

**The Methods of Producing and Analyzing Polarized Neutron Beams for HYSPEC at the SNS**

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**Abstract**

*The Hybrid Spectrometer (HYSPEC), under construction at the SNS on beam line 14B, is the only inelastic scattering instrument designed to enable polarization of the incident and the scattered neutron beams. A Heusler monochromator will replace the graphite crystal for producing polarized neutrons. In the scattered beam it is planned to use a collimator - multi-channel supermirror bender array to analyze the polarization of the scattered beam over the final energy range from 5 – 20 meV. Other methods of polarization analysis under consideration such as transmission filters using He<sup>3</sup>, Sm, and polarized protons are considered. Their performance is estimated and a comparison of the various methods of polarization is made.*

**1. Introduction.**

HYSPEC is an abbreviation for Hybrid Spectrometer, a unique direct geometry inelastic scattering instrument under construction at the Spallation Neutron Source at Oak Ridge National Laboratory [1]. The hybrid nature stems from the use of a focusing crystal, normally used in crystal spectrometers at continuous sources, and the time-of-flight (TOF) analysis of the energy of the scattered neutrons. A Fermi chopper will be used to monochromate the beam before it strikes the focusing crystal. This combination of monochromating the beam and using a crystal is a more efficient way of focusing a large beam to a small size (2x2 cm<sup>2</sup>) than using convergent guides. It will be situated at beam line 14B, which looks at a liquid hydrogen coupled moderator. The instrument is designed to operate in the incident energy range of 3.6 to 90 meV with a variable energy resolution  $2\% < \Delta E/E < 10\%$ . Importantly, HYSPEC will be capable of polarizing the incident beam and analyzing the polarization of the scattered beam – a unique capability for inelastic instruments at a pulsed source [2].

**2. Instrument Description**

An engineering drawing of HYSPEC is shown in Fig.1 [3]. The beam emerging from the liquid hydrogen coupled moderator at beam line 14B will pass through a T0 and frame overlap chopper, which will stop the very fast neutrons and neutrons from other frames, respectively. The neutrons will traverse a long curved supermirror (m=3) guide to an external building where it will pass through Fermi and order suppressor choppers. The monochromatic beam will then strike a focusing crystal placed inside a well-shielded drum. The beam emerging from the drum will strike the sample, which is external to the detector bank. The sample area should be accessible to the experimenter and can accommodate standard or exotic sample environments. The scattered beam first passes through a radial collimator, then a coarse 3° collimator and finally to the detector bank located 4.5m from the sample. The detector bank covers an angle of 60° horizontal and 15° vertical and is moveable inside a shield to cover a two-theta scattered angle range of 0-120°. There will be 160, 1.2m high position sensitive He<sup>3</sup> detectors arranged in 20 banks of 8 counters. There will be a choice of several radial collimations available to the experimenter and these will be manually interchangeable.

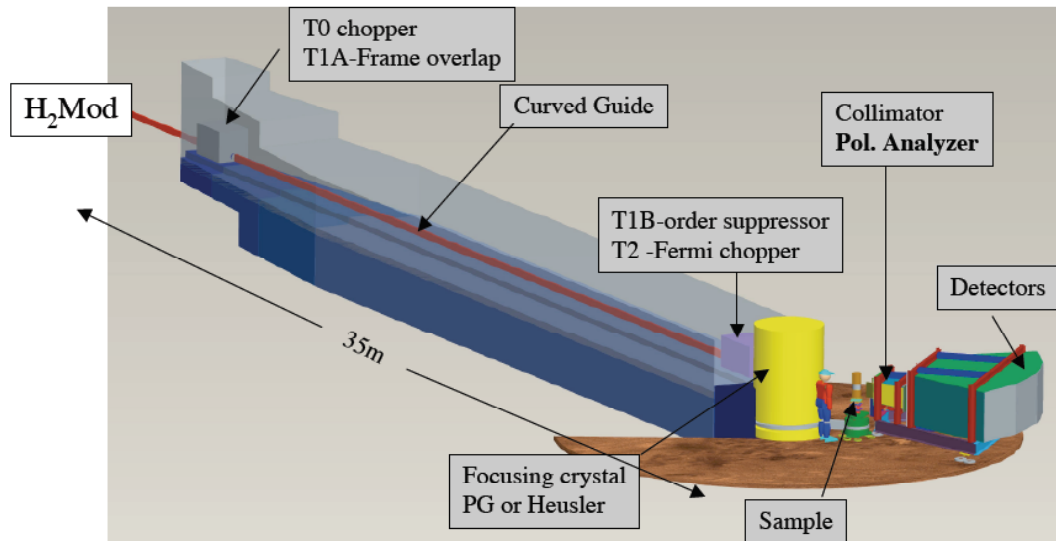


Figure 1: Engineering drawing showing the components of the HYSPEC instrument. The sample placed 35 m from the moderator. The focusing crystal, sample area and detector bank will be located in an external building.

