3.2.12

A model for non-thermalized neutron spectra emitted from para-hydrogen

T. Schönfeldt[1,2], **K. Batkov**[2], **E. B. Klinkby**[1,2], **B. Lauritzen**[1], **F. Mezei**[2], **A. Takibayev**[2], **P. K. Willendrup**[3] **,L. Zanini**[2]

1: Center for Nuclear Technologies, Technical University of Denmark, Roskilde, Denmark
2: European Spallation Source, Lund, Sweden
3: Department of Physics, Technical University of Denmark, Lyngby, Denmark

Abstract. At spallation and reactor cold neutron sources, neutrons are cooled by moderators. At high power neutron sources, such as the Japan Proton Accelerator Research Complex (J-PARC), European Spallation Source (ESS) and the Spallation Neutron Source (SNS) only few moderator materials are practical, due to the high radiation environment near the moderator and cooling demands. One of the very popular materials, used at J-PARC and planed for ESS, is the spin singlet state of H_2, para-hydrogen. This study assesses the non-Maxwellian neutron spectral structure achieved in para-hydrogen moderators, which is due to the complexity of the inelastic scattering cross section below 50 meV. The analytical description of a thermalized spectrum with slowing down components are discussed, then a formula is developed which is a good description of this non-equilibrium para-hydrogen neutron spectrum.

These analytical descriptions are fitted to the thermal and cold neutron spectra expected at the European Spallation Source according to the baseline configuration, as described in the Technical Design Report (TDR). The results of the fits have been implemented in McStas 2.0 and is used throughout the ESS instrumentation community. Though not shown here it is worth noting that the spectra for different heights of moderators in the more recent ESS geometry have also been fitted to this para-hydrogen spectrum model, the fits have been implemented and released in McStas 2.1.

1. Introduction

According to the TDR (see [1]) the European Spallation Source (ESS) will produce neutrons by spallation, driven by a 5 MW, 2.5 GeV proton beam impacting on a massive rotating tungsten target wheel. The target will be surrounded by a moderator reflector system, where the neutrons will be thermalized in an ambient temperature light water moderator and cooled further in a 20 K cylinder of liquid para-hydrogen. The moderators will be surrounded by an inner reflector made from beryllium, which in turn is surrounded by an outer reflector made of steel, as shown in Figure 1.

Neutron production and moderation is simulated via the Monte Carlo method using MCNPX [2]. From these simulations it is possible to predict the expected brightness spectrum, as shown in Figure 2.

The spectral brightnesses from the cold and thermal moderators are plotted in Figure 2. The figure also shows the overall brightness expectation from bispectral extraction, which is calculated from the cold and thermal spectrum respectively taking into account expected transmission and reflection factors [3].

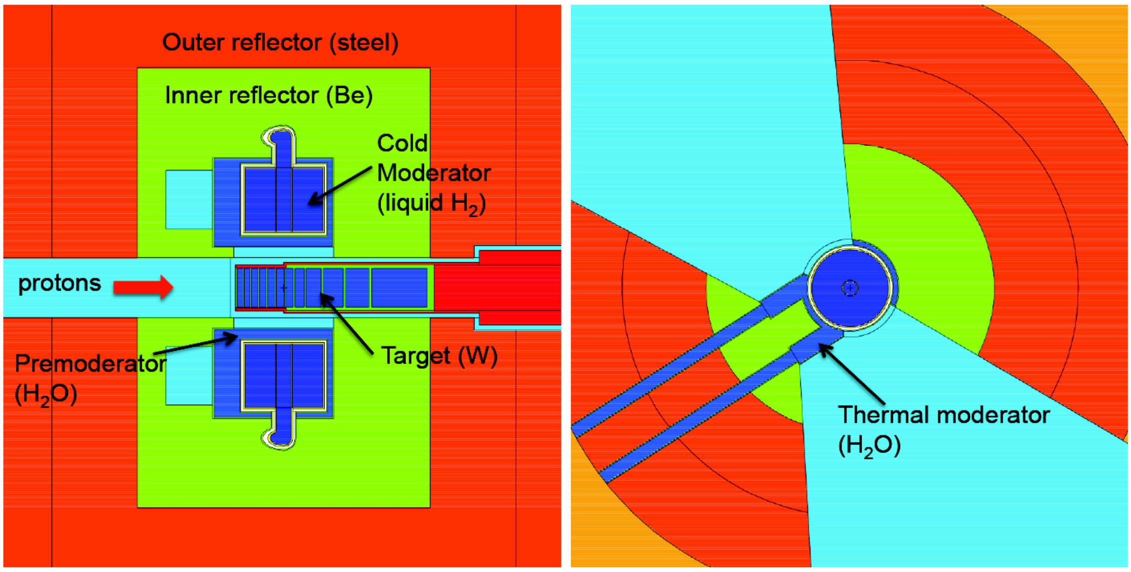

Figure 1: Target-Moderator-Reflector system, the TDR MCNPX model [1].

