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Instrument developments and recent scientific highlights at the J-NSE

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Abstract. The J-NSE neutron spin echo spectrometer faces now 10 years of successful user operation at the FRM II research reactor at the Heinz Maier-Leibnitz Zentrum (MLZ). We present scientific highlights and instrumental developments of the last decade, for example the development of grazing incidence neutron spin echo spectroscopy (GINSES) at the J-NSE and investigations of the dynamics at solid-liquid interfaces with this new option. Polymers in confinement have been a prominent topic, as well as the internal dynamics of proteins. The scientific questions also triggered instrumental developments such as a new polarizer and a new neutron guide concept. Finally, the future of the J-NSE will be addressed with a short presentation of the current upgrade program with superconducting main coils with reduced intrinsic field integral inhomogeneity.

1. Introduction

Neutron spin echo spectroscopy (NSE) provides the highest energy resolution of all neutron scattering techniques. It has been first proposed by Ferenc (Feri) Mezei in 1972 [1]. The first instrument of this kind was the IN11 at ILL, put into operation in 1977 [2]. Neutron beam monochromaticity and resolution are decoupled in NSE spectroscopy by encoding velocity changes during the scattering process in a change of polarization of a polarized neutron beam. NSE spectroscopy measures the normalized intermediate scattering function \(S(q,t)/S(q,t=0)\), which is on the one side the Fourier transform from energy to time of the scattering function \(S(q,\omega)\), and on the other hand the Fourier transform in space of the van-Hove correlation function \(G(r,t)\), which can be extracted e.g. from particle trajectories in computer simulations. NSE accesses length scales in the range of some nm and Fourier times of 0.1-100’s of ns, translating in an energy resolution in the sub-\(\mu eV\) region. Thermal fluctuations in soft matter systems, such as membrane fluctuations in microemulsions or vesicles, internal domain motion of proteins or polymer motion in a melt are prominent examples, where the length- and energy-scale of the systems are exactly in the working region of NSE spectroscopy [3-7]. In this contribution we show the scientific field of use of the J-NSE spectrometer and the modifications and upgrades of the last decade and give a short perspective on the major main coil upgrade planned for the near future.

2. Instrument upgrades
The J-NSE spectrometer has been transferred to the FRM II reactor at MLZ in 2006 after 10 years of operation at the DIDO reactor in Jülich [8-9], involving an upgrade of the electronics and with the advantages of a neutron guide end position. During the 10 years of operation at the FRM II the spectrometer has experienced some smaller instrumental improvements. The most prominent ones were the efforts for better correction coils for an improved field integral homogeneity. Each main solenoid is equipped with 3 correction coils which provide radially symmetric corrections to the field integral and are essential for achieving the required homogeneity.

The currently installed design are “Pythagoras”-coils first proposed at the ILL. Instead of the originally installed spiral coils the new design consists of 2 rectangular coils, each providing a quadratic correction in one direction, \(x^2\) or \(y^2\), providing a \(x^2 + y^2 = r^2\)-correction when mounted with 90° with respect to each other.

![Pythagoras correction coils at the J-NSE](image)

**Fig. 1**: Pythagoras correction coils at the J-NSE (left). The horizontal coils is visible, a second one perpendicular to it is on the back side. The schematic drawing (right) shows the effect of the two perpendicular coils, a \(x^2\) and \(y^2\) correction leading to a radially symmetric \(r^2\) correction of the magnetic fields.

This correction coil design has the disadvantage compared to the spiral Fresnel coils that only quadratic corrections can be realized, higher order corrections nonetheless still play a role, especially for the largest correction coil.

The advantage on the other hand is the better mechanical precision due to the easier cutting scheme, the small amount of material in the beam, increasing the transmission significantly, and at the same time the good heat removal, since the path of each current zone to the side frame is much shorter as in the case of the spiral Fresnel coils.

The polarization of the neutron beam has been done in two steps, for short wavelengths (\(\lambda < 8\text{Å}\)) in a bent part of the neutron guide, for longer wavelengths by a single reflection in a second polarizer at the instrument. The change between the two operation regimes involved a rotation of the whole spectrometer by 4°. The polarization concept has been modified by a new polarizer with significantly better performance, which polarizes the whole wavelength band from 4.5-17 Å used at the J-NSE. The rotation of the instrument became obsolete, simplifying the operation significantly with a slightly better polarization as before.
The renewal of the bent part of the neutron guide has been started, since first signs of degradation became visible. It is now replaced by a non-polarizing guide, leaving the whole polarization work to the new single polarizer in front of the main solenoids.

