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How to polarise all neutrons in one beam : a high performance polariser and neutron transport system

D. Martin Rodriguez[a], P. M. Bentley[a,c], C. Pappas[b,*]

[a]*European Spallation Source ESS ERIC, Box 176, 221 00 Lund, Sweden*
[b]*Faculty of Applied Sciences, Delft University of Technology, Netherlands*
[c]*Department of Physics and Astronomy, University of Uppsala, Uppsala, 751 20, Sweden*

Abstract

Polarised neutron beams are used in disciplines as diverse as magnetism,soft matter or biology. However, most of these applications often suffer from low flux also because the existing neutron polarising methods imply the filtering of one of the spin states, with a transmission of 50% at maximum. With the purpose of using all neutrons that are usually discarded, we propose a system that splits them according to their polarisation, flips them to match the spin direction, and then focuses them at the sample. Monte Carlo (MC) simulations show that this is achievable over a wide wavelength range and with an outstanding performance at the price of a more divergent neutron beam at the sample position.

Keywords: neutron guides, neutron polarisers, Monte Carlo simulations

1. Introduction

Polarised neutron beams fully exploit the strength of neutron in investigating the structure and motion of atoms and molecules in the bulk. This leads eventually to a broad range of applications and a high demand for the highest possible intensities. The usual polarisation methods involve polarising supermirrors [1, 2, 3], ^{3}He polarisers [4, 5, 6] or Heussler monochromatos [7]. All these methods, however, act as spin filters, i. e. they transmit the part of the neutron beam that has the *correct* spin state while discard all neutrons with the *wrong* spin state. Therefore and in order to maximise the neutron intensity, it would be highly beneficial to design a neutron polarising system that uses the full beam and after some manipulation brings all neutrons in the same spin state and recombines them at the sample position.

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[*] Correspondig author
Email address: `damian.rodriguez@esss.se` (D. Martin Rodriguez)

Such a device has been proposed by Badurek et al. [8], who showed that by applying the dynamic polarisation technique it is possible to polarise the full neutron beam and reach a high polarisation. However, this solution requires either a highly monochromatic beam, or a time-of-flight polychromatic beam with high time resolution. In both cases the neutron intensity is severely reduced, which is a major drawback. Therefore, for general purpose applications a different, more versatile, solution is required with an approach, which overcomes the limitations of conventional neutron polarisers.

2. Principle and description of the system

The principle of the proposed system consists in separating the neutron beams according to their spin states using a supermirror polarisering cavity. The neutrons are then converted in to the same spin state by adequate use of spin flippers and finally focussed and recombined at the sample position of an instrument. A schematic drawing of the setup is given in fig. 1. The starting point and key component is a V-shaped supermirror polarising cavity, which separates the neutron beams according to their spin states. Such a device has been realised at the Helmholtz Zentrum Berlin (previously Hahn-Meitner Institute) and provided polarised neutron beams to two instruments: the transmitted beam with a polarisation $|-\rangle$ was serving the reflectometer V6 while the reflected beam with a polarisation $|+\rangle$ was directed to the neutron-spin-echo spectrometer V5 [9]. The solution adopted here is a variant of the Berlin setup and is schematically shown shown in fig. 1-3. It includes a cavity consisting of m=2.5 (supermirrors) and m=1 (Ni) coated Si wafers inserted in the

