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HFM-EXED - the high field facility for neutron scattering at HZB

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Abstract.

Helmholtz-Zentrum Berlin is launching a high magnetic field facility for neutron scattering. Its two main components are the High Field Magnet, a 26 T hybrid magnet built specially for neutron scattering applications, and a dedicated Extreme Environment Diffractometer. The magnet is now in the final stage of commissioning and will be installed at the instrument in the near future. The neutron instrument itself has been in operation (without the magnet) for some time as a general purpose time-of-flight diffractometer. As the magnet will be permanently installed on EXED, the instrument capabilities have been expanded to include small angle scattering (Low-Q) and direct time-of-flight Spectroscopy. The elastic modes of operation have already been implemented whereas the inelastic one is under construction. In this paper we give an overview of the HFM-EXED facility with the main emphasis on its neutron scattering part.

1. Introduction

In order to gain a thorough understanding of the properties of modern functional materials, diverse characterization techniques must be employed. Among them is the material response to external perturbations such as temperature, pressure or magnetic field. In this respect, the combination of a microscopic probe such as neutrons and non-ambient sample environment conditions contributes considerably to the understanding of the physics and chemistry of new materials, and their functionality. Even more crucially, neutron scattering serves as one of the tools to unravel the details of fundamental physical phenomena and thus plays a significant role in understanding the laws of nature in general. Very often such investigations are performed under extremely non-ambient conditions. For instance, magnetic fields in the range of 30 T have led to the discovery of unexpected phenomena of fundamental importance, such as the Quantum Hall Effect and the Fractional Quantum Hall Effect [1, 2].

While different characterization techniques (e.g. measurements of static bulk properties, optical spectroscopy, nuclear magnetic resonance and electron spin resonance) benefit from the availability of magnetic fields of the order of tens of teslas, and up to one hundred tesla in pulsed regime, the existing neutron facilities do not have the capacity to access fields of a comparable magnitude. This is an obvious drawback as the microscopic details of magnetic correlations in time and space can be uncovered only by means of neutron scattering.

The Helmholtz-Zentrum Berlin (HZB) has always stayed in the forefront of the neutron scattering under extreme conditions. It still holds the world record of 17.4 T DC field combined with neutron experiments at its BERII research reactor. Now, an ambitious project of extending this range significantly beyond 26 T is close to completion. The High Field Magnet (HFM) and a dedicated Extreme Environment Diffractometer (EXED) are two counterparts of the new high magnetic field facility for neutron scattering. With HFM-EXED, the HZB ensures its leading position in researching the most topical issues in physics, chemistry, and material science. These include unconventional superconductors, heavy Fermions, quantum and molecular magnets, low-dimensional systems, frustrated and topological systems, multifunctional materials and others. In this contribution we describe briefly the HFM and focus on the neutron-scattering capabilities of the facility.

