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Neutron spin echo spectroscopy

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Body

Abstract

Neutron spin echo (NSE) **spectroscopy** is a powerful technique used to probe the internal dynamics and diffusion processes within matter, allowing researchers to quantify how materials respond to changes in external conditions. To fully understand the bulk properties of a material, it is often crucial to investigate dynamic processes occurring on nanometre length scales and nanosecond timescales. NSE **spectroscopy** provides an exceptional capability to measure such dynamics across a broad spectrum of condensed matter systems, ranging from proteins and quantum magnets to catalysts. In this Primer, we present an overview of NSE **spectroscopy**, highlighting the instruments used, methods of data collection and representative applications in both soft-matter and hard-matter sciences.

Neutron spin echo spectroscopy investigates internal dynamics and diffusion in materials, using advanced instruments and data collection techniques. In this Primer, Faraone et al. discuss how **neutron spin echo spectroscopy** can be used in both soft-matter and hard-matter sciences.

Introduction

Thermal **neutron** beams produced at **neutron** sources offer several valuable characteristics for probing the structure and dynamics of materials at the nanoscale (Supplementary Note 1). Their wavelength and energies closely match interatomic distances and the energies associated with atomic, molecular and magnetic excitations, as well as fluctuations. Because **neutrons** carry no charge, they are not scattered by electron clouds and can therefore penetrate deeply into bulk samples, making it possible to use complex sample environments and study materials under unusual or extreme conditions. **Neutrons** interact primarily with atomic nuclei, with scattering strengths that depend on the isotope, and with magnetic inhomogeneities. As a result, **neutron** scattering provides detailed information about the relative positions and motions of pairs of atoms and unpaired electrons, and, for certain atoms — most notably hydrogen — can reveal single-particle dynamics.

The primary experimental observable in a **neutron** scattering experiment is the double differential scattering cross-section, $\frac{d^2\sigma}{d\Omega dE}$. This quantity represents the probability that a **neutron** is scattered by the sample into a solid angle between Ω and $\Omega + d\Omega$, while transferring an energy between $E = E_i - E_f = \hbar\omega$ and $E + dE = \hbar(\omega + d\omega)$, in which E_f and E_i are the scattered and incident **neutron** energies, respectively. Integrating the double differential scattering cross-section over all scattering angles and exchanged energies, the total scattering cross-section, σ , representing the probability that a **neutron** is scattered by the sample, is recovered: $\sigma = \int \frac{d^2\sigma}{d\Omega dE} d\Omega dE$. The double differential scattering cross-section is directly related, through the dynamic structure factor, $S(\mathbf{Q}, E)$, to the structure and dynamics of the sample — for example its amount and chemical composition, the relative positions and motions of the nuclei, and magnetic inhomogeneities:

in which, $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$, is the scattering vector, $\mathbf{k}_f$ and $\mathbf{k}_i$ are the scattered and incident **neutron** wavevectors and k_f and k_i their magnitudes, respectively, and N is the total number of scatterers. Although $\mathbf{Q}$ is a vector, for isotropic samples, the dynamic structure factor and its derived quantities depend only on its magnitude: $Q = |\mathbf{Q}|$. In the remainder of this paper, we assume samples are isotropic and simply use Q , except in those few cases (for example, when we discuss magnetic scattering) for which the vectorial nature of $\mathbf{Q}$ needs to be considered.

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Q and E are inversely related to the inter-scatterer distance and time, respectively. Hence, indicatively, measuring at low/high Q implies probing long/short distances, with the caveat that the exact relationship is a Fourier transform. Similarly, the capability to appreciate small energy changes, E , that is, good energy resolution, implies the capability to measure long relaxation processes.

Traditional neutron spectroscopy^{1,2} relies on a relatively simple scheme: producing a monochromatic neutron beam and analysing the scattered beam energy distribution as a function of the scattering angle. However, thermal neutrons cannot easily be accelerated or slowed down, nor can they be directly detected as a function of energy. As a result, both monochromatization and energy analysis are achieved by filtering, selecting only those neutrons whose energies fall within a very narrow tolerance. Achieving higher energy resolution requires narrowing this tolerance further, which substantially reduces the number of usable neutrons. Although no fundamental limit prevents arbitrarily high resolution, the counting times required would quickly become impractical. Currently, even at the most intense neutron sources, the highest achievable resolution with reasonable counting time is obtained with backscattering instruments³, which reach energy resolutions of approximately 0.1 μeV to 1 μeV .

In 1972, Ferenc Mezei introduced the foundational principles of neutron spin echo (NSE) spectroscopy^{4, 5–6}, a technique that revolutionized high-resolution neutron scattering. NSE uses a polarized neutron beam — taking advantage of the intrinsic neutron spin — to encode and measure extremely small energy changes. Rather than directly determining the neutron's energy before and after scattering, NSE detects the subtle change in neutron velocity (or energy) within a well-defined magnetic field by measuring the change in beam polarization before and after the sample. NSE transfers the energy analysis from the neutron beam itself to the spin precession phase, allowing the resolution to be determined by the magnetic field homogeneity rather than by the width of the neutron energy distribution of the incoming and detected beam. This method provides unprecedented sensitivity to slow dynamics (Fig. 1a).

Fig. 1

Fundamentals of NSE spectroscopy.

a, Neutron spin echo (NSE) spectroscopy dynamic window. **b, Schematic of an NSE spectrometer.** (1) The neutron velocity selector narrows down the incoming wavelength band to an appropriate range of 10–20% width of the wavelength distribution/mean wavelength ($\Delta\lambda/\lambda$). (2) The polarizer selects one spin state, in this case, along the x direction. (3) The first $\pi/2$ -flipper turns the neutron spin to the z direction. (4) The neutron spin precesses within the magnetic field created by the first precession coil. (5) The π -flipper turns the neutron spin by 180° around the z axis. (6) The neutron beam is scattered by the sample. (7) The neutron spin precesses within the magnetic field created by the second precession coil. (8) The second $\pi/2$ -flipper turns the neutron spin to the scattering plane (xy). (9) The analyser transmits neutrons with a probability proportional to the cosine of the precession angle, ϕ . (10) The detector counts the neutrons. **c, Evolution of the neutrons' spin direction through an NSE spectrometer.** **d, Echo signal measured by NSE.** The continuous line is the fit using equation 6. **e, In an NSE experiment, the echo is measured for different Fourier times (t_F).** **f, The decay of the normalized echo amplitude with t_F determines the normalized intermediate scattering function, $FNSE(Q, t_F)/FNSE(Q, 0)$, which is the result of an NSE measurement.** σ_v , width of the echo envelope; A_{echo} , echo amplitude; A_v , average intensity; Q , magnitude of the scattering vector; T_{echo} , echo period.

