EPJ Web of Conferences **298**, 05001 (2024) https://doi.org/10.1051/epjconf/202429805001
UCANS-10

A high brilliance low-frequency spallation source optimized for one single instrument

Mina Akhyani[1*], *Henrik M.* Rϕnnow[1], and *Luca* Zanini[2]

[1]Laboratory for quantum magnetism (LQM), Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
[2]European Spallation Source, Lund, Sweden

Abstract. Conducting neutron scattering experiments in the presence of high pulsed magnetic fields provides valuable information about the magnetic structures of materials. However, these experiments are challenging and time-consuming because the neutron count is typically low, due to the asynchronization between the neutron and magnetic pulses. In this paper we investigate the idea of having an optimized dedicated source, i.e. a second target station at the European Spallation Source (ESS). This involves extracting protons from the same linear accelerator (linac) as the first target, synchronizing their frequency with the magnetic pulse frequency. The lower frequency contributes to a considerable decrease in the average heat load and provides greater flexibility in positioning neutron optics due to reduced radiation damage. Through an analytical approach, we investigated the effect of the moderator size and the guide distance on the sample flux, and compared it to the current ESS design.

1 Introduction

Neutron scattering under very high magnetic fields (above 40 T) plays a crucial role in investigating the behavior of magnetic systems at a microscopic level [1]. These experiments are currently conducted at facilities such as Institut Laue-Langevin (ILL) [2], the Spallation Neutron Source at US (SNS) [3], Japan Proton Accelerator Research Complex (J-PARC) [4] and are expected to be conducted at ESS in the near future [5]. Presently, very high magnetic fields can only be generated using pulsed normal conducting copper coil magnets. However, with each pulse, the magnet heats up and requires a cooling period of approximately 10-30 minutes, depending on the strength of the magnetic field [6] - [7]. As a result, the neutrons generated at a frequency of some tens of Hz in spallation sources, or continuously in reactors will remain unused during these cooling intervals.

We face technological limitations in reducing the frequency of magnet pulses, prompting the concept of designing a dedicated source for this instrument. This dedicated source could potentially act as a second target station within an existing neutron facility, such as ESS. Proton bunches extracted from the linac, synchronized with magnet pulses, would involve the use of a dipole magnet and an extraction line. The reduced frequency would substantially

* Corresponding author: mina.akhyani@epfl.ch

decrease the average heat and radiation loads by approximately three orders of magnitude. Moreover, this second target station is designed to accommodate just one instrument. These two reasons enable the guides to initiate closer to the source, unlike at ESS where neutron optics typically start at 2 meters. This allows to optimize the source to the needs of only one single instrument—a neutron diffractometer/spectrometer which utilize both thermal (20-100 meV) and cold (1-20 meV) neutrons. The typical sample size is 1 cm², with a divergence of approximately 1 degree for thermal neutrons and up to a maximum of 2.5 degrees for cold neutrons. These limitations stem from challenges in transporting different neutron energies inside the neutron guides. The sample is located at minimum 40 cm distance away from the guide exit, due to cryogenic installations.

This paper aims to examine the potential gain factors achievable in sample flux through the utilization of cold neutron spectra. Our comparison will be centered around ESS, acknowledged as the brightest neutron source globally and envisioned as the most efficient option for similar experiments in the near future. The adjustable parameters in this proposed dedicated source include the moderator's geometry and the distance between the source and neutron transport system. We intend to analytically investigate how these two parameters influence the sample flux.

2 FoM for the optimization

In most neutron scattering experiments, the primary objective is to maximize the neutron count rate on the sample. Achieving this involves incorporating neutron production in the target and simulating the transport of neutrons from the source to the neutron guides and ultimately to the sample. Monte Carlo simulation codes, such as PHITS [8], utilized for detailed modelling of neutron production and transport, require substantial computing resources. This limitation can restrict their application, particularly in the context of large-scale neutron sources. Consequently, it becomes advantageous to break down and independently optimize various subsystems, such as the source, transportation to guides, and transportation to the sample.

For a specific energy range, brightness refers to phase space (PS) density, calculated as the number of neutrons per second divided by the PS volume [9]-[10]. Using this terminology, Liouville's theorem asserts that for conservative force fields, the PS density—i.e., brightness—remains constant [11]. In mathematical terms:

$$\emptyset_s = \int B_s \cdot dV_s = \int B_M \cdot dV_M = \int B_M \cdot k \cdot dV_s \quad (1)$$

Here $\emptyset_s$ is the sample flux, B_s is the brightness at the sample, V_s and V_M are the PS volume at the sample and moderator, respectively, B_M is the brightness at the moderator, and k is a factor for the efficiency of PS volume transportation. This factor depends, on one side, on the losses in Neutron Transport System (NTS)[†], namely Brilliance [‡] Transfer (BT), and on the other side, the under- or over-illumination of the NTS entrance and the sample, which we call *illumination factor*.

