^2 \, dV = \frac{1}{2\pi}^3 (vdt)d\sigma \tag{2.16}$$

FIGURE 2.4: The volume element dV that a beam occupies passing through an area $d\sigma$ in time dt

Relating this probability to the probability of a particle being scattered into solid angle $d\Omega$ with equal velocity v per unit time dt.

$$dP = |\Psi_s|^2 \, dV = \frac{1}{2\pi}^3 \frac{\left| f(\boldsymbol{k'}, \boldsymbol{k}) \right|^2}{r^2} (vdt) r^2 d\Omega \tag{2.17}$$

Equations (2.16) and (2.17) can be solved for the differential cross section

$$\frac{d\sigma}{d\Omega} = \left| f(\boldsymbol{k'}, \boldsymbol{k}) \right|^2 \tag{2.18}$$

2.2.5 Scattering Amplitude

While equation (2.15) defines the magnitude of the outgoing spherical wave, it is defined implicitly in terms of the unknown ket $|\Psi^+\rangle$. The solution to this problem in the case of sufficiently weak scatterers is to use the first Born approximation

$$\left\langle \boldsymbol{x'} \,\middle|\, \Psi^+ \right\rangle \to \left\langle \boldsymbol{x'} \,\middle|\, \Phi \right\rangle = \frac{e^{i\boldsymbol{x'}}}{(2\pi)^{3/2}} \tag{2.19}$$

Combining (2.19) and (2.15) results in the first-order Born amplitude

$$f^{(1)}(\boldsymbol{k'}, \boldsymbol{k}) = -\frac{m}{2\pi\hbar^2} \int d^3 x' e^{i(\boldsymbol{k} - \boldsymbol{k'}) \cdot \boldsymbol{x'}} \mathcal{V}(\boldsymbol{x'}) \tag{2.20}$$

As the potentials that will be dealt with are spherically symmetrical, further approximations can be made utilizing $\boldsymbol{q} \equiv \boldsymbol{k} - \boldsymbol{k'}$ and

$$\left| \boldsymbol{k} - \boldsymbol{k'} \right| \equiv q = 2k \sin\left(\frac{\theta}{2}\right)$$

as seen in fig(2.5) The spherical symmetry can be used to integrate explicitly the angular component of the scattering magnitude.
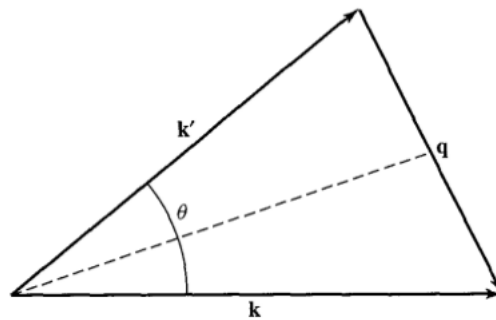

FIGURE 2.5: Scattering amplitude as a function of θ where $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k'}$

$$f^{(1)}(\theta) = -\frac{m}{2\pi\hbar^2}\int_{r=0}^{\infty}\int_{\phi=0}^{2\pi}\int_{\theta'=0}^{\pi}e^{i|q||r|cos(\theta')}sin(\theta')r^2\mathcal{V}(r)d\theta'd\phi dr$$

$$= -\frac{1}{2i}\frac{2m}{\hbar^2 q}\int_0^{\infty}r\mathcal{V}(r)(e^{iqr}-e^{-iqr})dr = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^{\infty}r\mathcal{V}(r)sin(qr)dr \tag{2.21}$$

Given a potential that has spherical symmetry it is now much more simple to calculate the scattering amplitude using (2.21).

2.2.6 Neutron-nucleus Scattering

Generally there are two interactions that an incident neutron on a material will experience. The interaction with the nucleus of the material atoms and which is referred to as nuclear scattering and the scattering due to interaction with unpaired electrons and their magnetic moments which is known as magnetic scattering. In practice nuclear scattering is more common as it allows the structure of solids to probed.

Given the assumptions that an incoming neutron beam will be elastically scattered and that the nucleus is fixed, the scattering will depend on the potential $V(\boldsymbol{r})$ between the nucleus and neutron. As this is interaction is due to the strong-force it is naturally occurring over a very short range, and is approximately zero at a distance of the order $\boldsymbol{r} = 10^{-15}m$. As this is much shorter than the wavelength of thermal and cold neutrons which are used in almost all scattering experiments, the nucleus acts as a point scatterer. A neutron beam can be represented as a plane wave a wave function described by (2.13) and the scattered wavefunction will take the form of (2.14,2.15).

Due to the magnitude of the difference between the wavelength of the incident neutrons and the effective acting distance of the strong-force neutron-nucleus interaction and its approximate spherical symmetry it is an acceptable approximation to use the Fermi pseudo-potential

$$\mathcal{V}(\boldsymbol{x}') = \frac{2\pi\hbar^2}{m}b\delta(\boldsymbol{x}') \tag{2.22}$$

as a scattering potential. Where b is known as the neutron scattering length and his units of meters. For the case of multiple nuclei the potential takes the form

$$\mathcal{V}(\boldsymbol{x}') = \frac{2\pi\hbar^2}{m}\sum_j b_j\delta(\boldsymbol{x}'-\boldsymbol{x_j}) \tag{2.23}$$

Using the spherical approximate Born solution for the amplitude (2.20) and the Fermi pseudo-potential the scattering amplitude can be found to be

$$f^{(1)}(\theta) = -\int d^3x'e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{x}'}\sum_j b_j\delta(\boldsymbol{x}'-\boldsymbol{x_j}) = -\sum_j b_je^{i(\boldsymbol{q}\cdot\boldsymbol{x_j}} \tag{2.24}$$

And in the case of a single scatterer at the origin reducing to

$$f^{(1)}(\theta) = -b \tag{2.25}$$

Therefore it can be seen that the completed neutron scattered wave form is

$$\langle \boldsymbol{x} \mid \Psi^+ \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\boldsymbol{k} \cdot \boldsymbol{x}} - \sum_j b_j e^{i(\boldsymbol{q} \cdot \boldsymbol{x_j}} \frac{e^{ikr}}{r} \right) \tag{2.26}$$

