A probabilistic description of neutron scattering in a polycrystalline material

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Abstract

The aim of this thesis is to give a statistical description of a neutron traversing a neutron detector system consisting of a polycrystalline support material. The material used as support material in this project is aluminium although the results are applicable to any polycrystalline material. A mathematical description of the possible interactions in the detector system will be given, from which the probabilistic nature of neutron scattering will be derived.

Alongside the main results there will also be a shorter mention of a different approach to finding the stochastic behaviour of the neutron scattering. This approach was however not fully pursued as it did not produce the expected simplifications and results. Last but not least there will be a discussion about the future work which can be done and how to continue this project as there is no complete solution to the entire problem.

Contents

1 Introduction

Neutron diffraction is the utilization of neutron scattering in order to determine the atomic and magnetic structures of a material. Neutron scattering renders a precise study of atomic level structures possible, as neutrons have a sufficiently small interaction with materials, allowing for materials being studied under extreme conditions such as high temperature or pressure, making it a very useful tool. Neutron diffraction is achievable by exposing a sample of a material to a beam of neutrons, which upon collision with the sample provides a diffraction pattern. Analyses of the diffraction patterns give insight into the properties of the material being examined. A necessary instrument for the performance of neutron diffraction is a neutron source which either is a nuclear reactor or a spallation source. As reactor based neutron imaging analysis is limited, there is a necessity of developing neutron sources that can further the applicability of neutron diffraction. The European Spallation Source (ESS) is a neutron (spallation) source based research centre currently under construction in Lund, Sweden, and will be operational in 2019. ESS will be fully operational in 2025 and will be able to produce neutron beams of an intensity which is 30 times larger than those produced in the existing neutron sources today. Neutron imaging is an extraordinary tool for examining materials on a molecular level with materials of interest ranging from computer chips, fuels, batteries, plastics to pharmaceuticals and medical devices, and the list continues. The more powerful the neutron source is, that is the larger the number of neutrons which can be produced by the neutron source, the more detailed and insightful the analyses become. This is where ESS will excel, enabling studies of even more complex problems. [6]

As the ESS will provide a significant improvement of the neutron source, the neutron detector systems will require similar enhancements. Previously, the neutron detector systems have been based on Helium-3 technology, however, a decreasing supply of Helium-3 has caused the need for a suitable replacement of technology used in the neutron detector system. A new promising technology is based on Boron-10, which will be used in the neutron detector systems of ESS.

A natural interest when constructing the neutron detector instruments is the effect of the neutron diffraction, that is, it is of interest to know where an incident neutron ends up after the interaction with the sample material. The path of the neutron travelling through the neutron detector system con-

stitutes a non-trivial statistical problem, which depends on various factors such as the geometry of the detector system, the nuclear interaction of the neutron and properties of the materials used in the detector system. The aim of this project is to give a mathematical description of the final position of the neutron, taking these factors into consideration.

2   The neutron detector system

The neutron detector systems considered in this project consist of a 10B4C (Boron-10) thin layer which is coated on a thicker substrate of support material. The single layer arrangement can be repeated with gas inbetween, forming a detector with several consecutive layers in order to make sure that even more neutrons will be detected. The reason for this construction is that for low energies of the neutrons, the direct detection of them is not possible. Instead, the Boron layer serves as a conversion step for the neutrons since there is a chance of the neutron being absorbed in the Boron layer. As the neutron is absorbed there is an emission of a lithium ion and an alfa particle in opposite directions. When these particles traverse the gas, the gas atoms are ionised, creating an electrical charge which can be detected. In this project, the case being considered is the one with aluminium as the support material. Moreover, it will be assumed that there is only a limitation in distance (denoted by D) in one of the directions whereas infinite lengths are assumed to hold for the other directions, see Figure 1.

The main thing of interest which will be investigated in this report is the following: given that the neutron enters the aluminium at a certain incidence angle, at what position and with what angle does it exit the aluminium? Before any calculations can be done, it is necessary to give a description of the physics in the aluminium.

3   A mathematical description of scattering and absorption in the aluminium foil

Inside the aluminium foil, there are two possible interactions between the neutron and the aluminium that can occur. These are absorption and scattering of the neutron. The exact meaning of what an absorption signifies does not need to be further investigated as the probability of an absorption
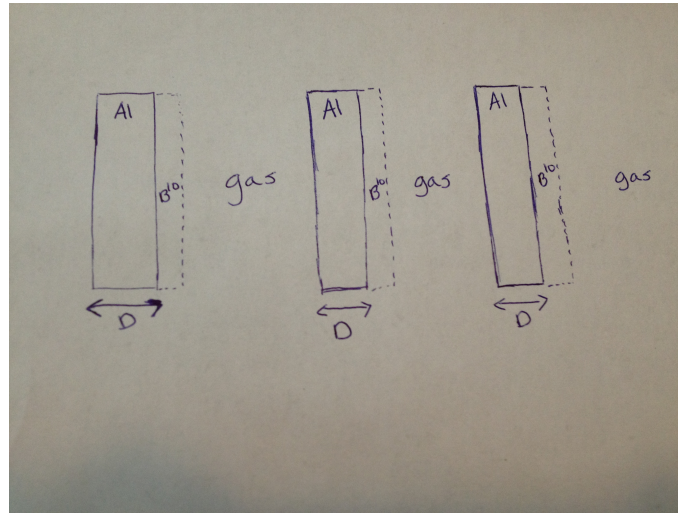
Figure 1: Neutron detector system

of the neutron inside the aluminium foil is small and will be neglected here, [4].