Today, several NSE spectrometers (Table 1) are available to users — typically via a proposal process — at neutron scattering facilities worldwide. The Institut Laue-Langevin (ILL) in Grenoble, France, hosts two complementary instruments, IN15 and WASP, optimized, respectively, for studying slow relaxation processes over large length scales and for probing slightly faster dynamics over a broader length-scale range. The Heinz Maier-Leibnitz Zentrum in Munich, Germany, operates the J-NSE Phoenix spectrometer. In the USA, both major neutron facilities — the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory and the National Institute of Standards and Technology Center for Neutron Research — provide NSE instruments, the SNS-NSE and the v-NSE, respectively. The iNSE spectrometer at the JRR-3 reactor (Japan Atomic Energy Agency, Tokai-mura, Japan) is another general-purpose instrument. These four spectrometers are designed to cover long timescales similar to those accessible on IN15, while also probing a broad range of length scales, although not as efficiently as WASP.

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When requesting beam time, users must carefully consider which spectrometer best matches the scientific objectives — for example, whether sensitivity to slow dynamics or broad length-scale coverage is the priority. Proposal reviewers generally expect reasonable evidence that the samples' relaxation processes fall within the NSE dynamic range (Fig. 1a), supported by complementary methods such as neutron spectroscopies, light scattering or computer simulations.

Table 1

Available NSE instruments, including information on the institute, reduction software and any other relevant remarks

Name	Institution	Remarks	Reduction software
<u>IN15</u>	ILL	Longest Fourier time	Custom set of Igor macros
<u>WASP</u>	ILL	Wide angle	Custom set of Igor macros
<u>J-NSE Phoenix</u>	FRM II	High resolution	DrSPINE242,243
<u>SNS-NSE</u>	SNS (ORNL)	Time-of-flight NSE	DrSPINE
<u>vNSE</u>	NCNR (NIST)	High resolution	DAVE244
<u>iNSE</u>	JRR-3 (JAEA)	Optimized shape	Custom scripts

In addition, Supplementary Note 2 reports a list of neutron resonance spin echo (NRSE) instruments. FRM II, Forschungs-Neutronenquelle Heinz Maier-Leibnitz; ILL, Institut Laue-Langevin; JAEA, Japan Atomic Energy Agency; JRR, Japan Research Reactor; NCNR, National Institute of Standards and Technology Center for Neutron Research; NIST, National Institute of Standards and Technology; NSE, neutron spin echo; ORNL, Oak Ridge National Laboratory; SNS, Spallation Neutron Source.

In this Primer, we review the operating principles, instrument characteristics and main applications of NSE spectrometers. Because of space constraints, we restrict ourselves to classical NSE instruments — such as those listed above — which use neutron spin precession in magnetic fields to encode energy changes. Readers interested in related techniques are referred to other sources for discussions of spin echo small angle neutron scattering^{7,8} methods that study large structures and detect changes in Bragg peak widths^{9, 10–11} or inelastic linewidths¹², and neutron resonance spin echo^{13,14}, which probes relaxational dynamics similar to NSE, but using a different technical realization of the spin manipulations using resonance spin flippers (Supplementary Note 2).

Experimentation

NSE spectroscopy encodes neutron velocity via the spin precession angle in a magnetic field^{4, 5–6}. Because the technique decouples the energy resolution of the incoming and outgoing neutrons from the resolution of the instrument, NSE can accept a relatively broad distribution of incident neutron energies while still achieving the highest energy resolution in neutron spectroscopy.

The neutron carries a spin angular momentum $\mathbf{S}$ whose z component S_z has two eigen values: $\pm \hbar/2$. The time evolution of the expectation value $\langle \mathbf{S} \rangle$ in a magnetic field $\mathbf{B}$ is

in which $\boldsymbol{\mu} = \gamma \hbar \mathbf{S}$ is the magnetic moment and γ is the gyromagnetic ratio. Therefore, when $\mathbf{B}$ has a component perpendicular to $\mathbf{B}$, the spins undergo Larmor precession.

Consider a polarized neutron with velocity v traversing a magnetic field of strength B and length l , with perpendicular to $\mathbf{B}$, the precession angle is

with the Larmor frequency $\omega_L = \gamma B$ and transit time $tT = l/v$.

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Now consider a neutron passing through a magnetic field of length l_1 and field B_1 , then a second region of length l_2 and oppositely directed field B_2 . A sample is placed between the two magnetic regions, where the neutron velocity changes from v to $v + \delta v$. If the field integral in the two regions are equal ($\int B dl$), then the net precession angle after both regions is

in which m is the neutron mass, we used $\lambda = h/mv$, and t_F is the Fourier time. Using the de Broglie relation (Supplementary Note 1), we obtain $t_F \propto \lambda^3$; hence, long wavelengths are required to reach long Fourier times, despite the associated loss in flux.

After a spin analyser, the neutron intensity is proportional to the expectation value $\langle 1 + \cos \phi \rangle / 2$, averaged over various energy transfers. Given that scattering with energy transfer $\hbar\omega$ and momentum transfer $\hbar Q$ is described by the dynamic structure factor, $S_{\text{NSE}}(Q, \hbar\omega)$ (Supplementary Note 1), and assuming $S_{\text{NSE}}(Q, \hbar\omega)$ is even in ω , we obtain

in which the first term is the unpolarized static structure factor (Supplementary Note 1), and the second term is the intermediate scattering function (ISF) (Supplementary Note 1). The superscript NSE highlights the fact that the relative weight of nuclear coherent, nuclear incoherent and magnetic neutron contributions depend on the specific instrument configuration.

Nuclear coherent and isotope-incoherent scattering do not flip the neutron spin. Spin-incoherent scattering flips the neutron spin with a probability of 2/3. Magnetic scattering¹⁵ produces a Q -dependent effect: in an NSE spectrometer, neutron spins at the sample lie in a plane perpendicular to the scattering plane; for isotropically distributed magnetic inhomogeneities (powder paramagnets), half the neutron spins undergo a π -flip about the z axis, perpendicular to the scattering plane ($\phi \rightarrow -\phi$), and half undergo a simple π -flip ($\phi \rightarrow \phi + \pi$)¹⁶.