From this approximate solution it is evident that the only difference between individual scatterers is their neutron scattering length b. The value b varies greatly among even neighbouring elements in the periodic table. Unfortunately the outlined theory is not strong enough to predict the scattering length and the parameters must be determined experimentally.
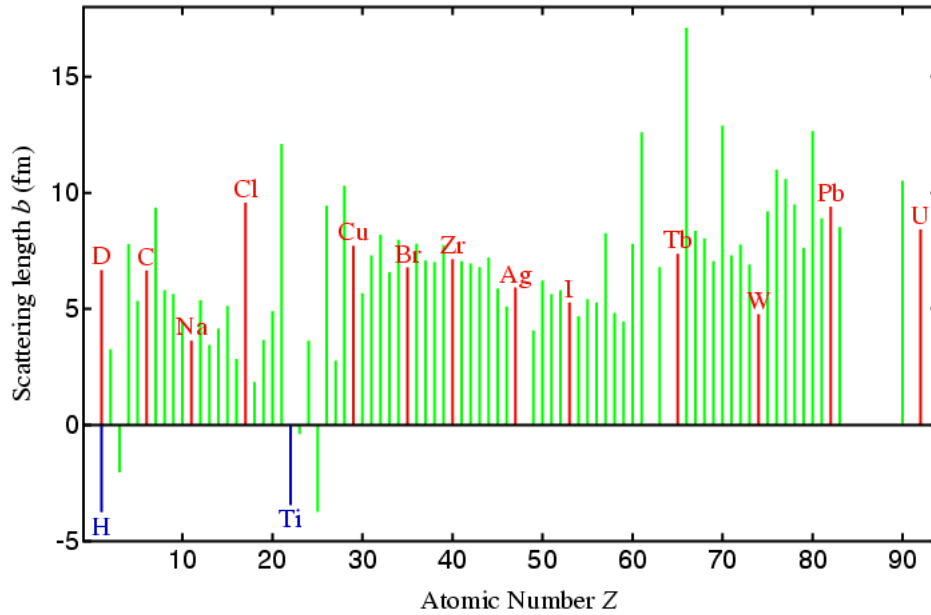

FIGURE 2.6: Neutron scattering lengths b for the elements of the periodic table

Inside a sufficiently large homogeneous material the Fermi pseudo-potential can be approximated to be

$$\mathcal{V}(\boldsymbol{x'}) = \frac{2\pi\hbar^2}{m} \sum_j b_j \delta(\boldsymbol{x'} - \boldsymbol{x_j}) \approx \frac{2\pi\hbar^2}{m} bN \tag{2.27}$$

Where N is the atom number density.

2.2.7 Neutron Optics

As the neutron beam is a wavefunction many analogies from classical optics hold. The index of refraction is defined as the ratio of the speed of neutrons experiencing no potential to the speed of neutrons affected by a potential. Compared to light the form is familiar

$$\frac{c}{n} = \frac{K}{k}$$

Where from Schrdinger's equation

$$\Delta^2 \Psi(\boldsymbol{x}) + \frac{2m}{\hbar^2}(E - \mathcal{V}(\boldsymbol{x})\Psi(r) = 0$$

$$K^2 = \frac{2m}{\hbar^2}(E - \mathcal{V}(\boldsymbol{x})) \tag{2.28}$$

$$n(\boldsymbol{x}) = \frac{K}{k} = \sqrt{\frac{E - \mathcal{V}(\boldsymbol{x})}{E}} = \sqrt{1 - \frac{\mathcal{V}(\boldsymbol{x})}{E}} \tag{2.29}$$

Given that the neutron scattering potentials are described by (2.27) the index of refraction can be approximated to

$$V(\boldsymbol{x}) = \sqrt{1 - \frac{\frac{2\pi\hbar^2}{m}bN}{E}} \tag{2.30}$$

In the case of magnetic materials the magnetic potential

$$\mathcal{V}_{mag}(\boldsymbol{x}) = -\boldsymbol{u} \cdot \boldsymbol{B_{eff}}$$

must be accounted for. This results in an index of refraction for magnetic materials such as Fe,Ni and Co of

$$n_{\pm}(\boldsymbol{x}) = \sqrt{1 - \frac{\frac{2\pi\hbar^2}{m}bN \mp \boldsymbol{u} \cdot \boldsymbol{B_{eff}}}{E}} \tag{2.31}$$

2.2.8 Neutron Wave Guides

Chapter 3

Contrast Improvement of Neutron Interferometry Measurements

3.1 Bayesian Markov Chain Monte Carlo Algorithms

Ever since Max Born presented what would become to be known as the Born interpretation, quantum mechanics has become a science of probabilities. The Born rule states that the probability of measuring an eigenvalue λ_i of an observable corresponding to a hermitian operator A will be

$$p(\lambda_i) = \langle \Psi \,|\, P_i \,|\, \Psi \rangle \tag{3.1}$$

This can be seen by applying the spectral theorem to A[?]

$$A = \lambda_1 P_1 + \lambda_2 P_2 \cdots \lambda_i P_i \tag{3.2}$$

Where P_i are the orthogonal projections of A onto the eigenspace corresponding to λ_i. As $I = P_1 + P_2 \cdots + P_i$ and $\langle \Psi \,|\, \Psi \rangle = 1$ given a probabilistic interpretation of the inner product.

$$\langle \Psi \,|\, I \,|\, \Psi \rangle = \langle \Psi \,|\, P_1 \,|\, \Psi \rangle + \langle \Psi \,|\, P_2 \,|\, \Psi \rangle + \cdots + \langle \Psi \,|\, P_i \,|\, \Psi \rangle = 1 \tag{3.3}$$

Given this result the interpretation may be made that

$$\langle \Psi \,|\, A \,|\, \Psi \rangle = \lambda_1 \langle \Psi \,|\, P_1 \,|\, \Psi \rangle + \lambda_2 \langle \Psi \,|\, P_2 \,|\, \Psi \rangle + \cdots + \lambda_i \langle \Psi \,|\, P_i \,|\, \Psi \rangle = \lambda_1 p(\lambda_1) + \lambda_2 p(\lambda_2) + \cdots + \lambda_i p(\lambda_i) = \bar{\lambda} \tag{3.4}$$

Therefore it is quite easy to see where the Born rule arises. It is therefore clear that the Born interpretation opens physics up to the world of statisticians and their probabilities. Using techniques from statistics it is possible that improvements in neutron interferometer contrast may be made.