Supercritical para-hydrogen is a favourite material for high cold neutron brightness at high power sources. However, as the para-hydrogen cross section drops off with two orders of magnitude around 15 meV neutrons are emitted prior to thermalizing. Due to this complexity of the inelastic scattering cross section below 15 meV the resulting spectrum cannot be described by a simple Maxwellian distribution.

The goal of this study is to provide a model for the cold spectrum from the para-hydrogen moderator; additionally, an analytical description of the thermal and slowing down components of an ordinary neutron spectrum will be discussed. In this study these analytical descriptions will be fitted to the simulated spectrum from the ESS baseline design [1], while in [4] the same function have, with great success, been fitted to the expected cold brightness from different heights of flat moderators [5].

2. Model

In this section analytical expression describing the wavelength distribution of the thermal and cold ESS neutron spectrum will be constructed from parts. In the end these constructed functions will be fitted to the wavelength spectrum obtained from simulations.

2.1. Slowing down

As neutrons are slowing down, at wavelengths (λ) below the thermal energy of the medium ($\lambda < 0.5$ Å) some of them will be emitted from the moderator. In this region the distribution is expected to fall off inversely proportional to the wavelength.

This is understood by looking at the flux as a function of lethargy, $\phi(u)$ ($u \propto \log(\frac{1}{E}) \propto \log \lambda^2$), which is well known to be a flat distribution at epithermal energies. From this one can easily derive the flux as a function of wavelength: $\phi(\lambda) = \phi(u- > \lambda)\frac{du}{d\lambda} = k\frac{du}{d\lambda} \propto \frac{1}{\lambda}$. As brightness is proportional to the flux it follows that the epithermal brightness is also proportional to $\frac{1}{\lambda}$.

When the neutron energy approaches the energy of the medium, the $\frac{1}{\lambda}$ term should disappear. Historically $(1 + e^{\alpha(\lambda - \lambda_{cf})})^{-1}$ has been used, where λ_{cf} and α are the parameters controlling the position and rate of the cut-off. By introducing an intensity parameter I_{SD} one can write the

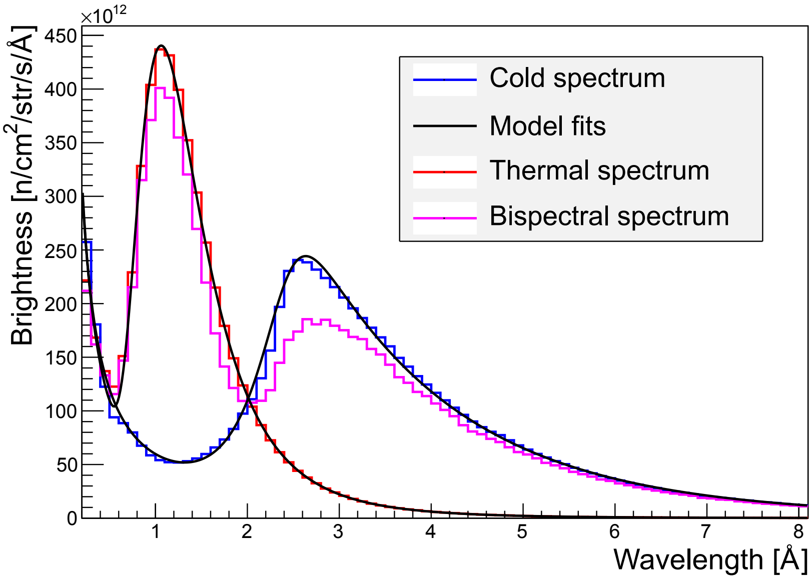

Figure 2: Expected peak brightness for cold, thermal and bi-spectral extraction, for the ESS, baseline configuration [1]. The peak brightness is calculated for the operational parameters described in the TDR: 2.5 GeV proton kinetic energy, average macro-pulse current of 50 mA, macro-pulse length of 2.857 ms, corresponding to a peak power of 125 MW and energy per pulse of 357 kJ.