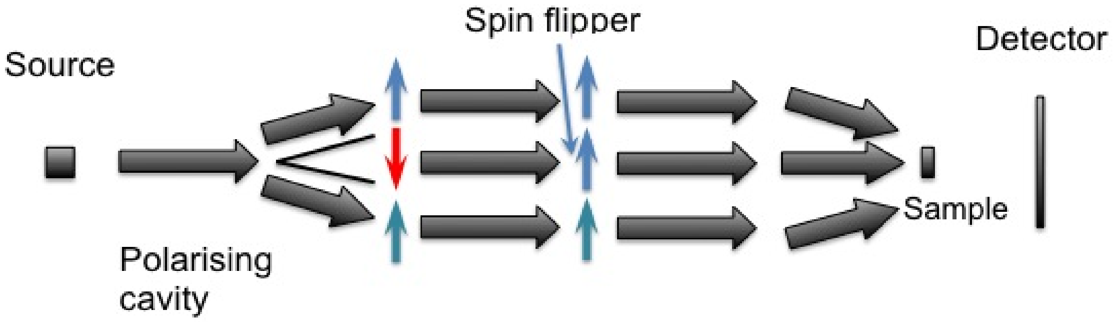

Figure 1: Principle of the beam transport system proposed in this work, illustrating the separation of the incoming depolarised neutron beam in three beams with different polarisations. Using spin flipper(s) all beams are converted into the same polarisation and finally recombined at the sample position.

neutron guide as specified in 2(b). The cavity splits the original neutron beam in three: a transmitted central beam with a polarisation $|-\rangle$, and two reflected lateral beams with a polarisation $|+\rangle$. After the cavity a guide system transports the central and lateral beams to the sample. Broadband RF flipper(s) as schematically shown in fig. 2(a) and in the artist's view of fig. 3 bring the three beams to the same polarisation state, e.g. in $|+\rangle$. Figures 2(a)-(b) and 3 illustrate the parameters on the basis of which the system was optimised using Monte Carlo simulations. If θ is the angle between the polarising supermirrors of the V-cavity and the central beam propagation axis, the reflected beams will be at an angle of 2θ, and for this reason at the sides of the cavity two curved guides take over with a respective inclination of

