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MONTE CARLO STUDY OF THE PERFORMANCE OF A TIME-OF-FLIGHT MULTICHOPPER SPECTROMETER

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ABSTRACT

The Monte Carlo method is a powerful technique for neutron transport studies. While it has been applied for many years to the study of nuclear systems, there are few codes available for neutron transport in the optical regime. The recent surge of interest in so-called next generation spallation neutron sources and the desire to design new and optimized instruments for these facilities has led us to develop a Monte Carlo code geared toward the simulation of neutron scattering instruments. The time-of-flight multichopper spectrometer, of which IN5 at the ILL is the prototypical example, is the first spectrometer studied with the code. Some of the results of a comparison between the IN5 performance at a reactor and at a Long Pulse Spallation Source (LPSS) are summarized here.

1. Introduction

Next-generation (> 1 MW) spallation neutron sources are currently being studied worldwide. The motivation behind the present flurry of activity stems partly from the desire to overcome the intensity "barrier" that presently limits many neutron scattering experiments, and partly from the rapidly increasing demand for neutrons as a tool for basic studies in many disciplines ranging from condensed matter physics to structural biology. In fact, the development of an accelerator-driven, 1 MW long-pulse spallation neutron source (LPSS), short-pulse spallation source (SPPS) for neutron scattering, and the upgrade of the existing short-pulse spallation source (LANSCE upgrade project) have been identified as main thrust areas at Los Alamos National Laboratory in the coming years.

Undoubtedly, the design, optimization, and analysis of new instruments for neutron sources is a major issue in the design of next-generation neutron sources. The complexity of these instruments coupled to the desire to optimize their performance as much as possible calls for design tools that go beyond traditional ray-tracing techniques. Simultaneously, the development of moderator simulation methods and recent advances in high-performance computing

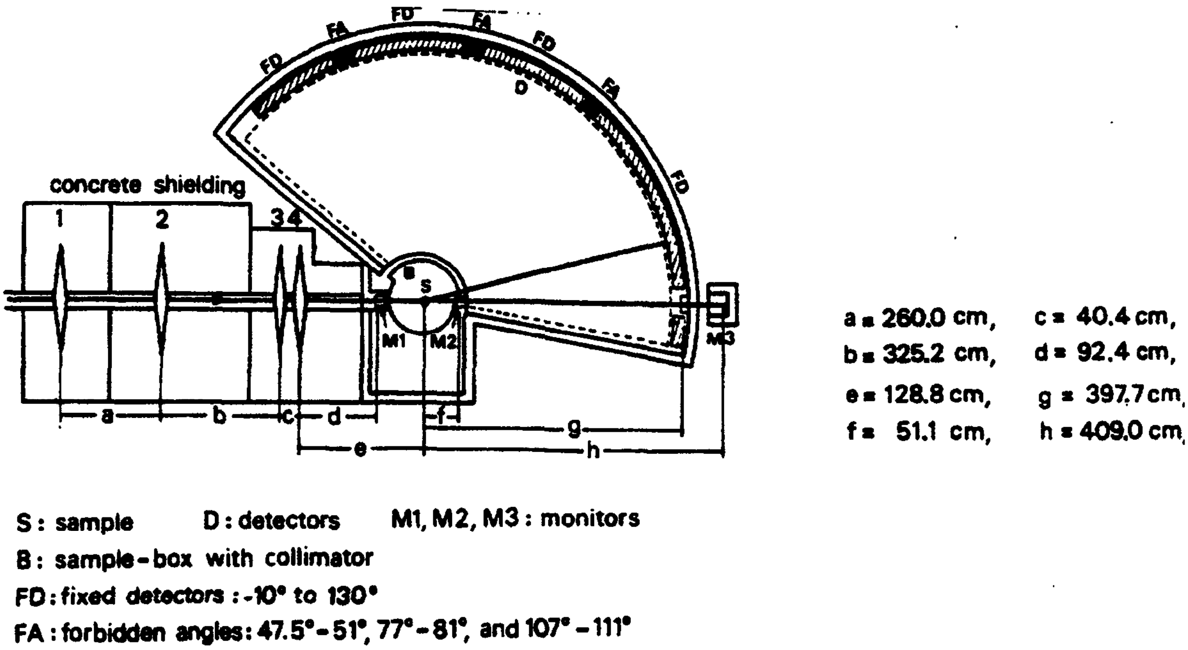

Figure 1: The IN5 spectrometer at the Institut Laue-Langevin.

make detailed moderator information (time and energy neutron pulse structure) available to the instrument designer. Quite often, the only way to make use of this information is in a computer simulation.

