McStas

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Polarised neutrons in McStas - Magnetic single crystal and SESANS

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Abstract

The Monte Carlo simulation package McStas[1] is a proven tool for instrument design and optimisation. Recently, the use of software of its kind has extended into the realm of virtual experiments, where sample models are included in the simulations[2]. Virtual experiments have been used interpret data, pinpointing the source of spurions as well as distinguishing between instrument resolution and peak broadening[3] by physical processes.

Thus far, virtual experiments using McStas have largely been limited to unpolarised instrumentation. An important recent development is support for polarisation analysis through the entire model of the instrument.

We present the first magnetic scattering component in McStas: A magnetic single crystal, generating structure factors from a list of atomic positions and scattering lengths in the unit cell of the crystal. This is to avoid having to generate a reflection list with structure factors in an external program, i.e. to simplify the use of the component.

Support for polarisation analysis includes tracking of beam polarisation through diverse components such as magnets (standard as well as user defined), spin flippers etc. Gravitational effects are, by design, handled natively by the kernel and is therefore handled by all supplied components.

A magnetic single crystal

The magnetic scattering cross-section for a sample with localised spin+orbital angular moment $g\mathbf{J} = (g_S + g_L)\mathbf{J} = 2\mathbf{S} + \mathbf{L}$ is [4]

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega_f \mathrm{d}E_f} = \frac{k_f}{k_i} \sum_{i,f} P(\lambda_i) \left| \langle \lambda_f \mid \sum_j e^{i\mathbf{Q}\cdot\mathbf{d}_j} U_j^{\sigma_i\sigma_f} \mid \lambda_i \rangle \right|^2 \delta(\hbar\omega + E_i - E_f)$$

where $\mid \lambda_i\rangle$ and $\langle\lambda_f \mid$ are the initial and final states of the sample with energies E_i and E_f respectively, $P(\lambda_i)$ is the distribution of initial states and

$$U_j^{\sigma_i\sigma_f} = \langle \sigma_f \mid b_j - m_j \mathbf{J}_{\perp j} \cdot \boldsymbol{\sigma} \mid \sigma_i \rangle$$

where $\mid \sigma_i\rangle$ and $\langle\sigma_f \mid$ are the initial and final spin states of the neutron (either up (+) or down (-)) and we have ignored the interaction between the neutron and the nuclear spin of the sample. $\boldsymbol{\sigma}$ are the Pauli spin matrices working on the neutron state. We consider the polarisation to be characterized in a coordinate system (ξ, η, ζ) and the incoming polarisation to be along the ζ axis $\mathbf{P} = (P_x, P_y, P_z) = P\boldsymbol{\zeta}$.Thus, the matrix elements of $U^{\sigma_i\sigma_f}$ can now be written

$$\begin{aligned} U^{++} &= b - mJ_{\perp\zeta} \\ U^{--} &= b + mJ_{\perp\zeta} \\ U^{+-} &= -m\left(J_{\perp\xi} + iJ_{\perp\eta}\right) \\ U^{+-} &= -m\left(J_{\perp\xi} - iJ_{\perp\eta}\right) \end{aligned}$$

where $m = \frac{r_0\gamma}{2} g f(\mathbf{Q})$ with r_0 the classical electron radius, $\gamma = 1.913$, g the Landé splitting factor and $f(\mathbf{Q})$ the magnetic form factor of a particular ion in the sample.

Features of Single_magnetic_crystal

We have constructed the component `Single_magnetic_crystal` which features

- Nuclear coherent scattering
- Nuclear incoherent scattering
- Electronic magnetic coherent scattering
- Absorption

The component calculates the scattering cross-sections (in barns) from a parametrised list of the atoms/ions in the unit cell such as

index	iontype	x	y	z	b_{coh}[fm]	g_S	S_x	S_y	S_z	g_L	L_x	L_y	L_z
1	Cu2+	0.5	0.5	0	7.718	2	0	-0.5	0	0	0	0	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Currently, all magnetic form factors are considered to be unity, and we assume that the polarisation does not precess inside the crystal. We also consider the mosaicity of the crystal and the relative uncertainty in lattice parameters to be isotropic.

Our plans are to further develop the model of the crystal to include:

- form factors for different ions from tabulated values[6].
- anisotropic mosaicity
- a temperature dependent magnetic ordering function making it possible to simulate the scattering of a magnetic phase transition.
- temperature dependent Debye-Waller factors.