Figure 1b shows a typical NSE instrument layout; Fig. 1c illustrates the evolution of the neutron spin orientation. The neutron velocity selector defines the wavelength distribution, and the polarizer prepares spins along the x axis, that is, along the neutron path. The first $\pi/2$ -flipper rotates spins to the z axis. Precession occurs in the yz plane in the first arm of the spectrometer. Because a region of zero magnetic field would depolarize the beam, the two magnetic arms use aligned fields, and a π -flipper between them performs the effective field inversion ($\phi \rightarrow -\phi$). For isotropic magnetic scattering, this π -flipper is omitted because the sample itself yields the required phase inversion for half of the magnetic scattering. Precession is 'unwound' in the second arm, and the second $\pi/2$ -flipper projects spins into the xy plane. The spin analyser transmits neutrons to the detector with probability $\cos^2 \phi$.

Therefore, NSE spectroscopy measures $S_{\text{NSE}}(Q, \hbar\omega)$; the accessible timescale (or instrumental resolution) is determined by the maximum Fourier time, t_F (Fig. 1f). Values up to $t_F \approx 1 \mu\text{s}$ have been achieved, corresponding to an energy resolution of $\approx 10\text{--}3 \mu\text{eV}$ (refs. 17, 18–19).

To illustrate the basic features of the NSE signal, we now develop a brief analytical description. Given that NSE experiments use neutron beams with a substantial velocity spread, the measured neutron intensity (equation 5) must account for the incoming velocity distribution $f(v, v_0, \sigma v)$, characterized by central velocity v_0 and width σv (typically given as the full width at half maximum, with $10\text{--}20\%$). Consider the situation in which the field integrals in the two arms are different. For simplicity, let $\int B_1 dl_1 = \int B_2 dl_2 + \delta J$, with δJ the phase offset. In addition, finite beam size and small deviations from field homogeneity along the neutron path introduce a constant offset in the precession angle, denoted as ϕ_{echo} . Under these assumptions, the final precession angle becomes $\phi + \phi_{\text{echo}}$. The resulting NSE intensity is

in which I_0 is the incident flux. The function $\mathcal{F}$ is the Fourier transform of the velocity distribution, centred at zero, and is a Gaussian-like function, centred at v_0 , with a width inversely proportional to σv . A perfectly monochromatic beam would produce an infinitely broad $\mathcal{F}$, whereas realistic velocity spreads produce a finite envelope for the echo oscillation.

Figure 1d shows a typical spin echo signal obtained by scanning the phase, δJ , via small magnetic field changes using the phase coil. The signal oscillates with δJ , and its period, τ , depends on the central velocity of the incoming beam. The echo amplitude, A_{echo} , and the average intensity, A_v , are proportional to the ISF and unpolarized static

scattering, respectively. The symmetry point, corresponding to the echo point, occurs at . The maximum (up) and minimum (down) signal levels are measured by turning off the $\pi/2$ -flippers, thus eliminating spin precession and yielding an effective $FNSE(Q,0)$. The up/down ratio is commonly referred to as flipping ratio.

Practical procedure for an NSE measurement

An NSE measurement begins with selection of the incident wavelength distribution. A set of Fourier times tF to be measured is then selected — typically ≈ 20 logarithmically spaced values within the dynamic range of the instrument. For each tF , the precession fields are set accordingly, and the phase coil is scanned to record the echo signal. The scanning protocol varies across facilities; common schemes include 19 points spaced by 45° or a compact four-point scan at 90° intervals. Before or after the scan, the up and down measurements are acquired. Given that the up and down do not depend on the intensity of the precession field, they can be measured at all, any or just some of the Fourier times, that is, precession field intensity, configurations.

Two main normalization procedures are used: nuclear scattering and isotropic paramagnetic scattering. For nuclear scattering, two measurements are performed with the $\pi/2$ -flippers off. These are the non-spin-flip (nsf) measurement (or up), performed with the π -flipper on, and the spin-flip (sf) measurement (down), performed with the π -flipper off. The normalization factor is $norm0 = nsf - sf$ (or up–down). For isotropic paramagnetic scattering, a full polarization analysis along three orthogonal directions (x , y and z) is required. The appropriate normalization is $norm0 = [2(znsf - zsf) - (xnsf - xsf) - (ynsf - ysf)]/2$. More complex magnetic scattering requires substantially more care and is not routinely performed on all instruments. In both nuclear and magnetic cases, the normalization corrects for detector efficiency, spin-flipper efficiency and finite beam polarization.

Once the phase scan and potentially the up/down measurements are complete, the instrument is set to the next Fourier time by adjusting the precession fields, and the process is repeated (Fig. 1e). Performing this sequence for all selected tF values yields the dependence of the ISF on tF .

Q-range, detector treatment and ISF extraction

The detector scattering angle — and, when applicable, the incident wavelength — may be changed to access different Q and tF ranges. For each configuration, the full measurement sequence (phase scan plus potentially the up and down measurements) is repeated at each Fourier time to obtain the normalized ISF.

NSE instruments rely on position-sensitive detectors. Because both $FNSE(Q,t)$ and ϕ_{echo} vary across the detector, the echo pattern differs with the position. Data from regions of the detector over which these quantities can be approximated as constant are summed to improve the statistics. Each echo is analysed to obtain the echo amplitude (Aecho) and the corresponding normalizing factor ($norm0$) as a function of detector region. After all echo scans at all tF , a normalized ISF can be assigned to each detector region. Finally, the ISF values are averaged over detector regions corresponding to the same Q , yielding the normalized ISF: $FNSE(Q,tF)/FNSE(Q,0)$ (Fig. 1f). In time-of-flight (ToF)-NSE, to which multiple wavelengths contribute, averaging is performed over both detector area and ToF bins.

Non-traditional NSE instruments

In this section, we discuss two NSE variations: ToF-NSE and wide-angle NSE, which still use precession coils to encode the neutron velocity.

ToF-NSE

The concept of an NSE instrument designed for pulsed sources was introduced by Mezei in 1979 (ref. 20), anticipating the use of ToF techniques in such a set-up^{21,22}. This concept is currently implemented only on the SNS-NSE^{23,24}.

The components and layout of a ToF-NSE instrument are essentially identical to those described above. However, although an NSE instrument at a continuous source typically uses a neutron velocity selector that accepts a wavelength band of $\Delta\lambda/\lambda = 10\text{--}20\%$, where $\Delta\lambda$ is the width of the wavelength distribution, centred at the mean

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wavelength λ , in ToF-NSE the wavelength distribution is time-dependent. It is defined by a chopper system and, when applicable, the pulsing of the neutron source. For the SNS-NSE, $\Delta\lambda$ is typically around 3 Å ($\Delta\lambda/\lambda \approx 50\%$) owing to the moderator–detector distance and the 60 Hz source frequency. At lower repetition rates (like at the European Spallation Source in Lund, Sweden or the SNS Second Target Station), $\Delta\lambda$ values as large as 8 Å are possible²².