The MCLIB package and its various appendages are described elsewhere in these proceedings [1,2]. The code is a Monte Carlo neutron transport code specifically designed to do neutron optics. The code originated at the Rutherford-Appleton Laboratory in the late 70's [3]. It was subsequently revised by Seeger in 1984 and extensively rewritten and expanded in 1994.

The work described below is one example of the application of the MCLIB tools to the study of a neutron scattering instrument at various sources: We compared the operation of IN5 at a reactor (continuous) source and at the proposed LPSS source. We chose to model IN5 first because of its simplicity and its importance for quasi-elastic neutron scattering, and because it is reasonably easy to convince oneself that it is an instrument that would perform very well at a LPSS [4]. While our simulations of IN5 at a reactor source confirmed, by and large, the performance predictions from simple analytical calculations, the simulations at an LPSS source revealed some new, interesting features that add to the flexibility and performance of IN5 at this type of source.

2. The IN5 spectrometer

The strucure of the IN5 spectrometer is well-known. The instrument has been described in detail elswhere [5,6]. The instrument consists essentially of four disk choppers (Fig.1). The first and last choppers are used to determine the incident wavelength on the sample by adjusting their relative phase. The second chopper eliminates higher-order contamination from the beam. The third chopper is essentially a frame overlap chopper; it controls the repetition rate of the neutron bursts, and hence the data collection rate and achievable bandwidth. Chopper

1, 2, and 4 rotate at the same speed, typically 20000 rpm (667 Hz), whereas chopper 3 rotates more slowly, typically by a factor of two or three. The choppers are 24.2 cm in radius with 2 cm wide slits. The burst width produced by the wavelength selection choppers at 20000 rpm is approximately 40 μs. The choppers can be rotated as slowly as 6000 rpm (100 Hz) to increase the intensity on sample, but this occurs, of course, at the expense of energy resolution. Nickel-coated glass neutron guides from the ILL liquid hydrogen moderator to the first chopper and between consecutive choppers help increase the flux on sample. A set of 1200 helium-3 tube counters located on a segment of a sphere 4 m in radius and centered on the sample completes the instrument. The detector covers approximately 110^o in the horizontal plane and has a total height of 2 m.

3. Simple Scaling Arguments

The IN5 instrument is simple enough that analytical calculations giving the instrument bandwidth, resolution, and intensity on sample can be performed easily without making drastic simplifying assumptions. This is useful for comparison with the Monte Carlo results, and so we will summarize the results of calculations by Lechner [5] for future reference. Notice however that while the analytical results provide a good description of IN5, the Monte Carlo simulations have uncovered a number of interesting features that would have been difficult to calculate, or even predict, from simple analytical considerations.

3.1 Bandwidth:

The bandwidth of the instrument is determined by chopper 4 and is given by:

$$\Delta E = \frac{h^3}{m^2}\frac{\tau_4}{L_{14}\lambda_0^3} \tag{1}$$

where τ_4 is the chopper open time, λ_0 is the incident wavelength, and L_{14} is the distance between chopper 1 and chopper 4.

3.2 Resolution:

For elastic scattering, Lechner obtained:

$$\delta E = C\frac{\tau_1^2 L_{4D}^2 + \tau_4^2 L_{1D}^2}{\lambda_0^3 L_{14} L_{SD}} \tag{2}$$

where L_{4D} is the chopper 4-detector distance, L_{1D} is the chopper 1-detector distance, L_{SD} is the sample-detector distance. A more general expression for the resolution at finite energy transfer is also given in Ref.[5] but will not be used here. It is interesting to remark that both ΔE and δE depend only on the relative phase and distance between chopper 1 and chopper 4, but not on their absolute distance from the source. Eqs.(1) and (2) are applicable to continuous and pulsed sources.

3.3 Intensity:

In Ref.[5] Lechner shows that:

$$I \propto \frac{\tau_1}{T_3} \times \frac{d\phi}{dE_0} \times \Delta E = \frac{1}{\lambda_0^3}\frac{d\phi}{dE_0}\frac{\tau_1\tau_4}{L_{14}L_{SD}} \tag{3}$$

where T_3 is the period of the frame overlap chopper, $d\phi/dE_0$ is the flux at the incident energy, $E_0 = h^2/(2m\lambda_0^2)$, and ΔE is the instrument bandwidth given by Eq.(1) above.

At a reactor source, the factor $d\phi/dE_0$ is *fixed* and constant for a given selected wavelength. At a pulsed source, however, the neutron energy spectrum incident on the first chopper depends on the *phase difference* between the neutron pulse and the first chopper. One might think that because of the fairly complex time-energy structure of the neutron pulse produced by, say, a coupled, reflected moderator at an LPSS, this additional complication is undesirable, but we will show below that it leads in fact to new, interesting results regarding the operation of IN5.

