ESSENSE: Ultra high resolution spectroscopy for the ESS

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Abstract. The instrument concept for a very high intensity neutron spin-echo spectrometer with ultimate resolution properties has been developed and submitted as an instrument proposal to ESS. Effective intensity gain factors up to 30 compared to the best current instruments are anticipated. In addition the resolution will be boosted to the technical limits by newly designed superconducting precession solenoids. The intensity gain results from the use of an optimized guide transporting the high flux from the ESS cold moderator on the one side and from the utilization of an extended wavelength frame of 8 Å yielding a multiplication of information collection rate on the other side. The instrument thus enables novel views on soft matter systems ranging from polymers, functional gels and more to to dynamics of biological molecules with relevance for MD development; the employment of new techniques for surface NSE (GINSE) may contribute to new knowledge in tribology and lubrication and other surface phenomena that currently are hampered by low intensity. New developments in “intelligent” polymers as e.g. self-healing, the properties of which depend on molecular mobility and dynamics, require observation at many 100 ns of correlation times with high intensity, which can be made with ESSENSE.

1. Introduction
In this article we present the salient features of the ESSENSE Neutron Spin-Echo(NSE)-instrument proposal for the ESS. The neutron spin-echo technique is a time-of-flight analysis that is sensitive to small changes of the neutron velocity; these changes are encoded into differences of the total Larmor-precession angle after the spin dynamics is inverted before and after the scattering. NSE measures the intermediate scattering function [1, 2, 3]. NSE is the only instrument type that enables effective energy resolution down to neV with a dynamical range that extends over 6 decades [4, 5]. Its resolution surpasses all other types of neutron spectrometers by three orders of magnitude. It will predominantly provide the dynamical window for the scattering from nano- and mesoscopic structures that are abundant in soft- and biological matter. The applications range from classical polymer topics and emerging new questions like e.g. the role of entanglements in macromolecules that differ from linear polymer chains or linear chains, which differ from ideal coils, to the interaction, diffusion and internal dynamics of proteins and other bio-molecules. Many of the relevant systems exhibit low concentrations of the mobile species and high background from the matrix material. They need very high intensity and high stability and reproducibility. The high resolution of a NSE spectrometer is expressed in terms of the maximum useful Fourier-time $t_{\text{max}} = \min(0.18 \, [\text{ns}/(\text{Tm} \, \text{Å}^3)] \times J_{\text{max}} \lambda^3, H \lambda^2)$. The proposed NSE has a maximum field integral...
$J_{\text{max}} \geq 1.5 \text{Tm}$ and a 2.5 times improved field integral homogeneity parameter \cite{5} $H \simeq 2.5 \text{ ns/Å}^2$. An effective gain of 30 is obtained by combining the high time-average intensity of the ESS with a larger guide cross section ($4 \cdots 6$ higher spectral neutron flux at the sample as compared to IN15 at ILL) and further gains of the order of $g = 5$ due to the wavelength frame width of 7 to 8 Å delivered by each pulse to the detector. The proper (secondary) spectrometer has a new magnetic design \cite{6} with improved field integral homogeneity allowing to perform many experiments with shorter wavelength than today and with shorter counting times due to the corresponding flux advantage.

At the time of this writing the NSE-instrument has priority 17 in the proposed list for 16 reference instruments.

2. Science case
The trends in condensed matter research, both fundamental and applied, are directed towards complex matter and mesoscopic time and length scales. A large fraction of the interesting complex systems pertain to “soft matter” and increasingly to “biological matter” from single protein molecules to assemblies and interacting collectives. Increasing focus is on responsive and functional materials in the “soft matter” class and understanding of pre-requisites and key properties for function in biological system \cite{7, 8, 9}. Here the use of scattering angles of only a few degrees (the “SANS-regime”) tunes the spatial resolution to the size of macromolecules, proteins or other mesoscopic structures and aggregates. Energy resolutions far beyond 1µeV or correlation times much larger than 1 ns are required. Among the neutron spectroscopic methods these are only reached by the spin-echo method. Correspondingly slow relaxations at shorter length scales (extending beyond the SANS regime) are observed in glass-forming systems as well as in materials with slow diffusion of small molecules or even atoms or protons. In “hard-matter” increasingly complex magnetic structures, possibly with coupling to electric fields, mechanical stress etc. will become candidates for novel electronic devices or examples for fundamental physics effects. Slow or critical (paramagnetic) fluctuations can be analyzed by NSE in a time domain from a few ps to many ns. Neutron scattering and in particular NSE, in combination with computer simulations, already proved to boost the potential to obtain detailed microscopic pictures of soft-matter and biological systems \cite{10, 11, 8}. Incoherent scattering (from protons) is also an important source of information on the transport properties of ions and protons in electrolyte and hydrogen storage materials that pertain to energy storage techniques in batteries or fuel cells, or in combination with hydrogen storage \cite{12}.