## 2. Polarized beam operations.

A vertical and horizontal focusing pyrolytic graphite(PG) crystal will be used in non-polarized beam operation. For polarized beam work, a vertical focusing Heusler ( $\text{Cu}_2\text{MnAl}$ ) crystal purchased from the Institute Laue Langevin (currently the only supplier of these crystals) will replace the PG crystal. The (111) reflection of this crystal will be used and a polarization of 95% is achievable when the Mn moments are fully aligned. For polarization analysis of the scattered beam, HYSPEC is designed with an array of

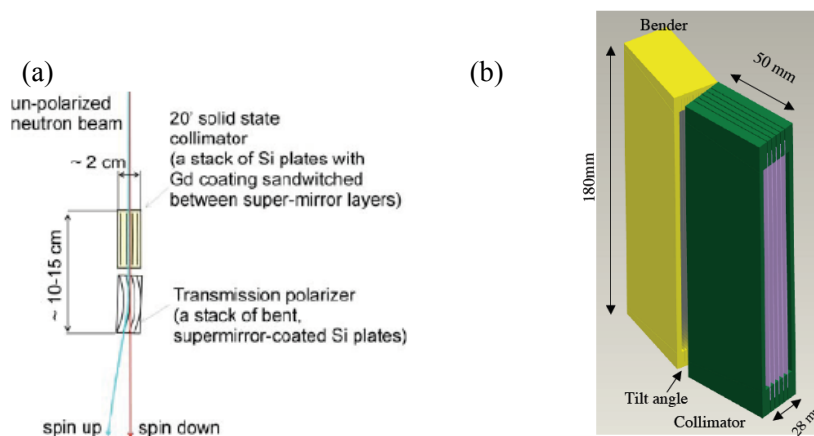


Figure 2: (a) Schematic of a single collimator-bender array showing the separation of the spin down(no-deflected) and the spin up (deflected) beams. (b) Drawing a single collimator bender array. The tilt angle in this figure is very exaggerated

supermirror bender transmission polarizers [4] that can be positioned where the radial collimator is located in the detector shielding. Figure 2a shows the schematic of one bender array. A 20 min. collimator will be placed before the supermirror bender to limit the divergence of the beam so the neutrons will strike the bender at angles less than the critical angle of the supermirror coating. Figure 2b shows a drawing of one collimator-bender array. There is a small tilt angle between the two that can be varied. The bender will consist of a stack of bent Si crystals with a supermirror coating of Fe-Si placed in a magnetic field to saturate the iron moments. For a magnetized film the spin state parallel to the polarized bender will be deflected and the spin state anti-parallel will be transmitted. It is thus possible to detect both spin states simultaneously on the detector. This concept has been tested and is in routine use at the NIST cold beam neutron reflectometer [5]. To assess the performance we performed Monte Carlo simulations using the NISP package from Los Alamos [6]. Figure 3a shows the result of the calculated intensity distribution on the detector bank for a 5 cm long bender with a radius of curvature of 5m, a tilt angle of  $0.3^\circ$  and a channel width of 0.025cm. (If a solid state Si collimator is used this would be the thickness of the individual plates.) The critical angles chosen are:  $\theta$  (spin up) =  $3.0 \theta_c^{(Ni)}$  and  $\theta$  (spin down) =  $0.6 \theta_c^{(Ni)}$ , where  $\theta_c^{(Ni)}$  is the critical angle for natural nickel. The sample-to-detector distance is 4.5m and the detector bank is 3.9 m from the polarizer's rear face. The two spin states are clearly separable. The spacing increases with increasing wavelength and become less resolvable for shorter wavelengths. The spacing also varies with tilt angle. It is envisioned to have two bender arrays optimized for 10 and 20 meV.