4. Monte Carlo simulations of IN5 on a reactor source

It is useful, as well as instructive, to compare the instrument characteristics mentioned in the preceding section with similar quantities calculated with MCLIB. To this effect, we mocked up IN5 reasonably accurately. For the sake of expediency, we did not include the neutron guides in our simulations. (Notice that Lechner also ignored the guides in his calculations.) We performed the simulations for the best achievable resolution, i.e., with the wavelength selection choppers rotating at 20000 rpm (667 Hz). The distances between source, choppers, sample, and detector, and their dimensions were chosen identical to those at IN5. The neutron source used in our simulations was a simple Maxwell-Boltzmann energy spectrum. Deviations from a strict Maxwell-Boltzmann spectrum are observable in practice, but they need not concern us here where our main purposes are to validate Lechner's scaling arguments (or, vice-versa, to validate the Monte Carlo simulations), and to explore more subtle effects particularly at pulsed sources rather than to design accurately a fully optimized instrument. The sample scatters with a fixed value of $\hbar\omega$. Energy resolution was measured by determining the broadening of the delta function scatterer in the time-of-flight spectrum. The counts of all the helium-3 tubes were summed to obtain the time-of-flight spectrum. We restricted the bandwidth to about 12 meV in our simulations, -2 meV $< \hbar\omega <$ 10 meV.

We repeated the simulation at several incident wavelengths for elastic scattering. The results are shown in Fig.2. While the Monte Carlo result is not identical to Lechner's result, it is fairly close. The agreement with Lechner's result gets better as the wavelength increases. The trend is clearly toward a decrease of δE as $1/\lambda_0^3$, but there appears to be additional, wavelength-dependent corrections to Lechner's result. Also indicated on the figure is one result for a vanadium sample at $6\mathring{A}$ incident wavelength. The measured resolution is between the Monte Carlo result and Lechner's result.

Equally interesting is a study of the energy resolution at finite energy transfer, i.e., for a delta scatterer sample scattering inelastically. Since in practice, there is no known material that mimics perfectly this behavior (unlike vanadium for the elastic scattering case), one is reduced to estimate computationally the resolution of the instrument for inelastic scattering. Fig.3 shows the results of our Monte Carlo simulations for three incident wavelengths. The lines are Lechner's result, Ref.[5]. Again, the trend for the analytical results and the Monte Carlo results is the same. As observed for the elastic scattering case, the agreement between