Finally we remark that the high intensity and the possibility to simultaneously cover a range of $q$ and $\tau$ values within one wavelength frame may enable kinetic observations focused on dynamic properties. For example the loss of mobility in the course of chemical or physical cross-linking or due to external stimuli, e.g. photochemical changes upon illumination or temperature or pressure jumps.

3. Layout of the instrument
The ultimate limit of resolution can only be reached by a combination of measures: 1. highest intensity at long wavelength, 2. lowest possible intrinsic effective field integral inhomogeneity, 3. best available correction for the unavoidable inhomogeneity, 4. stability over sufficiently long counting times. At the spectrometer side intensity can only be increased by using sufficient divergence for the illumination of an as-large-as-possible sample area, low intrinsic inhomogeneity can only be achieved by an optimized effective field shape. ESSENSE relies on the latest fully optimized implementation of these criteria.
Figure 1. Overview of the whole spectrometer with the dimensions and its main components. The insert (lower left) shows the polarizing kink bender in more detail, the red line represents the polarizing mirror.

3.1. Primary spectrometer: beam transport
The neutron guide of ESSENSE for a cold flat “pancake” moderator of 3 cm height starts at a distance of 2 m from the moderator, has a 3.4° kink with a polarizing FeSi multilayer mirror in order to avoid direct sight into the moderator and then extends to 27 m.

The spectrometer itself consists of two main superconducting solenoid sets on the same carriers that also host the flippers, the auxiliary coils, the polarization analyzer and the detector, the latter positioned at 35···36 m from the moderator. This distance yields a wavelength frame-width of $\Delta \lambda = 7 \cdots 8 \text{Å}$, which is sufficient to effectively harvest the pulse gain factor. Due to the finite width of the pulse the wavelength-spread at any instant is 0.3 Å. The layout of the transport system, the positions of the chopper system and of the polarization device are shown in Figure 1.

3.2. The chopper system
Frame selection is realized by a system of 4 disc choppers in the distance range between 14 m and 23 m (e.g. C1 at 14 m, C2 at 16.7 m, C3 at 20.12 m, C4 at 23 m). With a rotation frequency of 14 Hz and sector openings of 110.9°, 138.7°, 173.8° and 203.5° respectively, the choppers make use of the whole pulse. This system is able to select any frame within (and beyond) the useful operation wavelength range between $\lambda = 3$Å and $\lambda \approx 25$Å without any contamination of neutrons with wavelengths shorter than 80 Å. A distance of 14 m for the first chopper is the largest distance that yields a viable frame selection with no more than 4 choppers. Optionally a pulse shaping chopper may be installed at a distance of 6···7 m. It consists of two closely spaced synchronously co-rotating disks each with two symmetrically placed 90° sectors. By phasing of the two disks any effective sector width between 0° and 90° can be set. The chopper opens twice per revolution, its frequency range is between $n \times 7$ Hz $\rightarrow 7 \cdot 168$ Hz, $n = 1, 2, \cdots 24$, allowing a wavelength-spread reduction to virtually any value between 0.03···0.3Å.
3.3. The neutron guide system
The sample has typical/maximal dimensions of 3 cm × 3 cm and is placed at 4 m from the end of the guide. A guide cross-section of 8 cm × 8 cm at the guide exit still guarantees efficient brilliance transfer for λ larger than a limit wavelength of about 4 Å within maximum illumination divergence at the sample of ±0.8°. Even if the flat moderator geometry is not optimal for

![Figure 2](image-url)