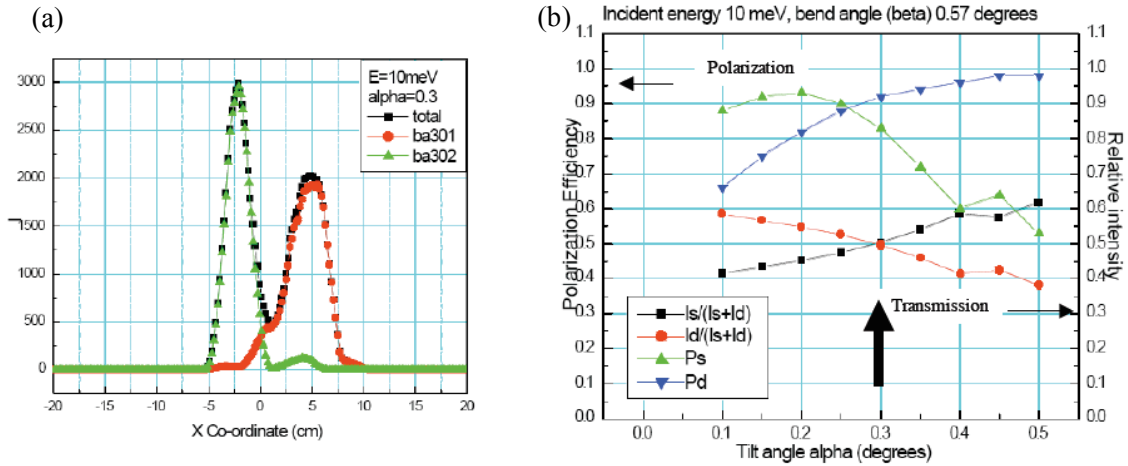


Figure 3: (a) Profile of neutron intensity at the detector determined by Monte-Carlo simulation using the NISP package. The red (green) curve is the spin up (down) polarization corresponding to the deflected (transmitted) beam. (b) The polarization efficiencies (upper two curves) and transmission (lower two curves) for the deflected and non-deflected beams

For this direct geometry instrument it would be possible to perform polarization analysis of scattered neutrons for energies from  $\sim 5 - 20$  meV. Figure 3 b shows the polarization efficiency and transmission of a bender for 10 meV neutrons as a function of tilt angle between the bender and the collimator. It is seen that the polarization efficiency is about 90% and an acceptable transmission of near 50% for a given tilt angle of  $0.3^\circ$ .

### 3. Transmission Polarizers.

HYSPEC will be built with the bender polarizer array discussed above. However, there are other options to produce and analyze polarized beams that have been considered and are currently under development. These are transmission polarizers, which have the advantage that they are suitable over a relatively broad energy range compared to crystals or multilayers. For the latter, diffraction plays the key role and the performance is very wavelength dependent. The transmission polarizers work on the principle

that one spin state is preferentially absorbed when passing through a medium of polarized nuclei [7]. We shall calculate the polarization and the transmission of three types of transmission polarizers: polarized protons, Sm and He<sup>3</sup>. Only the latter is under intense development and currently in use at several facilities, mainly reactor based. The compound nuclear state of a neutron when it is resonantly captured by a nucleus has either a spin  $I+1/2$  or  $I-1/2$ , where  $I$  is the spin of the nucleus before neutron capture. The spin dependent neutron cross section,  $\sigma$ , for the combined system was worked out by Rose [8] many years ago:

$$\sigma = \left(\frac{1}{2I+1}\right)(1 - f_n f_N) \sigma_{I-1/2} + \frac{I+1}{2I+1} \left(1 + \frac{I}{I+1}\right) f_n f_N \sigma_{I+1/2} \quad (3.1)$$

$f_n$  and  $f_N$  are the neutron and nucleus polarization, respectively, and  $\sigma_{I-1/2}$  and  $\sigma_{I+1/2}$  are the cross sections of the different spin states of the compound nucleus. From this the neutron polarization,  $P_n$ , and the combined transmission,  $T_n$ , of the two spin states are:

$$\begin{aligned} P_n(f_N, N\tau) &= \tanh(N\tau\sigma_p f_N) \\ T_n(f_N, N\tau) &= \exp(-N\sigma_0\tau) \cosh(N\tau\sigma_p f_N) \end{aligned} \quad (3.2)$$

$N$  = the number of atoms/volume in the neutron beam

$\tau$  = the length of the filter

$\sigma_p = (I/(2I+1))(\sigma_{I+1/2} - \sigma_{I-1/2})$

$\sigma_0 = (I/(2I+1))\sigma_{I-1/2} + (I+1)/(2I+1)\sigma_{I+1/2}$

Equations 3.2 were used to calculate the polarization and transmission of the three types of transmission polarizers.