2. High Field Magnet

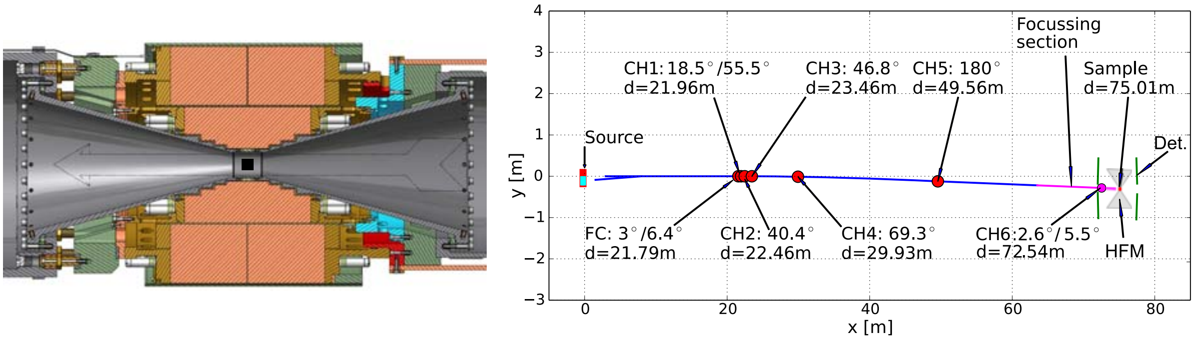
The HFM is a "first of its kind" hybrid magnet system that is capable of producing fields above 26 T, making it by far the strongest DC field available for neutron scattering experiments worldwide. It has been built in collaboration with the National High Magnetic Field Laboratory (Tallahassee, Florida). The magnet is designed as a series connected hybrid system. With the aid of resistive insert coils, which are mounted in the room-temperature bore of a superconducting solenoid, fields between 26 and 32 T can be obtained for the cooling power of the resistive coil 4–8 MW [3]. In the initial stage of its operation the HFM will use 4 MW power, producing fields of about 26 T. To operate the hybrid system a complex technical infrastructure is required. It includes a 20 kA power supply for both coils connected in the series, a helium refrigerator for cooling the superconducting coil and a water cooling system for the resistive coil. The commissioning of the magnet, which is now close to completion, shows good results and the achieved B_{max} of about 26.3 T is in perfect agreement with the expectations.

The scattering space of the magnet is rather simple as shown in Fig. 1a. It is a solenoid with 30° conical openings at both ends, envisaged for neutron scattering, and a 50 mm room-temperature bore. The neutrons enter the magnet through one of the cones and their scattering is limited by the angular dimensions of both cones. In other words, only forward and backward scattering directions are accessible. Rotation of the magnet around its vertical axis allows to achieve a scattering angle as high as $2\theta=30°$ (150° in backscattering), however, the vertical acceptance approaches zero for $2\theta \rightarrow 2\theta_{max}$.

In order to perform experiments at low temperatures, a special ^{3}He/^{4}He cryostat which is inserted into one of the magnet cones has been developed and is currently being tested. The cryostat should allow experiments with temperatures down to 0.5 K, with sample cross-section up to $\approx 13\times 13$ mm^2. The details of the magnet and its sample cryostat are presented in a separate contribution of this meeting.

3. Extreme Environment Diffractometer

In order to compensate for the angular limitations imposed by the magnet, EXED uses a polychromatic (time-of-flight (TOF)) technique. A sketch of the instrument is given in Fig. 1b and details of the instrument design can be found in Refs. [4, 5]. Access to a wide neutron-wavelength band is achieved by means of a multispectral extraction system [6]. This system feeds neutrons from the thermal and cold moderators into the same neutron guide. The supermirror guide itself is essentially straight (100×60 mm^2 cross section) with a kink designed to remove neutrons with $\lambda < 0.7$ Å. The last 7.5 m of the guide are elliptically converging down to 50×30 mm^2, focusing the beam onto the sample located about 75 m from the neutron source. This focusing section is displayed in Fig. 2a. The m-values of the supermirrors vary across the



a)

b)

