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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:

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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

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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

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

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 $939.56Mev$. 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),

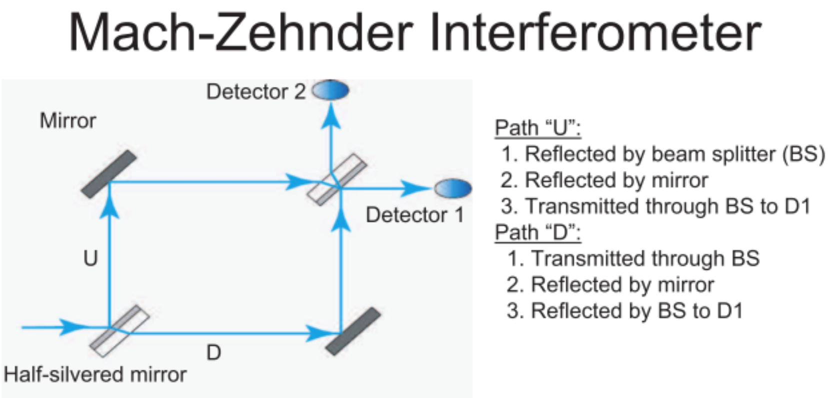

FIGURE 2.1: The Mach-Zehnder interferometer

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.[**?**]

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.[**?**]

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 $\left|\Psi\right\rangle \rightarrow \left|\Phi\right\rangle$ as $\mathcal{V} \rightarrow 0$. 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

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

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

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

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

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

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 $|\boldsymbol{x}| >> \left|\boldsymbol{x}'\right|$.

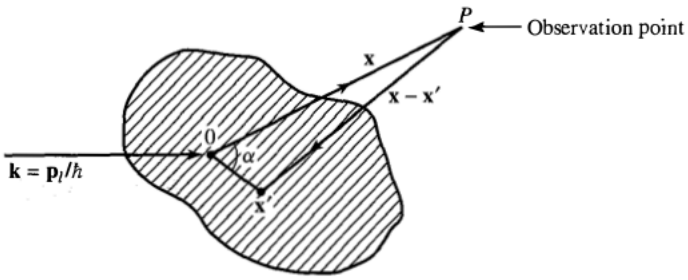

FIGURE 2.2: The finite range scattering potential. Any observations via detectors will be outside the range of the potential and therefore approximations can be made when evaluating (2.8).

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 $|\Phi\rangle \rightarrow |\boldsymbol{p}\rangle$ 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

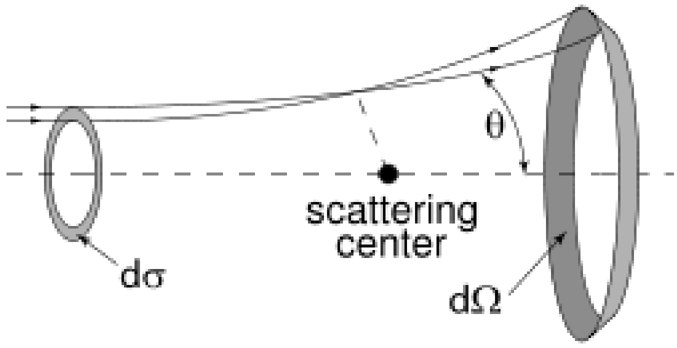

FIGURE 2.3: The differential cross section is the relationship between incident particles travelling through area $d\sigma$ to scattered particles crossing through the solid angle $d\Omega$

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

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

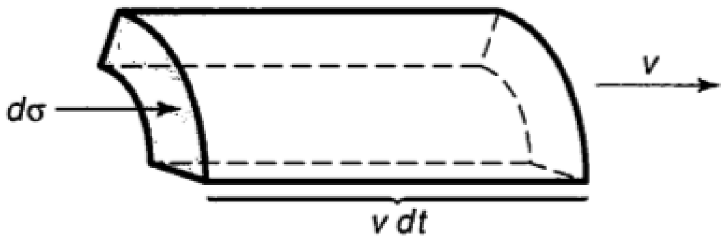

FIGURE 2.4: The volume element dV that a beam occupies passing through an area $d\sigma$ in time dt

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

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

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

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

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

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

. The spherical symmetry can be used to integrate explicitly the angular component of the scattering magnitude.

$$f^{(1)}(\theta) = -\frac{m}{2\pi\hbar^2} \int d^3x' e^{i(\boldsymbol{k} - \boldsymbol{k}')\cdot\boldsymbol{x}'} \mathcal{V}(\boldsymbol{x}') = -\frac{m}{2\pi\hbar^2} \int_{r=0}^{\infty} \int_{\phi=0}^{2\pi} \int_{\theta'=0}^{\pi} e^{i|q||r|cos(\theta')} sin(\theta') r^2 \mathcal{V}(r) d\theta' d\phi dr$$

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

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 $V(\mathbf{r})$ 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 $\mathbf{r} = 10^{-15}m$. 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 with the wave-function

$$\Psi_i = e^{ikz} \tag{2.22}$$

As the nucleus is a point scatterer as in section(**??**) the outgoing scattered wavefunction will be spherically symmetric of the form

$$\Psi_s = -\frac{b}{r}e^{ikr} \tag{2.23}$$

$b \in \mathbb{C}$ is the *nuclear scattering length* of the nucleus and is dependent on the composition of the nucleus. The imaginary component of b only plays a role for nuclei that have a high absorption coefficient. For a three dimensional group of nuclei the resultant outgoing scattered wave will be of the form

$$\Psi_s = -\sum_i \frac{b_i}{r}e^{ikr}e^{i\mathbf{q}\cdot\mathbf{r}} \quad \mathbf{q} = \boldsymbol{k_i} - \boldsymbol{k_s} \tag{2.24}$$

Where $\boldsymbol{k_i}, \boldsymbol{k_s}$are the wavevectors of the incoming and scattered waves respectively.

2.2.7 Neutron Wave Guides

Chapter 3

Experimental Setup

3.1 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.

3.1.1 NIST

3.1.2 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.

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

If the perpendicular component of the neutron energy incident on the guide is less than the potential of the guide it will be reflected.

3.1.3 Motors and Actuators

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