This fact limits a possible interaction to scattering of the neutron, which is either elastic or inelastic. For an elastic scattering process, the energy of the incident particle does not change when a scattering occurs whereas for an inelastic scattering process, the neutron either loses or gains energy. Henceforth, it is assumed that the scattering process is elastic. Furthermore, the length traversed by the neutron until there is a scattering is assumed to follow an exponential distribution with parameter λ. The reason for this is the following:

We start by defining the intensity for a continuous random variable X with probability density function f and distribution function F as

$$\lambda(x) = \frac{f(x)}{1 - F(x)} \quad .$$

The interpretation of this is apparent from the following:

$$
\begin{aligned}
\lambda(x)dx &= \frac{f(x) \cdot dx}{1 - F(x)} \\
&= \frac{P(x < X \leq x + dx)}{P(X > x)} \\
&= P(X \leq x + dx \,|\, X > x).
\end{aligned}
$$

The second equality follows from the definition of the probability of an event $X \in A$, which says that for an event $X \in A$, where A is a Borel set in $\mathbb{R}$, the probability of the event is equal to the integral over A of the probability density function of the continuous random variable X. In other words,

$$
P(X \in A) = \int_A f_X(x)dx
$$

where f is the probability density function of X. In the case above, the length of A is simply dx. Since we are dealing with infinitesimal values, the integral can be approximated by the product of the length of the interval A and the probability density function f evaluated at the starting point of A, obtaining $f(x)dx$. The third equality has simply made use of the definition of conditional probability.

Now assume that the intensity is constant $\lambda(x) \equiv \lambda$. This means that

$$
\lambda = \frac{f(x)}{1 - F(x)} = -\frac{d}{dx} \log(1 - F(x))
$$

Integrating both sides over the interval $[0, t]$ gives

$$
\begin{aligned}
\lambda \cdot t &= \int_0^t \lambda \cdot dx \\
&= -\int_0^t \frac{d}{dx} \log(1 - F(x))dx \\
&= -[\log(1 - F(t)) - \log(1 - F(0))] \\
&= -\log(1 - F(t))
\end{aligned}
$$

Since X is the distance traversed by the neutron, it is obvious that $F(0) = 0$ has to be fulfilled. The equality above is therefore equivalent to

$$
\begin{aligned}
e^{-\lambda t} &= 1 - F(t) \Leftrightarrow \\
F(t) &= 1 - e^{-\lambda t}
\end{aligned}
\tag{1}
$$

We recognize (1) as the exponential distribution, and so X is an exponentially distributed random variable.

Assuming the intensity function to be constant means that for any $u, v > 0$

$$P(v < X \leq v + dx \,|X > v) = P(u < X \leq u + dx|X > u)$$

This means that given that the neutron has already travelled some distance, the probability of it travelling some further distance dx is the same no matter where in the aluminium the neutron is located. Writing the above equality as a function of the intensity, this implies that

$$\lambda(v) \cdot dx = \lambda(u) \cdot dx \Leftrightarrow$$
$$\lambda(v) = \lambda(u) \ \forall \, (u, v) > 0.$$

Note that since there are not any variations in neither the atomic structure of the aluminium nor any other parameters as the neutron is traversing the aluminium, it is a valid assumption that λ is constant. Note also that $\frac{1}{\lambda} = E(X)$, that is, the expected or mean length to scattering is $\frac{1}{\lambda}$.

The value of the scattering intensity λ for aluminium is known and is given by

$$\lambda = \Sigma_{Al} = n_{at} \cdot \sigma_{Al} \, ,$$

where n_{at} is the atomic density $((cm)^{-2})$ of aluminium and σ_{Al} is the probability of a scattering in one aluminium atom. As it is rather vague what scattering in a single atom means, the concept of cross section needs to be introduced in order to explain this. The cross section, in our case the cross section for aluminium σ_{Al}, is a hypothetical area around the aluminium atom which can be thought of as a surface surrounding the atom. The cross section determines whether any sort of interaction will occur between the incident particle and the atoms of the material at which the particle is sent. If the particle hits the cross section of the atom, there is a 100 % chance of interaction whereas there is a 0 % chance of interaction if the particle misses the cross section. There are various types of cross sections but the one interesting in our problem is the scattering cross section. This can be calculated, and multiplied with the atomic density of aluminium as above,the scattering intensity λ is obtained. Since it is assumed that the scattering is elastic, there is no change to any of these parameters after a scattering and thus the distance travelled by the neutron until the next scattering is exponentially distributed with the same parameter λ.

Every time a scattering happens, although the energy of the neutron remains unaltered, there is a change in the direction in which the neutron is travelling. Since the direction is uniquely determined by the angle, the direction of the neutron after the scattering depends on the scattering angle. This is a 2-dimensional random vector, the distribution of which depends on the support material in the detector system. Having aluminium as the support material leads to coherent scattering which means that the scattering angle can only assume a finite number of values. One of the angles will be uniformly distributed on $[0, 2\pi]$ and the other will be a discrete random variable, which has a distribution that depends on the energy of the neutron. The probability mass function of the discrete random variable θ is given by
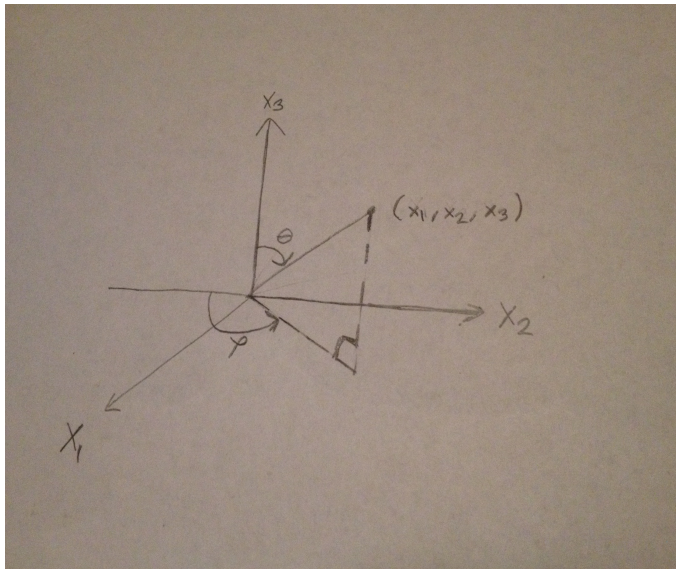

