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BAMBUS: a new inelastic multiplexed neutron spectrometer for PANDA

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Abstract. We report on plans for a multiplexed neutron analyser option for the PANDA spectrometer. The key design concept is to have many analysers positioned to give a large coverage in the scattering plane, and multiple arcs of these analysers to measure different energy transfers simultaneously. The main goal is to bring intensity gains and improved reciprocal-space and energy mapping capabilities to the existing cold triple-axis spectrometer.

1. Introduction

The study of magnetic excitations is important in understanding the emergent properties in a range of heavy fermion, superconducting and low dimensional materials. Neutron triple-axis (TAS) and time of flight (TOF) spectroscopies are valuable tools for probing excitations, as they are able to pick out magnetic excitations with spatial information.

The geometry of triple-axis spectroscopy experiments, that allows measurements within a given scattering plane, are well suited for setups with sample environments (as these often restrict the outgoing neutron trajectories out of the scattering plane). Hence, TAS instruments are often interesting for a range of condensed matter applications, for example studies with magnetic field, pressure, etc. However, it is a technique that only measures a single point (of a 4D momentum-energy space) per instrument setting and has long counting times. One solution to this is to have many analysers and detectors; for example FLATCONE at the ILL, MACS at the NCNR and RITA2 at PSI [1–3]. Recently, other multi-analyser projects are also planned, such as CAMEA at the ESS [4], Multi-FLEXX at HZB [5] and CAMEA at PSI. The basic concept is to have multiple analysers that cover a greater solid angle to increase the data acquisition rate and the reciprocal space coverage per instrument position.

This paper details plans for a multiplexed analyser and detector option (BAMBUS) for the PANDA cold triple-axis spectrometer at FRM-II, Garching.

2. Existing cold triple-axis spectrometer: PANDA

PANDA is a cold triple-axis spectrometer and is designed as a high flux instrument with low background [6, 7]. A wide range of energy transfers can be covered and different sample conditions are accessible, e.g. temperatures down to 50 mK and fields up to 15 T.