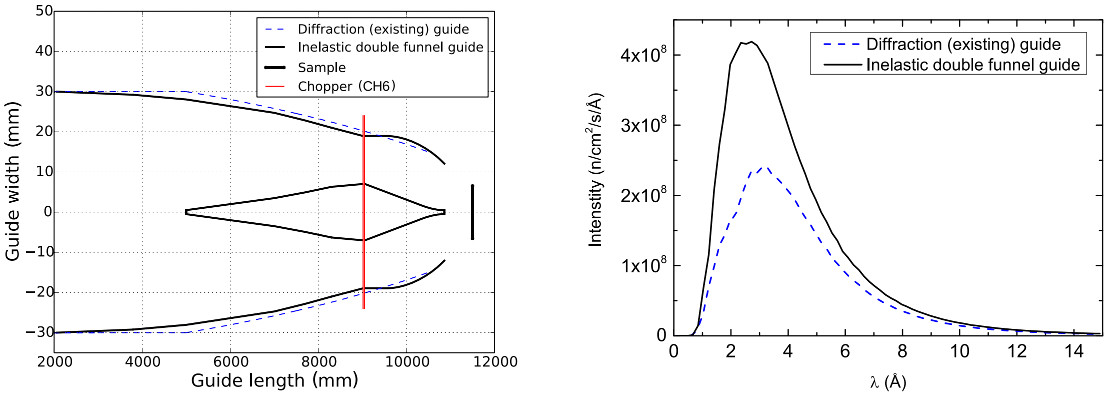
Figure 1. a) Scattering geometry of the HFM. The picture shows the magnet cross section with the room temperature bore and the sample (black square), the magnet cones for neutron scattering access and the resistive coils. b) Schematic layout of EXED. The neutron source is composed of thermal (red) and cold (cyan) moderators. The bi-spectral extraction system feeds the thermal and cold neutrons into a single guide (blue solid line); the choppers FC, CH1-CH5 (red dots) constitute the currently existing chopper system. Angular sizes of their windows together with the distances from the source are also given. After the implementation of the inelastic mode (see below in the text), there will be a new focusing guide (magenta solid line) and a monochromatising double-disc chopper CH6 (magenta dot). The detector positions are indicated by green solid lines, and the magnet coils are outlined in gray.

guide reaching $m = 3$ for the extraction and focusing sections, while $m = 1.5$ for the straight parts [4, 5]. The resulting neutron spectrum is illustrated in Fig. 2b. It has a maximum around 3 Å, a cutoff at 0.7 Å and a shoulder below 2 Å. The latter two represent the effect of the kink and the thermal source contribution, respectively.

The instrument chopper system is complex. EXED is equipped with a Fermi chopper (FC), a double disc (CH1) and four single disc (CH2-CH5) choppers (Fig. 1b) [4, 5]. The first two are pulse generating choppers for high or medium/low resolution applications, respectively. They can provide a primary time resolution covering about 3 orders of magnitude (from μs to ms range). The other four choppers ensure there is no frame-overlap and define the wavelength band. Since the effective frequency of the whole chopper system is variable from 5 up to 120 Hz, the instrument operation becomes very flexible, ranging from a broad wavelength band (up to 14.4 Å) down to a short one (0.6 Å).

The entire instrument sample area is built out of nonmagnetic materials. There are four detector banks which are positioned in a way reflecting the geometry of the magnet: two in forward and two in backward scattering direction. Each detector bank is equipped with 48 position sensitive ^{3}He detector tubes with 1/2"-diameter. The effective length of the tubes is 0.9 m with 1% position resolution, resulting in 19200 detector pixels. Each of them produces a dataset of intensity vs. time.

The data acquisition system on EXED is event-recording-based, with precise timing and integration of external trigger sources. The external signals come from the choppers, the beam monitor in front of the sample and (optionally) the sample environment, containing information e.g. about the current sample temperature or magnetic field. The processing of the data is a two-step process. In the first step, a specially developed eGraph software identifies the opening time of the first chopper and, based on that, calculates TOF using the neutron detection time. After that it selects the appropriate neutron events and bins them in TOF and position coordinates and, finally, allows visualizing the data. In the second step, the software package Mantid is used



a)

b)

Figure 2. a) Geometries (in the horizontal plane) of the existing diffraction guide and the new double funnel guide. The position and size of the sample are indicated by a vertical black line. The position of the monochromatising CH6 in the inelastic guide is marked by a vertical red line. b) Neutron wavelength spectra at the sample position as simulated using VITESS neutron ray-tracing software package [7]. The plot compares the data obtained using the diffraction guide (dashed blue line) with the one expected for the double funnel guide.

for further data manipulation, reduction and analysis [8].