Figure 2: Angle Orientation

$$p_\theta(\theta) = \sum_{i=1}^{n(E)} a_i \delta(\theta - \theta_i)$$

where $n(E)$ denotes the number of different angles. The value of $n(E)$ is a function of the energy E of the neutron which determines the number of possible directions. The coefficients a_i satisfy $a_i \geq 0 \, \forall i$ and $\sum_{i=1}^{n(E)} a_i = 1$ and δ is the Dirac function, see appendix, cf. [3].

4 An approach to the problem of scattering in the aluminium foil

The main objective is to be able to determine the position of a neutron using probability theory, or rather the probability of the neutron ending up at a given position. Also, we would like to know the angle at which the neutron exits the aluminium foil. In order to do this, we consider the cartesian coordinates X_1, X_2, X_3 and thus want to find the probability density functions of X_1, X_2, X_3. Since the position of the neutron and its travelling angle depend on the number of scatterings in the foil, the law of total probability is going to be used:

$$P(A) = \sum_{i=0}^{\infty} P(A|B_i) \cdot P(B_i)$$

where A is an event and $B_i \cap B_j = \emptyset \,\forall i \neq j$ and $\bigcup_{i=0}^{\infty} B_i = \Omega$, where Ω is the sample space. In our setting, A is the event that the neutron ends up at a certain position and we are going to condition on the number of scatterings that can occur in the aluminium foil. This means that we are going to choose

$$B_i = \{w \in \Omega : \text{the number of scatterings} = \text{i}\}$$

where i=0,1,2,... Consequently, $A|B_i$ is the conditional event that the neutron ends up at a certain position given that i scatterings have taken place in the aluminium foil. It is important to include the case $i = 0$, which corresponds to 0 scatterings, since this is a possible event and we have to consider all possible events. Thus the sample space Ω, corresponding to $\bigcup_{i=0}^{\infty} B_i$, simply means that the possible outcomes are 0,1,2,... scatterings in the aluminium foil.

5 Description of the geometry

Now assume that the distance travelled by the neutron is exponentially distributed and that the scattering angle, which is a 2-dimensional random vector, consists of one continuous random variable, φ, and one discrete random variable, θ, assumed to be independent of each other. The fact that the latter angle is a discrete random variable is due to the choice of support material of which the foil consists. Recall that we are dealing with aluminium, which is a polycrystalline material. For a polycrystalline material, the atomic

structure can be thought of as the atoms lying in different planes with some distances $d_1, ..., d_n$ (in the case of n different planes) between the atoms in each plane. Considering a fixed plane of atoms, for incident neutrons with a certain energy, corresponding to a certain wavelength, and a given incident angle relative to the plane, there will occur constructive and destructive interference. Constructive interference occur only when the relation $k\lambda = 2d \cdot sin\theta$ where k is an integer, λ the wavelength of the incident neutrons (this is not to be confused with the scattering intensity), d is the distance between the atoms in the plane and θ the angle between the incident waveplane and the plane of atoms. This relation is known as the Bragg law, demonstrated in Figure 3 below. The multiple planes of atom layers ensure for a multiple although finite number of scattering angles, implying a discrete distribution for the second angle. [1]
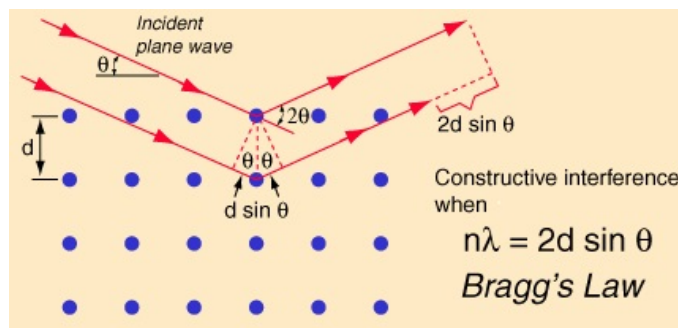

Figure 3: Bragg's law

To begin with, we are going to investigate the length travelled by the neutron until the first scattering, the length travelled by the neutron from the first scattering to the second, and so on. For this reason, we want to find the distributions of the distances from one scattering position to another. First of all the corresponding distribution in the X_1-direction will be considered and later the X_2- and X_3-directions as well.