**Figure 2.** Left: Optimization study for a flat moderator (3 cm height) for λ = 8 Å. The picture shows two possible solutions for the vertical profile of the beam transport optics that are results of the optimization: a tapered and an elliptic. A third solution consisting of a mixed guide layout is also possible and it has been investigated by Mads Bertelsen. Such a solution would provide an average gain of 1.5 between 3 and 7 cm. The displayed neutron intensity ratio is calculated with respect to the original TDR moderator (12 cm × 12 cm²). Right: Figure of merit (FOM) for a tapered channel analyzer with FeCoV supermirror with m_up = 3 (right). The angle of inclination is explained in the text. The FOM is the product of the polarization times the square root of the transmission (Q = P√T).

the NSE requirements, the neutron guide system can collect up to 50% of the threefold gain depending on the degree of guide adaption, see left of Figure 2. The polarizing device consists of an inclined polarizing mirror (kink). With a total length of 2.7 m, it is a sufficiently compact insert that can be placed between the 8 m after the moderator and shutter and before the first chopper at 14 m. As supermirror a coating with Fe/Si (m=4 ··· 5) multilayers is envisaged. With the inclination of θ = 1.7° and a length of the polarizing mirror of 2.7 m the kink provides a polarization of more than 95% up to a wavelength λ ≥ 15 Å dropping to 80% at 20 Å and it effectively avoids direct view from guide exit to moderator. To improve the polarisation for wavelengths beyond 15 Å an additional transmission polarizer (FeSi on silicon mirror, inclined 4.6°, preceded by a broadband adiabatic RF flipper) is inserted to improve P at wavelengths larger than 11 Å.

3.4. Analyzer
The challenge for the analyzer is to accept the divergence from the sample and to cope with a broad wavelength band Δλ = 8 Å simultaneously. The analyzer in front of the detector has the dimension of the detector (30 cm diameter). The design parameters are 40 cm length with 4 mm wide and 30 cm high channels with (FeCoV multilayer coating with m_up = 3 or higher and m_down = 0.35) on both vertical walls of each channel. An optimization of the angle of
inclination of the channels (i.e. the orientation towards a source positioned at some centimeters off the real one) is needed in order to maximize the polarization after the analyzer (aimed > 95% polarization at 25 Å). The expected performance is shown in Figure 2.

3.5. Detector
A detector 30 cm × 30 cm and with a moderate (2D) position resolution (better than 3 cm or 1 inch), high efficiency and high maximum count rate (better than 5 KHz/cm²) is required. A robust possible solution would consist of an array of 100-200 front-end counting tubes (³He) with square cross-section (∼ 15 l ³He).

3.6. Instrument layout: Secondary (proper) spectrometer
The proper spectrometer is of the generic IN11 type [4, 13], but with a new sophisticated magnetic design in order to extend the technical limit for the Fourier-time (τ) given by the residual field-integral inhomogeneity, which remains after the action of correction elements in the beam paths (“Fresnel” correction coils). The present state-of-the-art correction elements seem to be resistant to further improvement, therefore the most promising means towards the ultimate limits of resolution is a reduction of the intrinsic inhomogeneity of the main solenoids, a measure that has been first selected at the ILL to enhance the IN15 properties within a currently conducted refurbishment. The potential of the application of this strategy is about a factor between 2 and 3 inhomogeneity reduction compared to existing instruments as may be expressed by an increase of the homogeneity parameter H from about 1 to 2···3 ns/Å². Reduction of intrinsic inhomogeneity is achieved by a somewhat enhanced field in the center of the solenoids (resembling C. Zeyen’s optimal field-shape solution for a narrow beam [14]) and enlargement of the solenoid diameter [6]. The latter, however, is limited by the requirement to avoid extensive fringe fields and to keep the total length of the instrument within feasible limits. Optimization consists in finding the best compromise among these contradicting requirements. By using superconducting partial solenoids, that are fringe field compensated in a similar way as the solenoids of the SNS-NSE spectrometer, these requirements can be fulfilled with a distance of 4 m from the sample to the π/2-flipper.

