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EXPERIMENTAL TEST OF CONSTANT **q** SINGLE CRYSTAL SPECTROSCOPY ON A TIME-OF-FLIGHT SPECTROMETER.

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Triple-axis spectroscopy (TAS) is the method of predilection for constant **q** single crystal spectroscopy on continuous sources. This method is not naturally adapted for pulsed sources and actually it has actually never been implemented on such a source. It has been argued that time-of-flight (TOF) spectroscopy can take over the role of TAS on pulsed facilities. TOF is actually well adapted for both pulsed and continuous neutron beams, but it is not an established method for constant **q** spectroscopy. In order to compare the data collection efficiency of both techniques, we have performed the same experiment on the same sample with the same resolution on instruments of both types at the same continuous reactor source at Hahn-Meitner-Institut, Berlin. The results show that, even on a continuous source, the TOF method is comparable to TAS if at least a few (<10) constant **q** points are to be explored in a single symmetry direction. It becomes superior or vastly superior if the fraction of **q** space expected to be explored contains more than the above small number of resolution elements, i.e. in the case of exploring isotropic phenomena. This observation implies, that on for TOF more favorable pulsed sources single crystal spectroscopy, including most demanding constant **q** scans, can be advantageously performed by this technique, and there is no need to adapt the TAS for pulsed sources.

1. Introduction

Constant **q** spectroscopy is a crucial tool in neutron scattering study of single crystals. Traditionally triple axis spectrometers (TAS) are used with great success for this purpose on continuous (CW) neutron sources. TAS spectroscopy, however, cannot take primary advantage of the time structure of pulsed sources and in actual fact it also has substantial drawbacks on CW sources, such as higher order contamination, "spurions" (e.g. diffuse scattering on the analyzer crystal) or the notorious complexity and limited reliability of determining absolute cross sections.

Time-of-flight (TOF) inelastic spectroscopy, a method practically never used for constant **q** spectroscopy by now, can be easily and – under the condition of making use of the recently

introduced repetition rate multiplication technique [1] – also efficiently transferred from CW sources to pulsed spallation sources. In addition, the TOF method does not suffer from the above mentioned drawbacks of TAS and in cases where its large solid angle capability can be made use of, e.g. with polycrystalline or amorphous samples it provides vastly superior data collection rates compared to TAS. Recently we have investigated with encouraging results the feasibility of constant **q** spectroscopy by TOF techniques using Monte-Carlo simulation [2, 3].

Our goal in the present study was to establish a real life experimental comparison of the data collection efficiency of the TAS and TOF approach in single crystal spectroscopy at the same CW source, on the same sample and with the same resolution. For this purpose we have used two up to date instruments, built at the same period of time (early 90's) following to the same high standards, and facing the same cold source at the BER-II research reactor at HMI, Berlin, namely FLEX and NEAT, respectively. In terms of counting rate vs. source flux both of these instruments substantially outperform their competitors worldwide, for the same sample and resolution the counting rate on FLEX is only 3 times less than on the best comparable ILL instrument, IN14, and on NEAT only 1.2 times less than on IN5, in spite of more than a factor of 10 difference in the cold source flux between the two sources.

2. Comparison for isotropic magnetic excitations.

For the purpose of this comparison we have measured a few spectra on the TOF instrument NEAT comparable to those taken previously on FLEX as part of an investigation of magnon renormalization near the Curie point T_c in EuO. The sample is not an easy one to work with, it absorbs about 90 % of the incoming beam. We have worked around the (000) reciprocal lattice point, at small scattering angles in the range of 5 – 15°. Fig. 1 shows typical spectra obtained at the same temperature below T_c. The experiment on NEAT only used beam time over a weekend which could not be filled in otherwise after a user no-show, so we had to live with the detector settings of the previous experiment, i.e. the lowest scattering angle was just above the highest on FLEX. This was, however, perfectly sufficient to establish the intensity ratio of the magnon signal on both instruments. Note that at $q = 0.3$ Å^{-1} the magnon signal is already nearly lost in the background on FLEX (in contrast to NEAT), so its intensity was actually determined by fitting the expected q dependence over the whole q range of the TAS experiment. The TOF scans in Fig.1 are at constant angle, not at constant q. We have also verified that the elastic energy resolutions are indeed the same in both cases. We have only considered TOF detector tubes centered around the horizontal scattering plane, which implies 5.5° vertical collimation, about 1.5 times larger than on FLEX.