It has been argued that the distances traversed by the neutron between scattering $i - 1$ and scattering i are exponential. It is of importance to bear in mind that the exponentially distributed distances travelled by the neutron is in some given direction, which does not have to coincide with the $X_1, X_2,$ or the X_3-directions. This distance will henceforth be denoted by T_i. Hence, depending on the incidence angle and the scattering angles, the

distances travelled by the neutron in the different directions are

$$\begin{cases} X_1^{(i)} = T_i \sin\theta \cos\varphi \\ X_2^{(i)} = T_i \sin\theta \sin\varphi \\ X_3^{(i)} = T_i \cos\theta \end{cases}.$$

It has to be taken into consideration that there are some restrictions to these variables due to the geometry of the detector system and the limitations of the thickness of the support material. As mentioned earlier, it is assumed that the thickness of the aluminium foil is D in the X_1-direction and infinite in the X_2- and X_3-directions. This implies that the maximum distance travelled by the neutron before a scattering occurs is a function of the angle at which the neutron is travelling, as well as the starting position of the neutron. The starting position refers to the position of the previous scattering, as the remaining distance that can be travelled depends on the position in the aluminium foil and the direction of the neutron.

Assume the position of the previous scattering $i-1$ is $X_1^{(i-1)}$. It is obvious that the remaining length in the forward direction is $D - X_1^{(i-1)}$ and in the backward case $X_1^{(i-1)}$. However, since the scattering angle is a random variable, the direction in which the neutron is travelling is unknown. For the given definition of the angles, the forward direction corresponds to the case $\varphi \in (-\frac{\pi}{2}, \frac{\pi}{2})$ and the backward case to $\varphi \in (\frac{\pi}{2}, \frac{3\pi}{2})$. This implies that the remaining length D_i is

$$D_i = \frac{D - X_1^{(i-1)}}{\sin\theta |\cos\varphi|} \mathbb{1}\{-\frac{\pi}{2} < \varphi < \frac{\pi}{2}\} + \frac{X_1^{(i-1)}}{\sin\theta |\cos\varphi|} \mathbb{1}\{\frac{\pi}{2} < \varphi < \frac{3\pi}{2}\}.$$

6 Derivation of the scattering distributions

6.1 Conditional distribution of $X_1^{(i)}$

We are going to find the conditional distribution of $X_1^{(i)}$ conditioned on the scattering angle at scattering number $i - 1$, denoted below by (θ, φ). We
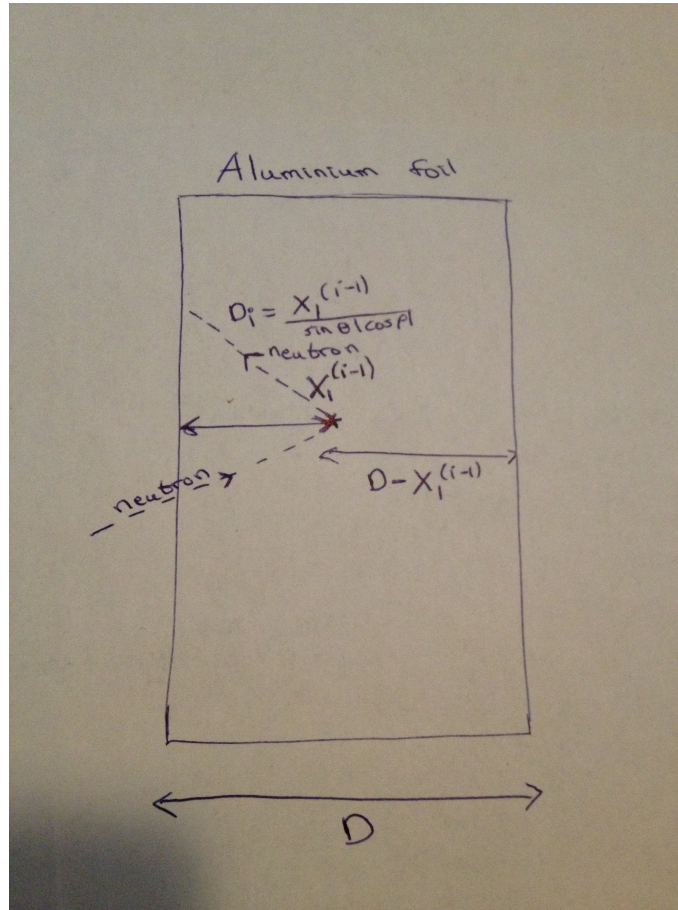
Figure 4: Remaining distance in the case of backscattering

obtain

$$
\begin{aligned}
F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) &= P(X_1^{(i)} \leq x|(\theta,\varphi)) \\
&= P(T_i \sin\theta \, \cos\varphi \leq x|(\theta,\varphi)) \\
&= P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \leq x|(\theta,\varphi)) \\
&= P(\{T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \leq x\} \cap \\
&\quad \{sign(\cos\varphi) > 0 \cup sign(\cos\varphi) < 0\}|(\theta,\varphi)) \\
&= P(\{T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \leq x \cap sign(\cos\varphi) > 0\} \cup \\
&\quad \{T_i \sin\theta \, |cos\varphi|sign(\cos\varphi) \leq x \cap sign(\cos\varphi) < 0\}|(\theta,\varphi))
\end{aligned}
$$

Since the two events in the union in the above expression are disjoint we get

$$
\begin{aligned}
F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \;=\;& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) > 0|(\theta,\varphi)) \\
+\;& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) < 0|(\theta,\varphi))
\end{aligned}
\tag{2}
$$