Not only does incorporating ToF methods into NSE enable a broader usable wavelength band, but it also allows determination of the neutron wavelength on an event-by-event basis via its measured time of flight. This yields a more precise determination of the scattering vector Q . The larger $\Delta\lambda$ also extends the Q coverage at a fixed scattering angle in a quasi-continuous manner. In addition, ToF-NSE enables a more accurate determination of the echo point ϕ_{echo} , given that its position is wavelength-independent, and the entire wavelength band contributes.

Despite these advantages, the ToF-NSE technique also presents challenges. Pulsed neutron sources generally provide lower average flux. Moreover, because the neutron flight time depends on the wavelength, the flipper currents in ToF-NSE must be synchronously and continuously ramped during each pulse to match the changing neutron wavelengths, while all other currents and magnets remain constant. Consequently, the measured Fourier time varies within each pulse. For example, at field integral of $J = 0.56$ T m and for a wavelength band of 5–8 Å, the Fourier time varies from about 15 ns to 50 ns.

Additional complexities arise in data collection and analysis. Some subtle differences exist in how relevant data are extracted, but these are generally handled within the instrument control and data-reduction software. The full potential of the ToF-NSE is therefore realized only when combined with advanced reduction software capable of handling this increased complexity²⁵.

Wide-angle NSE

As explained above, most NSE instruments use two identical precession coils with rotational symmetry along the beam direction. These long cylindrical coils provide very low magnetic-field inhomogeneity, yielding high energy resolution (long Fourier times t_F). However, their geometry restricts the angular coverage of the neutron detector to about $3^\circ \times 3^\circ$. To cover a wider Q range, the detector arm position must therefore be scanned in several steps.

The now decommissioned IN11C instrument²⁶ at the ILL was the first to use a flattened 30° -wide precession coil after the sample, together with a 30° -wide detector bank. Extending this approach further — up to 360° — causes the coil to separate into two disks (top and bottom), which generate magnetic fields in opposite directions, forming an anti-Helmholtz configuration. This design principle formed the basis of the SPAN instrument²⁷ at the Hahn-Meitner-Institut in Berlin, and ultimately of WASP²⁸. In theory, such instruments could achieve almost full 360° detector coverage. In practice, WASP currently covers 130° and may reach up to 160° in the future.

IN15 and WASP at the ILL are complementary instruments. IN15 is optimized for the low Q range of 0.02 Å^{-1} to 0.2 Å^{-1} , whereas WASP excels at high Q , covering the range between 0.2 Å^{-1} and 3.5 Å^{-1} . IN15 accesses NSE times from 5 ps to 1,000 ns, whereas WASP covers 0.5 ps to 10 ns. For incoherent scatterers, glassy systems or any case in which the full detector area provides useful signal, WASP achieves a count rate up to $100\times$ higher than that of other NSE instruments.

Sample environment

One of the key advantages of neutron scattering instruments is their ability to accommodate complex sample environments, enabling studies under a wide range of, and sometimes extreme, conditions. In principle, NSE spectrometers can use the same sample environment as other neutron instruments, but a few important limitations apply.

The first limitation is sample size. NSE spectrometers typically use a relatively large neutron beam, about 3 cm in diameter. For an optimal NSE experiment, both the sample environment and the sample volume must therefore be larger than in standard diffraction or small-angle-scattering experiments. For liquids, sample volumes of 1 ml to 4 ml are typical. Most samples are placed into standard quartz cells or aluminium cans. When quartz cells are used, in

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situ dynamic light scattering measurements can be useful — both for determining the low- Q limit of the diffusion coefficient and for monitoring the stability of delicate samples²⁹. In situ dynamic light scattering measurements are currently available on IN15 and J-NSE Phoenix²⁹.

Another constraint is the limited space around the sample, given that the π -flipper must be positioned close to the sample.

The sample environment must be non-magnetic to preserve beam polarization. Even though ensuring non-magnetic construction can be as simple as replacing steel screws with titanium or aluminium ones, challenges arise when motors are needed close to the beam. Conventional iron-core electric motors cannot be used close to the sample. Instead, piezo motors, pneumatic actuators or motors positioned sufficiently far from the beam path are suitable alternatives.

High-pressure experiments on NSE are especially challenging, because strong steels are ferromagnetic, and therefore unusable³⁰. The large beam size also necessitates large windows in the pressure cell, limiting the maximum achievable pressure. Nevertheless, several high-pressure NSE studies have been reported^{31, 32, 33–34}, and, in situations in which high pressure is essential, a smaller neutron beam can be used, albeit at the cost of reduced signal intensity.

Other sample environments — such as rheometers³⁵, humidity-controlled³⁶ or gas-absorption chambers^{37,38}, and electric cells³⁹ constructed from aluminium or copper — have been implemented on NSE instruments.

Experiments that require magnetic fields at the sample position or investigations involving ferromagnetic samples are difficult but not impossible. In such cases, the ferromagnetic NSE or intensity modulated NSE option must be used, although it comes with a reduction in intensity^{6,40}. Currently, these options are only available on IN15.

Results

As in any neutron scattering experiment, NSE data must be corrected for scattering from the sample container and sample environment, as well as for background signals arising from neutrons that reach the detector but have not been scattered by the sample. Accordingly, two additional measurements are required: an empty-cell measurement (no sample) and a background measurement, performed with an absorber (such as cadmium or boron) in place of the sample. These contributions must be subtracted from both the echo amplitude and the normalizing static signal after weighting by the transmission ratio $Tr = T_{\text{sample}}/T_{\text{empty}}$:

in which the superscript m denotes measured (uncorrected) quantities.

For magnetic scattering, this correction is usually not needed, as the empty and background contain no magnetic signal. If the empty and/or background contributions are negligible, the correction may also be omitted. In solution measurements, the solvent can be considered part of the empty measurement, provided the sample's solute volume is properly accounted for.

The dynamic response of the instrument — that is, the loss of polarization due to the nonideality of the instrument — must be taken into account. This loss is mainly caused by echo smearing: neutrons hitting the same detector pixel but following slightly different trajectories experience different magnetic field integrals, shifting their echo points. The measurement used to capture this effect is routinely called the resolution, and it is obtained using a sample with no dynamics within the probed dynamic range. It is important that the resolution sample reproduces the sample geometry so that the neutron trajectories are the same.