full slowing down function SD as a function of wavelength:

$$SD(\lambda) = I_{SD}\frac{1}{\lambda}\frac{1}{1+e^{\alpha(\lambda-\lambda_{cf})}} \tag{1}$$

2.2. Thermalization

At low energy the neutrons will begin to equilibrate around the thermal energy of the moderating medium and the thermal spectrum can be described by a Maxwellian (M):

$$M(\lambda) = \frac{2k_{Th}^2}{T^2\lambda^5}e^{-\frac{k_{Th}}{T\lambda^2}} \tag{2}$$

Where $k_{Th} = \frac{2\pi^2\hbar^2}{m_n k_B} \approx 949$ KÅ^2 and T is the temperature. It is well known that at low energy the cross section increases with speed, hence it also increases with wavelength. As this increase is mainly due to absorption longer wavelength neutrons have lower probability of survival in a moderator, this results in a suppression of long wavelength neutrons. The most common approach is to increase the temperature parameter T of the model above that of the system. Another way of modelling this is by increasing the power of the wavelength, i.e. $\lambda^{-5} \to \lambda^{-(5+\chi)}$, where χ is often in the order of 0-1. However, in this study only the temperature increase was adopted while the later correction (the χ part) was neglected.

The full thermal moderator wavelength spectrum (S_{Th}) can now be assembled from the above pieces:

$$S_{Th}(\lambda) = I_{Th}\frac{2k_{Th}^2}{T^2\lambda^5}e^{-\frac{k_{Th}}{T\lambda^2}} + I_{SD}\frac{1}{\lambda}\frac{1}{1+e^{\alpha(\lambda-\lambda_{cf})}} \tag{3}$$

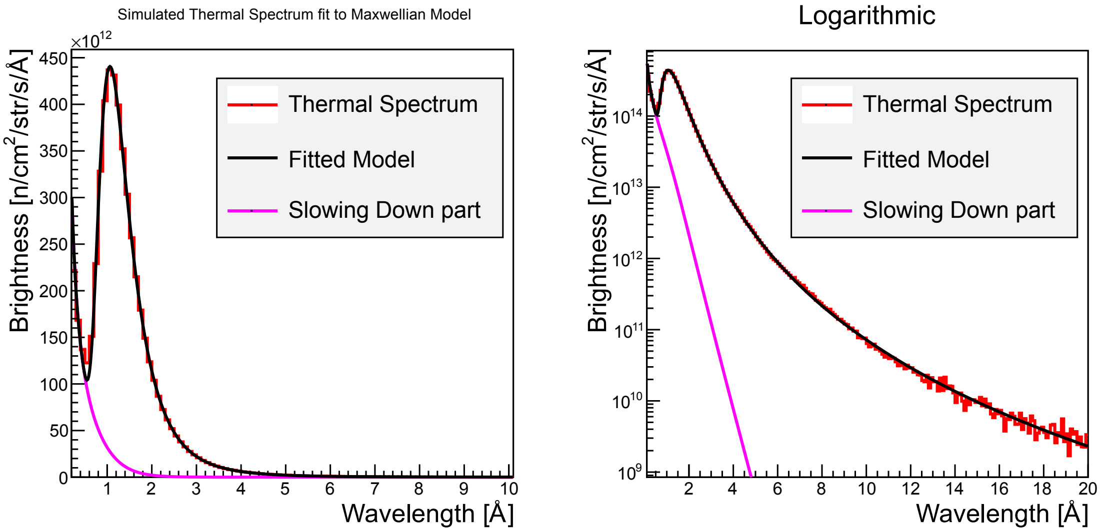

Figure 3: Expected ESS peak brightness from thermal moderator (linear left, logarithmic right), fitted to Eq. 3, parameters are shown in Table 1. The *SD* part is plotted in purple in the background.

where I_{Th} is the intensity of the thermal Maxwellian. This model (Eq. 3) have been fitted to the simulated brightness spectrum of the thermal moderator, shown in Figure 3. The obtained parameters are shown in Table 1.

Table 1: Parameters used in Figure 3; only I_{Th}, I_{SD} are fitted, the remaining parameters are fixed to the values obtained in an earlier study [6].