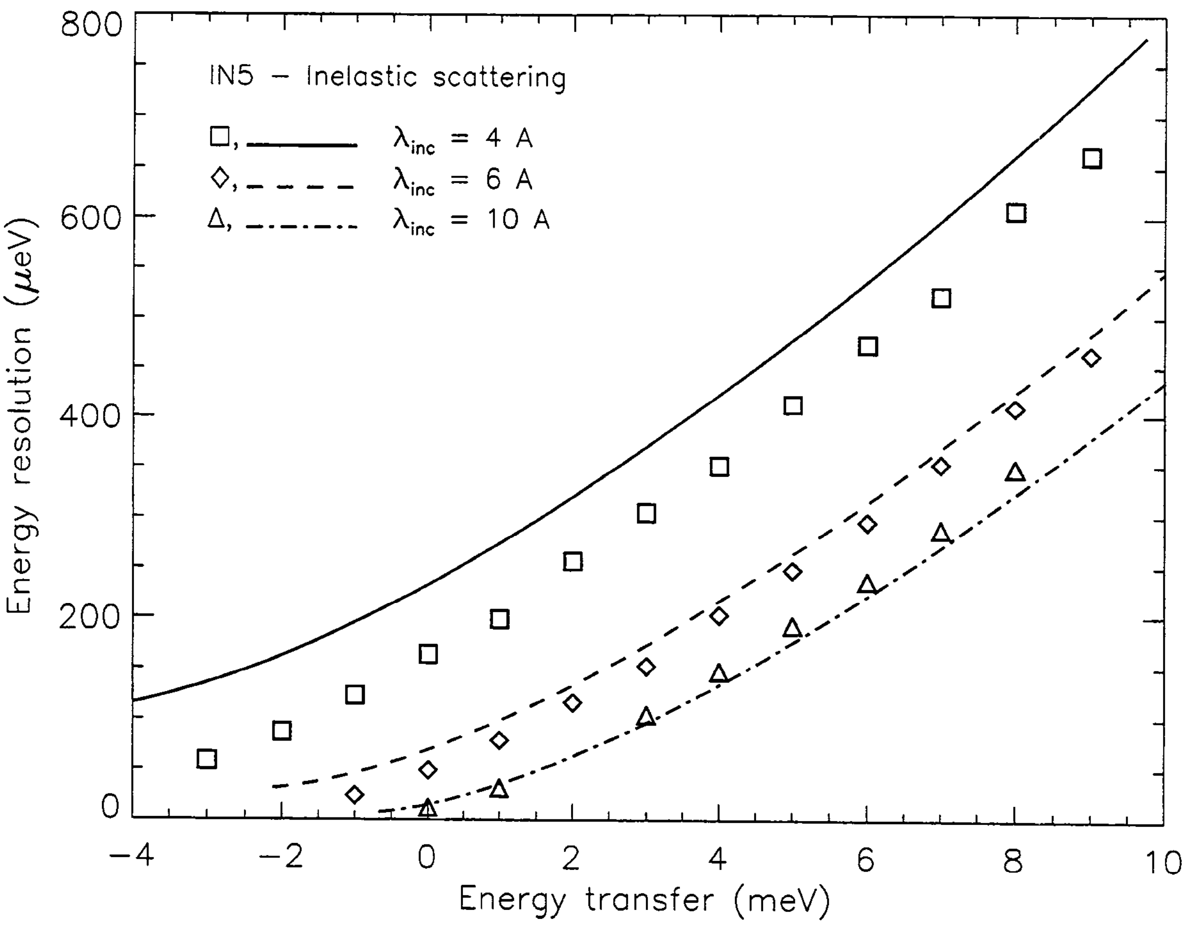

Figure 2: Monte Carlo calculation of the energy resolution for elastic scattering at IN5 with a continuous source. The solid line is a third degree polynomial fit to the data. The dashed line is Lechner's result, Eq.(3).