We study the first term in this expression first:
Since $T_1^{(i)}, \sin\theta, |\cos\varphi|$ are all positive quantities, if $sign(cos\varphi > 0)$, this implies that the product of these four factors is positive. Hence, the intersection is nonempty for $x > 0$, whereas for $x < 0$, the intersection is the empty set and the probability is equal to zero. Therefore, the first term is

$$
\begin{aligned}
& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) > 0|(\theta,\varphi))\mathbb{1}\{x \ge 0\} \\
=\;& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) > 0 \\
& \cap ((\theta,\varphi) \in I_1 \cup (\theta,\varphi) \in I_2)|(\theta,\varphi))\mathbb{1}\{x \ge 0\} = \\
=\;& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) > 0 \cap (\theta,\varphi) \in I_1)|(\theta,\varphi)) \\
& \cdot \mathbb{1}\{x \ge 0\} + \\
+\;& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) > 0 \cap (\theta,\varphi) \in I_2)|(\theta,\varphi)) \\
& \cdot \mathbb{1}\{x \ge 0\}
\end{aligned}
$$

where the sets I_1, I_2 are given by

$$
I_1 = \{(\theta,\varphi) : \theta \in \Theta, \varphi \in (-\frac{\pi}{2}, \frac{\pi}{2})\},
$$
$$
I_2 = \{(\theta,\varphi) : \theta \in \Theta, \varphi \in (\frac{\pi}{2}, \frac{3\pi}{2})\}.
$$

Note that

$$
sign(\cos\varphi) = \begin{cases} > 0 & \text{for } (\theta,\varphi) \in I_1\,, \\ < 0 & \text{for } (\theta,\varphi) \in I_2\,. \end{cases}
$$

We will use the fact that for any events A and B

$$
0 \le P(A \cap B) \le P(B)\,.
$$

Hence

$$
\begin{aligned}
0 \;\le\;& P(T_i \sin\theta \,|\cos\varphi|sign(\cos\varphi) \le x \cap sign(\cos\varphi) > 0 \cap (\theta,\varphi) \in I_2|(\theta,\varphi)) \\
\le\;& P(sign(\cos\varphi) > 0 \cap (\theta,\varphi) \in I_2|(\theta,\varphi)) \\
=\;& 0
\end{aligned}
\tag{3}
$$

Thus the first term in (2) becomes

$$P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, sign(\cos\varphi) > 0$$
$$\cap \, (\theta,\varphi) \in I_1)|(\theta,\varphi))\mathbb{1}\{x \ge 0\} + 0$$
$$= \quad P(T_i \sin\theta \, | \cos\varphi| \le x \, \cap \, (\theta,\varphi) \in I_1)|(\theta,\varphi))\mathbb{1}\{x \ge 0\}$$

Next, we study the second term of (2): This distribution holds for $x < 0$ and is equal to 0 elsewhere, due to the fact that the intersection of the two terms implies that the quantities are both negative and hence, the probability of getting a positive value is 0. So for $x < 0$,

$$P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, sign(\cos\varphi) < 0|(\theta,\varphi))\mathbb{1}\{x < 0\}$$
$$= \quad P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, sign(\cos\varphi) < 0$$
$$\cap \, ((\theta,\varphi) \in I_1 \, \cup \, (\theta,\varphi) \in I_2)|(\theta,\varphi)\mathbb{1}\{x < 0\} =$$
$$= \quad P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, sign(\cos\varphi) < 0$$
$$\cap \, (\theta,\varphi) \in I_1)|(\theta,\varphi))\mathbb{1}\{x < 0\} +$$
$$+ \quad P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, sign(\cos\varphi) < 0$$
$$\cap \, (\theta,\varphi) \in I_2)|(\theta,\varphi))\mathbb{1}\{x < 0\}$$
$$= \quad 0 + P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, sign(\cos\varphi) < 0$$
$$\cap \, (\theta,\varphi) \in I_2)|(\theta,\varphi))\mathbb{1}\{x < 0\}$$
$$= \quad P(T_i \sin\theta \, | \cos\varphi|sign(\cos\varphi) \le x \, \cap \, (\theta,\varphi) \in I_2)|(\theta,\varphi))\mathbb{1}\{x < 0\}$$
$$= \quad P(T_i \sin\theta \, | \cos\varphi| \ge -x \, \cap \, (\theta,\varphi) \in I_2)|(\theta,\varphi))\mathbb{1}\{x < 0\}$$

The first equality follows from (3) with changes in $sign(\cos\varphi) > 0$ and $(\theta,\varphi) \in I_2$ to $sign(\cos\varphi) < 0$ and $(\theta,\varphi) \in I_1$ which gives similar results.

Consequently

$$F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \quad = \quad \begin{cases} P(T_i \le \frac{x}{\sin\theta \, |\cos\varphi|} \, \cap \, (\theta,\varphi) \in I_1)|(\theta,\varphi), x > 0 \\ P(T_i \ge \frac{-x}{\sin\theta \, |\cos\varphi|} \, \cap \, (\theta,\varphi) \in I_2)|(\theta,\varphi), x < 0 \end{cases}$$

$$= \quad \begin{cases} \mathbb{1}\{(\theta,\varphi) \in I_1\} \cdot P(T_i \le \frac{x}{\sin\theta \, |\cos\varphi|}), x > 0 \\ \mathbb{1}\{(\theta,\varphi) \in I_2\} \cdot P(T_i \ge \frac{-x}{\sin\theta \, |\cos\varphi|}), x < 0 \end{cases}$$

$$= \quad \begin{cases} \mathbb{1}\{(\theta,\varphi) \in I_1\} \cdot (1 - e^{-\frac{x}{\sin\theta \, |\cos\varphi|}}), x > 0 \\ \mathbb{1}\{(\theta,\varphi) \in I_2\} \cdot e^{-(-\frac{x}{\sin\theta \, |\cos\varphi|})}, x < 0 \end{cases}$$