If we can assume that the scattering features, e.g. magnon dispersion relation is isotropic enough for the purpose of the experiment, it is sufficient to take TOF spectra with a single sample orientation, and it is a standard procedure in TOF spectroscopy to convert the directly observed constant scattering angle data into constant $q = |\mathbf{q}|$ spectra. For the comparison of the two methods we have required that for the lowest intensity magnon group in the TAS study ($q = 0.3$ Å^{-1}) the same number of neutron counts are registered in both cases. (This requirement actually favors TAS, in view of its worse signal to noise ratio equal counts in the signal in reality mean lesser amount of information.) With TOF all q's will then be measured simultaneously for the same length of time (assuming that there are indeed detectors placed at the smaller angles required here, of course). In the actual TAS experiment 7 q values were studied, namely the

higher intensity signals for shorter time (see Fig. 3) and the total measuring time for the 7 points was 8500 min. In comparison, in the TOF experiment 700 min was found to be sufficient to provide equal signal around q = 0.3 $Å^{-1}$, and superior ones at smaller q's.

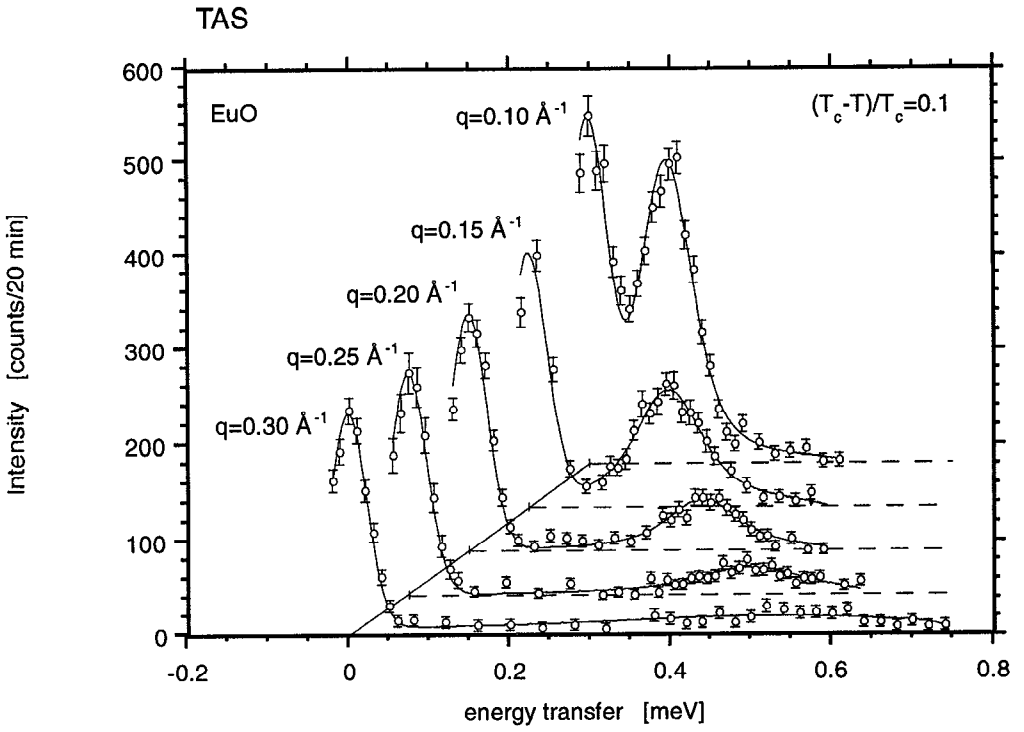

Figure 1. TAS constant **q** scans measured on FLEX for exploring the magnon in the q range of 0.1 – 0.3 $Å^{-1}$.

The conclusion from this comparison is therefore, that if an experiment is aimed at collecting information at least at 5 - 10 different q's (e.g. determining a fraction of an excitation dispersion relation) and it is acceptable to observe the scattering function $S(\mathbf{q},\omega)$ along a set of **q** trajectories in the scattering plane determined by neutron kinematics rather than by the symmetry of the sample crystal, TOF as represented by NEAT is more than an order of magnitude more efficient than TAS as represented by FLEX. This situation applies to all isotropic samples and phenomena, but it can also be the case for single crystals if the theoretical models used for the interpretation of the data can be evaluated for any **q**, not only for those in symmetry directions.