The resolution measurement is also used to determine the echo period T_{echo} , the echo envelope width σ_v , and the echo point, ϕ_{echo} , for every area of the detector (phase map). In fact, all these parameters are sample-independent. Knowledge of these parameters from the resolution sample facilitates the determination of Aecho for the sample, empty and background measurements.

The correction for the resolution can be carried out as a simple division in the time domain, whereas for other spectrometers working in the energy domain, the fitting function has to be convoluted with the resolution.

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The resolution defines the dynamic window accessible to the spectrometer. When the ratio becomes too small (a precise threshold does not exist, but $\approx 1/e$ is a reasonable estimate), uncertainties increase, and the measurement becomes impractical⁴¹. Instrument developments aim to minimize field-integral inhomogeneities through improved precession-coil geometries and correction coils⁴². Field integrals of 1.2 T m are now possible, which, at an incident wavelength of ≈ 20 Å, provides access to $tF \approx 1$ μs (ref. 17).

For a sample with only nuclear scattering, the normalized ISF measured by NSE is⁴³:

Equation 9 demonstrates that the measured ISF is a weighted sum of coherent and spin-incoherent contributions (Supplementary Note 1), in which the weights depend solely on their respective static intensities.

Despite the use of a polarized neutron beam, coherent and incoherent scattering contributions cannot be experimentally separated in the standard NSE set-up⁴⁰. Ideally, neutron experiments should be designed to isolate coherent or incoherent scattering, but structural modulation in Q often prevents this. Consequently, at certain Q values, coherent and incoherent contributions coexist and evolve on different timescales. As a result, can demonstrate seemingly unusual behaviours, including values above one or even negative values. These effects follow directly from equation 9.

For a sample with isotropically distributed magnetic inhomogeneities, measured without a π -flipper, the normalized ISF measured by NSE is:

in which $FM(Q, tF)$ is the ISF of the magnetic scattering. Therefore, removing the π -flipper yields an echo signal that depends only on magnetic scattering.

Applications

Among the many methods available to study dynamical processes in materials, NSE offers several unique capabilities. Like all neutron spectroscopic techniques, NSE is sensitive to magnetic inhomogeneities and to light atoms — particularly hydrogen — as well as to isotopic composition, enabling the use of isotopic substitution and contrast-variation methods. These characteristics distinguish NSE from X-ray-based techniques, in which scattering arises from the electron cloud and therefore scales with the atomic number.

As with all scattering methods, NSE simultaneously provides information on the timescale and the geometry — through Q — of the probed dynamics. This sets NSE apart from spectroscopic methods such as dielectric spectroscopy⁴⁴, susceptometry⁴⁵ or nuclear magnetic resonance (NMR)^{46,47}, which typically offer detailed temporal information but limited spatial resolution. NSE uniquely covers length scales from the Ångström to tens of nanometres, and timescales from picoseconds to hundreds of nanoseconds. Other neutron spectroscopies reach shorter timescales and smaller length scales, whereas light scattering^{48,49} probes processes in the hydrodynamic limit⁵⁰ at much larger length scales. A related technique, pulse gradient spin echo NMR^{47,51}, is also powerful for measuring diffusion but probes macroscopic length scales on the order of micrometres.

X-ray-scattering methods can access length scales similar to those of neutron scattering, but the accessible timescales differ markedly. Inelastic X-ray scattering^{52, 53, 54–55} typically achieves energy resolutions of ≈ 1 meV, corresponding to timescales of only a few picoseconds. With recent advances in beam coherence and detector technology at modern synchrotron sources, X-ray photon correlation spectroscopy (XPCS)^{56,57} can probe correlation times ranging from tens of seconds down to microseconds, and potentially shorter for selected samples⁵⁸. Resonant γ -ray techniques such as time-domain interferometry^{59, 60–61} and multiline spectroscopy quasielastic γ -ray scattering⁶² access timescales from sub-nanoseconds to hundreds of nanoseconds. These developments mean that modern X-ray-scattering methods now cover timescales adjacent to, and in some cases overlapping with, those accessible by NSE. They therefore provide naturally complementary methods. However, it is important to emphasize that the key characteristics of neutron scattering — sensitivity to magnetic scattering, hydrogen and isotopic composition — distinguish NSE from time-domain interferometry, XPCS and related X-ray-based approaches. In practice, NSE is most powerful when used in combination with these other experimental methods.

Thanks to these capabilities, NSE provides unique insight into a range of science problems and fields. Here, the main applications are discussed.

Liquids, glasses and confined molecules

As shown in the following, NSE is widely used to study amorphous molecular systems such as liquids, glasses and molecules confined within^{63,64} or adsorbed on solid matrices⁶⁵. These studies are performed at Q values beyond the small-angle region, in which the coherent scattering from large (>1 nm) structures, if present, would otherwise be dominant. This Q range is also accessible using other quasi-elastic neutron scattering (QENS) techniques, namely ToF and backscattering spectrometers. However, these instruments are generally limited to probing timescales up to ≈ 1 ns. At these length scales, the incoherent scattering contribution is often dominant, particularly for hydrogenated samples⁶⁶. NSE can therefore be used in combination with other QENS spectrometers to extend the explored dynamic range, for example as a function of temperature^{64,65} or timescale^{64,65,67}.

When incoherent scattering is dominant, NSE probes the single-particle dynamics, providing access to translational diffusion, as well as rotational or localized motions. Typical applications include studies of confined water^{63,68} and proton-conducting materials^{69, 70, 71, 72–73}. It should be noted, however, that in NSE the spin-incoherent scattering signal is reduced by a factor of three. In addition, the NSE signal is obtained as the ratio between Aecho and the static normalization factor that is approximately proportional to the static structure factor intensity. Consequently, small dynamic signals superimposed on a strong static component can be difficult to resolve⁶⁸. By contrast, ToF and backscattering QENS spectrometers exhibit peak signal-to-noise ratios on the order of 104 to 105 (defined as the ratio between the elastic peak intensity and the background for the resolution sample)^{74, 75, 76, 77–78}, making them better-suited to probe small signals^{79,80}. Additionally, $\Delta\lambda/\lambda$ is relatively large in NSE, resulting in limited Q resolution. For these reasons, studies of incoherent dynamics at wide scattering angles have historically been inefficient using conventional NSE. This situation has changed substantially with the advent of wide-angle NSE instruments, such as WASP at ILL, which compensate many of these limitations with a flux on the sample much larger than that on other ToF or backscattering spectrometers, and a detector coverage much larger than that of other NSE spectrometers.