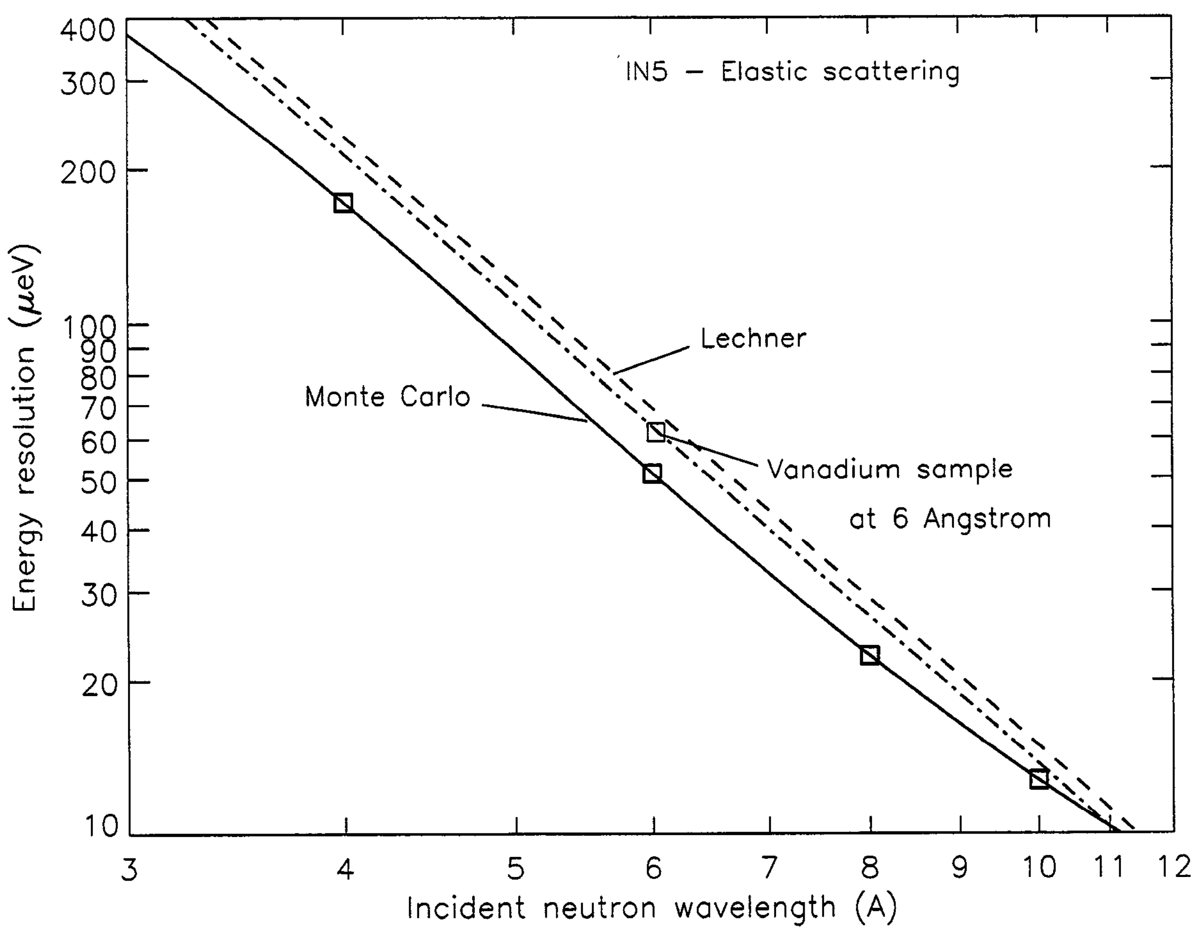

Figure 3: Monte Carlo calculation of the energy resolution for inelastic scattering at IN5 with a continuous source. The sample is a delta scatterer. The lines are Lechner's result, Ref.[5]; The symbols are the results of our Monte Carlo simulations.

Lechner's result and the Monte Carlo result seems to improve greatly with increasing wavelength. Altogether, the agreement between the two results is quite reasonable, even at shorter wavelengths, but it would be interesting to pursue this study and try to understand the exact origin of the discrepancy.

5. Monte Carlo simulations of IN5 on an LPSS source

As pointed out above, the IN5 would perform in a very similar way at a reactor and a pulsed source. However, we also remarked that the pulsed nature of the neutron source at an LPSS leads to the added complication of having to determine a *global* chopper phase with respect to the accelerator (or neutron) pulse, in addition to the *relative* phases between choppers. To study the impact of this global phase on the performance of IN5 at an LPSS, we varied this phase systematically by varying the t_{shift} parameter defined in Fig.4(a). The pulse shape in Fig.4(a) is typical of a coupled liquid hydrogen moderator at an LPSS. The cusp indicates the end of the 1 ms proton pulse on the neutron production target. The 370 μs decay constant of the exponentially decaying "tail" is also typical of a coupled, cold moderator at an LPSS. We used the Ikeda-Carpenter formula [7] to generate a source term for an LPSS in our simulation. Again, the emphasis is on understanding and exploring rather than on the production of a final, optimized design for an actual source. The Ikeda-Carpenter result is analytically expressible in a simple way, and lends itself to analytical treatment. In addition, its use allowed us to change moderator parameters rapidly and to explore systematically the effect of these changes on the instrument performance.

One disadvantage of using an accelerator to produce neutron pulses for IN5 is that the chopper rotaional frequency has to be equal to (or at least a multiple of) the accelerator frequency. We chose 120 Hz as a typical number in our simulations. It is trivial, however, to rescale the results for other frequencies. Similarly, at 120 Hz, the data collection rate is less than or equal to that achievable at ILL, so one must be careful in comparing intensities, resolution, and bandwidth between the two sources. The relative simplicity of the instrument, however, should allow the reader to perform comparisons that are meaningful for the particular situation at hand.

The effect of varying t_{shift} systematically between a negative value (-1 ms to 0 ms, i.e., when the proton pulse is "on") and a positive value ($>$ 0 ms, proton pulse "off") on the detected intensity and elastic resolution is shown in Figs.4(b) and (c), respectively. The simulations were performed for two different wavelengths, 4 and 10 $\AA$ corresponding to the typical range of wavelengths used in practice by most IN5 users. The sample was again a delta scatterer (zero energy transfer, i.e., elastic scattering). Clearly, the results are not as simple as one might have imagined. At a given incident wavelength, intensity and resolution "peak" at different values of t_{shift}. We intuitively expect the intensity to peak near $t_{shift} = 0$ since the longer we wait, the larger the population of thermalized neutrons in the moderator. Notice also that neutron thermalization times are wavelength-dependent, and the neutron flux in the moderator will "peak" at a time depending on the neutron wavelength. This is a degree of freedom offered by the (t,E) structure of the neutron pulse at an LPSS that can be taken advantage of: It should always be possible to adjust the global pulse-choppers phase to "ride" the peak intensity at the desired wavelength.