![Figure of merit](image)

**Fig. 2:** Figure of merit (polarization x intensity$^{1/2}$) from McSTAS simulations for the new instrument configuration with the second polarizer only compared to the initial configuration.

### 3. Scientific usage of J-NSE

The scientific topics of the last decade came mainly from the domains of soft matter and biology. The development of the grazing incidence NSE technique (GINSES), where the near-interface dynamics is probed with an evanescent wave opened a new field of NSE experiments, where the influence of a rigid wall on surfactant membrane fluctuations [3-4] or microgels adsorbed at the interface [5] have been studied. Currently, efforts are made for increasing the applicability of this technique by different measures of intensity improvements. Polymer dynamics, one of the primary research fields for NSE, evolved towards complex systems where e.g. confinement effects play a crucial role [6]. The internal fluctuations of sub-domains in proteins has been studied with the J-NSE for example in immunoglobulin, a Y-shaped human antibody protein [7]. NSE allows to study the proteins in a physiologically relevant temperature range in solution.

### 4. Major upgrade project

Recent developments at the ILL and the proposed NSE instrument for the ESS [10] aimed for a configuration of the main precession coils with lower field-integral intrinsic inhomogeneity. This has been achieved through an optimization of the magnetic field shape and a consequent minimization of
the amount of required additional corrections. The 2.5-times improved homogeneity makes higher Fourier times possible than those previously accessible, by equal wavelengths. Instead of a single main precession coil the optimized configuration consists of a set of five pairs of superconducting coils with different diameter that are fringe field compensated in a similar way as the solenoids of the SNS-NSE spectrometer. The new design is based on an extension of the Zeyen and Rem [11] approach and it uses a combination of analytical calculations and numerical simulations to shape the magnetic field to an optimal form that minimizes the first order terms in an expansion of the intrinsic integral field homogeneity.

Assuming in the simulations linearly increasing radial current density at the position of the correction elements (e.g. Fresnel coils), the new layout allows reaching a residual inhomogeneity of 1 ppm with only two (radial) correction coils (instead of three like in the NSE’s at MLZ and SNS). An optimization of the currents and of the positions of these elements shows that higher homogeneity of the field integral translates into weaker corrections and hence into weaker current in the outset (and most significant) large correction element.

Therefore the conclusion is that the final resolution of the spin echo spectrometer will be higher - even if corrections coils are used – because of the reduced intrinsic inhomogeneity of the coil.

**Fig. 3:** Top: Magnetic field strength along the flight path of the neutrons (from right to left). Bottom: corresponding coil configuration for the intrinsically more homogeneous field configuration, with the neutrons coming from the right. The sample position is in the middle in the region of low field strength, the detector is at the left side.
Fig. 4: Deviation of the field integral of a neutron path, $\frac{\delta J}{J_0}$ as a function of distance $r_3$ from the central axis at the flipper position, for the current configuration (red, top point cloud) and the configuration with optimized field shape (black, bottom point cloud). The deviation should be as small as possible also for off-axis flight paths ($r_3 \neq 0$).

5. Conclusion – NSE – Quo Vadis?

The spatial and temporal domain of nanometers and 1-1000 nanoseconds will be also the future domain of spin echo spectroscopy. The technique will be an indispensable tool with the capabilities provided at the modern facilities which cannot be replaced by other means. The tendency will be to observe smaller effects and changes in line shape accessible with the new capabilities of the upgraded NSE instruments. As an example, proteins in solution, i.e. in its natural environment show in addition to normal diffusion also the contribution of internal protein subdomain motions. Small effects have to be measured in this case up to several 100’s nanoseconds, in order to properly determine the internal contribution to the dynamics (see e.g. [7] for the internal dynamics of Immunoglobulines). Dynamics at an interface, e.g. of polymers [5] or membranes [4] may also be a field where NSE can contribute a lot if high precision and sufficiently long Fourier times are provided. The domain of soft matter, with polymer melts, complex liquids and composite materials tends to go into the direction of more complexity of the systems (confinements, multi-component systems). The dynamics, e.g. the “nanorheology” in these samples, will remain an important issue. Also some structural changes in multicomponent soft matter systems may only be visible by its effects on the dynamics of the system. There NSE will provide unique information on these systems, which can be combined with other structural information, e.g. from small angle scattering, to provide a complete view of the sample. The currently upgraded J-NSE spectrometer with its new main coils and the increased dynamic range is therefore well prepared for the future scientific challenges in the field of slow dynamics.
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