In general, NSE data on liquids and glasses are analysed using an exponential or stretched-exponential model (equations 20 and 21 in Box 1). The dependence on Q and temperature of parameters such as amplitude, relaxation time and, when applicable, stretching exponent are examined^{81,82}. To reduce the number of free parameters, simplifying assumptions are often adopted; for example, the amplitude and stretching exponent may be assumed to be independent of Q and/or temperature⁸². The temperature dependence of the relaxation time is frequently parameterized according to viscosity^{82, 83, 84–85} or the timescale obtained using other methods such as, for example, dielectric spectroscopy⁸⁶ (Fig. 2a,b). If warranted by data quality, the presence of multiple relaxation processes can be accounted for using sums of exponential or stretched-exponential functions^{81,87} (equations 22 and 23).

Fig. 2

Normalized ISFs from liquid samples obtained by NSE and extracted parameters.

a, Normalized intermediate scattering function (ISF), $FNSE(Q,t)/FNSE(Q,0)$, of fully deuterated glyceline, a deep eutectic solvent composed by choline chloride and glycerol with molar ratio 2:1, measured at the structure factor peak, $1.4 \text{ \AA}^{-1}$, as a function of temperature. Continuous lines are fitted to a stretched exponential function⁸⁶ (equation 21). **b**, Data from part **a** form a master curve when the horizontal axis is scaled by the relaxation time (τ) measured in glycerol by dielectric spectroscopy⁸⁶. **c**, Normalized ISF of *m*-toluidine, measured by neutron spin echo (NSE) at the prepeak, the valley between the prepeak and the main structure factor peak, and at the main structure factor peak. Lines are fitted to a stretched exponential⁸² (equation 21). **d,e**, Normalized ISF of glass former $\text{CaO}_4\text{K}_0.6(\text{NO}_3)_{1.4}$ measured using the WASP spectrometer at various magnitude of the scattering vector (Q) values (part **d**) and temperatures (part **e**). Curves are fitted using the sum of an exponential and a stretched exponential function (equation 22, with $\beta_1 = 1$), with all parameters free⁸¹. **f**, Dependence of the fit parameters for $\text{CaO}_4\text{K}_0.6(\text{NO}_3)_{1.4}$ on temperature and Q , showing a modulation in phase with the structure factor⁸¹. β , stretching

exponent for the slowest relaxation process; τ_{slow} , relaxation time of the slowest relaxation process; f , amplitude of the slowest relaxation process; $I(Q,t)/I(Q,0)$ and $F(Q,t)/F(Q,0)$, normalized ISF; tF , Fourier time; $S(Q)$, static structure factor. Parts **a** and **b** reprinted with permission from ref. 86, AIP. Part **c** reprinted with permission from ref. 82, AIP. Parts **d–f** reprinted from ref. 81, CC BY 4.0.

Given the characteristics and limitations outlined above, NSE is most effectively used to study, in deuterated samples, the structural relaxation — commonly referred to as α -relaxation — which corresponds to the slowest relaxation process in amorphous systems^{83,84}. Here, structural relaxation is understood as the timescale associated with the rearrangement of molecular configurations over specific length scales. Typically, this relaxation is studied at the main peak of the static structure factor, which reflects the average interparticle distance and the dominant local structural motif. Nevertheless, NSE studies have been performed at other features of the structure factor, such as the prepeak⁸² (Fig. 2c) and the second structure factor peak^{81,82,88} (Fig. 2d–f).

Traditional NSE spectrometers are well-suited to probing coherently scattered dynamics at selected Q values over a broad time window. Such studies aim to elucidate how molecular structuring affects macroscopic transport properties, including mass transport (viscosity)⁸³ and charge transport (conductivity)^{89,90}. In many cases, the dynamics measured at the structure factor peak correspond to the same α -relaxation process observed using other techniques, and scale with the viscosity of the system. NSE thus provides valuable insight into the molecular origins of relaxation processes, including secondary relaxations also detected by other spectroscopic methods, such as dielectric spectroscopy⁸⁸. For example, it has been shown that dynamics associated with the prepeak are linked to the rearrangement of hydrogen bonds in transient molecular associates. These processes can give rise to weak dielectric signals, which are also observable via NMR relaxation^{91,92}. Moreover, such associate dynamics have been demonstrated to play a substantial role in determining the macroscopic viscosity of the system^{93, 94, 95, 96–97}. Many technologically and societally relevant liquids — including battery electrolytes^{98,99}, ionic liquids^{87,100,101} and deep eutectic solvents⁸⁶ — exhibit nanoscopic structural heterogeneities arising from molecular transient associates^{87,100,101}. NSE has been used to characterize the relaxation dynamics of these domains at intermediate length and timescales between the nanoscopic and macroscopic regimes^{82,86,87,91,97, 98, 99–100}. Information on the lifetime, diffusion and rearrangement of these associates is essential for understanding transport properties such as viscosity and conductivity, as well as emergent collective behaviour.

Structural relaxation dynamics has also been extensively investigated in polymer systems^{88,102}. For instance, NSE studies of polybutadiene at the first and second structure factor peaks enabled detailed modelling of secondary, localized dynamical processes¹⁰³. Measurements at the structure factor peak have also provided critical experimental benchmarks for theoretical descriptions of the glass transition^{82,83,85,103,104}. More recently, these concepts have been extended to lipid bilayer systems, for which NSE measurements of acyl-tail correlation dynamics at the structure factor peak have been shown to relate directly to membrane viscosity¹⁰⁵.

The WASP spectrometer has recently enabled NSE studies of molecular systems in a wide Q and tF range with unprecedented granularity. This makes it possible to probe dynamics not only at the peaks but also at the valleys of the static structure factor (Fig. 2d–f). New analytical strategies based on isotopic substitution allow coherent and incoherent scattering contributions to be disentangled, enabling, for example, selective studies of bulk water¹⁰⁶ or distinct components in ionic liquid mixtures¹⁰⁷. These advances have led to the identification of new dynamical processes in molecular liquids¹⁰⁸ and the observation that the temperature dependence of molecular dynamics varies with length scale and with the type of molecular rearrangement being probed⁸¹ (Fig. 2d–f). It has also been demonstrated that enhancements in ionic conductivity upon dilution of ionic liquid electrolytes are directly correlated with increased mobility at both microscopic and macroscopic length scales^{98,99}. Finally, the complementarity between wide-angle NSE and ToF spectroscopy has been highlighted in recent studies of collective and self dynamics in van der Waals liquids such as tetrahydrofuran^{98,99,109}.