Similarly, it should be intuitively obvious that for $t_{shift} > 0$, we are making use of a heavily thermalized neutron population corresponding to a smaller energy range (ideally determined by the Maxwell-Boltzmann distribution) than during the transient period following the irradiation

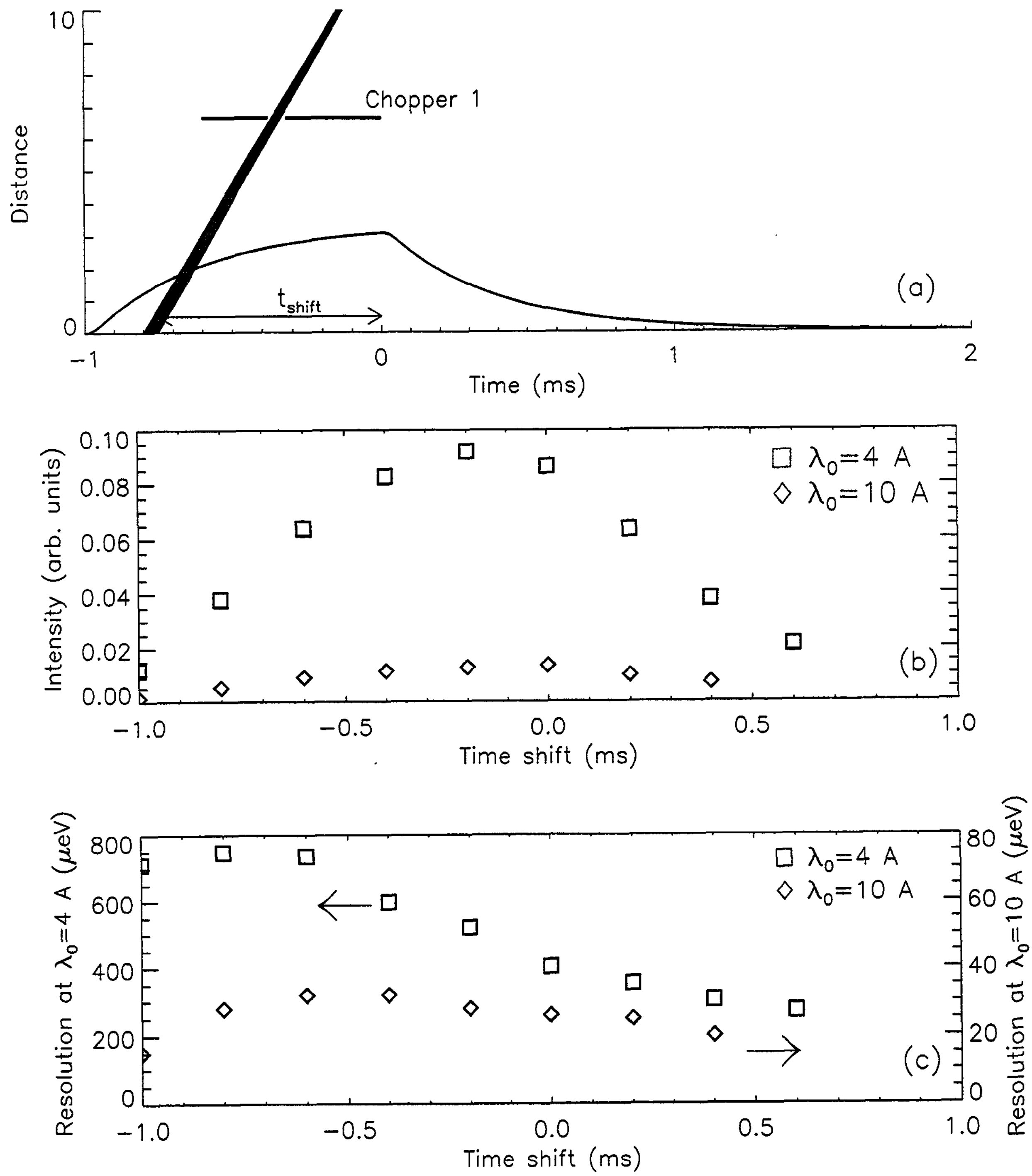

Figure 4: (a) Definition of t_{shift} and typical neutron pulse shape at an LPSS. The moderator decay time is 370 μs; the proton pulse duration is 1 ms; the accelerator frequency is 120 Hz; the choppers rotate at 120 Hz. (b) Detected intensity as a function of t_{shift} for two extreme wavelengths, 4 and 10 Å. (c) Corresponding elastic energy resolution as a function of t_{shift}.