Testcase of Single_magnetic_crystal

As testcase the anti-ferromagnetic La_2CuO_4 was used. The orthorhombic unit cell is shown in Figure 1

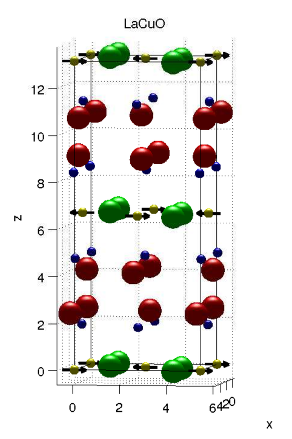

Figure 1: The orthorhombic unit cell of the antiferromagnetic La_2CuO_4

Polarised Laue setting

In Figure 2 our set-up to test the magnetic single crystal is shown. It consist of a low-divergence source with a flat distribution of wavelengths between 0.1Å and 7.9 Å, the magnetic single crystal sample and two PSD detectors covering all 4π space. These register the neutrons' spin component parallel and antiparallel to the incoming polarisation $\mathbf{P}$, i.e. non spin-flip (NSF) and spin-flip (SF), respectively.

In the case where $\mathbf{P} \parallel \mathbf{Q}$ all magnetic scattering from the reflection $\mathbf{Q}$ is SF. All nuclear scattering is NSF hence this configuration is optimal for studying anti-ferromagnets. Figure 3 shows the NSF and SF 4π Laue patterns in case of an unpolarised beam $\mathbf{P}$=0. Figure 4 shows the NSF and SF 4π Laue patterns in case of a polarised beam $\mathbf{P}$=(PX,PY,PZ).

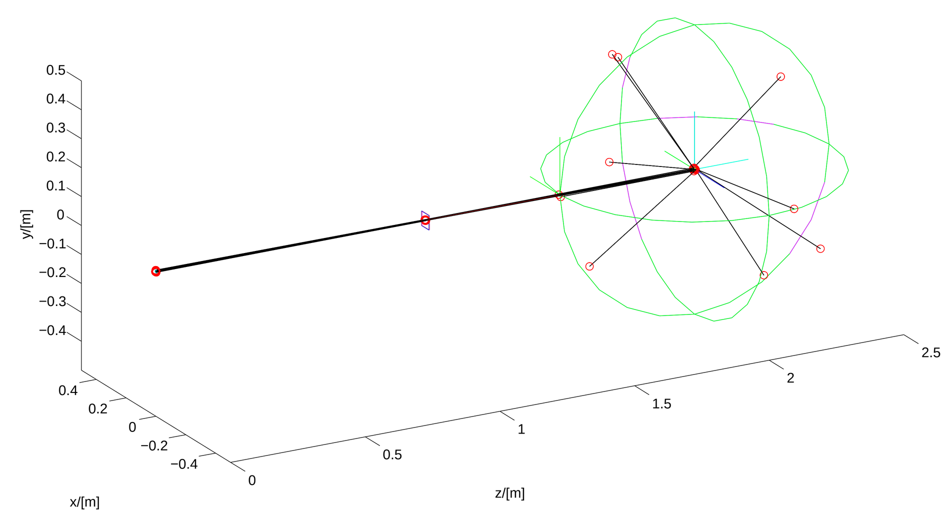

Figure 2: A screendump of the idealised neutron Laue scattering instrument featuring 4π detectors with polarisation option used for testing `Single_magnetic_crystal`

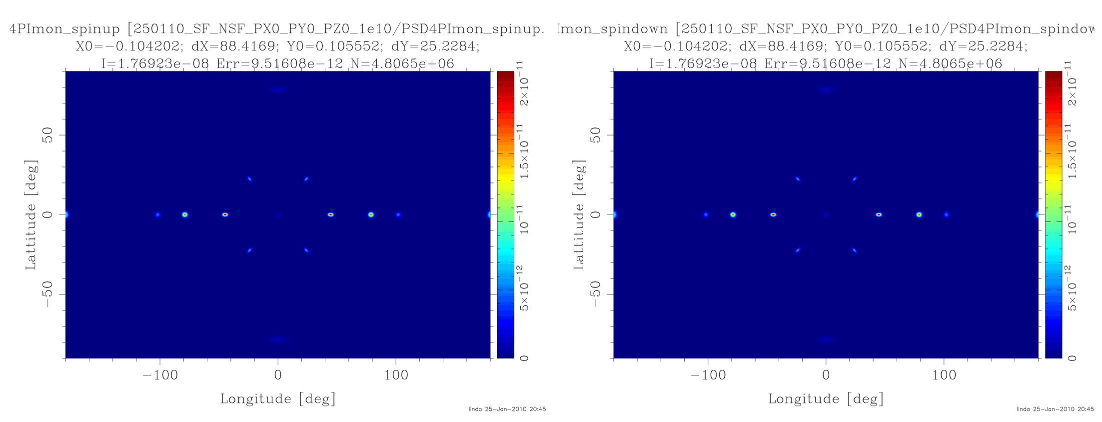

Figure 3: The nuclear and magnetic coherent scattering in case of unpolarised incoming beam. Left detector is NSF, right detector is SF. Reflections are seen to be equally distributed in both channels.