$$(4)$$

This implies that the conditional probability density function of $X_1^{(i)}$ is

$$
\begin{aligned}
f_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) &= \begin{cases} \mathbb{1}\{(\theta,\varphi) \in I_1\} \cdot \frac{1}{\sin\theta|\cos\varphi|}e^{-\frac{x}{\sin\theta|\cos\varphi|}}, x > 0 \\ \mathbb{1}\{(\theta,\varphi) \in I_2\} \cdot \frac{1}{\sin\theta|\cos\varphi|}e^{\frac{x}{\sin\theta|\cos\varphi|}}, x < 0 \end{cases} \\[2mm]
&= \begin{cases} \mathbb{1}\{(\theta,\varphi) \in I_1\} \cdot \frac{1}{\sin\theta|\cos\varphi|}e^{-\frac{|x|}{\sin\theta|\cos\varphi|}}, x > 0 \\ \mathbb{1}\{(\theta,\varphi) \in I_2\} \cdot \frac{1}{\sin\theta|\cos\varphi|}e^{-\frac{|x|}{\sin\theta|\cos\varphi|}}, x < 0 \end{cases}
\end{aligned}
$$

6.2 Unconditional distribution of $X_1^{(i)}$

In order to obtain the unconditional distribution function of $X_1^{(i)}$, we integrate over all possible values of (θ,φ) by the law of total probability. As before, the random variables are assumed to be independent. We begin with the case $x > 0$:

$$
\begin{aligned}
F_{X_1^{(i)}}(x) &= \int_\theta \int_\varphi F_{X_1^{(1)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_{\theta,\varphi}(\theta,\varphi)d\theta d\varphi \\
&= \int_{I_1} \int F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_\theta(\theta)f_\varphi(\varphi)d\theta d\varphi + \\
&\quad \int_{I_2} \int F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_\theta(\theta)f_\varphi(\varphi)d\theta d\varphi \\
&= \int_{I_1} \int F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_\theta(\theta)f_\varphi(\varphi)d\theta d\varphi + 0 \\
&= \int_\theta \int_{\varphi=-\frac{\pi}{2}}^{\frac{\pi}{2}} F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi))f_\varphi(\varphi)f_\theta(\theta)d\varphi d\theta \\
&= \int_\theta \sum_{\theta_i} a_i \delta(\theta-\theta_i) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi))\frac{1}{2\pi}d\varphi d\theta \\
&= \sum_{\theta_i} \frac{a_i}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi
\end{aligned}
$$

Here the first equality follows from the continuous version of the law of total probability, conditioning on the scattering angle which is a 2-dimensional random vector. The second equality follows from the independence between the two angles, θ, φ, and the use of the partition $I_1 \cup I_2$ of I. The third equality is a consequence of (4). The fourth equality is due to the fact that θ is a

discrete random variable with probability mass function p_θ. The penultimate equality has used the expression of the probability mass function of θ, with the probability mass function of θ being a sum of Dirac functions. The last equality follows from the property of the Dirac function.

For $x < 0$:

$$
\begin{aligned}
F_{X_1^{(i)}}(x) &= \int_\theta \int_\varphi F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_{\theta,\varphi}(\theta,\varphi)d\theta d\varphi \\
&= \int_{I_1} \int F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_\theta(\theta) f_\varphi(\varphi)d\theta d\varphi + \\
&\quad \int_{I_2} \int F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_\theta(\theta) f_\varphi(\varphi)d\theta d\varphi \\
&= 0 + \int_{I_2} \int F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \cdot f_\theta(\theta) f_\varphi(\varphi)d\theta d\varphi \\
&= \int_\theta \int_{\varphi=\frac{\pi}{2}}^{\frac{3\pi}{2}} F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) f_\varphi(\varphi) f_\theta(\theta) d\varphi d\theta \\
&= \int_\theta \sum_{\theta_i} a_i \delta(\theta - \theta_i) \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} F_{X_1^{(i)}|(\theta,\varphi)}(x|(\theta,\varphi)) \frac{1}{2\pi} d\varphi d\theta \\
&= \sum_{\theta_i} \frac{a_i}{2\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi
\end{aligned}
$$

The calculations in this case correspond to those in the case $x > 0$ with the only difference in the third equality which is due to (4) with corresponding changes to match the case of $x < 0$. Thus

$$
F_{X_1^{(i)}}(x) = \begin{cases} \sum_{\theta_i} \frac{a_i}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi & , 0 < x < D - Y_1^{(i-1)} \\ \sum_{\theta_i} \frac{a_i}{2\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi & , -Y_1^{(i-1)} < x < 0 \end{cases}
$$

The limits in the two cases depend on the position of the previous scattering, $Y_1^{(i-1)}$ $(Y_1^{(i-1)} = X_1^{(1)} + X_1^{(2)} + ... + X_1^{(i-1)})$. If the neutron continues forward, the remaining distance is $D - Y_1^{(i-1)}$. If the neutron travels backwards, the remaining distance becomes $Y_1^{(i-1)}$. The distribution of $F_{X_1^{(i)}|(\theta_j,\varphi)}(x|(\theta_j,\varphi))$ depends on, besides the scattering angle of course, the position of the previous scattering which in this case corresponds to $Y_1^{(i-1)}$.