### 3.1 Polarized protons:

Polarized protons have been used for many years as targets in high energy physics experiments so the technology is well established [9]. A high degree of polarization is obtained by using the technique of dynamic nuclear polarization (DNP). In this method the sample is cooled to low temperatures (<1 K) in a homogeneous magnetic field to polarize the paramagnetic spins. A microwave field is applied to equalize the population of the two spin states and to transfer the polarization to the nuclear spins via dipole—dipole coupling. Several different proton targets have been used such as ammonia, lanthanum-magnesium nitrate doped with neodymium (LMN), and butanol. We have chosen to study butanol ( $\text{CH}_3(\text{CH}_2)_3\text{OH}$ ), doped with paramagnetic centers, as the source of polarized protons. Figure 4a gives the results of the calculations with a 90% proton polarization and a density length corresponding to  $N_h\tau=4.2 \times 10^{22}$  atoms/cm<sup>2</sup>. This shows the broad-band nature of the filter. The polarization is greater the 75% over the energy range of 3.6-90 meV. The transmission is also very high for neutron spins polarized parallel to the proton polarization (spin-up). It is low for spins anti-parallel to the proton polarization so one would have to do two measurements in order to get a complete picture of the polarization of the scattered neutrons from the sample.

### 3.2 Nuclear polarized Sm:

<sup>149</sup>Samarium is particularly useful as a polarizer. It has a broad 98 meV resonance and a highly spin-dependent cross section, which enables a high degree of polarization. The nuclei have to be cooled to very low temperature to get them to order and a modest field is needed to orient the atomic moments. Because of the very high hyperfine field of Sm (335 T), a high degree of nuclear polarization can be achieved. There were several studies of Sm compounds to test its feasibility as a neutron polarizer. One study [10] used a filter of Sm-doped cerous magnesium nitrate. Because this material is an insulator it was difficult to maintain the low temperatures necessary for maintaining the nuclear polarization. Another study used fine particles of SmCo<sub>5</sub>, a high remnance ferromagnet [11]. The difficulty with this material for neutron polarization was the magnetic alignment of all the small particles. This misalignment leads to a depolarization of the neutron beam. We chose a foil of <sup>149</sup>Sm<sub>0.4</sub>Y<sub>0.96</sub>Al<sub>2</sub>, to study since this is either a paramagnet or weak ferromagnet at millikelvin temperatures and the problem associated with domains in the other Sm magnets does not exist. The amount of nuclear polarization is determined by the (low)

temperature and the size of the holding field. The results calculated from equations 3.2 are shown in Fig.4b for an achievable nuclear polarization of 90% and a thickness of the foil of 0.7mm. Over the range of energy (3.6 – 90 meV) the neutron polarization is very high (>80%). However, the transmission of the spin-up state varies due to the rapid variation of the spin-dependent cross section and averages around 40%. The transmission for the other spin state is very low so two measurements would be required to study both spin states of the scattered neutrons.

