Figure-of-Merit for a Cold Coupled Moderator at the SNS Second Target Station suited for Direct Geometry Inelastic Spectrometers

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Abstract.
The suite of moderators for the Second Target Station (STS) at the Spallation Neutron Source (SNS) in Oak Ridge is currently undergoing the planning stage at which various options and configurations are being considered. The current plans for the instrument suite include two direct geometry inelastic spectrometers, CHESS and HERTZ, which will receive beam from cold moderators and work mostly in the 1-20 meV incident energy range. CHESS will be a relatively short (wide bandwidth) instrument that is dedicated to studying small samples (\(\sim\) mm\(^3\)) with coarse energy resolution (2.5 – 5% of \(E_i\)). HERTZ on the other hand will be designed to achieve very good energy resolution, 1 – 3% of \(E_i\), using a long secondary flightpath with a \(\sim 4 \times 4\) cm\(^2\) beam on sample. In this contribution, we will discuss the implications of these design requirements for the optimal moderator pulse width, and for the repetition rate that would be best suited for the spectrometers.

1. Introduction
One of the most important limitations of the neutron scattering technique is that it requires, in comparison to x-ray scattering, relatively large samples, in particular for inelastic scattering. It is thus a priority to use the latest advances in source and instrumentation technology to design instruments that can overcome this limitation. Being able to study smaller samples will not only widen the range of an instrument for possible uses but will also enable inelastic neutron scattering to make important contributions earlier in the development process for new materials.

Direct geometry inelastic spectrometers are workhorse instruments at each major neutron scattering facility. They are very flexible and powerful instruments that can address a wide range of scientific problems in condensed matter physics, chemistry and biology. To address an area of critical importance, the first instrument of this kind, named CHESS, to be constructed at the Second Target Station (STS) will specifically aim to enable inelastic scattering experiments with \(\sim\) mm\(^3\) samples. It will focus a small beam of high (and tunable) divergence on the sample.
Naturally, the energy resolution has be rather coarse, and $\sim 2.5 - 5\%$ of $E_i$ appears to be a reasonable target range for the energy resolution.

The high peak brightness of STS is achieved by compressing the linac output using the accumulator ring to produce a short proton pulse [1]. For CHESS this has the consequence that it needs to be a rather short instrument, $\sim 30$ meters from source to sample, because otherwise the source pulse will be sharper than optimal for the anticipated resolution range.

A second instrument that is being planned, called HERTZ, will use the high source brightness to achieve very good energy resolution. This is often needed at high scattering angles to study phonons. Better resolution means that this instrument is optimally somewhat longer (which has advantages for the optics design) and that it will operate with smaller bandwidth than CHESS.

This paper will discuss the consequences of these design requirements for the optimal moderator pulse width, and for the repetition rate that would be best suited for the spectrometers. We will establish a figure of merit that can be used to optimize the moderator performance for these instruments.

This paper is organized as follows: In section 2 the main terms governing the energy resolution are discussed and the conclusions one can draw from the resulting matching conditions. It will also be discussed how one can increase the flux on sample by relaxing the resolution at low incident energies. Section 3 discusses the main figure of merit for the moderator which will be expressed as the wavelength dependent product of pulse width and neutron speed at a particular neutron wavelength. Section 4 summarizes the paper.

2. Energy Resolution

A direct geometry inelastic spectrometer at a spallation source employs one or two high speed choppers, which define the working neutron wavelength (energy) through their phase relative to the source pulse timing, and the resolution via the burst times. These are often referred to as the $P$-chopper (pulse shaping chopper) and the $M$-chopper (monochromating chopper), respectively. The $P$-chopper is optional if the source pulse is short enough in the working energy range of the spectrometer so that it does not need to be cut further. This is typically the case for thermal neutrons but not for cold neutrons, because the moderator pulse width increases with neutron wavelength [2, 3, 4].