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In order to obtain the probability density function of $X_1^{(i)}$, the probability distribution function is differentiated which leads to the following:

$$f_{X_1^{(i)}}(x) = \begin{cases} \frac{d}{dx}\left(\sum_{\theta_i} \frac{a_i}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi\right) & , 0 < x < D - Y_1^{(i-1)} \\ \frac{d}{dx}\left(\sum_{\theta_i} \frac{a_i}{2\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi\right) & , -Y_1^{(i-1)} < x < 0 \end{cases}$$

$$= \begin{cases} \sum_{\theta_i} \frac{a_i}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{d}{dx}\left(F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))\right)d\varphi & , 0 < x < D - Y_1^{(i-1)} \\ \sum_{\theta_i} \frac{a_i}{2\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} \frac{d}{dx}\left(F_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))\right)d\varphi & , -Y_1^{(i-1)} < x < 0 \end{cases}$$

$$= \begin{cases} \sum_{\theta_i} \frac{a_i}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} f_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi & , 0 < x < D - Y_1^{(i-1)} \\ \sum_{\theta_i} \frac{a_i}{2\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} f_{X_1^{(i)}|(\theta_i,\varphi)}(x|(\theta_i,\varphi))d\varphi & , -Y_1^{(i-1)} < x < 0 \end{cases}$$

$$= \begin{cases} \sum_{\theta_i} \frac{a_i}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{\sin\theta_i|\cos\varphi|} e^{-\frac{|x|}{\sin\theta_i|\cos\varphi|}} d\varphi & , 0 < x < D - Y_1^{(i-1)} \\ \sum_{\theta_i} \frac{a_i}{2\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} \frac{1}{\sin\theta_i|\cos\varphi|} e^{-\frac{|x|}{\sin\theta_i|\cos\varphi|}} d\varphi & , -Y_1^{(i-1)} < x < 0 \end{cases}$$

The fact that the differentiation can be moved inside the integral function is a result of the following theorem, as the conditional distribution of $X_1^{(i)}$ satisfy the assumptions of the Leibniz theorem, cf [2]:

Let K be a compact set in $\mathbb{R}^n$ and $s \in E$ where $E \subseteq \mathbb{R}$. Furthermore, let

$$I(s) = \int_K f(x, s)dx$$

and assume that f is partially differentiable with respect to s and that f and f_s' are continuous in $K \times E$. Then $I(s)$ is continuously differentiable in E and

$$I'(s) = \int_K f_s'(x, s)dx.$$

7 Further work

The work which so far has been done has led to the derivation of the unconditional probability density functions for the distances in between scatterings, where the probability density functions depend on the position of the previous scattering $Y_1^{(i-1)}$. It should be noted that the derived probability density

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functions only apply to the first coordinate X_1, which is the restricted axis. However, it is possible to use the same method in order to compute the probability density functions for distances in between scatterings also in the X_2- and X_3-directions. What has to be taken into consideration then are for which values of the angles that the X_2- and X_3-coordinates are positive and negative respectively. Another difference is that there are no limitations of the size of these latter coordinates as infinite lengths have been assumed in these directions. Once the unconditional distribution functions are calculated, one might use convolution in order to obtain the probability density function of the total distance travelled.

Let us denote the total distances travelled in each of the directions

$$
\begin{aligned}
Y_1 &= X_1^{(0)} + X_1^{(1)} + X_1^{(2)} + X_1^{(3)} + \dots \\
Y_2 &= X_2^{(0)} + X_2^{(1)} + X_2^{(2)} + X_2^{(3)} + \dots \\
Y_3 &= X_3^{(0)} + X_3^{(1)} + X_3^{(2)} + X_3^{(3)} + \dots
\end{aligned}
$$

Without having proved it yet, it can be stated that there is a very small possibility of having more than two scatterings. The estimated probabilities of the different number of scatterings have actually been calculated from ESS data, although this was in the case when vanadium was the support material, cf [5]. Even though there might be a dependence of the material, it is quite believable that the same results hold in our case, as the two problems are closely linked. For this reason, one could use the law of total probability to give a very good approximation using only the few first terms and use convolution in the cases of one or two scatterings. By construction, for k scatterings there will be $k + 1$ distances as there is also a distance from the last scattering until the neutron exits the aluminium foil. However, having conditioned on k scatterings using the law of total probability, $X_j^{(k+1)}$ will not be a random variable but a deterministic event as it will always be determined by the position of the last scattering and the last scattering angle. This can be expressed mathematically as $X_j^{(k+1)}$ having the Dirac function with the corresponding parameters as its probability density function.

8   A Poisson process approach

In the early stages of the project, when it was still unclear which approach to follow, the idea of using a Poisson process approach was introduced. This

was due to the fact that since the distances in between scatterings are exponentially distributed, there might have been a possibility to model the number of scatterings as a Poisson process since the time between events in a Poisson process are exponentially distributed.

Furthermore, the main reason for choosing the Poisson model is, by using the law of total probability conditioning on the events of having i scatterings before the neutron exits the aluminium foil, the probability can be approximated by limiting the number of possible scatterings to only a few. However, the summation to infinity will be kept for now. The notation $X_1^{(1)}$ is introduced for the distance in the X_1-direction until the first scattering. Thus, according to the law of total probability

$$F_{X_1^{(1)}}(u) = P(X_1^{(1)} \leq u) = \sum_{i=0}^{\infty} P(X_1^{(1)} \leq u | N(D) = i) P(N(D) = i)$$

In other words, the distribution of the distance to the first scattering is calculated by conditioning on all the possible events, that is, 0,1,2,... scatterings until the neutron exits the aluminium foil. In order to generalise this model for the distribution of any distance between scattering number $k - 1$ and k, some knowledge of the properties of a Poisson process is required.