Parameter	Value
I_{Th}	4.35915×10^{14} cm^{-2}sr^{-1}s^{-1}
I_{SD}	7.48017×10^{13} cm^{-2}sr^{-1}s^{-1}
T	325 K
α	2.5 Å^{-1}
λ_{cf}	0.88 Å

2.3. Para-hydrogen

The cold moderator consists of 20 K pure para-hydrogen. The neutron scattering cross section drops off (with almost two orders of magnitude) near the excitation energy of the ortho (triplet) spin-state (para is the singlet state), around 15 meV. As a result para-hydrogen becomes transparent (or translucent; cold neutrons mean free path is 10 cm to 15 cm, which is very long compared to the mean free path of a few mm for thermal neutrons) to neutrons with wavelengths longer than 2.32 Å. It should be noted that this happens before the neutrons are at thermal equilibrium (i.e. 15 meV corresponds to 174 K), hence the cold spectrum can not be described by a Maxwellian. This is confirmed by looking at Figure 4, which amongst other things includes a fit of a Maxwellian to the distribution. This transparency also results in a number of geometrical effects, some of which can be found in [7]. Due to this anisotropy it is worth mentioning that the spectrum fitted in this study is the neutron spectrum observed at the center of one of the four 60° extraction windows, directly in front of the cold para-hydrogen moderator.

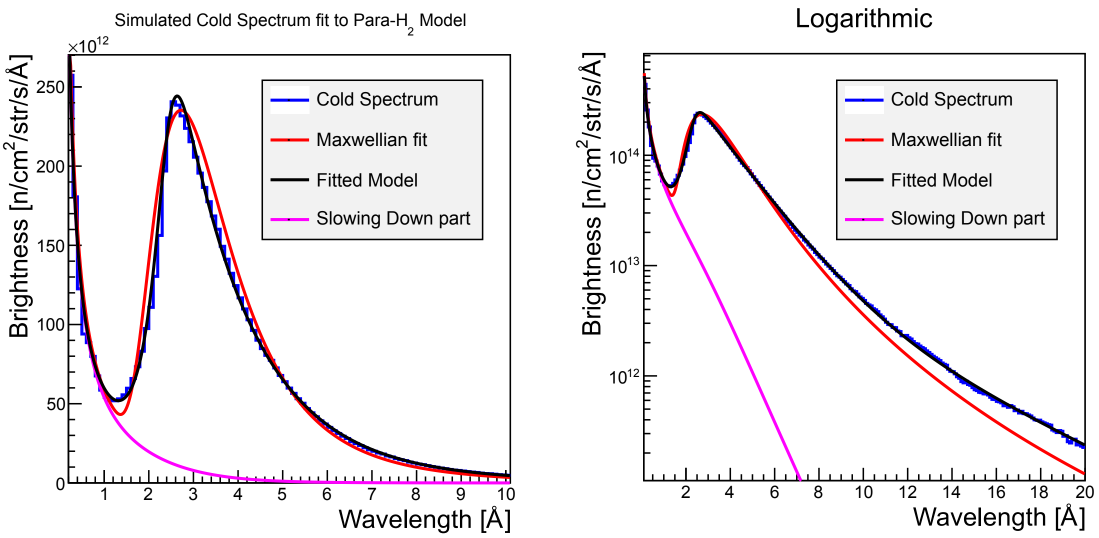

Figure 4: Expected ESS cold peak brightness (linear left, logarithmic right), fitted to Eq. 4 with parameters as shown in Table 2. The slowing down part is shown in purple and a Maxwellian fit is shown in red. Note that the Maxwellian description is inadequate both near the peak of the distribution (∼3 Å) and at long wavelengths ($\lambda > 7$ Å).

Thermal neutrons entering the cold para-hydrogen will very quickly (most often in a single scatter) be cooled below this 15 meV threshold energy and be transmitted from the moderator. This means that the spectrum from a para-hydrogen, at wavelengths above 2.3 Å will look like the spectrum of an inelastic down scatter, which on the tail can be fairly well described by an exponential.

But para-hydrogen is not fully transparent; in fact cold neutrons have 10 cm to 15 cm mean free path, which means that a few neutrons will re-scatter, even below the 15.2 meV limit. These neutrons mainly scatter on the intermolecular para-hydrogen spin state which has much lower scattering cross-section and a energy around 5 meV. These second scatters can be modelled by a second exponential with lower intensity and slower decay rate.