3.1.1 Baye's Theorem

Baye's theorem is a very interesting statistical method that is useful for predicting the accuracy of statistical models given event data. The generic form of Baye's Thereom is

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \tag{3.5}$$

What this says is that given an event B occurring from a set of events $\mathcal{E}$, the posterior probability that the model A describing it is the most likely model in the set of models $\mathcal{M}$ is the probability of event B occurring according to model A multiplied by the prior likelihood of model A and normalized by the total probability of event B occurring according to all models in set $\mathcal{M}$.[?]

This is an incredibly powerful theorem as it allows a set of models to be analysed statistically to determine the correct model with an actual likelihood of correctness given event data. A broad range of models can be tested and as more data rolls in the likelihood of the correct model to describe the system will rise.

There are discrete and continuous forms of Baye's theorem, however in this case only the discrete form is of interest.

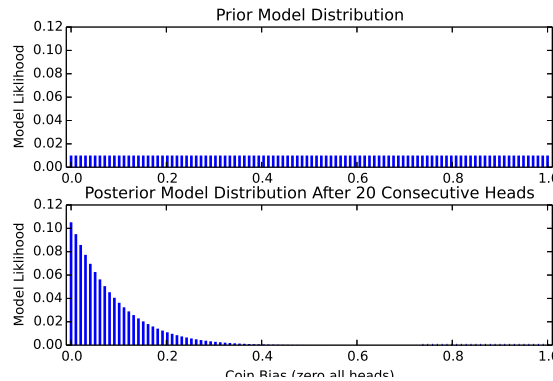$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{\sum_j P(B|A_j)P(A_j)} \tag{3.6}$$

FIGURE 3.1: Example prior and posterior distribution for a set of coin flip models that samples 10 heads flips in a row

3.1.2 Markov Chain Monte Carlo Methods

Often when attempting to fit a model it is computationally infeasible to explore the entire model space. This can be due to having a large number of possible models, models having a large number of parameters and the fact that most physical process parameters are described by real numbers and it is therefore impossible to explore the entire parameter space. A way to deal with model selection in this case is known are Markov Chain Monte Carlo (MCMC) methods. Given a set of models

$$\mathcal{M} = \{\mathbf{M}(x_1, x_2, \cdots, x_i; y_1, y_2, \cdots, y_i) : y_j \in \mathcal{F}\} \tag{3.7}$$

where x_j are input variables to the model and y_j are model parameters, it is desired to find and approximate ideal model. MCMC methods will select an original set of possible model parameters

$$\mathbf{P} = \{(y_{11}, y_{12}, \cdots, y_{1i}), \cdots, (y_{j1}, y_{j2}, \cdots, y_{ji})\}$$

and assign a prior distribution to these models $\mathcal{D}_{prior}$. Given a set of inputs

$$\mathbf{I} = \{(x_{11}, x_{12}, \cdots, x_{1i}), \cdots, (x_{j1}, x_{j2}, \cdots, x_{ji})\}$$

the posterior distribution $\mathcal{D}_{pos}$ can be evaluated using (3.6). In order to explore the parameter space, the algorithm must select a new set of parameters. One method of doing this is to select some $\subset \mathbf{P}$ and generate a new set of models and posterior distributions according to some utility function[?]

$$\mathcal{M}_{pos}, \mathcal{D}_{pos_2} = f(\mathcal{M}, \mathcal{D}_{pos}) \tag{3.8}$$

It is useful to think of the set of selected model parameters as a large number of points in space, in practice these are often referred to as points. By re-sampling model parameters as in (3.8) it is possible to select points throughout the parameter space and ideally zero in on the optimal model. However, due to the nature of sampling normally being non-deterministic and numerical precision errors, it is crucial examine the convergence of the model to experimental data.

3.1.3 Fisher Information and the Cramer-Rao Lower Bound

The Cramer-Rao lower bound is hugely important in statistics as it provides a lower bound on the variance of an unbiased estimator

3.1.3.1   Covariance Matrix

The covariance matrix in statistics is a measure of how a random vector of variables changes together. Two random variables are related by their covariance $\sigma(x,y) = E_x\left[(x - E[x])(y - E[y])\right]$, where $E[x]$ denotes the expectation value of x. As an example, in quantum mechanics the expectation value according to the Born interpretation is as in (3.4). The covariance of two random variables can be generalized to that of a random vector of estimated coefficients $\mathbf{X}$ where [12]

$$cov(\mathbf{X})_{ij} = cov(X_i, X_j) = E[(X_i - E[X_i])(X_j - E[X_j])] \tag{3.9}$$

Which in matrix notation takes the form

$$\mathbf{\Sigma} = cov(\mathbf{X}) = [(\mathbf{X} - u)(\mathbf{X} - u)^T] = E(\mathbf{X}\mathbf{X}^T) - uu^T \tag{3.10}$$

Where $u = E(\mathbf{X})$. It is prudent to note that the elements of the diagonal of the covariant matrix $\sum ii$ are the variances of the elements of the vector $\mathbf{X}$. When $\sigma(x,y) > 0$ the relationship between the two variables tends to be similar, ie. when one grows the other grows and similarly when $\sigma(x,y) < 0$ when one variable grows the other will tend to show the opposite behaviour.[12]

3.1.3.2   Cramer-Rao Lower Bound

The Cramer-Rao lower bound states that the variance of an unbiased estimator $\hat{\theta}$ is lower bounded by the reciprocal Fisher Information $I(\theta)$.[?]