8.1 Properties of the Poisson process

Let $N(D) = k$ denote the event of having k scatterings until the neutron exits the aluminium. Moreover, let $(T_1^{(i)}, T_2^{(i)}, ..., T_k^{(i)})$ denote the times of the first, second, ..., kth scattering where the superscript i refers to the distribution of the distance between scattering number $i - 1$ and i. Then, with i being equal to one for the distribution of the length until the first scattering, and assuming the neutron enters the aluminium perpendicularly, $(T_1^{(1)}, T_2^{(1)}, ..., T_k^{(1)}) | N(D) = k$ are independent $U[0, D]$ where $U[0, D]$ denotes the uniform distribution. For the ordered sample, that is,

$$T_{(1)}^{(1)}, T_{(2)}^{(1)}, ..., T_{(k)}^{(1)} = \text{sort}(T_1, T_2, ..., T_k)$$

the probability distribution function, when having an arbitrary incident angle, is given by

$$F_{T_{(1)}|N(D)=k}(t) = 1 - (1 - F_{U^{(1)}}(t))^k \text{ where } U^{(1)} \in U[0, D_1].$$

where
$$D_1 = \frac{D}{sin\theta cos\varphi}$$

Since $T_{(1)}$ is the distance traversed by the neutron in some direction, the distance in the X_1-direction can be obtained by suitable scaling depending on the incident angle.

Second scattering:

The same arguments are made for the length travelled in the X_1-direction until the second scattering. However, the conditions have changed. Depending on the position of the first scattering and the resulting scattering angle $(\theta^{(1)}, \varphi^{(1)})$, the distance D_2, up to the length of which the neutron can travel at most, will be restricted as to make sure the neutron stays within the aluminium foil (due to the assumptions of infinite length in X_2, X_3-directions, D_2 will depend on (X_1, θ, φ)). So, with the same assumptions as before but with D_2 replacing D from the previous calculations, we obtain

$$(T_1^{(2)}, T_2^{(2)}, ..., T_k^{(2)}) | N(D_2) = k \text{ independent } U[0, D_2]$$

and the ordered sample is now

$$T_{(1)}^{(2)}, T_{(2)}^{(2)}, ..., T_{(k)}^{(2)} = \text{sort}(T_1^{(2)}, T_2^{(2)}, ..., T_k^{(2)})$$

Thus, the conditional distribution becomes

$$F_{T_{(1)}^{(2)} | N(D) = k}(t) = 1 - (1 - F_{U^{(2)}}(t))^k \text{ where } U^{(2)} \in U[0, D_2].$$

The distributions of the lengths until the third, fourth,... scattering are determined in a similar way as for the second.

Although a lot more work was done using this approach, it suffices to say that the results were derived in a similar way as in the main approach. More precisely, the derivation of the results in this latter was rather a modification/improvement on the calculations based on the Poisson model. The principal cause for changing approaches and finding another model is that the Poisson process model did not simplify calculations as hoped. Thus there was no reason to use this latter model as it gave an approximation instead of the true probability, which also was easier to determine.

9   Conclusion

To summarize, using neutron diffraction as a research tool requires not only powerful neutron sources but also advanced neutron detector systems. Considering a detector system which uses a polycrystalline material as support material, the distributions of the lengths inbetween scatterings inside the support material have been derived. These depend on the position of the previous scattering as well as limitations implied by the geometry of the detector system. Using a general approach in the calculations in the limited case, this approach can also be applied to the cases which are not subject to geometrical restrictions, with appropriate modifications.

The path of the neutron inside the neutron detector system is arguably a large problem with many parameters to consider. The pursuit of a complete mathematical description of the problem was stopped due to a shortage of time, although there were ideas how to do this. Hopefully this project can be continued based on these results and the ideas suggested, or other ones which might provide an accurate description.

A   The Dirac (generalised) function

In order to treat the Dirac generalised function rigorously, one needs to be acquainted with either distribution theory or measure theory, as the Dirac function belongs to the class of generalised functions. Instead of doing this, some of the more basic properties and in particular useful and needed results for this project will be introduced. Having said that, the Dirac function, also known as the delta function, can be thought of as the function defined on the real line which is constantly equal to zero for every point except at the origin where it is infinitely large. This is expressed as

$$\delta_0(x) \;=\; \begin{cases} \infty & , x = 0 \\ 0 & , x \neq 0 \end{cases} \;.$$

The function description above is merely an aid to get some intuitive idea of the behaviour of the Dirac function. Mathematically, the Dirac function, δ_0, is defined as a linear functional $C_0^\infty \longmapsto \mathbb{R}$ taking any $g \in C_0^\infty(\mathbb{R})$ to $g(0)$, where $C_0^\infty(\mathbb{R})$ is the set of functions that are infinitely many times continuously differentiable and that have compact support. This can also be

written as

$$\int_{\mathbb{R}} g(x)\delta_0(x)dx = g(0) \tag{5}$$

A consequence of this is, since $g(x) \equiv 1 \in \mathbb{R}$ is infinitely many times continuously differentiable, that $\int_{\mathbb{R}} \delta_0(x)dx = 1$. In relation to probability theory, a random variable with cumulative distribution function

$$H(x) = \begin{cases} 1 & , x \geq 0 \\ 0 & , x < 0 \end{cases}$$

would have the Dirac function as its density function. Thus for random variables which assume only a single value with probability 1, the Dirac function can be used as the probability density function to describe this point mass.

The delta function can be translated to some other point $a \in \mathbb{R}$ so that

$$\delta_a(x-a) = \begin{cases} \infty & , x = a \\ 0 & , x \neq a \end{cases}$$

with the corresponding change in (5) to

$$\int_{\mathbb{R}} g(x)\delta_a(x)dx = g(a)$$

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