Minimizing the NTS losses has been facilitated by advancements in neutron guide manufacturing over recent decades, combined with the adoption of Monte Carlo simulation

[†] Any elements situated between the moderator and sample is called the neutron transport system (NTS), which may include neutron guides, focusing mirrors, lenses, monochromators, entrance and exit slits, Soller collimators, etc.

[‡] "brilliance" or the spectral brightness, defined as the number of neutrons emitted from an area onto a specified solid angle within a certain energy range over a given time. Integrating this quantity over the energy range yields the brightness definition used in the context described.

packages such as McStas [12]. This advancement allows us to focus our efforts on optimizing the PS density at the entrance of the neutron transport system and separate the neutron source optimization problem into two distinct aspects: the source brightness and, the everything on the guide system happening between the source and the sample, which contribute to the BT and the illumination factor [9], [13], [14].

In this analytical approach, we assume an NTS with negligible losses and employ approximations for both the source brightness and the illumination factor. These approximations are based on optimal and full sample illumination (OFSI) conditions [14]. Through this comprehensive geometrical approach, we aim to estimate the maximum achievable gain factor in the sample flux compare to the sample flux at ESS, presently under construction in Lund, Sweden, which stands as the brightest neutron source globally. Hence, conducting high magnetic field experiments on ESS beamlines, e.g. at BiFrost, inherently provides a gain factor compared to the currently available instruments. Consequently, our decision to benchmark our results against those from ESS was made.

When deliberating between cold and thermal moderators, we opted for the gain offered by the cold spectrum. This choice stemmed from the directional nature of cold neutrons emanating from the parahydrogen moderator, providing higher directionality compared to thermal neutrons. Therefore, a higher gain in the cold spectrum is anticipated.

3 Sample flux gain factor: analytical approach

Considering an ideal NTS with negligible loss ($BT \approx 1$), the k factor will only depend on the illumination conditions which can be explained by the intersection of PS shapes at each location and can be segmented into two terms.

First, from the moderator surface to the entrance of the NTS, represented as the ratio of the PS shape at the moderator (V_M) accepted by the entrance PS volume of the NTS (V_{in}). The second term involves the fraction of the PS shape at the NTS exit (V_{out}) accepted by the sample's PS shape (V_s). Mathematically, this is expressed as follows:

$$illumination\ factor = \frac{V_{in} \cap V_M}{V_{in}} \times \frac{V_{out} \cap V_s}{V_s} \quad (2)$$

As can be seen the maximum of illumination factor can reach 1. Analytical formulas for this quantity can be derived using a fully geometrical calculation method, as detailed in [14]. This method conceptualizes the NTS as a black box and is built upon the sample PS requirements. In this context, an NTS exit capable of fully and optimally illuminating the sample is referred to as PS focusing exit. On the other hand, an NTS entrance that can accept neutrons from the moderator in a shape transportable to the NTS focusing exit shape is called PS focusing entrance. Since, we assumed a lossless transport in the NTS system, based on Liouville's theorem, the density will remain conserved, although its shape can change during the transport. Obviously, a PS non-focusing exit has a shape that does not match the PS shape of the sample after transport from the guide exit to the sample position, and PS non-focusing entrance means that the PS shape provided by the moderator cannot be fully transported by the NTS system.

Based on the four configurations of PS focusing/non-focusing at both the NTS entrance and exit, along with the other parameters, such as distances between the NTS entrance and the moderator (L_{in}), the distance between the NTS exit and the sample (L_{out}) and the shape of the sample's PS volume (rectangular or parallelogram), 1D PS volumes (as the unit [cm.sr]) for the NTS exit, entrance and the moderator surface can be derived analytically.

Among the cases, we selected the NF-F (entrance-exit) case due to its resemblance to elliptic guide designs commonly utilized. The PS volume at the sample in our instrument is rectangular (notated as n=1 in the paper) with the two sizes of 1 cm.deg and 2.5 cm.deg.

Based on the selection of this configuration, the results are independent of L_{out}. Detailed mathematical calculations are available in Appendix C of [14].

In designing this dedicated source, there are two adjustable factors open for optimization. At ESS, the moderator height remains fixed at 3 cm, a result of numerous optimizations catering to the requirements of various instruments [13]. Additionally, the guide entrance is constrained to a position at 200 cm due to accommodation of all instrument suites and radiation safety. In our source design, optimization aims to meet the needs of only one single instrument, allowing for variations in the moderator size in comparison to the fixed ESS specifications. Moreover, given the relatively low average heat load resulting from the infrequent proton pulses, the NTS can be positioned closer to the source. These alterations influence the PS volume at the moderator surface, essential for fully illuminating the sample PS volume.