$$var(\hat{\theta}) \geq \frac{1}{I(\theta)} \tag{3.11}$$

The Fisher Information is the expectation value of the square of the first moment of the log likelihood function for some probability density function $p(\mathbf{X};\theta)$. The log-likelihood of the probability density function is defined as $\updownarrow(\mathbf{X};\theta) = log(p(\mathbf{X};\theta))$ Therefore the Fisher information is

$$I(\theta) = E\left[\left(\frac{\partial}{\partial\theta}log(p(\mathbf{X};\theta))\right)^2 \Big| \theta\right] = -E\left[\frac{\partial^2}{\partial\theta^2}l(\mathbf{X};\theta)\Big|\theta\right] \tag{3.12}$$

The Fisher Information is the variance of the statistical score of the probability density function. Geometrically it is a measure of the amount of curvature of the log-likelihood function. It is a measure of the amount of information an observable $\mathbf{X}$ carries about an unknown parameter θ of which the probability of $\mathbf{X}$ relies on according to the function

$p(\mathbf{X}; \theta)$. In multiple dimensions the Fisher Information matrix takes the form

$$\mathbf{I}(\theta) = E_D[\nabla_\theta log(P(D|\theta)) \cdot \nabla_\theta^T log(P(D|\theta))] \tag{3.13}$$

The Cramer-Rao lower bound establishes a lower limit on the amount of information an unknown parameter of a probability distribution carries.[13] This is very useful in determining the fit of a set of model parameters as shall be seen. It is important to keep in mind that this only holds for unbiased estimators and may be violated by biased estimators.

3.2 Robust Online Hamiltonian Learning

The construction of a large scale quantum information processor is an extremely difficult challenge. Before error correcting codes and algorithms can be applied to such a system, the full characterization of the system is required. This is normally achieved via statistical estimation of Hamiltonian parameters via tomography. In quantum tomography the process is normally carried out on the device as a *black box* and a set of measurements is chosen such that the parametrization of them will allow the output of any input state to be predicted.[14] Full tomography is computationally complex and requires the simulation of the behaviour of the quantum system. As the systems being simulated grow in complexity, it is no longer possible for classical computer to simulate.[15]

In practice there is often more information available about the form of the Hamiltonian of a given system and this allows the number of parameters that need be estimated to be reduced. This is known as partial process estimation or partial tomography. The goal of the experiment proposed in this thesis is to provide experimental verification of the algorithm proposed in the 2013 paper "Robust Online Hamiltonian Learning" by Chris Granade at the University of Waterloo.[16]

An additional benefit to the algorithm of focus is that in quantum mechanics, often future measurement results depend on prior measurements. The use of MCMC methods allows model parameters to be estimated for such time dependent measurements. As given a set of estimated models for the hamiltonian it is possible to predict the probability of a future measurement d_{N+1} given a future set of experimental controls c_{N+1}.

$$P(d_{N+1}|D; c_{N+1}, C) = E_{\mathbf{x}|D;C}[P(d_{N+1}|\mathbf{x}; c_{N+1}] \tag{3.14}$$

3.2.0.3 Algorithm Specifics

3.2.0.4 Bounding the Error of an Estimator

Given a set of future experimental controls and their potential outcome probabilities it is useful to quantify the measurements usefulness. This is just the utility function as described in section (3.1.2). An often used measure is that of information gain, or in other words the expectation value of the logarithm of the estimator.

$$U(d_{N+1}; c_{N+1}) = E_{\mathbf{x}|dN+1,D;c_{N+1},C}[log P(\mathbf{x}|d_{N+1}, D; c_{N+1}, C)] \tag{3.15}$$

Maximizing the utility function is equivalent to minimizing the entropy of the posterior distribution.

The quality of an estimator $\hat{\mathbf{x}}$ for a set of observed data D and experimental controls C can be quantified by using the quadratic loss function

$$L_{\mathbf{Q}}(\mathbf{x}, \hat{\mathbf{x}}(X, X)) = (\mathbf{x}, \hat{\mathbf{x}}(D, C))^T \mathbf{Q}(\mathbf{x}, \hat{\mathbf{x}}(D, C)) \tag{3.16}$$

Where $\mathbf{Q}$ is a chosen positive definite matrix deciding the importance of model parameters in the quadratic loss function. The quadratic loss is used to define the risk of an estimator by taking the expectation value of the quadratic loss over all possible outcomes of the experiment.

$$R(\mathbf{x}, \hat{\mathbf{x}}; C) = E_{D|\mathbf{x};C}[L(\mathbf{x}, \hat{\mathbf{x}}(D, X))] \tag{3.17}$$

The Bayes risk is the average risk of the risk function with respect to a prior distribution $\pi(\mathbf{x})$

$$r(\pi; C) = E_{\mathbf{x}}[R(\mathbf{x}, \hat{\mathbf{x}}; C)] = \int \pi(\mathbf{x}) R(\mathbf{x}, \hat{\mathbf{x}}; C) d\mathbf{x} \tag{3.18}$$

Here $\hat{\mathbf{x}}$ is taken to be the unique Bayes estimator, which is the estimator that minimizes the total risk. The utility function is chosen as the negative Bayes risk as this corresponds to minimizing the Bayes risk for chosen set of parameters.

Remembering the Fisher information matrix as defined in (3.13) we call the Bayesian information matrix[17]

$$\mathbf{J}(\pi; C) = E_{\mathbf{x}}[\mathbf{I}(\mathbf{x}; C)] = \int \pi(\mathbf{x}) R(\mathbf{x}, \hat{\mathbf{x}}, C) d\mathbf{x} \tag{3.19}$$

From Bayesian information matrix a lower bound on the risk function called the Bayesian Cramer-Rao bound can be placed [18]

$$r(\pi; C) \geq \frac{1}{\mathbf{J}(\pi; C)} \tag{3.20}$$

This is used rather than the Fisher Information as in the case of an experiment giving no information about a parameter set, the Fisher Matrix I is singular and therefore its inverse is undefined, this is resolved via the Bayesian Cramer-Rao Lower Bound (3.20).