In summary, the tail of the para-hydrogen spectrum can be written as: $(I_1 e^{-\alpha_1 \lambda} + I_2 e^{-\alpha_2 \lambda})$, where I_1 and I_2 are intensities of the first and the second scatter respectively and α_1, α_2 are the decay rates of the primary and secondary scatter exponential respectively. Note that $I_1 >> I_2$ and $\alpha_1 >> \alpha_2$.

The two exponentials should only exist at energies larger than the transparency energy, around 15 meV, this can be described by a function growing from 0 to 1 fast enough, i.e. faster than the two exponentials fall off. A good description of this turns out to be: $(1 + e^{\alpha_l (\lambda - \lambda_l)})^{-\frac{1}{\gamma}}$, where γ and α_l governs the rate at which the transparency sets in and λ_l govern the position.

The full ESS para-hydrogen cold spectrum model (S_{cold}) becomes:

$$\begin{aligned} S_{cold}(\lambda) = \\ \frac{1}{(1 + e^{\alpha_l (\lambda - \lambda_l)})^{\frac{1}{\gamma}}} (I_1 e^{-\alpha_1 \lambda} + I_2 e^{-\alpha_2 \lambda}) \\ + I_{SD} \frac{1}{\lambda} \frac{1}{1 + e^{\alpha_{SD} (\lambda - \lambda_{SD})}} \end{aligned} \tag{4}$$

where I_{SD}, α_{SD} and λ_{SD} are the intensity, the cut off rate and cut off position of the slowing down function (similar to the one from the thermal spectrum). α_l and γ govern the rate and

Table 2: Parameters from the fit shown in Figure 4. Note that $\lambda_{SD}, \alpha_{SD}$ have been taken from [6].

Parameter	Value
I_{SD}	7.22356×10^{13} cm^{-2}s^{-1}sr^{-1}
α_{SD}	0.9 Å^{-1}
λ_{SD}	2.444 Å
α_l	-6.71404 Å^{-1}
λ_l	2.42099 Å
γ	2
I_1	1.2634×10^{15} cm^{-2}sr^{-1}s^{-1}Å^{-1}
α_1	0.617494 Å^{-1}
I_2	2.01876×10^{13} cm^{-2}sr^{-1}s^{-1}Å^{-1}
α_2	0.2237 Å^{-1}

structure of the region where the transparency sets in and λ_l relates to the position (λ_l should be in the order of 2.3 Å). Figure 4 shows a fit of Eq. 4 to the expected cold spectrum, which reveals the parameters shown in Table 2. Note that the fit uses $\gamma = 2$ corresponding to a square root, which is descriptive for a large bulk moderator as the one investigated in this study. However, further studies have shown that for more advanced moderator designs, e.g. the flat moderators described in [5], a square root is an inadequate description.

3. Conclusion

A fit of expected ESS baseline, thermal and cold, neutron spectra have been carried out. While the thermal spectrum fits nicely to a Maxwellian, it has been shown that the common Maxwellian description of the para-hydrogen neutron spectrum is inadequate. Therefore a new formula (Eq. 4) has been developed, which fits the simulated ESS para-hydrogen spectrum very accurately in the range from 0.01 Å to 20 Å. The results of the fits have been implemented in McStas 2.0 and is used throughout the ESS instrumentation community.

References

[1] S. Peggs, editor. *ESS Technical Design Report.* April 2013.

[2] L. S. Waters, G. W. McKinney, J. W. Durkee, M. L. Fensin, J. S. Hendricks et. al. The MCNPX Monte Carlo radiation transport code. *AIP Conf.Proc.*, 896:81, 2007.

[3] Mezei, F. Private communications, 2013.

[4] T. Schönfeldt et al. Phenomenological study of expected cold and thermal brightness phase-space at ESS. *In review, NIMa*, 2014.

[5] K. Batkov, A. Takibayev, L. Zanini and F. Mezei. Unperturbed moderator brightness in pulsed neutron sources. *Nucl. Inst. Meth.*, 729(0):500, 2013.

[6] Mezei, F. Internal report: Ess target - moderator performance estimates, 2010.

[7] T. Schönfeldt et. al. Optimization of cold neutron beam extraction at ESS. *AccApp Conf. Proc. (2013).*