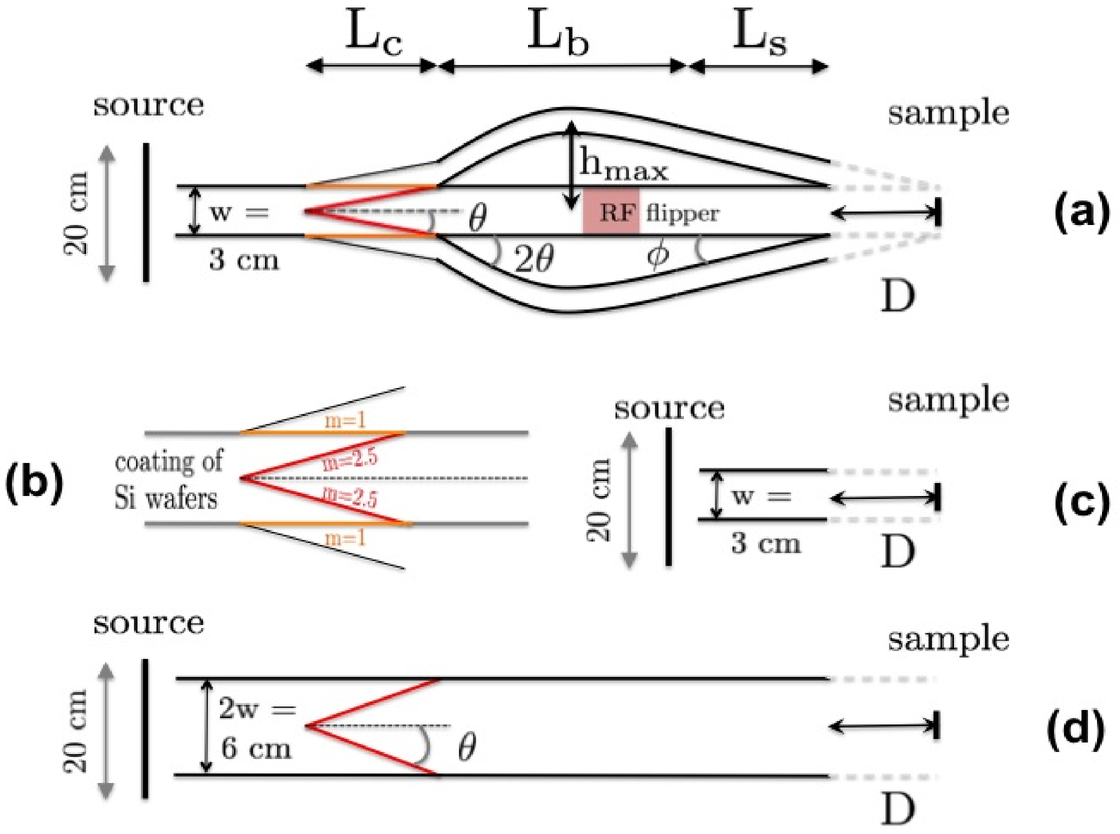

Figure 2: (a) Schematic representation of the system illustrating the fixed dimensions and the free parameters (angles θ and ϕ, lengths h_{max}, L_b and L_s) used for the Monte Carlo simulations. The elements in orange and red designate the parts that are reflecting and also transmitting neutrons. In a real setup these would be consisting of Si wafers coated with m=2.5 suppermirrors (red lines) and m=1, i.e. Ni (orange lines), as illustrated by the closeup view of (b). The reference setup used to normalise the neutron intensities at the sample is shown in (c). The performance of the system (a) has been compared with that of a double width polarising cavity shown in (d). All drawings are not in scale.

2θ. The curved guide sections have a linear length of L_b and separate the beams by h_{max} by following an arc with an angular opening of $2\theta+\phi$, where ϕ is determined by :

$$\phi \approx \tan\phi = \frac{3}{4}\frac{W}{D} \tag{1}$$

with W the width of the initial beam and D the distance between the end of the guide and the sample position. Finally, a straight guide with an inclination of ϕ with respect of the central guide direction, transports the lateral beams to the sample. Obviously the width of the lateral guides is half that of the central beam and the successful implementation of the concept relies on the optimum design of the lateral beam sections. The system potentially uses all incoming neutrons, but at the price of a more divergent beam. The successful implementation of the device requires the optimum superposition of the three beams at the sample with a smooth beam profile and a homogeneous angular divergence. We will show that this is feasible. Furthermore, the system provides the flexibility to block the lateral beams and use only the less divergent central beam if required.

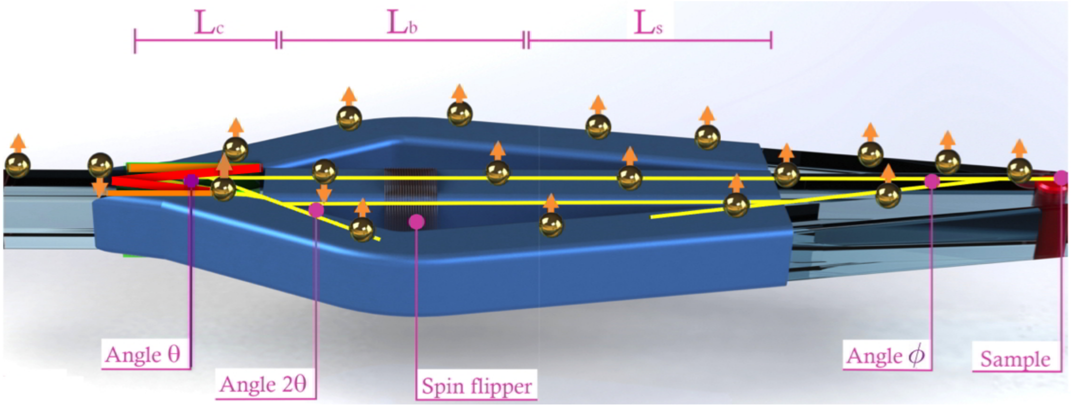

Figure 3: Artist's view of the setup of fig. 2 illustrating the geometry and an RF flipper positioned at the central beam. The drawing is not in scale.