Box 1 Fitting functions for the ISF measured by NSE

Exponential decay:

Stretched exponential decay:

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Double stretched exponential decay:

Double stretched exponential decay and constant:

Fickian diffusion:

Effective diffusion:

Polymers

Rouse:

in which l is the segment length, N is the number of segments, D is the polymer chain diffusion coefficient, τ_R is the Rouse time and W is the Rouse rate.

Rouse and reptation:

in which d is the reptation tube diameter.

Membranes' bending

Zilman and Granek modelling

in which α is a factor close to unity originating from averaging the angle between the wave vector and a vector normal to the bilayer surface. κ is the effective bending modulus measured by neutron spin echo (NSE), which is identified with the unrelaxed bending rigidity as^{208,209} follows:

in which κ_r is the relaxed, equilibrium bending modulus obtained by other, more macroscopic methods; d_{bilayer} is the hydrophobic bilayer thickness; and dn is the neutral surface height, which takes values between half and full monolayer thickness. Recent results suggest that dn is close to the monolayer thickness, implying that (ref. 19).

A scaling form can be obtained for the intermediate scattering function (ISF)

Thickness fluctuations:

in which Q_0 and ξ denote the Q value at which membrane form factor minimum appears and the width of the extension of the thickness fluctuations, which relates to the thickness fluctuation amplitude.

Sample geometry

Samples of liquids, glasses and confined molecule systems are typically measured in a wide angular range, and hollow cylindrical aluminium sample holders are commonly used. When single-particle dynamics in hydrogen-rich samples are of interest, fully hydrogenated materials are used to maximize the incoherent scattering signal^{1,110}. Partial deuteration can be used to selectively probe the single-particle dynamics of specific molecular moieties or transient associations^{82,86,97,111}. In such cases, careful selection of the probed Q range is required, as deuteration can substantially increase the coherent contribution. Conversely, full or partial deuteration may be used to enhance the coherent scattering signal at selected Q values in studies of collective dynamics^{82,92,112,113}. In all experiments, the possible mixing of coherent and incoherent scattering should be carefully considered, and measurements should be designed to favour one contribution whenever possible.

The sample thickness is usually constrained by neutron transmission requirements. To minimize multiple scattering effects in incoherent scattering experiments, a transmission of approximately 90% is typically targeted, so that the ratio between the probability of double-scattering and single-scattering events is 1:10, implying that roughly only 10% of the detected signal arises from double-scattering events¹¹⁰. The validity of this approximation must be carefully assessed for each experiment. As an illustrative example, for liquid water, a slab thickness of 0.3 mm yields approximately 90% transmission, whereas an annular geometry would require thickness of around 0.1 mm.

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Given a typical beam size of approximately 3 cm, less than 0.5 g hydrogenated material is generally sufficient. The optimal sample thickness scales with the hydrogen atom density.

For studies focusing on coherent scattering, the signal of interest is often localized within specific Q ranges, and the transmission requirements can be somewhat relaxed. As multiple scattering tends to be distributed broadly in Q , transmissions as low as 70% are sometimes acceptable. Nevertheless, the effects of multiple scattering must always be carefully evaluated, for example to ensure that double scattering from a structure factor peak does not generate a spurious peak. For these experiments, sample amounts of the order of few grams should be targeted.

For resolution measurements, either a null-scatterer such as $\text{Ti}_2\text{O}_8\text{Zr}$, which exhibits nearly Q -independent scattering, or the sample itself measured at sufficiently low temperature, is commonly used.

Magnetism

The scattering of thermal **neutrons** from electronic magnetic dipoles involves non-trivial rotations of the **neutron spin** about Q . Accounting for these rotations requires additional complexity in the experimental implementation of an NSE spectrometer. However, this complication comes with an important benefit: magnetic and nuclear scattering contributions can be separated experimentally in an unambiguous way, without relying on model assumptions. As a result, in materials with weak magnetic moments, the signal-to-noise ratio can be markedly improved, often making such studies feasible in the first place^{5,16,114}.

Historically, early applications of NSE **spectroscopy** to magnetism focused on the dynamics of **spin** glasses and the critical dynamics of isotropic ferromagnets near their phase transitions, topics that were of considerable interest at the time. Subsequently, geometric frustration emerged as a means to engineer magnetic materials exhibiting unusual low-temperature behaviour¹¹⁵. Examples include delayed freezing upon cooling or residual **spin** dynamics at low temperature, phenomena that arise from a macroscopically degenerate ground state commonly found in such materials. In this context as well, NSE **spectroscopy** provided key insights, as its time window overlaps more closely with the relevant energy scales than conventional inelastic **neutron** scattering techniques using triple-axis or ToF spectrometers, which typically probe dynamics in the terahertz range, appropriate for most internal processes in condensed matter³.

Spin ice materials $\text{Dy}_2(\text{Ti},\text{Sn})_2\text{O}_7$ and $\text{Ho}_2(\text{Ti},\text{Sn})_2\text{O}_7$ have attracted sustained interest as paradigmatic examples of geometrically frustrated magnets. The low-temperature **spin** dynamics — in which NSE can contribute most effectively — has largely been investigated with susceptometry⁴⁵, because this technique accesses comparable timescales. By extending **neutron** scattering sensitivity to slow **spin** dynamics (microseconds to nanoseconds), NSE measurements were able to approach the relevant low-temperature timescales in **spin** ices¹¹⁶. Because dysprosium has a large absorption cross-section for thermal and cold **neutrons**, most **neutron** scattering studies have focused on holmium-based **spin** ice systems (Fig. 3).

Fig. 3

Normalized ISF from magnetic scattering for **spin ice $\text{Ho}_2\text{Sn}_2\text{O}_7$ measured using the IN11C spectrometer.**

Curves are fitted using an exponential function (equation 20). The inset demonstrates the temperature dependence of the relaxation time (τ in equation 20). Data obtained from IN11C are complemented by backscattering data obtained using the backscattering silicon spectrometer (BASIS)⁷⁶ at the Spallation **Neutron** Source²⁴⁵. ISF, intermediate scattering function; Q , magnitude of the scattering vector; $S(Q,t)/S(Q,0)$, normalized intermediate scattering function. Reprinted with permission from ref. 245, IOP.