At the STS, the lengths (moderator to detector) of CHESS and HERTZ will be defined by the coarsest energy resolution setting to which the instruments will be optimized to operate in. This is $\Delta E/E_i = 5\%$ for CHESS and 3\% for HERTZ. These numbers are derived from operating experience: It is often found that data become much less informative if the resolution is relaxed beyond 5\%. However, targeting small samples, it will be important for CHESS to be able to relax the resolution with adequate intensity gain, that is to say, one will want to increase the $P$- and $M$-chopper burst times until the full source pulse width is used at $\Delta E/E_i = 5\%$. For the discussion that follows, it is therefore convenient to write down the energy resolution as if there was no $P$-chopper and the natural source pulse width was used. Assuming elastic scattering (incident and final neutron velocities are equal, $v_i = v_f = v$), one has three terms that add in quadrature [5, 6]

$$\Delta^2 E = \frac{m^2 v^6}{L_1^2} \cdot \left(1 + \frac{L_2}{L_3}\right)^2 \cdot \Delta^2 t_S + \frac{m^2 v^6}{L_1^2} \cdot \left(1 + \frac{L_1 + L_2}{L_3}\right)^2 \cdot \Delta^2 t_M + \frac{m^2 v^6}{L_3^2} \cdot \Delta^2 t_D, \tag{1}$$

where $L_1$ is the distance from the source to the $M$-chopper, $L_2$ is the distance from the $M$-chopper to the sample, $L_3$ is the distance from the sample to the detector, $\Delta t_S$ is the source pulse width, $\Delta t_M$ is the burst time of the $M$-chopper, and $\Delta t_D$ is the uncertainty in time-of-flight between the sample and the detector (which is related to the pixel and sample sizes). This approximation neglects line shape effects on the energy resolution but for the present purposes
it is accurate enough. For best “value” (intensity vs resolution), the three contributions have to match. One of the matching conditions that one can derive is

$$\frac{\Delta t_S}{\Delta t_M} = \frac{L_1 + L_2 + L_3}{L_2 + L_3}.$$  

Traditionally chopper systems have been designed to deliver burst times that are independent of wavelength (energy) although they can be changed between instrument settings such as “high flux” and “high resolution”. In such a scenario one can read off of eq. (1) that \(\Delta E \propto v \cdot E_i\), which means that the relative energy resolution \(\Delta E/E_i\) becomes better (smaller) as \(E_i\) decreases, approximately like \(\Delta E/E_i \propto E_i^{1/2}\) [6, 7, 8]. This is only an approximation because the last term \(\Delta t_D = \Delta L_3/v\) makes a constant contribution to \(\Delta E/E_i\).

At a modern spallation source that features a low frequency and emphasizes slow long-wavelength neutrons, direct geometry spectrometers are nowadays designed to employ repetition rate multiplication (RRM) [8, 9, 10]. This means that a number of incident neutron energies are used to measure separate spectra simultaneously. In such a scenario it is often more convenient to achieve an approximately constant resolution \(\Delta E/E_i\) that is independent of energy. Practical experience at high resolution instruments such as LET [11] and CNCS [12] also shows that at

Figure 1. Performance comparison of two moderators for STS that have been optimized to different specifications. Moderator 1 was optimized for peak brightness which resulted in pulse widths of \(v \cdot \Delta t_S \sim 0.12\) m in the range of interest, \(\lambda \sim 2 - 12\) Å. Moderator 2 was optimized for integral brightness, which resulted in a larger size and \(\sim 2\) times broader pulses. Left panel: pulse width multiplied with neutron speed. For each moderator two traces are given, which represent optima for different viewing areas. Note, that even moderator 2 still delivers less pulse width on average than what CHESS could use in its coarsest resolution setting. Center panel: peak brightness that one would pick off from a \(2 \times 2\) cm\(^2\) area (this is about what CHESS would need). The source brightness is normalized to 500 kW at 15 Hz with 1.3 GeV proton energy. One can see that a moderator optimized for a smaller viewing area gives a higher peak brightness, which is expected. Also, moderator 1 is better with this figure of merit because it was optimized for it. Right panel: Pulse brightness integrated over full width of the pulse, which is better approximating what a direct geometry inelastic instrument would accept as a beam. This shows that moderator 2 performs about 50% better. Again, a moderator optimized for a smaller viewing area yields a higher brightness.
low energy, $E_i \sim 2$ meV and lower, the resolution is often too good and it would be preferable to be able to trade coarser resolution for higher intensity. In this energy range the brightness of a cold moderator goes rapidly down with increasing wavelength, approximately as $\propto \lambda^{-5}$ [1]. The issues of a variable $\Delta E/E_i$ and too good resolution at low energies can be mitigated with a chopper system that is able to deliver wavelength-dependent pulse widths, which obey the condition

$$\Delta t_P, \Delta t_M \propto \nu^{-1} \propto \lambda,$$

where $\Delta t_P$ is the burst time of the $P$-chopper. This would ensure constant $\Delta E/E_i$ and a more balanced resolution at low energy. Recently it has been shown how this can be done with a “blind” chopper system [13].