3. Simulation procedure and results

The simulations were performed with the VITESS program [10], assuming the ILL_cold_2011 neutron source. The source had a diameter of 20 cm, large enough to fully illuminate with full divergence and at all wavelengths the neutron guides considered in this work. At 2 m from the source a 10 m long guide was placed with a width of W=3 cm, a height of 6 cm and all walls coated with m=1 (Ni). After this straight guide section the V-shaped polarising cavity was placed as shown in fig. 2(b). The coating of the polarising supermirrors corresponded to Fe/Si multilayers with m=2.5, while the rest of the mirrors was coated with m=1. An important element for the successful implementation of the concept are the m=1 coated Si wafers, sketched by the orange lines in fig. 2(a)-(b) and 3, which were also included in Berlin setup [9]. The curved lateral parts had a non-polarising coating of m=2 for the outer walls and m=1 for the rest. The central guide was also coated with m=1 over the whole length. The sample had a cross-section of 2 x 2 cm^2 and was placed at D = 4 m from the end of the guide assembly.

The results of the simulations will be discussed in two sections, in which the performance of the proposed system (from now on named *the system*) is discussed as a function of its total length and the geometry of the polarising cavity respectively. The neutron intensities at the sample were normalising the corresponding intensity of the reference setup shown in fig. 2(c), which corresponds to the arrangement of fig. 2(a) without the polarising system: i.e. at 2 m from the source a 10 m long guide is placed with a width of W=3 cm, a height of 6 cm and all walls coated with m=1 (Ni). This normalised neutron intensity together with the polarisation, horizontal profile and divergence of the neutron beam at the sample position were used to assess the performance of the system.

3.1. Length of the device

The length of the system depends on the length of the cavity ($L_c = W/2 \tan\theta \approx W/2\,\theta$) and the requirements to redirect the lateral beams to the sample. With the angles defined as in fig. 2 the angular length of the arc is fixed to $2\theta+\phi$. However, the length depends on the radius of curvature ρ, which can be obtained following a well established geometrical approach [11]. For the assessment of the performance three extreme cases were considered by comparing the position of the curved section exit window with respect to the line-of-sight (LOS) of the entrance window : (a) half in the LOS (b) exactly out of LOS and (c) twice out of LOS. The parameters used for the simulations are summarised in table 1.

The results are given in fig. 4 and show that in all cases the polarisation is high and the normalised neutron intensity, which in this case can be associated with the transmission of the system, higher than 50 %, reaching even 80 %. The