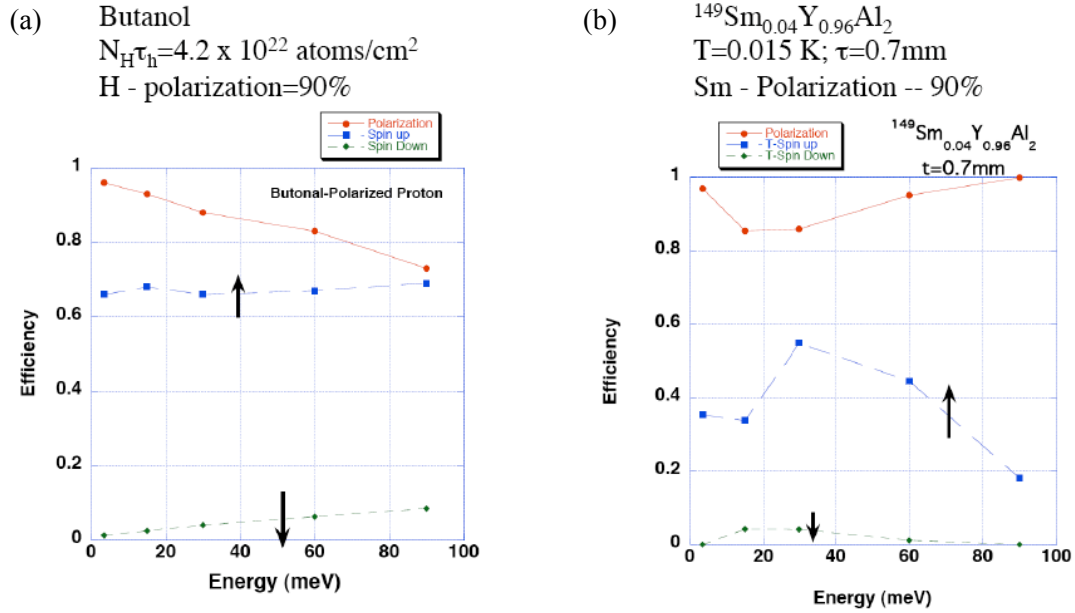


Figure 4: Calculated polarization and transmission of (a) Butanol and (b)  $^{149}\text{Sm}$  transmission polarizers

### 3.3 $\text{He}^3$ Transmission Polarizer:

The transmission polarizer that shows the greatest promise for applications in pulsed neutron beams is  $\text{He}^3$ . It is under intense development at ILL [12] and NIST [13] and is currently being used on the diffractometers D1B and D3 at ILL [14]. For the neutron polarization parallel to the  $\text{He}^3$  spin direction the absorption is nearly zero, whereas for the neutron spin anti-parallel the absorption cross section is very large. The cross section is directly proportional to the wavelength or  $1/\sqrt{E}$ . Polarized  $\text{He}^3$  is produced by two optical pumping methods: spin-exchange (SEOP) [15] and metastability-exchange (MEOP) [16]. Figure 5 shows the calculated polarization and transmissions for a  $\text{He}^3$  nuclear polarization of 75% and 90%. In Fig. 5a, the nuclear polarization is 75%, which is the current state of the art for  $\text{He}^3$  polarization. The neutron polarization varies from 100% for low energies (~3.6meV) to a low of 60% for 90 meV. The transmission of the spin-up state is quite low at low energies and increase to 80% for 90 meV. As with all transmission filters the down-spin state is low over the entire energy range. If the  $\text{He}^3$  polarization can be increased to 90% (Fig. 5b), there is a marked improvement in performance. The polarization is greater than 65% over the entire energy range and the transmission is greater than 60%, a truly suitable performance. A central filling station would be required and  $\text{He}^3$  has the attractive feature that it would be relatively easy to change the gas pressure of the cell and thus change the transmission and the polarization depending upon the energy range of the experiment.

## 4. Comparison of different polarization analysis methods

Table 1 summarizes the advantages and disadvantages of the four types of polarization methods discussed above. For the benders the clear advantage is that the technique is well established and maintenance free. You can also measure both spin states simultaneously. Importantly the device is