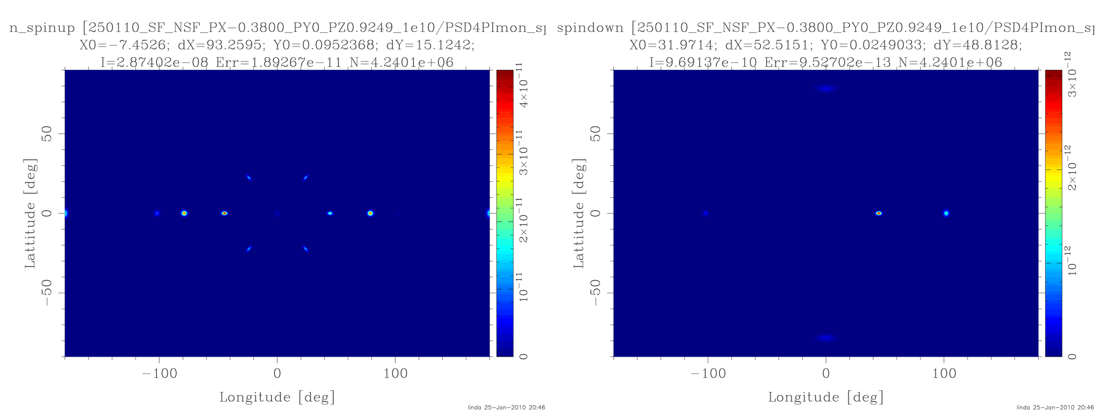

Figure 4: The nuclear and magnetic coherent scattering in case of polarised incoming beam. Left detector is NSF, right detector is SF and it is seen that the magnetic reflection with $\mathbf{P} \parallel \mathbf{Q}$ is only in the SF channel.

Precession of polarisation in McStas

As a neutron bunch traverses a magnetic field its polarisation vector precesses around a vector parallel to the local field, with an angular frequency given by:

$$\omega = \gamma\mathbf{B}, \quad \gamma = -\frac{eg}{2m} \approx 2\pi\, 29.164 MHzT^{-1}$$

In McStas, neutrons are propagated in the time-domain by Δt. In the presence of a magnetic field in McStas, a neutron is propagated through the field using the following algorithm:

1. $t_{target} = n_t + \Delta t$
2. `while` $n_t < t_{target}$
   (a) `store neutron`
   (b) `sample magnetic field:` $\mathbf{B}_1 = \mathbf{B}(n_x, n_y, n_z, n_t)$
   (c) `propagate neutron "non-magnetically" by` $\delta t (< \Delta t)$
   (d) `sample magnetic field:` $\mathbf{B}_2 = \mathbf{B}(n_x, n_y, n_z, n_t)$
   (e) `if` $\mathbf{B}_1 \angle \mathbf{B}_2 < \theta_{threshold}$:
      i. `restore neutron`
      ii. $\delta t := \delta t / 2$
      iii. `goto 2c`
   (f) `else:`
      i. `rotate polarisation` $n_{\mathbf{P}}$ `by` ω `around` $\frac{\mathbf{B}_1 + \mathbf{B}_2}{2}$
      ii. `goto 2`

This simplistic algorithm ensures that stepsizes adapt to the the magnetic field in each neutron's flightpath, provided δt is chosen sufficiently small to avoid aliasing. No other formal limit is imposed on the magnetic fields, which, e.g. allow field descriptions to be nested inside each other.

SE-SANS

To evaluate the performance of the precession allgorithm we have chosen to implement a model of a Spin-Echo Small Angle Neutron Scattering set-up. In particular the model is set up to mimic that of the SE-SANS machine at Delft[7][8]. We have built a model of the SE-SANS machine, complete with guide systems, slits, etc. Inserting an idealised sample at the sample position of the instrument we may record an ideal modulation of the polarisation signal as shown in figure 5.

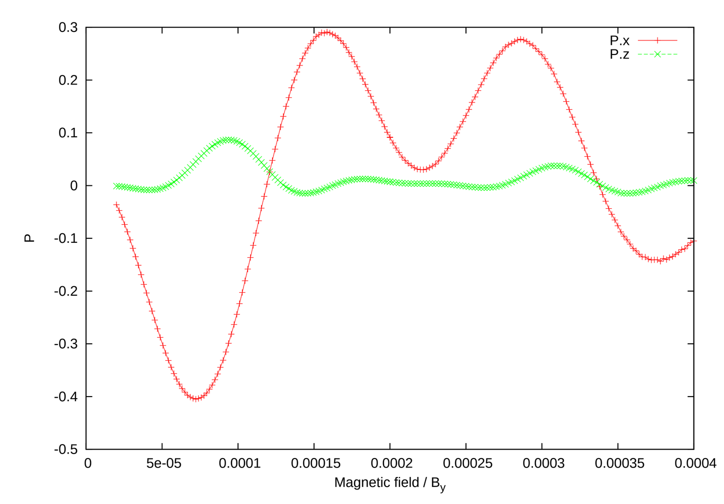

Figure 5: Modulation of polarisation at the detector of a model SE-SANS instrument, using an idealised scatterer.

References

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Keywords: McStas, Monte Carlo sim., Software,Polarisation,Neutrons, Instruments