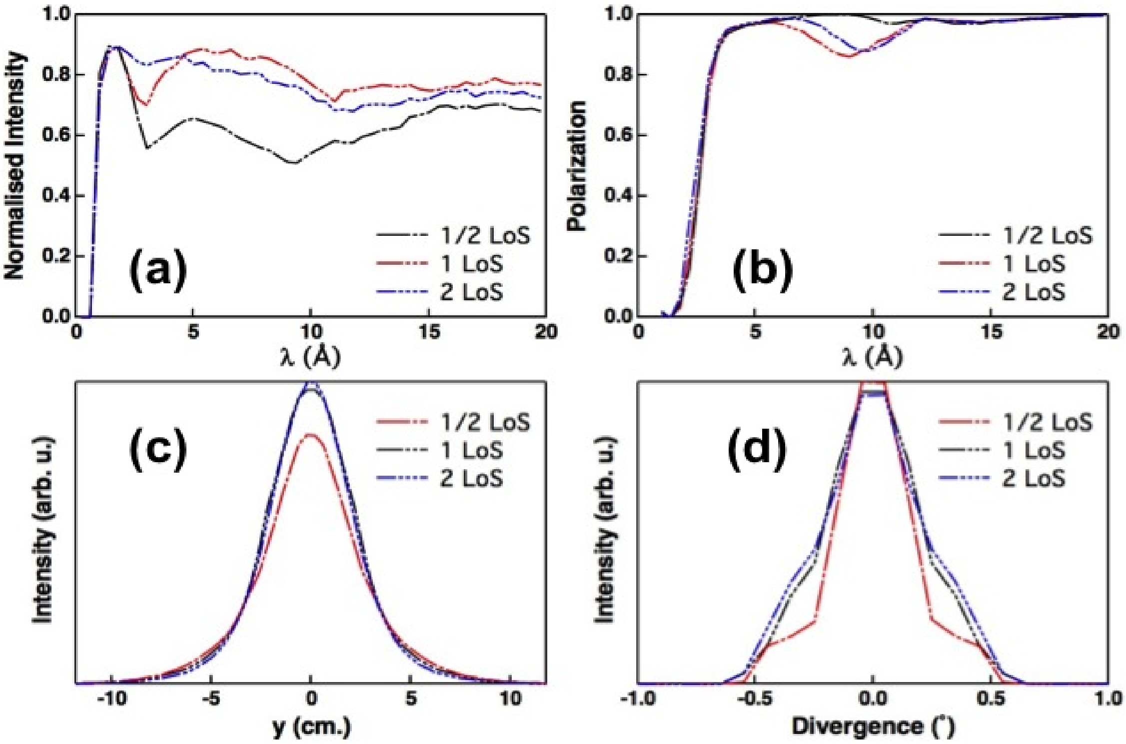

Figure 4: Normalised neutron intensity (a), polarisation (b), horizontal beam profile (c) and divergence (d) of the system for three positions of the curved section exit window with respect to the line-of-sight (LOS) of the entrance window. The characteristic lengths used in the simulations are given in Table 1.

Table 1: Parameters of the systems simulated in 3.1.

θ [°]	ρ [m]	$L_c [m]$	L_b [m]	L_s [m]	Remarks
0.6	44.34	2.86	1.16	1.84	1/2 LOS
0.6	177.38	2.86	4.61	7.25	1 LOS
0.6	709.51	2.86	19.65	20.78	2 LOS

cases“1 LOS” and“2 LOS” give very similar results. It is also noticeable that the polarisation of the lateral beams goes through a minimum at about 9 Å for the “1 LO” and “2 LOS” cases but not for “1/2 LOS”. This effect should therefore be brought in relation with ρ and the reflectivity of the outer walls, which are m=2 for both spin states and thus not polarising. The higher values of ρ lead to lower incident angles of the neutrons on the outer walls, which increases the transmission for all neutrons including those with the wrong spin state that are not completely filtered out by the polarising cavity. It is indeed known that such a “leakage” exists for the reflected beams [12], which is closely related with the geometry of the cavity and will be discussed in the following sub-section. The “leakage” could be eliminated by a polarising supermirror coating of the outer walls, as it was suggested in [12] and realised in Berlin [9].