In Eq. (1) and Eq. (2), assuming a constant value for B_M, then $\emptyset_s$ will be equivalent to the k variation. In this approach, BT is equal to one, therefore k represents only the illumination factor. Fig. 1 illustrates the illumination factor concerning various combinations of moderator extraction window (D_M) and NTS entrance size (ω_{in}) for two different L_{in}. The graph demonstrates that as proximity to the source increases, smaller moderators and NTS entrances fully and optimally illuminate the sample. This presents an opportunity to utilize low-dimensional moderators, resulting in higher brightness [15].

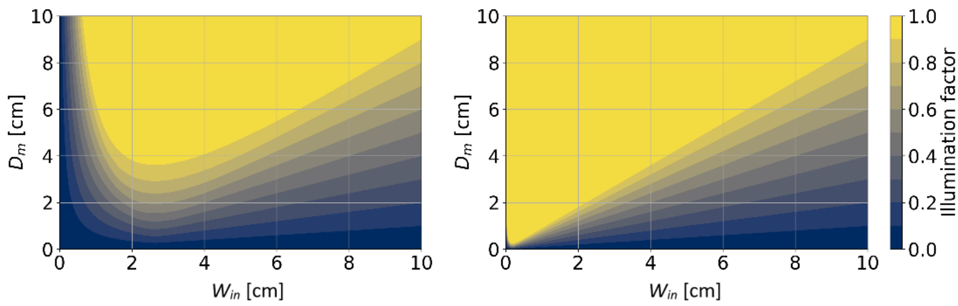

Fig. 1. Illumination factor for different sizes of moderator extraction window (D_m) and the NTS entrance size (w_{in}) for the sample PS volume 1 cm.deg; Left: $L_{in} = 200\ cm$, Right: $L_{in} = 1\ cm$

In the case of parahydrogen, research indicates that its brightness significantly depends on its size [10]. Utilizing the findings from Figure 18 in [10], we performed calculations for the sample flux. Fig. 2 illustrates the flux map for the parahydrogen moderator geometry at ESS. The results are for the illumination factor equal to 1 as in Fig. 1 for $L_{in} = 200\ cm$. It is evident that the highest flux occurs within a range of 2 to 4 cm at the moderator height and the NTS entrance (ESS utilizes a 3 cm moderator height). Incorporating the brightness function, the gain amounts to a 2.4-fold increase, indicating the potential for achieving higher flux by optimizing the source geometry.

Fig.3 depicts the maximum gain factor in sample flux relative to the ESS sample flux (moderator height equal to 3 cm and L_{in}= 200 cm) plotted against L_{in} for two distinct instrument requirements. Notably, at the closest L_{in}, a small sample PS volume of $d_s = 1\ cm$ and $\alpha_s = 1°$ achieves a maximum gain factor of 2.9, by setting both the moderator extraction window and NTS entrance to 0.35 cm. On the other hand, for a larger sample PS volume of $d_s = 1\ cm$ and $\alpha_s = 2.5°$, the maximum gain factor is 3.7, observed when the moderator extraction window and NTS entrance are both set at 0.5 cm.

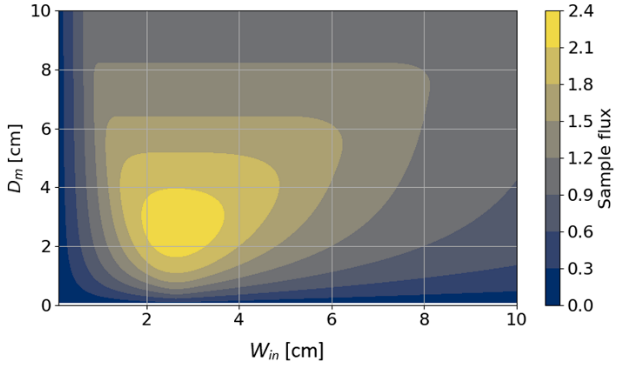

Fig. 2. Sample flux for the parahydrogen moderator for different sizes of moderator extraction windows (D_m) and the NTS entrance sizes (w_{in}) for the sample PS volume 1 cm.deg and $L_{in} = 200\ cm$. The flux is normalized to maximum in Fig.1, i.e. illumination factor=1.