3. Desirable Moderator Performance

It is instructive to plug in some numbers in the equation above, rearranging for the source term contribution to the energy resolution,

$$\frac{\Delta E_{(S)}}{E} = \frac{0.05}{\sqrt{3}} = \frac{2v}{L_1} \cdot \frac{L_2 + L_3}{L_3} \cdot \Delta t_S.$$

Using the following reasonable length estimates for CHESS, $L_1 = 28$ m, $L_2 = 1.5$ m, $L_3 = 2.5$ m, one gets for matching conditions a moderator pulse width $v \cdot \Delta t_S \sim 0.25$ m, which is expressed as the product of the pulse width and the neutron speed, $v$, at the corresponding neutron wavelength. HERTZ would view the same moderator, and the better energy resolution $\Delta E_{(S)}/E \sim 0.03/\sqrt{3}$ would be achieved by making the instrument longer, $L_1 = 37.5$ m, $L_2 = 1.5$ m, $L_3 = 5$ m.

The original design of a compact cold coupled moderator for STS, that was optimized for peak brightness over a viewing area of $3 \times 6$ cm$^2$, led to a figure $v \cdot \Delta t_S \sim 0.12$ m averaged over the range of interest, $\lambda \sim 2 - 12$ Å [1]. This is shown in Fig. 1 (left panel). With a diameter of $\sim 10$ cm, and only few cm tall, this moderator is quite compact. On the other hand, a moderator optimized for integral brightness produces pulse widths much closer to the figure above, $v \cdot \Delta t_S \sim 0.23$ m on average (also in Fig. 1). This moderator is larger, diameter $\sim 20$ cm, and delivers $\sim 25\%$ less brightness at the peak, but integrated over the useful peak width it performs nearly 50% better than the smaller moderator.

It would be difficult if not impossible to shorten the incident flight path of CHESS until the moderator figure $v \cdot \Delta t_S \sim 0.12$ m is matched, and still optimize the neutron guide and leave adequate room for choppers, polarizer and other components. Furthermore, an instrument that is too short will also have to use an excessive bandwidth.

4. Conclusion

It can be concluded that direct geometry inelastic instruments at STS with energy resolution requirements as laid out above are best served with a moderator optimized for integral brightness. An appropriate figure of merit is $v \cdot \Delta t_S \sim 0.25$ m for the pulse full width at half maximum multiplied by the neutron speed at the corresponding wavelength. In the case studied above, an optimization for peak brightness alone results in lower, by $\sim 1/3$, useful flux on sample.

The source frequency also enters the discussion via the bandwidth of incident wavelengths that such an instrument would use in a single pulse. No matter what the moderator will ultimately look like, CHESS is going to be a rather short instrument. This is necessary to match the source pulse width to the resolution needs. In fact, with $L_1 \sim 28$ m and $L_1 + L_2 + L_3 \sim 32$ m it is about as short as one can build it without seriously compromising neutron transport. At this length and $f = 15$ Hz, the bandwidth will be $\sim 7$ Å after factoring in that the edges of the spectrum need to be cut off in order to avoid frame overlap. By all measures, this is a
wide bandwidth for this type of instrument, and all reasonable instrument configurations will always measure at least one pulse around $E_i \sim 1$ meV or lower. The HERTZ instrument will be somewhat longer, $L_1 + L_2 + L_3 \sim 46$ m, but the bandwidth will still be rather wide, $\sim 5$ Å after accounting for frame overlap. For a direct geometry inelastic spectrometer, a wide bandwidth is a-priori not a disadvantage [14]. The science program at such an instrument will focus on exploration type experiments in which a wide energy range of dynamic responses in the sample is probed simultaneously. In the case of STS, where the source frequency is constrained to be a divider of 60 Hz, the choice between 10 Hz, 15 Hz, or 20 Hz results in incremental changes to the bandwidth, while increasing the repetition rate will give a corresponding increase in the useful flux across the range of incident energies used. Thus, both CHESS and HERTZ would benefit from a higher source frequency, and a broader moderator pulse width that more closely matches the resolution needs of the instruments.

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