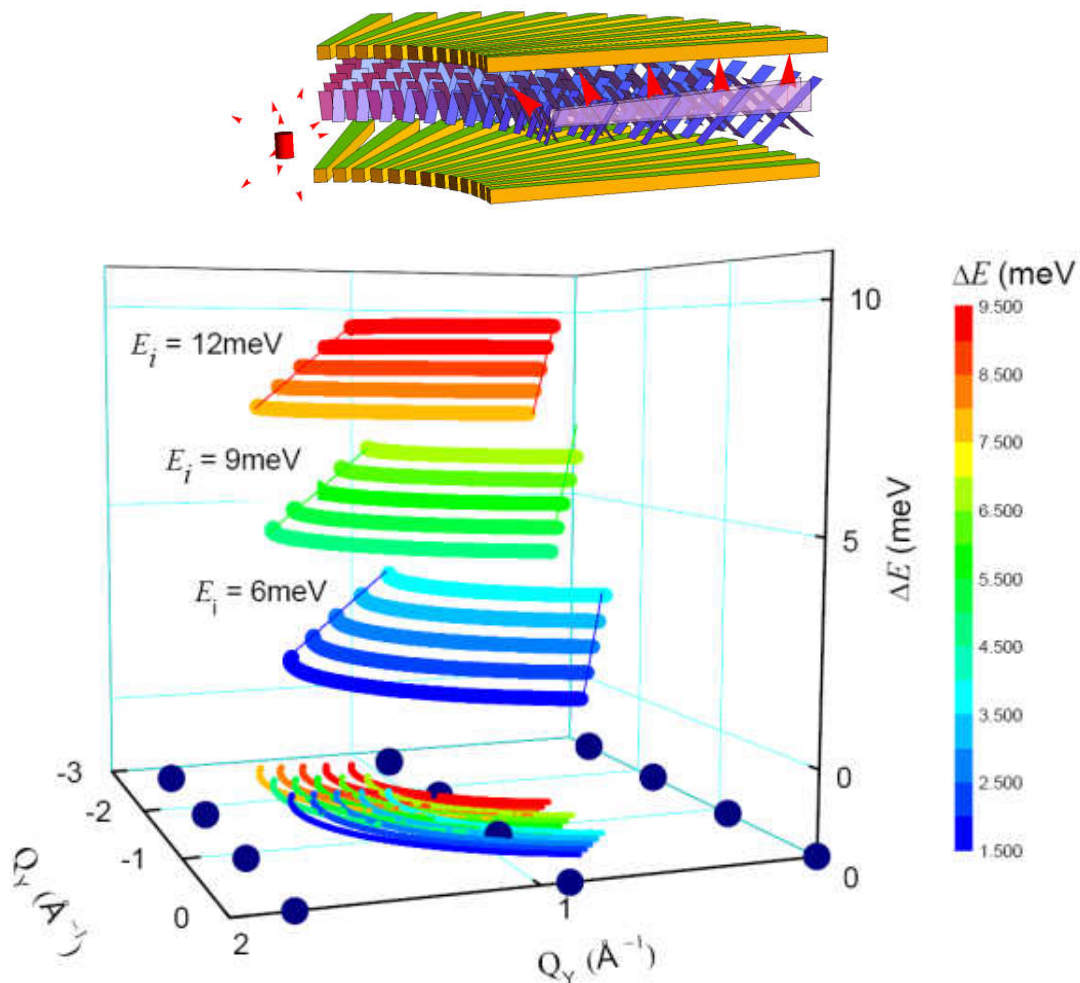


Figure 1. Top: a schematic of the BAMBUS secondary spectrometer showing the analyser positions. The red cylinder represents the sample, the tilted blue plates are analysers, arrows show the neutron trajectories from the analysers and the yellow/green rods represent the detectors. Bottom: the accessible $(\vec{Q}, E)$ space for three different incoming energy settings for a fixed sample position.

The key features of the spectrometer are the relatively short source to monochromator distance (7.8 m) and large doubly focusing monochromator and analyser. It is in this framework that a multiplexed analyser and detector secondary spectrometer is planned. Here the main aim would be to complement the existing setup, by having many detectors at fixed final energy to quickly build up momentum transfer maps simultaneously for a number of energy transfers. Also by changing the incoming neutron energy, different energy transfers can be accessed and therefore energy scans across a range of momentum transfers can be realised.

3. Design concept

The key design concept behind the BAMBUS analyser system is to use many vertically scattering analysers around the sample, giving a large coverage of in-plane scattering. These are complemented by multiple concentric analyser arcs to increase the number of energy transfers measured at once at every given 2θ angle. The planned upgrade would bring improved reciprocal space mapping capabilities at a number of discrete low energy transfers. A schematic of this

layout and reciprocal space coverage is shown in Fig. 1.

The design criteria and main goals for the BAMBUS multiplexed spectrometer have been identified:

i) To cover a broad range of reciprocal space and allow measurements of broad and diffuse features and also parametric studies (e.g. with temperature, field etc.) of excitations.

ii) A simple and robust multi-analyser module is desired. It should require little alignment during an experiment and be readily accessible by any of the wider inelastic neutron scattering community, in terms of simplicity of experimental use and analysis.

iii) The module should complement and work alongside the current triple-axis spectrometer on PANDA. The large $(\vec{Q}, E)$ coverage supports mapping capabilities and parametric studies (e.g. against temperature or magnetic field), however sometimes conventional TAS mode is also required. It is planned that it should be possible to switch between conventional TAS and the multiplexed module in the same experiment.

iv) The resolution between different analysers should be comparable (relative to the features studied) to allow straightforward interpretation of the data.

v) The spectrometer should have a simple, well understood background and good signal to noise performance.

The BAMBUS project therefore lies between conventional TAS (which measures point by point and has some flexibility over the resolution ellipsoid) and TOF spectroscopies (which obtain large $(\vec{Q}, E)$ mappings but have a lower incident flux and typically have geometrical sample environment constraints) and therefore is capable of providing alternative insights into a range of strongly correlated condensed matter systems.