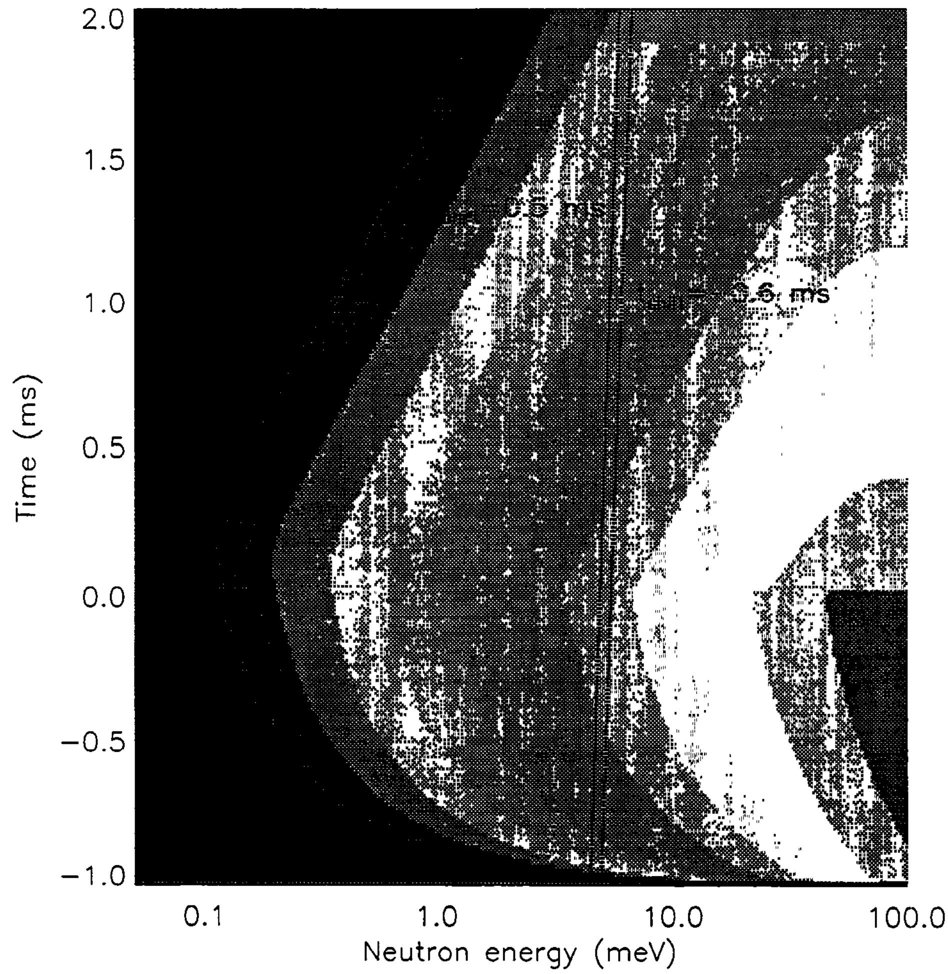

Figure 5: Ikeda-Carpenter time-energy distribution of the neutron pulse for the parameters given in the caption of Fig.4(a). The two curves are given by Eq.(4) for the values of t_{shift} indicated on the figure. The pulse is typical of a liquid hydrogen moderator at 20 K. The contour intervals are logartihmic.

of the neutron production target by the proton pulse since during this period, one has to deal with a more energetically diverse neutron population in the moderator as the neutron gas comes into thermal equilibrium with the moderating medium.

It is instructive to pursue this point a little further. It should be clear that neutrons emitted with energy E at time $t_{emission}$ such that

$$t_{emission} = t_{shift} + \frac{L_{M1}}{\frac{h}{m\lambda_0}} - L_{M1}(\frac{m}{2E})^{1/2}, \tag{4}$$

where L_{M1} is the moderator-to-chopper 1 distance (equal to 20.5 m in our simulations) and λ_0 is the selected incident wavelength all arrive at the first chopper at the same time. The second term in the above equation is the time-of-flight of a neutron with the nominal wavelength. (Neutrons with energy E slightly less than E_0 but leaving the moderator slightly before neutrons with energy E_0 can arrive at the chopper at the same time, as do slightly faster neutrons leaving the moderator somewhat later. Thus, neutrons whose time-of-emission and