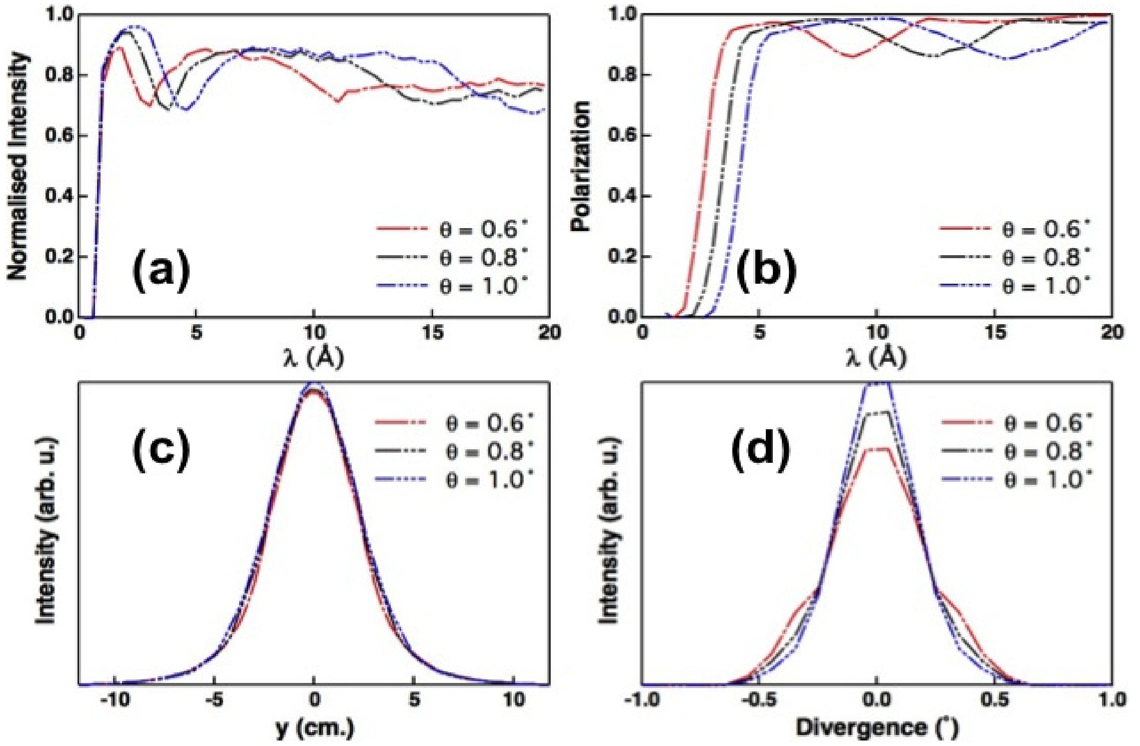

Figure 5: Normalised neutron intensity (a), polarisation (b), horizontal beam profile (c) and divergence (d) of the system for three values of the angle θ for the polarising cavity. The simulations correspond to the case “1 LOS” assuming the characteristic lengths given in Table 2.

3.2. Geometry of the polarising cavity

The performance of polarising cavities depends on the combination of the angle θ and the supermirror coating [12, 3]. In this work we fixed the supermirror coating to m=2.5 as shown in fig. 2b and changed θ to 0.6°, 0.8° and 1.0°, while keeping the "1 LOS" configuration for the lateral beams with the lengths given in Table 2. The deduced performance is given in figure 5, where similar trends and similar shapes are found for these three cases. As expected, the higher values of θ shift the optimum performance towards longer wavelengths and the "leakage" seen in the polarisation occurs at longer wavelengths as well.

Table 2: Parameters of the systems simulated in 3.2.

θ [°]	ρ [m]	L_c [m]	L_b [m]	L_s [m]	Remarks
0.6	177.38	2.86	4.61	7.25	1 LOS
0.8	111.47	2.15	3.66	8.75	1 LOS
1.0	76.48	1.72	3.03	10.00	1 LOS

4. Discussion

The system can efficiently split the incoming neutron beam in three polarised beams, and after proper spin manipulation with spin flippers, it has the potential to redirect them to the sample position. In this way the intensity is practically doubled with respect to what would have been delivered only by the supermirror cavity in transmission, i.e. by the central beam of the system shown in fig. 2a. In the following we will show that this result is in many aspects similar to what would have been obtained by doubling the dimensions of the central beam as shown in fig. 2d. The performance of the different setups (always at the sample position) is given in fig. 6 for the $\theta = 0.6°$ and "1 LOS" case. All setups lead to a highly polarised beam. On the other hand, the intensity at the sample is the lowest for the central beam alone and is practically doubled either by doubling the width of the guide or by using the proposed system. A similar trend is found on the divergence of the beam, which is the lowest for the central beam alone and broader but with a similar distribution both for the double width and the proposed system cases. The beam profile in the horizontal direction is different for each of the cases: it is the broadest for the double width beam whereas it shows a sharp profile for the proposed system illustrating its focusing effect.