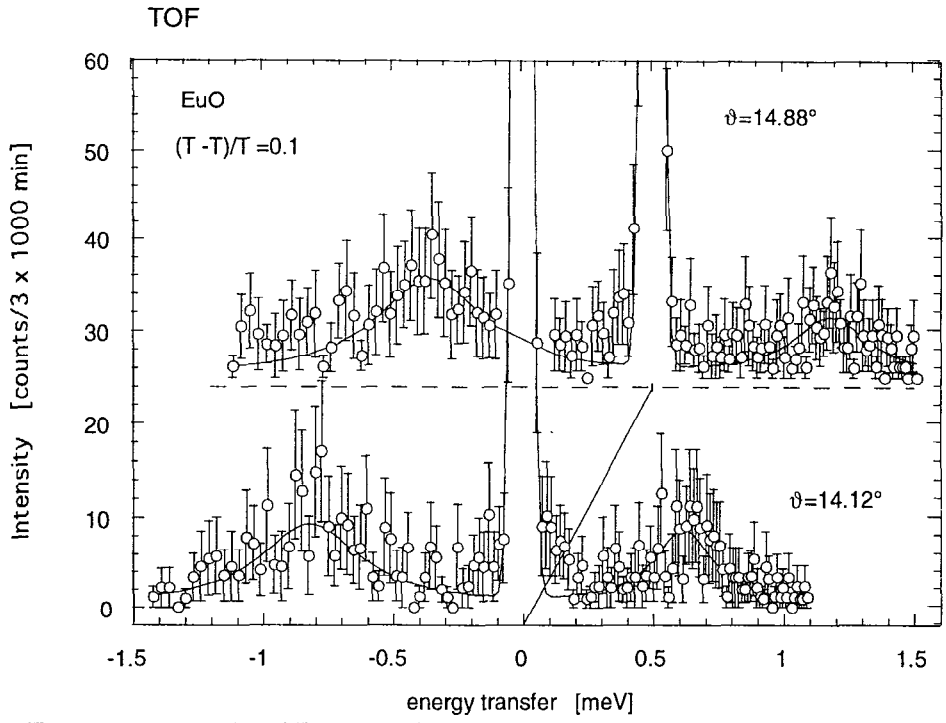

Figure 2: TOF scans measured on NEAT on the same EuO single crystal sample. The constant scattering angle ϑ spectra measured at a fixed sample orientation correspond to q values between 0.32 and 0.35 $Å^{-1}$

3. Comparison in exact constant q spectroscopy in a single symmetry direction.

The worst case for the TOF approach is exact constant **q** (vector) data collection in a single prescribed crystal symmetry direction. At a given sample orientation from the vast 2 dimensional data set (angle and time-of-flight) collected by TOF we only can at best only use infinitesimal 1 dimensional locus. This is illustrated in Fig.4. For example, the set of points at the upper boundary of the area covered by dots shows for each of the 18 detector tubes placed between about 2.5 and 15.5° scattering angle the energy value of the single bin in the collected histogram, which belongs to a **q** vector pointing in the given symmetry direction of the crystal. The area covered by points in the figure shows the (**q**,ω) domain (**q** in the [110] symmetry direction) which can be covered by rotating the sample over a 65° range. In order to explore this range with a similar density as in the TAS experiment, we would need to take data at 34 different rotational position of the single crystal sample. Under the requirement of collecting equal number of signal counts in the lowest intensity group considered, we find that the TOF instrument would need about 11000 min time, quite similar to the 8500 min actually used on FLEX.

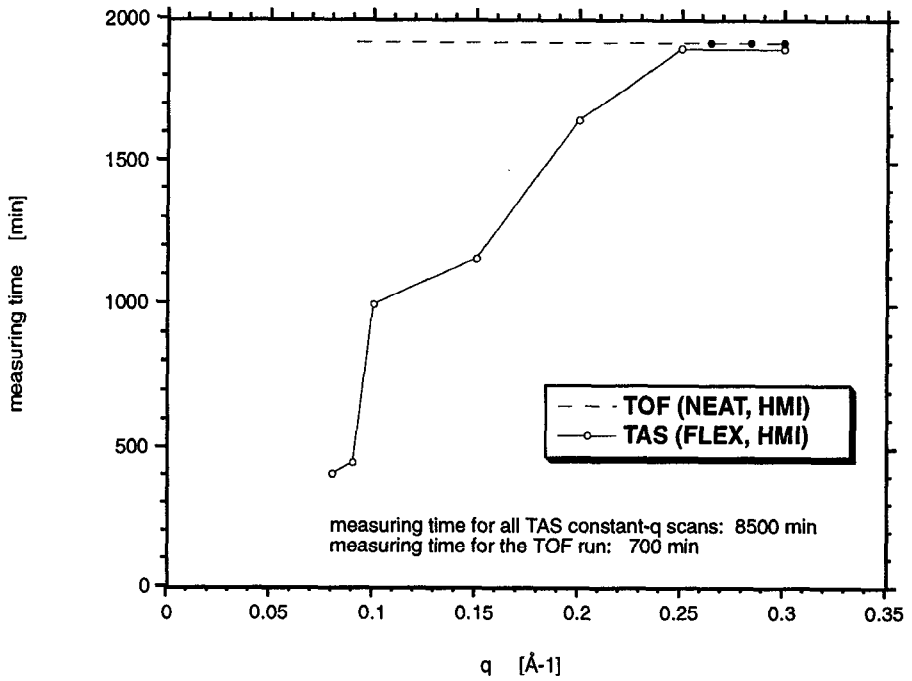

Figure 3: The measuring times needed for the various TAS constant-**q** scans shown in Fig. 1. In comparison, the dashed line indicates the relative intensity of the collected signal in a 700 min TOF run (not constant-**q**) expressed as equivalent TAS data collection time at each q.