$$N\tau = 3.14 \times 10^{20} \text{ atoms/cm}^2$$

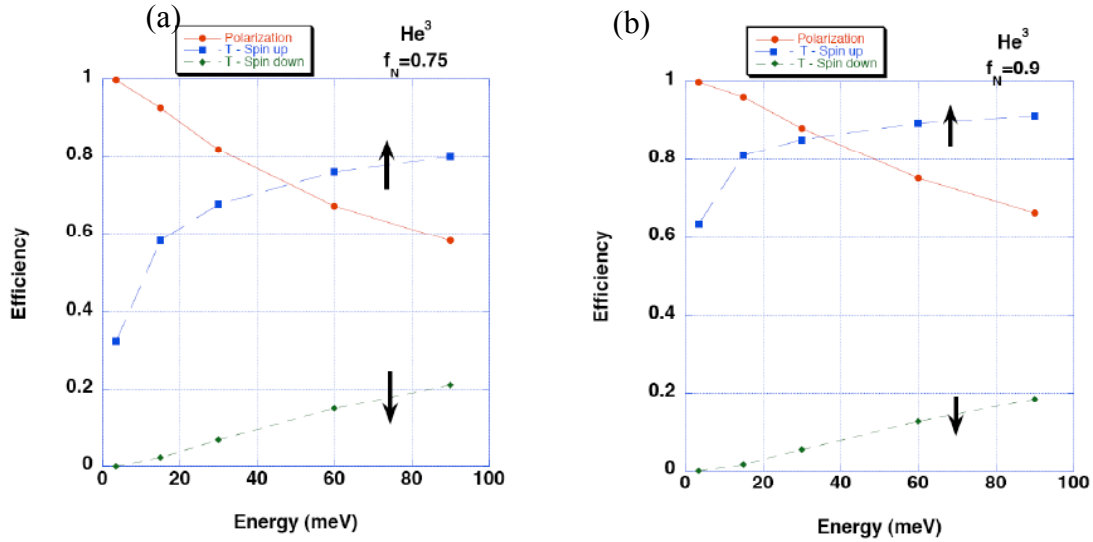


Figure 5: Calculated polarization and transmission for He<sup>3</sup> spin filters with nuclear polarization (a)  $f_N=75\%$  and (b)  $f_N=90\%$ .

insensitive to stray magnetic fields. Its disadvantages include a limited energy range of applicability and also that the tilt angle for optimum performance depends on the neutron energy. Also, all counters will not be used in a single measurement. Moreover, there is considerable transmission loss in the 20 minute collimator needed to limit the divergence of the beam striking the bender.

For the He<sup>3</sup> transmission polarizer the distinct advantage is its broad band nature with a high polarization efficiency, which can be varied with pressure to suit the energy range of the experiment. One can also cover a wide angular range with a single cell or a number of different cells. However, the He<sup>3</sup> polarization cells are very sensitive to magnetic field gradients and its use may be limited to studies not involving high sample magnetic fields where stray fields will affect the performance. To cover the angular range of HYSPEC, a large He<sup>3</sup> volume is required. Also, a central facility is required to fill and polarize the He<sup>3</sup> nuclei in the cells and this adds greatly to the cost of the technique and requires a significant facility infrastructure.

There are also tradeoffs for the less well known methods of polarizing neutrons. For the Sm filters, a high degree of polarization can be achieved and this is magnetic field insensitive. However, very low (mK) temperatures and a holding magnetic field are needed to maintain the Sm nuclear polarization. Also, the polarization efficiency, once fixed, cannot be varied. For the polarized proton transmission filter a high degree of polarization can be achieved and it performs well over a broad energy range. The means of producing polarized protons has been studied over many years by the high energy community. Its disadvantages are the complicated nature of the technique in that mK temperatures and a microwave pumping field are needed to maintain the proton polarization. Also, it, too, is sensitive to magnetic field gradients around the device and the polarizing efficiency, once fixed, cannot be varied.

## 5. Summary and conclusions

HYSPEC is unique instrument at a pulsed source and will be the only inelastic instrument at SNS with a designed-in capability to do full neutron polarization. Other methods using transmission polarizers, whose transmission and polarization depend upon the absorption of one spin state and transmission of the other, are more broad-band in nature. There are clear trade-offs to be considered in each of these systems. The collimator-bender polarizer is the chosen method to be used in HSYPEC because it has been demonstrated to work and is maintenance free. He<sup>3</sup> transmission polarizers are under intense investigation and would be

desirable if a number of hurdles can be overcome. The feasibility of using Sm and polarized protons has been demonstrated, but more R&D would have to be undertaken to establish this method as competing techniques for polarization analysis.

Table 1: Advantages and disadvantages of four polarization techniques discussed in this paper

BENDERS	He <sup>3</sup>	Sm	Polarized Protons
<b>ADVANTAGES</b>			
Established technique Maintenance free Measure both spins Magnetic field insensitive	High polarization efficiency Vary polarization efficiency with pressure Wide angular acceptance Broad-band	High polarization efficiency Magnetic field insensitive	High polarization efficiency Broad-band Established technology
<b>DISADVANTAGES</b>			
Polarization depends upon energy Limited energy range Not all detectors used Transmission loss in collimators	Magnetic field sensitive Large He <sup>3</sup> volumes required Need central facility	Very low temperatures required Polarization efficiency is fixed	Low temperatures required Microwave pumping needed Magnetic field sensitive

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