A pre-requisite for the optimum performance of the system is the possibility

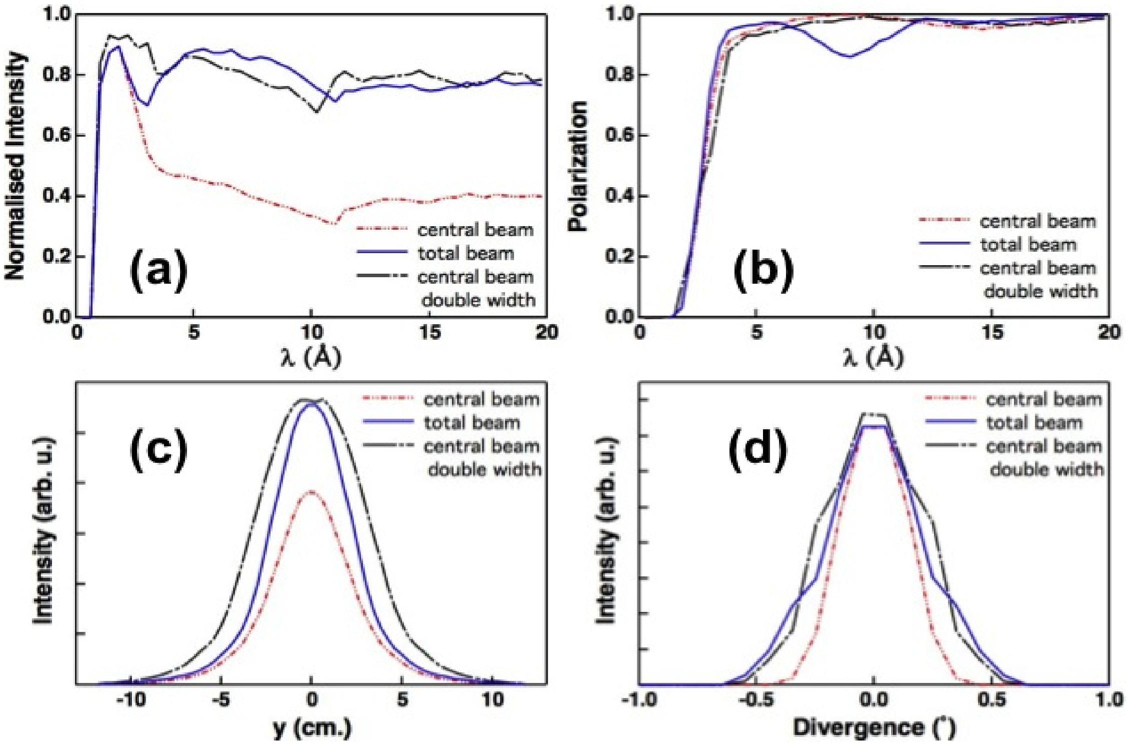

Figure 6: Comparison of (a) the normalised intensity, (b) the polarisation, (c) divergence integrated over the full spectrum and (d) beam profile in the horizontal direction (y) at the sample position for three cases: the central beam of the system shown in fig. 2a, the combined central and lateral beams of fig. 2a, and for the double width central beam with the polarising cavity in transmission shown in fig.2d. All results refer to the sample position, and to the case of “1 LOS” with $\theta = 0.6°$.

to apply magnetic fields over the whole length of the device. The magnetic fields should be high enough to polarise the beam at the cavity and then sufficient to guide and maintain the beam polarisation. In fact several realisations of polarised cavities have addressed this point [14, 13] and a variety of solutions have been successfully adopted involving either coils or the strong permanent magnets available nowadays.

The design of the device implies that the strong magnetic fields needed to saturate the supermirrors and polarise the neutron beam are applied only at the cavity and thus far away from the sample position. This is an advantage for applications, like in Neutron Spin Echo spectroscopy, where a high magnetic field homogeneity is required. and any cross-talk with other magnetic fields must be minimised.

Last but not least the performance of the device depends on the capability to flip the beam polarisation of the central and/or the lateral beams with a high efficiency over a broad wavelength range. For this purpose RF adiabatic flippers [15] can be used, which combine a compact design with broadband high flipping efficiency [13, 16]. These flippers consist of a longitudinal RF coil, which can practically have the dimensions of the neutron guide and can even slide along the guide [16], and a vertical magnetic field, with a longitudinal gradient, which can be realised by placing permanent magnets below and above the device as a whole.

To conclude, from todays perspective there are no technological risks in adopting the proposed design for future polarised neutron instruments, in particular neutron spin echo spectrometers. In this way it is possible to improve the performance of beam extraction systems by polarising also those neutrons that are usually discarded.

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