4. The BAMBUS secondary spectrometer

The complete design details are still to be finalised, however some of the key features of the planned BAMBUS secondary spectrometer will now be discussed.

The primary spectrometer of PANDA makes use of Liouville's theorem and has large intensity gains from focusing optics [6, 8] and this governs many of the flux and resolution properties of the secondary multiplexed analyser. In order to make best use of the available neutrons, BAMBUS plans to place analysers to cover the $2^\circ \times 2^\circ$ vertical and horizontal divergences from the sample position. Vertical slits at the entrance of the secondary spectrometer could also match smaller sample volumes and reduce background.

A large simultaneous in-plane scattering coverage is planned. The different $|k_f|$ channels (sample 2θ in TAS nomenclature) are 2° wide (with 1° angular dead-space between channels) giving an angular coverage over 75° in sample 2θ . The analysers will scatter alternatively up/down for adjacent sample 2θ , to allow complete shielding between these channels with a small angular dead-space.

The high reflectivity and transmission properties of pyrolytic graphite (PG) make this an attractive option for a multiplexed design [4, 9]. Carbon has a relatively low incoherent scattering cross-section (0.01 b) which is desirable for a good signal to noise ratio.

Whilst the reflectivity profile against wavelength does not vary much for PG, the transmission profile is heavily dependent on the incoming and outgoing energies [10]. There is strong drop in transmission at the elastic condition where the Bragg condition results in a reduction in the number of transmitted neutrons ($< 50\%$). The width of this feature in energy (approximately 0.5 meV) sets the minimum energy spacing for an array of analysers, such that there is little depletion in neutron flux in transmission from one analyser to the next. Also below an incoming energy of approximately 5 meV, the transmission remains high ($> 90\%$) away from the elastic condition: here there are few inelastic processes that can close the triangle. This serves to define an upper final energy working range of the spectrometer to maximise the neutron flux and limit spurious.

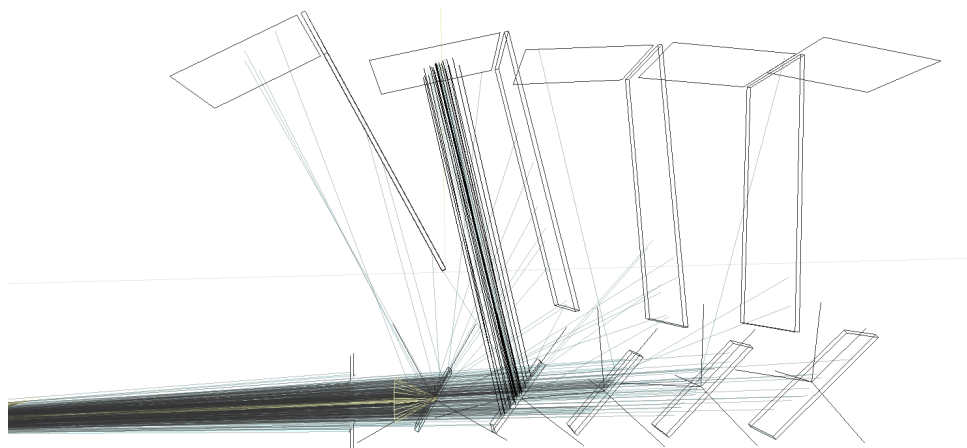


Figure 2. Monte Carlo neutron ray tracing of a set of analyser elements at a given sample 2θ . The incoming rays (which have an energy centred around 3.5 meV) primarily results in Bragg reflection by the second analyser, although the neutron beam is incident on all analysers and so other scattering processes are possible. Vertical shielding elements are necessary to isolate each analyser-detector pair.