Figure 3. Left: horizontal section of the secondary spectrometer. Each pair of lines delimits the contour of a magnetic coil, see e.g. in the right arm the inner red coils (+NI) and the corresponding concentric, outer compensating coil (−NI/2) in blue. The superconducting main coils are between 0.96 and 3 m. Right: Profile of the magnetic field (solid line) along the axis for both arms of the coil. Dashed line: B × 40, point-dashed line: B × 40 for a configuration with an extra free sample space of 30 cm radius.
3.7. The coil assembly.
The superconducting main coil assembly is about 2.4 m long with a maximum coil radius of 0.68 m and consists of five fully compensated, superconducting parts. The magnetic field optimizations were performed with a $\pi$ flipper positioned between 10 cm to 20 cm from the sample. If required by bulky sample environments or special setups more sample space can be supplied thanks to the possibility of including extra distance pieces between spectrometer arms and sample stage. The coils of Figure 3 have an intrinsic inhomogeneity $\sqrt{\langle \Delta J^2 \rangle}/J_0 = 3.4 \times 10^{-4}$ for a neutron beam with 10 cm radius at the $\pi/2$ flipper. Figure (3) also shows the magnetic field along the axis for both arms; the typical asymmetric triangle shape that is common to all optimized solutions is visible. The still necessary corrections will be performed by two correctors at optimized positions in each of the main solenoid sets. The full dipole moment compensation of the main solenoids allows easy access to large scattering angles, e.g. for 45 degrees the computed corrected inhomogeneity (by 2 quadratic ideal current distribution type correctors) is increased by magnetic cross-talk between both spectrometer arms merely from 1ppm to 4ppm. By solely shifting the correctors by less than 0.5 mm this can be reduced to 2ppm again. Further, the fringe fields are compatible with a magnetic shielding enclosure [5]. In the design optimization and assessment of the main coils it was assumed that ideal radial coils with quadratic correction effects are in place. That allows for a correction of the uniformity of the precession field to less than 1 ppm, i.e. the deviation of the main field from quadratic errors are sufficiently low and the necessary quadratic correction strength is reduced, corresponding to the reduced intrinsic inhomogeneity properties of the new coil design.

3.8. Short times option
The ultimate short time limit of the spectrometer in standard configuration is around 50 ps. In order to extend this down to 1 ps two methods may be used. Both require a few additional smaller coils and two additional flippers.

(i) A “small” version of an NSE setup within the sample space comprising two $\pi/2$-flippers and auxiliary “main” solenoids. The rest of the instruments just supplies the guide field.

(ii) Inserting extra $\pi$-flippers between the main coil ends and the “normal” $\pi/2$-flippers and adding short extra coils in the space between these flippers will enable an operation where, the effective field integral, i.e. the Fourier-time can be set to arbitrary small values. This is achieved by inverting the precession angle in the second $\pi$-flipper thus subtracting the field integral inside the main coil (at very low current) from that generated by the short extra coil. This mode has already been proven at the SNS-NSE spectrometer. The shortest time here is not given by the arbitrarily small effective field integral but rather by the condition that the field integral $\delta J_\pi$ variation, necessary to probe at least 1/2 echo oscillation is less than 10% to 20% of $J_{\text{eff}}$, which yields $\tau_{\text{min}} = (J_{\text{eff}}/\delta J_\pi)(m_n/2h)\lambda^2$, about 1 ··· 2 ps at $\lambda = 4 \text{ Å}$.

The second option leaves more open room in the sample space.

3.9. Magnetic shielding
The coil design is compatible with a magnetic shielding around the spectrometer. If realized it would consist of a double walled mu-metal enclosure with a space of about 0.3···0.5 m between the layers (thickness $\approx$1.5-2 mm). The walls must be 2 m apart from the magnetic axis. The space in-between can host the radiation shielding around the spectrometer [5].

4. Performance
Concerning the expected performance of the instrument there are two main distinct but still entangled aspects: effective flux and resolution. The resolution issues do not depend on
the nature of the neutron source and are independent from its pulse structure. However, a high neutron intensity at long wavelength is essential to reach the highest Fourier-times. The longest useful wavelength largely depends on available intensity and together with field integral homogeneity and/or the maximum available field integral, determines the largest Fourier time. The resolution of a NSE spectrometer is expressed in terms of the maximum Fourier time or better by the range where the resolution function $R$ is still larger than $1/e$. 

$$R \approx \exp\left(-\frac{\tau}{(H\lambda^2)^2}\right),$$

where $H$ is a measure of the relative field integral homogeneity.