For a limited period of time EXED was available for internal and external users as a general-purpose TOF diffractometer combined with standard HZB sample environment. With the HFM installation, it will be transformed into a high field facility for neutron scattering. A special feature of this facility will be its multi-purpose operation. Indeed, because of the magnet size and complex operational infrastructure, the HFM cannot be transferred to other instruments like the standard superconducting magnets. As a result, to match the scientific case, the functionality of EXED has been extended. The existing Diffraction mode of operation is complemented by small angle (Low-Q) and Spectroscopy modes.

4. Modes of HFM-EXED operation

In this section we briefly describe the foreseen modes of EXED operation. They include the Diffraction and the Low-Q, both already implemented, as well as the Spectroscopy, which is currently under construction.

4.1. Diffraction

Since EXED had been designed as a diffractometer, the Diffraction is the most natural mode of the HFM-EXED operation. In this regime, HFM-EXED offers a broad range of applications ranging from high resolution to medium and low resolution (high flux) powder and single crystal diffraction in high magnetic fields. Some examples of powder diffraction experiments, performed on EXED during its initial operation, can be found in Refs. [9, 10, 11, 12]. One has to stress the high flexibility of the Diffraction mode as a general feature of a chopper instrument. It allows almost continuous relaxation of resolution (resulting in a corresponding flux gain) and selection of the wavelength band as requested by the experiment. This is extremely important as the HFM does not offer much flexibility in the secondary instrument. The main characteristics of the Diffraction mode are collected in Table 1.

Table 1. The main characteristics of HFM-EXED facility

Parameter	Diffraction	Low-Q	Spectroscopy
Wavelength range	0.7 - 15 Å	4 - 18 Å	1.8 - 7 Å
Angular range	5° - 30°, 150° - 170°	$< 10°$	$< 30°$
Q-range	$0.1 < \mathrm{Q} < 12$ Å^{-1}	$\mathrm{Q} \gtrsim 0.01$ Å^{-1}	$\mathrm{Q} < 1.8$ Å^{-1}
Resolution	$\Delta\mathrm{Q}/\mathrm{Q} > 10^{-3}$	$\Delta\mathrm{Q}/\mathrm{Q} < 0.1$	$\Delta\mathrm{E}/\mathrm{E} \gtrsim 10^{-2}$

From the experimental point of view, the magnet angular constraints are not a serious issue for randomly oriented powders or single crystals isotropic with respect to the magnetic field direction. The TOF method combined with the 15° magnet rotation enables gapless coverage of momentum transfer Q-range from about 0.1 up to 12 Å^{-1}. A proper combination of the field orientation and the choice of wavelength range allows bringing reflections of interest into forward- or backscattering banks. The former are important for the observation of magnetic scattering while the latter are mainly used for the nuclear scattering. For anisotropic systems, however, the magnet angular constraints become an issue as the field orientation along a given crystallographic direction is then the main defining factor for the accessible range in the reciprocal space. It turns out that in the forward scattering banks the accessible scattering range will be mainly perpendicular to the field, while in the backscattering it is along the field (see Fig. 3 and explanations below).

As the restricted geometry of the instrument implies the importance of careful experiment planning, a software tool, EXEQ (EXED (E,q)-range calculator), has been created to assist the users of HFM-EXED in finding the optimal sample orientation [13]. The software uses pre-defined information about the neutron wavelength spectrum, detector geometry and positions and obstacles limiting the scattering angle. The user input defines the sample unit cell, sample orientation, instrument wavelength band and the desired wavelength resolution. The main output of EXEQ are the reciprocal space coverage maps as shown in Fig. 3. They illustrate the extent of the reciprocal space, in the units of sample Miller indices (h, k, l), that can be accessed using the given set of instrument parameters. The intensity reflects the actual instrument spectrum, multiplied by the duty cycle of the chopper system at the current resolution and bandwidth settings.