Given (3.20) the lower bound on the Bayes risk can be iteratively monitored.

$$r(\pi; C_{N+1}) \geq \frac{1}{\mathbf{J}_{N+1}(C_{N+1})} \tag{3.21}$$

where

$$\mathbf{J}_{N+1}(C_{N+1} = \mathbf{J}(\pi; C_{N+1}) + J_N(C_N) \tag{3.22}$$

3.2.0.5 Resampling

Utilizing sequential monte carlo methods the costly posterior distribution are approximately calculated by approximating the distribution as a set of particles or points distributed over the parameter space, each with weight w_i and with the sum of all weights being $\sum_i w_i = 1$. Therefore the probability distribution is

$$P(\mathbf{x}|D) \approx \sum_{k=1}^{n} w_k(D)\delta(\mathbf{x} - \mathbf{x}_k)$$

with the weights being iteratively updated according to

$$w_k(d_{j+1} \cup D) = \sum_{k=1}^{n} P(d_{j+1}|\mathbf{x}_k)w_k(d_j)$$

As with MCMC algorithms the accuracy can be made arbitrarily high by increasing the number of particles. The initial weights are chosen to simply be $w_k = 1/n$. Using this approximate distribution, Bayes updates can be performed and an accurate estimator approached.

Since any particle estimate will only ever approach the true parametrization, all weights will tend to zero. This can be postponed by re-sampling and updating weights at intervals. The basic idea is too select some n most likely particles and choose new particles around these likely particles according to some distribution to replace unlikely particles. Re-sampling will be performed when $n_ess = 1/\sum_i w_i^2 > 0.5$ where 0.5 is the re-sampling threshold. After re-sampling the weights are reset.

The algorithm to be tested adds the additional step of a random normally distributed perturbation vector $\epsilon = \mathcal{N}(0, \sum)$ to the position of a random selected point. This is to

further increase the size of the parameter space explored.[16]

$$pos(\mathbf{x}') = \sum_i w_i \frac{1}{\sqrt{(2\pi)^k |\sum|}} exp\left(-\frac{1}{2}(\mathbf{x}' - \mathbf{u_i})^T \mathbf{\Sigma}^{-1}(\mathbf{x}' - \mathbf{u_i})\right) \qquad (3.23)$$

Where k is the number of model parameters. This distribution is known as a mixture distribution. The mean u_i of each particle is chosen using a linear combination of the form

$$\mathbf{u}_i = a\mathbf{x}_i + (1 - a)\mathbf{u} \qquad (3.24)$$

Where $\mathbf{u} = E[\mathbf{x}]$. Therefore re-sampling consists of sampling from the distribution described by (3.23) for the $k = N - n$ unselected particles and then resetting all weights to $w_i = 1/n$.

3.2.0.6 Region Estimation

It is not just important to have an accurate estimator for the system, but also crucial to be able to quantify the error in the estimator and how much it differs from the Bayesian Cramer-Rao lower bound. This is achieved by finding a region of the parameter space $\hat{\mathbf{X}}$ such that the probability of the true parameter set $\mathbf{x_0}$ is contained within $\hat{\mathbf{X}}$ is maximized, while the volume $V(\hat{\mathbf{X}})$ is minimized.[16]

The probability of the true model being within a region $\hat{\mathbf{X}}$ can be expressed as

$$P(\mathbf{x_0} \in \hat{\mathbf{X}}) = E[1_{\hat{\mathbf{X}}}] \qquad (3.25)$$

Where $1_{\hat{\mathbf{X}}}(x) = 1$ if $\mathbf{x} \in \hat{\mathbf{X}}$ and otherwise $1_{\hat{\mathbf{X}}}(x) = 0$. The probability of a region can then be calculated from the particle weights from section (3.2.0.5).

$$E[1_{\hat{\mathbf{X}}}] \approx \sum_i w_i 1_{\hat{\mathbf{X}}}(\mathbf{x}_i) = \sum_{i,\mathbf{x_i} \in \hat{\mathbf{X}}} w_i \qquad (3.26)$$

Therefore a region $\hat{\mathbf{X}}$ must be found such that (3.26) is sufficiently large, while $V(\hat{\mathbf{X}})$ is sufficiently small. Under the assumption that after a reasonable amount of data the posterior distribution is approximately normally distributed according to $\mathcal{N}(\mu, \mathbf{\Sigma})$, from the definition of the normal distribution it follows that the inverse covariance matrix Σ^{-1} describes an ellipse of dimension d where 0.682^d of the probability mass is contained within the ellipse. Where, d is the number of model parameters. The volume of the ellipse can be found to be

$$V(\mathbf{\Sigma^{-1}}) = \frac{\pi^{d/2}}{\Gamma(d/2 + 1)} det(\mathbf{\Sigma^{-1}}) \qquad (3.27)$$

In order to determine the fit of the region found, it is important to compare the found covariance ellipse to the optimal one according to the Bayesian Cramer-Rao lower bound

$$E_\pi[cov(\hat{\mathbf{x}})] \geq \mathbf{J}(\pi; C)^{-1}$$

3.3   Q-Infer

3.3.1   Interaction with NI-Engine

3.3.2   GPU Implementations of Likelihood functions

Chapter 4

Experimental Setup

4.1 The Neutron Interferometer

The neutron interferometer that this thesis refers to is located at the Neutron Interferometry and Optics facility (NIOF) at the National Institute of Standards and Technology (NIST) in Gaithersburg, MD.

4.1.1 NIST

4.1.2 Reactor

NIST operates a 20MW split-core research reactor. Neutrons of approximate energy $1MeV$ are emitted during ^{235}U fission and then thermalized using heavy water (D_2O) as a moderator. This brings the neutrons to room temperature as discussed in (2.1.2). At the reactor core the peak thermal neutron flux is $4 \times 10^{14} neutrons/cm^2$. The reactor is operated on a seven week cycle during which it is operated at full power for 38 days and then followed by 11 days of refuelling and maintenance operations.