Combining the new coil design with the present performance of the correction elements we expect a parameter $H = 2 \cdots 2.5 \text{ns/Å}^2$ leading to a maximum Fourier time of $800 \cdots 1000 \text{ns}$ at $\lambda = 20 \text{Å}$ ($1200 \cdots 1600 \text{ns}$ at $\lambda = 25 \text{Å}$) and of $H\lambda^2 = 40 \text{ns}$ for $\lambda = 4 \text{ Å}$. The number of scattered neutrons depends on the flux at the sample and the sample size. It has huge influence on the data quality that can be obtained. The average flux (from McStas simulation [15]) at the sample for the new ESS cold source model is given in table 1. The simulated fluxes are multiplied by attenuation factors coming from the (assumed) 4 cm Al, 5 m He and 1 m air that the neutrons will inevitably find on their path in the real instrument. Finally the larger frame width yields

| $\lambda$/Å | simulated $\Phi$ ($10^8$ n/s/cm$^2$/Å) | attenuation factor | $\Phi$ [ESSENSE] ($10^8$ n/s/cm$^2$/Å) | $\Phi$ [IN15] ($10^8$ n/s/cm$^2$/Å) |
|-----------|-----------------|-----------------|-----------------|-----------------|
| 6.3       | 1.3             | 0.77 x 0.84 x 0.98 | 0.82           | 1.1±1.2        |
| 7         | 0.9             | 0.76 x 0.81 x 0.97 | 0.54           | 0.76±0.81      |
| 17        | 0.025           | 0.56 x 0.73 x 0.94 | 0.01           | 0.01±0.015     |

Table 1. Fluxes at the sample position (31m) for polarized neutrons. (*) Courtesy of B. Farago.

a gain factor, $g$, compared to reactor based instruments which is $g = \ln(\lambda_{\text{max}}/\lambda_{\text{min}})/w$, where the effective relative selector width of the reactor instrument is $w$. Assuming $w = 0.15$ for an instrument with 15% resolution like IN15 and a wavelength window from 7 to 14 Å the gain factor is $g \approx 5$. Thus, the new high-resolution NSE will have an effective intensity gain factor around 30 with respect to IN15. In Figure 4 these relations are illustrated by a complete experimental cycle with the scattering intensity computed for standard polymer samples from h/d mixtures of polyethylene simulated with the data of new ESS spectrometer and for the new IN15. Resolution functions were modeled by the Gaussian approximation given above, assuming $H=2.5 \text{ ns/Å}^2$. The integrated detector area was 100 cm$^2$ in all cases, i.e. 1/6 of the full detector. Figure 4 shows simulated incoherent scattering from a fully protonated PE sample with 0.5 mm thickness (size 3 cm x 3 cm) and it demonstrates the advantage of a large wavelength frame. The larger average intensity yields more than two times smaller error bars in the corresponding ESS curve (red points). In both cases the field-integral range was 0.001-1 Tm (ESSENSE) or 0.001-0.25 Tm (IN15, pertains omission of the last 4 tau-points). The dynamical features were assumed to be simple Rouse type polymer dynamics, in detail real polymers will show somewhat different, yet similar $S(Q,t)$ behavior. The comparisons show that beyond the larger average flux ratio of 3-4 a big advantage of the ESS spectrometer lies in the fact that between 7 and 3 effective experiments, all yielding useful data, are performed simultaneously. The significant increase in error bars at the large Fourier-time side are due to the approach of the resolution limit (residual inhomogeneity of the main coils).

5. Conclusion
An ultra high-resolution NSE is indispensable to extend the dynamic range of the ESS spectroscopic suite thus enabling measurements with 1000 times smaller energy transfer than
Figure 4. Simulations of an experiment with polyethylene (molecular weight 10, sample thickness d=0.5mm), for incoherent scattering (contrast ratio Phi=1) at the future ESS spectrometer (left) and at IN15 (right) with either the optimized (for ESS) or the IN15 specifications of the instrument, both cases with 15% wavelength-band resolution using data from 100 cm$^2$ detector area. The assumed counting times (ctimes) per field-integral setting for the ESS and the IN15 cases were equal; the total time (runtime) for the simulated experiment differs. We considered 20 phase points, 5 for spin up and 3 for spin down (npaths). In the left panel the curve at the top corresponds to the lowest q=0.104 Å$^{-1}$, the one at the bottom to the highest one. The curve corresponding to q~0.16 Å$^{-1}$ -comparable to the one in the right panel - is marked with red symbols.

any other spectrometers. ESSENSE is the high-resolution NSE (of the IN11-type) proposed to the ESS with an innovative design of the precession coils that would allow such measurements.

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