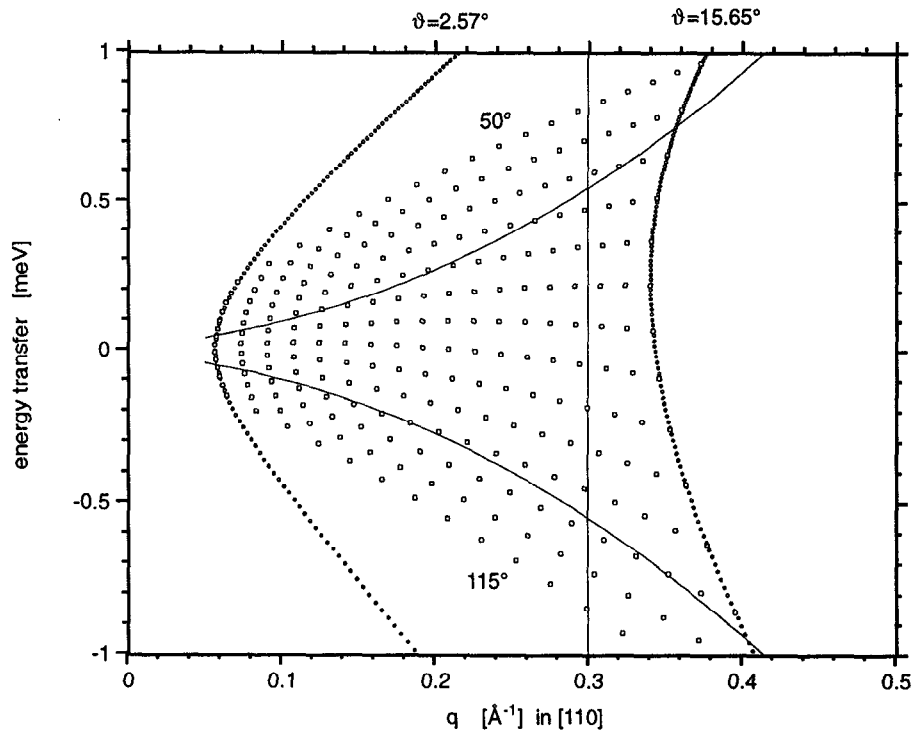

Figure 4: Mapping a symmetry direction cut of the (**q**,ω) variable space by the TOF technique. One dot represents one of 18 detector tubes between and one of 14 sample orientations shown. The continuous lines show magnon the dispersion relation in EuO at the chosen temperature.

4. Conclusion

The real life comparison between data collection times on two instruments of the same generation at the same CW source at HMI, Berlin shows, that the TOF approach is about equally efficient compared to the conventional TAS technique in constant **q** spectroscopy in single crystal samples, assuming that at least some 5-10 different points in the reciprocal space are of interest. Our comparison was very conservative, in favor of the conventional TAS approach, e.g. we did not take into account the possibility of detecting neutrons by TOF on both sides of the incoming beam and that the TOF technique usually provides data in more than one symmetry directions simultaneously. In experiments in which information corresponding to **q**'s outside the symmetry directions is also of value, the TOF technique becomes superior, by up to more than an order of magnitude. This means that, even on a CW source, TOF spectrometers (adapted to the requirement of being able to align a single crystal sample in any direction) are comparable or superior in efficiency to TAS in typical inelastic experiments in single crystals. The TOF technique can obviously take more advantage of the time structure of pulsed beams on a pulsed spallation source than TAS. Therefore we can conclude that there is no need to trying to implement TAS on pulsed sources: the job can be better done by TOF spectroscopy. Actually we believe, that we might end up with virtually the same situation on CW sources too, once TOF spectrometers are built with keeping single crystal spectroscopy in mind.

References

[1] F. Mezei, Proc. ICANSXIII (PSI 1995) 400.
[2] S. Schorr, F. Mezei, J. Stride and C. Guy, J. Neutron Research 6 (1997) 113.
[3] S. Schorr and F. Mezei, Physica B, **241-243** (1998) 166