As the longer wavelength of cold neutrons ($\lambda > 1.8\mathring{A}$ and $E < 25meV$) is often desired for condensed matter study there is a cold moderator installed next to the core. The thermal neutrons scatter with liquid hydrogen at $20K$ and exit with a Maxwellian distribution of characteristic temperature of $34K$.

There are eight thermal neutron ports available for lab use. The neutrons are transported to the instruments in the NCNR hall using neutron guides. The neutron interferometer facility is located on the NG7 guide shown in figure (??). The guides are of a rectangular cross-section and are produced by gluing together meter long sections of $100nm$ thick

^{58}Ni optically-flat borated glass plates. ^{58}Ni is used due to its large neutron reflective potential.

$$V = \frac{2\pi * \hbar^2}{m}\rho = \frac{2\pi\hbar^2}{m}\frac{1}{V}\sum_i b = 335 neV$$

4.1.3 Motors and Actuators

The neutron interferometry lab uses a variety of motors and actuators that allow experimental parameters to be controlled over the wire. Depending on the device communication is achieved via analog or digital protocols.

4.1.3.1 Newport 301

The Newport ESP301 is a three axis motion controller and driver.[19] It can drive both DC servo motors and 2-phase stepper motors at up to 3 amps. It has a 1000x microstep resolution per axis which allows very fine grained control of movements which is necessary for precision measurements. The Newport ESP 301 is primarily used to drive servo motors that orient the phase flag in the neutron interferometer. Precise angular control is a must as this is one of the primary experimental parameter. The device can also be used to control the interferometry stage to orient it.

The Newport device utilizes encoder feedback built into servos to obtain precise positional feedback. While most Newport brand motors will automatically supply their configuration information, the equipment at NIST is not necessarily compatible in such a way. Therefore advanced configuration must be supplied by the device programmer.

The ESP301 is controllable via a fairly extensive language of approximately 100 commands, a large portion of which are necessary for the device to be controlled successfully. Valid configuration information must be supplied. Commands are transmitted via ASCII characters according to the selected protocol. Supported protocols are serial RS232C, USB and IEEE488 with delays of $7 - 30ms$, $3.5ms$ and $1ms$ respectively.

4.1.3.2 Kepco Power Supply

Kepco series ATE power supplies are used to control a variety of devices in the interferometry lab. Specifically the 15-6M and 36-15M models are used and are rack mounted. The models are rated at $(0\text{-}15V, 0\text{-}6A, 50W)$ and $(0\text{-}36V, 0\text{-}15A, 500W)$ respectively.[20] The models are controllable via an analog input line that sets the supply output as a linear function of the input from 0-10V. Additionally there is a crowbar voltage controller
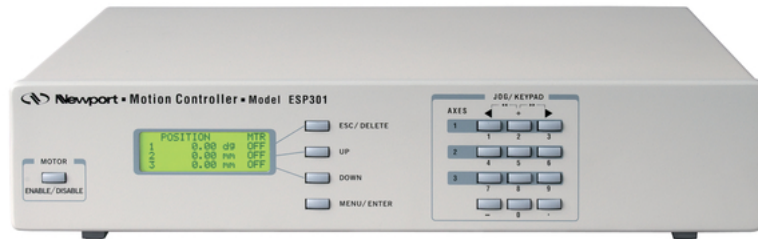
FIGURE 4.1: Newport ESP301 three axis motion controller

which allows a maximum voltage to be set in a similar manner. The Kepco supplies are controllable via DACs which are managed via a LabJack.

4.1.3.3   LabJack

The LabJack is a low cost measurement and automation platform. Specifically NIST will use the U3-LV variant. The U3-LV provides up to 16 analog inputs, 2 analog outputs and up to 20 digital I/O pins. The analog inputs accept voltages from $0\text{-}3.6V$ and the onboard DACs outputs from $0\text{-}5V$. The LabJack devices are easily controlled via a Python API.

In Addition to the LabJack the LJTick-DACs, a DAC made to be digitally controlled by LabJack devices are used to provide control inputs to devices such as the Kepco power supplies. The LJTick-DAC outputs $\pm10V$ controllable by the LabJack pins in which it is inserted too. Each LJTick-DAC provides two DACs.

FIGURE 4.2: Labjack U3 with LJTick-DAC

4.1.4 Sensors

As the likelihood method for the contrast measurement is a function of the temperature and humidity of the interferometer chamber, a variety of measurements must be taken using many different sensors.

4.1.4.1 EI1050 Temperature and Humidity Probe

The EI1050 is a digital temperature and humidity probe produced by LabJack. While its protocol is open source, it has been designed to be used with a LabJack device and sample code has been provided. The device is not especially accurate as it is rated at $\pm 0.5°$ and $\pm 3.5\%$ humidity at ranges from $-40\text{-}120C$ and 0-100% humidity. It is still useful to provide a quick and easy measurement.

4.1.4.2 Stanford Research Systems CTC100 Temperature Controller

The SRS CTC100 is a cryogenic temperature controller. It provides four sensor inputs, four analog outputs and six feedback control loops. Temperature readings are made by thermistor sensors and heating is provided by resistive heaters. The device is programmable using USB, Ethernet and either GPIB or RS-232 inputs. Commands are provided via ASCII commands. The thermistor temperature readings are very accurate with an accuracy of $\pm 0.25\Omega$ for a 300Ω thermistor. The CTC100 automatically supplies the mean and standard deviation of sampled temperatures.

FIGURE 4.3: Stanford Research Systems CTC100: Cryogenic Temperature Controller

4.2 NI-Engine

The current system at the NIST interferometry lab uses an Excel spreadsheet connected via ActiveX to closed source controller code. This system only controls the bare minimum of experimental hardware and is very inflexible. The system is not easily extensible and the software design principles are very poor. As the contrast improvement experiment requires many different sensor inputs and system controllability for many different measurement cases, it would have been a tremendous task to implement into the current system.

Ni-Engine attempts to solve the problems of the previous system for the proposed experiment and future lab researchers. NI-Engine is an experimental neutron interferometry control system programmed in Python using open source libraries and software design principles.