4.2. Low-Q

In order to enable the investigation of matter in the nanoscale range, such as the vortex state in type-II superconductors as a function of external magnetic fields, a special Low-Q setup had been built ($\mathrm{Q}_{min} \approx 10^{-2}$ Å^{-1}). It comprises a pin-hole collimation section with variable apertures which replaces the last 5.5 m of the focusing guide. Two EXED detector banks are positioned at 6 m away from the sample and cover an in-plane angular range of about 2θ = -4.5–1.5° and 2.5–8.5°. A He-filled detector chamber in front of the detectors is used to suppress air scattering. The entire chopper system can run at a low frequency (5-10 Hz) as the wavelength resolution requirements in small angle scattering experiments may be relaxed. The wavelength band is typically centered at $\lambda > 4$ Å. The main characteristics of the Low-Q mode are given in Table 1.

The Low-Q mode was commissioned using a silver behenate powder sample, and flux-line lattice measurements on a Nb single crystal. Both confirm its feasibility and are in a good agreement with published data [14, 15].

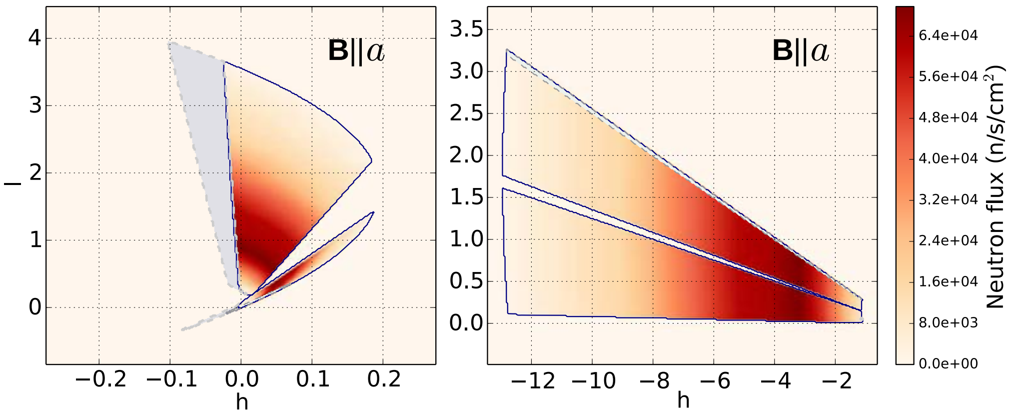


Figure 3. The instrument Q-coverage in Diffraction mode. The ($h0l$)-map is calculated with EXEQ for an "artificial" sample aligned with its a-axis parallel to the field and the c-axis perpendicular to the field in the equatorial plane, with the magnet rotated by 14° with respect to the incident beam. The wavelength band was set to 0.7–7.9 Å and the wavelength resolution to $\delta\lambda/\lambda$=0.1%. The detector panels located in forward (backward) scattering direction are grouped in the left (right) plot. The coverage of each detector panel is delimited by a blue solid contour line. The gray areas with a dashed-line contour in each plot correspond to the part of a detector panel that is shadowed by either the magnet cone, beam stop or guide housing.

4.3. Spectroscopy

The Spectroscopy mode will add a very important component to the scientific portfolio of HFM-EXED: It will allow studying dynamics of materials with magnetic degrees of freedom in high magnetic fields. For the purpose of performing inelastic experiments, EXED will operate as a direct TOF spectrometer. Here, a pulsed monochromatic neutron beam impinges onto the sample and TOF is used to analyze the change in the energy of the scattered neutrons. This is the most efficient way of performing inelastic experiments when taking into account the geometry and constraints of the magnet. Limited sample size inside the HFM and weak inelastic scattering cross sections imply the necessity to optimize for signal strength and low background conditions. The former will be achieved by enhancing the flux at the sample using a novel focusing guide, while the latter will be provided by means of a shielded and evacuated detector chamber. Below we briefly describe four main components of the Spectroscopy mode: i) an evacuated detector chamber for forward scattering with a built-in ii) ^{3}He detector array, and iii) a new focusing guide section that accommodates iv) a monochromatising double disc chopper.