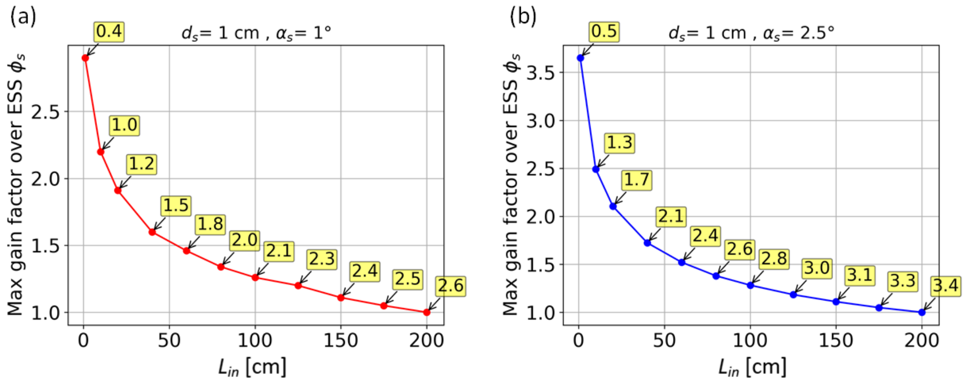

Fig. 3. Maximum gain factor over ESS sample flux (D_m= 3 cm, L_{in}= 200 cm) as a function of L_{in}. Each point on the figures are the optimal D_m and ω_{in} for the selected L_{in} and their value is equal and written in the yellow text box next to each point; (a) sample PS: $d_s = 1\ cm$, $\alpha_s = 1°$; (b) sample PS: $d_s = 1\ cm$, $\alpha_s = 2.5°$

4 Conclusion

Using an analytical approach, we estimated the achievable gain factor in comparison to ESS for a dedicated neutron scattering source operating under very high pulsed magnetic fields. The results revealed a maximum 3.7-fold gain for a large sample PS volume (2.5 cm.degree) and 2.9-fold for a small PS volume (1 cm.degree). However, in this calculation, we did not constrain the angular acceptance of the NTS entrance. This means that, according to the assumptions of this analytical framework, any neutrons originating close to the moderator's surface would be transported by NTS. In reality, this is not accurate, as the angular acceptance of the NTS restricts such transport. Consequently, the actual gain factors in close proximity to the source are likely lower than the reported values. With $L_{in} > 20$ cm being more reliable in terms of this framework, the maximum gain factor is more likely to be around 2.

Additionally, these calculations were based on the ESS geometry and the size-dependent brightness of parahydrogen. Changes in moderator material or geometry could potentially yield different outcomes. Moreover, the one-dimensional nature of this analytical method does not fully represent reality, as both the height and width of the moderator impact the brightness value. Hence, conducting Monte Carlo simulations becomes crucial for a more accurate estimation of the maximum gain factor on the sample flux.

The authors would like to thank Petr Konik for the precious discussions and valuable inputs. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 754354.

References

[1] M. Motokawa and M. Arai, Physica B: Condensed Matter, **213–214**, 1017–1021, (1995)
[2] F. Duc *et al.*, Review of Scientific Instruments, **89**, 053905 (2018)
[3] G. E. Granroth, D. H. Vandergriff, and S. E. Nagler, Physica B, Condensed Matter, 1104–1106 (2006)
[4] M. Watanabe, T. Kihara, and H. Nojiri, Quantum Beam Science, **7** (2023)
[5] https://www.fysik.dtu.dk/english/research-sections/nexmap/research/instruments-at-large-scale-facilities
[6] E. Fogh *et al.*, Phys. Rev. B, **101**, 024403 (2020)
[7] H. Nojiri *et al.*, Phys. Rev. Lett., **106**, 237202 (2011)
[8] K. Niita, T. Sato, H. Iwase, H. Nose, H. Nakashima, and L. Sihver, Radiation Measurements, **41**, 1080–1090 (2006)
[9] M. Bertelsen and K. Lefmann, Nim A, **830**, 313–324 (2016)
[10] L. Zanini *et al.*, Nim A, **925**, 33–52 (2019)
[11] Landau, Lev Davidovich, Course of Theoretical Physics, **5**. Pergamon Press, (1958)
[12] P. Willendrup, E. Farhi, E. Knudsen, U. Filges, and K. Lefmann, Journal of Neutron Research, **17**, 35–43 (2014)
[13] K. H. Andersen *et al.*, J Appl Crystallogr, **51**, 264–281 (2018)
[14] P. Konik and A. Ioffe, Nim A, **1056**, 168643 (2023)
[15] L. Zanini, F. Mezei, K. Batkov, E. Klinkby, and A. Takibayev, J. Phys.: Conf. Ser., **1021**, 012009 (2018)