4.2.1 Design Requirements

The core design requirement of NI-Engine are to be a complete, easy to use neutron interferometry experimental control system. In order fulfil this core requirement the software had to fulfil these requirements:

- Be able to communicate with and control a large range of hardware in a manner that allows powerful functionality while hiding the inherent complexity.

- Handle experimental setup and configuration via configuration files such that an experimental setup is easily repeatable given an identical configuration.

- Handle the collection and storage of experimental data. Experimental data will be large, possible into the $10 + GB$ range. Should allow for multiple identical experiments to be performed sequentially.

- Execution of software functionality must be fast and allow for experiment running times to be dominated by hardware measurement and control, rather than software running time.

- Software must be able to run for long periods of time with consistent memory requirements.

- Data should be collected and stored with units available to avoid confusion.

- Should be modular. Outside researchers should be able to modify software to their own requirements. ie. addition of new hardware, file formats, data types.

- Software must have extensive documentation and example code. Researchers should be able to utilize without extensive outside help.

These design requirements had to be taken into account when designing and programming Ni-Engine

4.2.2 Language and Software Library Choices

4.2.2.1 Language

Given the design requirements outlined in (4.2.1) it is clear that the system required is quite extensive. Python[21] was selected as the development language for Ni-Engine. Python was selected for a variety of reasons including

- Python is very easy to learn and use. Its syntax style allows newcomers the ability to quickly write code, while still allowing experts powerful expressibility.

- Python's code is extremely legible and the nature of its syntax naturally generates readable code.

- Python has many powerful libraries available that when used allow rapid development of complex software without the complexity of rolling ones own solution.

- Python has a large and help community.

- It is very easy to interface with C based code if performance is desired.

- Python is object oriented which when used correctly allows simple creation of modular and extensible software.

- Python is dynamically typed and evaluated which allows rapid iteration and ease of use at the cost of performance and security.

While the use of python does come at some costs, namely memory and CPU performance, on a whole the choice of language provided enormous benefits.

4.2.2.2 Software Libraries

Due to the nature of an experimental system composed of heterogeneous hardware there is a lot of complexity in communicating with hardware over different communication channels. To overcome this challenge the library InstrumentKit[**?**] was used. InstrumentKit allows identical commands to be sent over a variety of different communication

channels at a high level of abstraction. It was a much more simple matter to contribute communication code for necessary sensors and hardware to InstrumentKit and then just utilize the library. As Ni-Engine must handle large volumes of data and manipulate this data, Numpy[?] was used for its efficent handling of arrays in Python and the variety of methods it provides. To store this data the first file format to be implemented was HDF5[?], which is a version of the Hierarchical Data Format. HDF5 was designed for the storage of large amounts of numerical data. Additionally, it provides an easily navigable hierarchical file system. Creation and manipulation of HDF5 files was facilitated by the memory efficient H5py[?] library for Python. Configuration data is in the YAML[?] format and is manipulated using PyYaml[?]. As the main goal of the system is to handle experimental data that is often associated with physical units of measurement Python units[?] was used. Units allows the wrapping of Python data types and Numpy arrays in physical units, and performs the necessary unit operations when performing operations between data types of units.

As extensive documentation is a core design requirement of Ni-Engine, it was essential that a documentation generation library be used throughout development. Sphinx[?], the De facto Python standard for documentation pulls in-code comments and generates relational documentation in a variety of formats including html and pdf formats.

4.2.3   System Architecture

Ni-Engine is split into several major components controlled by the main NiEngine object. Major components are the configuration, hardware, controllers, sensors and storage sections.

4.2.3.1   Design Patterns

Due to the complexity of Ni-Engine it was necessary to use object oriented design patterns. The main NiEngine class controls the execution and control flow of the experimental system. During execution of an experiment all commands initially must go through the NiEngine class. Ni-Engine follows a chain of responsibility pattern and has a strict hierarchy with NiEngine sitting at the top.

Ni-Engine divides the software into five separate components, each of which attempts to be as modular as possible, allowing the modification of internals without the affecting the behaviour of the system as a whole. The main sections are the configuration, hardware, controller, sensors and storage sections. The NiEngine object reads in the experimental configuration via the Configuration object and supplied file. From there, it dispatches

creation of experimental software components HardwareManager, ControllerManager, SensorManager and DataHandler objects which are responsible for their self-descriptive duties.
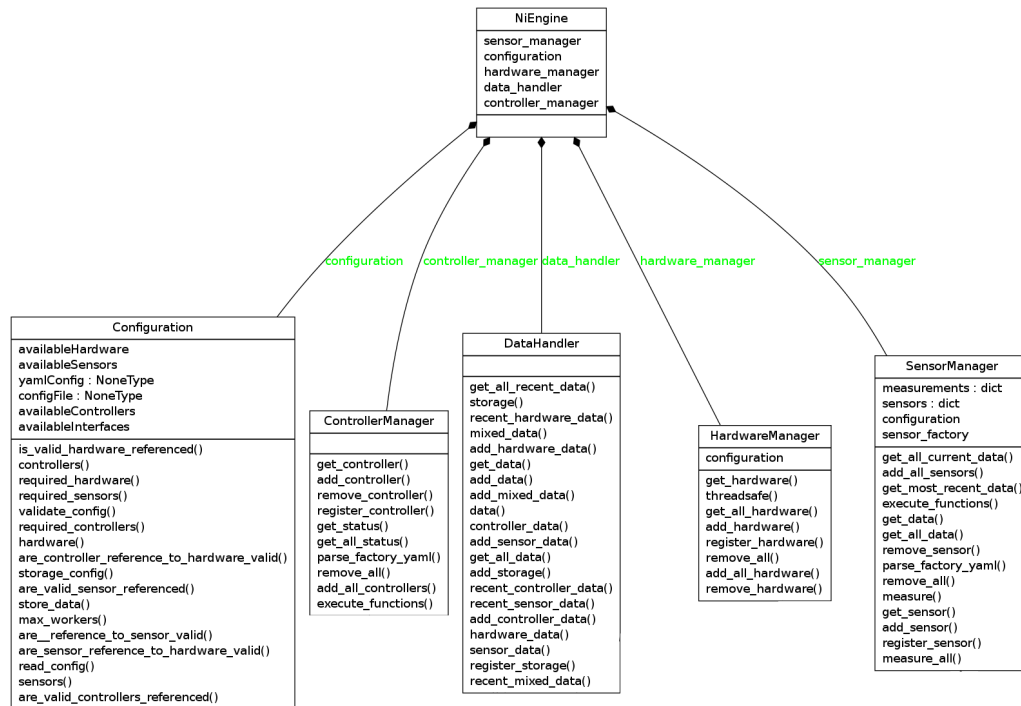