The detector chamber will be connected directly to the forward-scattering cone of the magnet, and rotated together with the magnet. The chamber rotation will be limited to -2°...+15°. The inner side of the chamber will be shielded with Cadmium-absorber, and the outer one will be covered with polyethylene and Boron-absorber. After evacuation, the chamber will provide almost window-free flight path from the sample to the detector. The latter is based on the IN5 (ILL) multi-tube design and being built in collaboration with the ILL (Grenoble). The detector modules with 0.75"-diameter position-sensitive tubes will cover the entire available 30° angle in- and out-of-plane at 4.5 m away from the sample.

A distinct feature of the design of inelastic mode is the rather slow (120-240 Hz) monochromatising chopper (CH6 in Fig 1b) supported by conventional ceramic ball bearings and positioned relatively far from the sample, at 2.45 m. These are the consequences of high stray magnetic fields close to the sample. As a result of the chopper speed limitations, it became necessary to reduce the size of the chopper window significantly. While the energy resolution is defined by the opening times of the first and last chopper and the corresponding chopper distances to the detector, the neutron flux depends also on the neutron transport system [16]. Therefore, the shape of the guide has been adjusted to the chopper windows and the sample size. For this we use a double funnel guide concept, first implemented at LET spectrometer at ISIS [17, 18]. Contrary to the LET design, however, the EXED guide does not expand after the chopper position, but is even further compressed because of the sample size limitations. As a result, the m values for the new guide reach 4.5. The new guide is visualized in Fig. 2a. In comparison with the existing diffraction guide the new guide provides over 60% integral intensity gain as can be derived from Fig. 2b.

The overall performance of the Spectrometer has been simulated using VITESS neutron ray-tracing software package and will be published elsewhere [7, 19]. Some results of the simulations including energy resolution and corresponding neutron flux for 5 Å wavelength (incident energy 3.3 meV) are summarized in Table 2. For comparison, the table comprises the relevant measured data from the ILL, FRM-II and NIST reactor-based disc chopper spectrometers.

After completion, the Spectroscopy mode will enable energy-resolved measurements over a limited Q-range (<1.8 Å^{-1}) with an energy resolution of a few percent and incident energy below 25 meV (Table 1). Planning of inelastic experiments, which is even more crucial than that of the elastic ones, will be covered by the inelastic version of EXEQ. It is being prepared and will be released in a due time.

Table 2. The expected performance of EXED Spectroscopy mode compared to existing neutron TOF spectrometers. The EXED data are simulated for 5 Å wavelength. The remaining data are the resolution and flux of the IN5 (ILL), TOFTOF (FRM-II) and DCS (NIST) spectrometers, measured with the same wavelength. Two different values of flux and energy resolution in case of TOFTOF, DCS and EXED correspond to their low and high resolution modes defined by use of different chopper windows.

Instrument name	Instrument setting	Flux (n/s/cm^2)	Energy resolution (μeV)
EXED	High flux	2.03×10^5	170
	High resolution	1.29×10^4	58
IN5 (ILL) [20]		6.83×10^5	100
TOFTOF (FRM-II) [21]	High flux	1×10^5	102
	High resolution	8×10^3	52
DCS (NIST) [22, 23]	High flux	2.6×10^4	115
	High resolution	6.7×10^3	55

5. Conclusions

HFM-EXED is a unique facility for neutron scattering in high magnetic fields. It will be the only instrument in the world where elastic (Diffraction and Low-Q) and inelastic neutron scattering experiments can be combined with steady-state magnetic fields as high as 26 T. The main characteristics of HFM-EXED operation modes are summarized in Table 1. The facility is open for accepting user proposals. The first experiments will start with the elastic modes and will be complemented by the inelastic one in the near future.

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