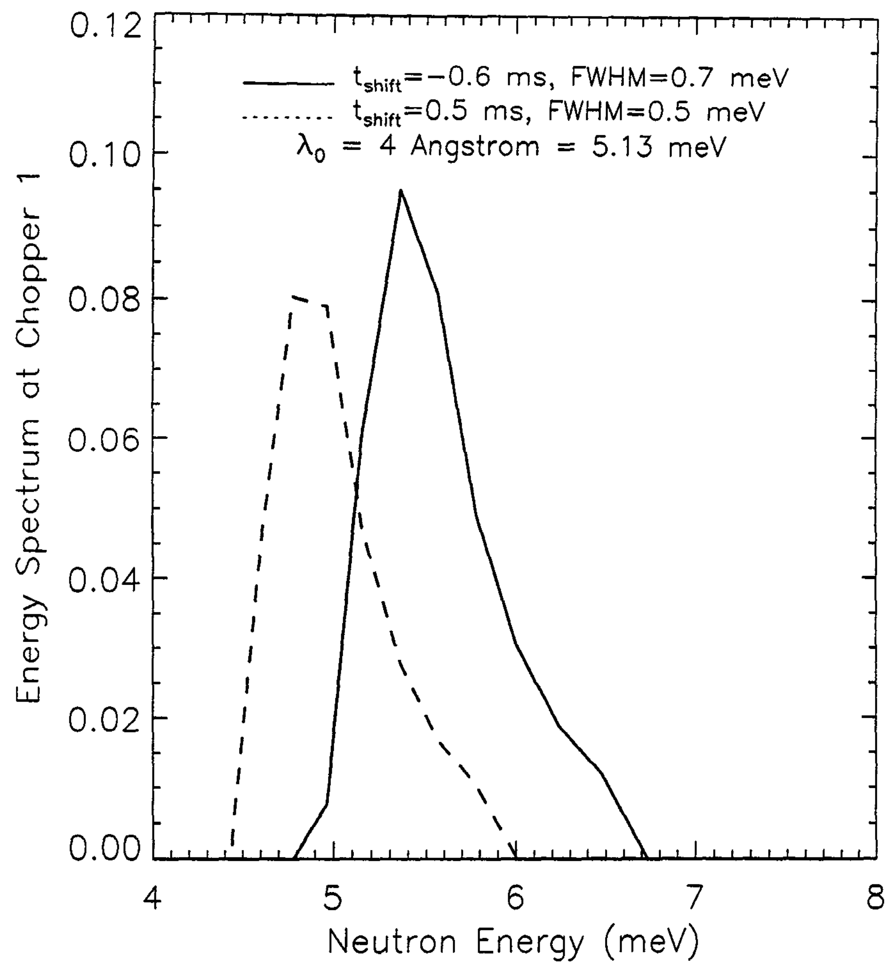

Figure 6: The neutron energy distributions corresponding to the two loci shown in Fig.5.

energy E are related via Eq.(4) arrive at the same time at the first chopper (and pass through the chopper). Eq.(4) determines a locus in the moderator (t,E)-space. Two of these curves are shown for two different values of t_{shift} in Fig.5. Changing t_{shift} amounts to shifting this curve vertically, along the energy axis, in the moderator (t,E)-plane; this does not change the shape of the curve. But the energy distribution of neutrons on two loci corresponding to two different values of t_{shift} are different: A larger t_{shift} corresponds to a greater degree of neutron thermalization and a narrower energy distribution (but also to less intensity when $t_{shift} > 0$, i.e., in the "tail"). The distribution of neutron energies for the two loci are show in Fig.6. Clearly the full-width at half-maximum of the two distributions is different, and it is not difficult to conclude the argument to explain the behavior of the elastic resolution as a function of t_{shift} shown in Fig.4(c).

It is also worth mentioning that by running IN5 at a reactor source with the choppers running at 120 Hz and all other things being equal, the resolution achievable at the reactor source is close to 1 ms, much worse than is possible at an LPSS by carefully "phasing" the pulse and the choppers.

6. Conclusions

We showed that the Monte Carlo results are in reasonable agreement with the simple scaling arguments advanced by Lechner. Clearly, there are some interesting deviations from the simple analytical arguments, and it would be interesting to explore this further.

The performance of an IN5-type instrument at an LPSS can be understood along the lines described in Ref.[5]. The global phasing of the proton (or neutron) pulse is an additional degree of freedom that is unique to the pulsed source and which can be taken advantage of to optimize the instrument performance or increase its flexibility.

An ideal moderator for IN5 at an LPSS would produce a neutron pulse with a long "tail" of highly thermalized neutrons (to improve the resolution), with as much intensity in the tail as possible (to increase the detected intensity). We have started to investigate the effect of varying the neutron pulse shape systematically (decay time, rise time, integrated and peak intensity, etc). The results will be reported elsewhere.

Many other aspects deserve to be investigated more closely, especially in view of the fact that they are not easily taken into account in simple analytical calculations. We have done some preliminary work on the effect of chopper jitter on the performance of IN5 at continuous and pulsed sources. The results show a modest improvement in energy resolution and a corresponding decrease in detected intensity. The relative loss of intensity at an LPSS seems to be somewhat less that the relative loss of intensity at a reactor. More work is needed to clarify the reason for this behavior.

Other, more complex chopper configurations can be considered. The fourth chopper, for instance, could be replaced by a pseudo-statistical chopper to measure several wavelengths simultaneously in one counting frame. Again, such ideas are best explored via the Monte Carlo technique.

7. Acknowledgements

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