These constraints then set natural limits for the analyser array: a maximum final energy up to 5 meV and consecutive analysers must be 0.5 meV apart to avoid reduced neutron transmission from consecutive analysers. For the PG 002 reflection, the minimum final energy (3.0 meV, corresponding to $2\theta = 102.4^\circ$) is also set by a maximum Bragg angle which would reasonably fit in this geometry. Therefore five PG 002 analysers, equally spaced at fixed final energy in the range from 3.0-5.0 meV, are proposed.

It is desirable that the resolution is similar between the different analyser arcs. This simplifies the scans, data analysis and interpretation. A consequence of this is that given similar resolutions (in addition to similar solid angle coverage) for the different analysers, the measured intensities will be comparable in all channels. In principle, an analyser at 2.5 meV is also geometrically possible ($2\theta = 117.2^\circ$), however this high angle take-off gives a small resolution ellipsoid, which results in limited flux with a resolution much different from the other analysers and is therefore not considered [5].

It should be noted that the energy spacing of the analyser (0.5 meV) is set by the neutron transmission profile in order to maximise flux throughout the analyser array and is much greater than the energy resolution for each analyser. Measurement of smaller energy steps, which approach the instrumental energy resolution, are achievable by simply adjusting the incoming energy at the monochromator (E_i).

In the proposed multiplexed design, there are many possible neutron trajectories in the secondary spectrometer: for example, scattering between analysers before reaching a detector. Furthermore, a large portion of the transmission losses come from scattering processes in graphite, which increases the likelihood of this multiple scattering scenario further. It is therefore important to understand and model these processes in order to achieve a low and well understood background.

The contributions to the multiple scattering background are from incoherent and coherent (and a mixture of both) scattering processes. The incoherent and mixed incoherent-coherent contributions within the analyser array are unavoidable, but are partly mitigated by the low incoherent scattering cross-section of carbon.

There also exist coherent-coherent neutron scattering trajectories. These can be naïvely

modelled by considering a white beam scattering from an analyser, generating a Laue pattern, that can then scatter from another analyser into a detector (if this second reflection fulfils the Bragg condition). The in-plane powder nature of pyrolytic graphite (perpendicular to stacking along the c -axis), generates Debye-Scherrer cones of scattering. A ray trace showing some neutron trajectories is illustrated in Fig. 2.

The beam entering the secondary spectrometer is not a white beam and, in general, will be made up of an inelastic contribution (material dependent) and also elastic incoherent scattering from the sample (which is set by the monochromator energy and equal to E_i). This will result in a limited number of systematic reflections/spurions compared to Laue scattering from a white beam; however, the complication arises that in operation of the spectrometer, E_i will be varied which means the set of spurions is now energy dependent.

To address this, we simulate a *pseudo* white beam (with energies set by the extremal values of $3 < E_i < 15$ meV for operation) entering and scattering in the secondary spectrometer to study these spurions using the MCSTAS Monte Carlo ray tracing program [11]. Each analyser then generates a Laue pattern (forwards or backwards) that can then reach and scatter from any other analyser: a process that is looped over to obtain the intensities at the detector.

The energy profile of neutrons reaching the detectors show a strong contribution at the Bragg condition for each respective analyser, in addition to a broad distribution of spurions above 7 meV from multiple Laue-type scattering processes described above. It should be noted that it is not possible to implement the intensity contribution of this spurion signal due to the complex reflectivity/transmission profile and this simulation gives a valid geometrical result only.

It is planned to operate the spectrometer with a wide-angle Be-filter (attenuation of neutrons > 5.1 meV) with radial collimation after the sample to eliminate the $\lambda/2$ contamination and also avoid cross-talk in this open geometry. This is important in fulfilling the design goal of a simple, easily interpretable background that is largely free of spurions.

5. Conclusions

We present plans for a flexible multiplexed secondary spectrometer option for the PANDA triple-axis instrument: with five concentric arcs of analysers, with each arc at a different fixed energy [3.0, 3.5, 4.0, 4.5, 5.0] meV. The focus at low fixed final energies (< 5 meV) means that in addition to Bragg scattering of the analysed energy, there is high transmission of neutrons and the possibility of limiting other spurious scattering processes.

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