FIGURE 4.4: NiEngine object control hierarchy

4.2.3.2 Configuration

A core tenet of the design of Ni-Engine was that it has to make experiments easily scriptable and repeatable. As experimental hardware requires many different configuration values to be set, that if set incorrectly can result in disastrous consequences it is infeasible to supply configuration via the command-line or as python based configuration. Therefore configuration is provided to Ni-Engine via Yaml configuration files which allows the specification of all runtime configuration options for Ni-Engine. This allows experiments to be run with the same initial settings consistently simply by passing Ni-Engine a predefined configuration file. Configuration is made simple thanks to Yaml's hierarchical data format, which is converted into a very simple to use Python dictionary by PyYaml.

4.2.3.3 Data Storage

Ni-Engine utilizes a storage format agnostic API. All storage communication is channelled through a DataHandler instance. At initialization time DataHandler is a passed its required configuration information as defined in the experiments configuration file. It is possible to utilize many different file formats provide a class that implements the AbstractPhysicalStorage is provided and it is registered with the main Ni-Engine class. This Builder pattern allows future extensibility and interaction, although at current time only the HDF5 file format is supported.

In Ni-Engine all measurements reside in memory as Data objects. Data objects are interesting in that they measurement meta-information with such fields such as measurement names, measurement types and the time the measurement was taken at. All the while Data objects behave as their value data-types in code. This allows measurements to be created with essential meta-information and than to be manipulated in a normal fashion as would integers,floats, arrays and other basic data-types.

Due to the slow nature of permanent storage devices, data to be written to storage are batched in order to limit the amount of write calls. When the buffer is filled it is flushed to the disk. A balance must be established between the amount of data stored in memory compared to how often it is written to disk. Of course any data in memory is ethereal and power failure / program crashes will cause the data to be lost.

4.2.3.4 Manager Objects

In Ni-Engine all control of physical hardware is managed by the HardwareManager,ControllerManager and SensorManager objects. Managers are responsible for initialization, configuration, data acquisition and object destruction. Upon initialization these manager classes are passed configuration information that contains all necessary information for the setup and control with all experimental hardware. Each manager object creates its own singleton factory object that is responsible for constructing either the hardware, controllers or sensors for the system depending on its type. Every controller and sensor object interacts with physical hardware through hardware objects. This is to ensure that each physical device is only instantiated once and prevents race conditions. Upon creation of these experimental equipment objects they are placed under management by their respective managers.

Measurement calls to devices are made via manager objects. Manager objects have the ability to measure individual devices or all devices at once. As differing devices have different latencies, sequential measurement can take an excessive amount of time.
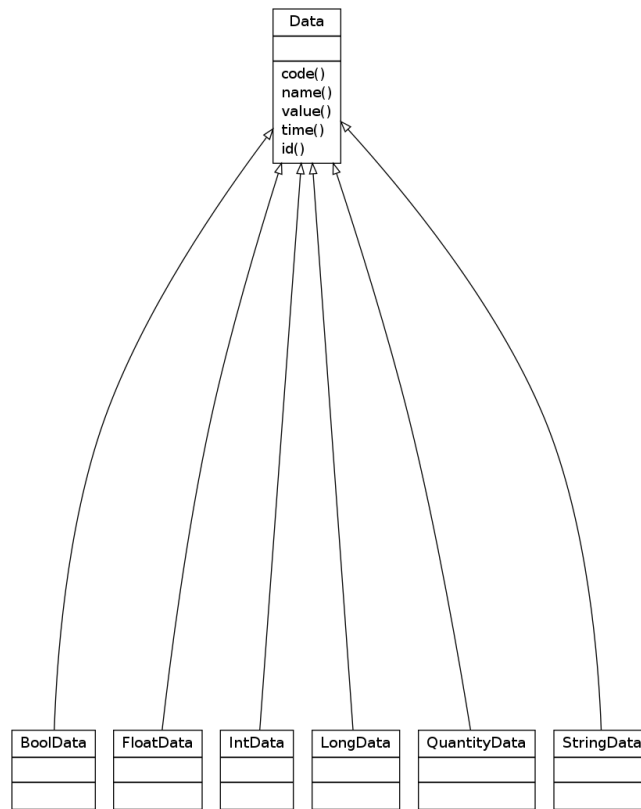
FIGURE 4.5: Datatype measurement class

Therefore measurement calls are threaded to allow measurements to be performed in parallel. Of course certain sensors and controllers may utilize the same hardware and therefore race conditions can result. It is therefore important for these to devices to implement thread locking at the hardware level for these objects. After measurements are made they are passed onto the DataHandler object for storage as well as returned to the function call.

4.2.3.5 Documentation

As the purpose of Ni-Engine is to be a general neutron interferometry experimental engine and not just to be used one time the neutron contrast experiment it is important that documentation be available for future researchers that may not have the luxury of a hands on introduction by the software designers. To increase the software ease of use

4.3 Q-Infer

4.3.1 Interaction with NI-Engine

4.3.2 GPU Implementations of Likelihood functions

Chapter 5

Discussion

5.1 Application to Quantum Information

5.2 Application to Quantum Fundamentals

5.3 Application to Materials Science

5.4 Outside of Neutron Interferometry

Chapter 6

Conclusion

6.1   Contrast Improvement with MCMC Methods

6.2   The Experimental Setup

6.3   Application of Findings

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