In broad terms, temperature-dependent **spin** dynamics in **spin** ice separates into two regimes: a high-temperature (temperature ≥ 10 K) thermally activated regime, and a low-temperature ice regime in which the dynamics are much slower, though not entirely frozen, and shows a much weaker temperature dependence. **Neutron** scattering experiments, including both NSE and ToF **spectroscopy**, identified the activation barrier in the high-temperature regime with the first crystal field excitation and established its origin in single-ion anisotropy. These measurements further demonstrated that **spin** dynamics is not collective, but single-ion and stochastic in nature¹¹⁶. In NSE

measurements of the ISF, this is reflected by single-exponential spin relaxation, an Arrhenius temperature dependence of the relaxation time, and a Q -independent characteristic timescale. Upon cooling into the low-temperature regime, the activation barrier becomes increasingly prohibitive; nevertheless, the spins do not freeze completely. This residual dynamics is understood in terms of creation and annihilation of emergent magnetic monopoles in a slowly fluctuating ambient field created by nearby spins.

As for the case of molecular liquids, the normalized ISF is typically fitted using either a simple exponential or stretched exponential function¹¹⁷ (equations 20 and 21). The dependence of the corresponding fit parameters on experimental conditions — most commonly Q and temperature — is then analysed.

Sample geometry

As a practical rule of thumb, NSE experiments on magnetic systems are generally feasible when the magnetic scattering contribution, under realistic experimental conditions, yields more than one count per second in the detector. Because nuclear scattering appears as depolarized scattering and therefore does not contribute to the NSE signal, a ratio of nuclear to magnetic scattering of roughly ≈ 10 to 50 can usually be tolerated. In practical terms, this typically requires sample masses of at least one gram and the complete absence of hydrogen, including trace amounts such as those arising from surface contamination. Even stoichiometric concentrations of deuterium, which has a small but not zero incoherent scattering cross-section, can render a magnetic spin echo experiment unfeasible.

Finding a suitable resolution sample is often very challenging, if not impossible, because the sample shape, size and neutron transmission must closely match those of the actual sample. Consequently, the most practical approach is usually to measure the sample itself at base temperature and to treat any dynamics within the NSE time window as effectively frozen. If observable residual dynamics persists down to base temperature, the conclusions that can be drawn from the experiment are correspondingly limited. In some cases, a non-magnetic analogue with the same geometry may be used as a reference, which is achieved by substituting the magnetic ion with a non-magnetic one. However, this approach requires the use of a π -flipper to recover an echo signal. Placing this flipper a few centimetres away from the sample can create an imbalance in the magnetic field integrals on either side of the sample, potentially introducing measurement artefacts that are difficult to correct.

Finally, partial depolarization of the neutron beam caused by strong internal magnetic fields within the sample constitutes an immediate experimental failure, because it affects the scattered polarization — the primary observable in NSE — in an unpredictable and uncontrollable manner.

Small-angle applications of NSE

NSE spectroscopy is often used to investigate the dynamics of large structures — such as polymer chains^{118, 119, 120, 121–122}, biological macromolecules^{7,119,123, 124–125} and self-assembled systems^{7,119,126} — on length scales of tens of nanometres. These experiments are typically performed in the small-angle scattering regime, in which coherent scattering from these mesoscopic structures is dominant. In this Q region, atomic granularity is less relevant, and it is therefore convenient to adopt a continuum description in terms of scattering length density (Supplementary Note 1), denoted as ρ_{sld} .

For a two-components system, the coherent ISF can be written as:

in which $\rho_{\text{sld},1}$ and $\rho_{\text{sld},2}$ are the scattering length densities of the two components, $K = (\rho_{\text{sld},1} - \rho_{\text{sld},2})$ is the contrast and V_1 is the volume occupied by component 1.

Assuming a collection of large scattering objects, the ISF may be expressed in terms of the position of their centres of mass ($\mathbf{r}_{\text{CM}}$) and the internal coordinates of constituent atoms, $\mathbf{b}_i$: $\mathbf{r}_i = \mathbf{r}_{\text{CM}} + \mathbf{b}_i$, $\mathbf{r}_i$ being the position of each atom. Within the decoupling approximation¹²⁷, this leads to:

in which

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The ensemble averages in equations 12, 13, 14 and 15 are taken over all orientations and configurations. The superscripts *coll* and *s* refer to collective and self-contributions, corresponding to correlations between different objects and within the same object, respectively.

For rigid, centrosymmetric macromolecules, the internal correlation simplifies to:

in which $P(Q)$ is the form factor, and equation 12 becomes:

which can be used to study the collective diffusion of nanoparticles or spherical proteins such as apoferritin¹²⁸. By identifying each monomer (or bead) as a scattering centre and using $P(0)=K^2V^2$, equation 17 can also be applied to investigate the internal (Rouse) dynamics of polymer chains.

For flexible and/or non-centrosymmetric macromolecules in the dilute limit, correlations between the motions of the centres of mass of different particles vanish, such that:

and consequently

which explicitly illustrates how NSE spectroscopy probes the internal dynamics of macromolecules.

Sample geometry

Experiments in the small-angle regime require prior knowledge of the scattering contrast between the sample and its background. Because scattering angles are small, flat sample geometries are typically chosen, with samples contained in quartz or custom-made flat cells with quartz, niobium or aluminium windows. Typical sample thickness ranges from 0.5 mm to 5 mm, depending primarily on the hydrogen content of the system, leading to sample volumes of 0.5 ml to 10 ml.

High hydrogen content reduces neutron transmission, necessitating thinner sample cells, whereas systems with low hydrogen content can be measured in thicker cells^{110,129,130}. Similar considerations to those used in small-angle neutron scattering (SANS)¹³¹ for optimizing sample thickness generally apply. Multiple scattering is usually not a concern, although very strong scattering at low Q or at the structure factor peaks can lead to double-scattering events and should be considered carefully.

In solutions, hydrogenated solutes are dissolved into deuterated solvents to maximize the coherent contrast while minimizing incoherent scattering. As in SANS¹³¹, contrast matching can be achieved by tuning the solvent scattering length density to match specific components of the sample, rendering them effectively invisible. This approach has been used, for example, to suppress scattering from nanoparticles, to investigate polymer nanocomposites^{132,133}, to mask selectively deuterated domains in proteins^{134,135}, to enhance scattering from surfactant films in microemulsions^{136, 137–138} or lipid headgroups in vesicles¹³⁹, and to isolate single-chain dynamics of polymers in complex macromolecular architectures^{140,141}. However, it should be noted that the use of mixed hydrogenated–deuterated solvents degrades neutron polarization and therefore reduces NSE signal quality.

Modern NSE spectrometers can perform successful experiments even in Q ranges in which the SANS scattering intensity is as low as 0.1 cm^{-1} , provided that coherent scattering dominates^{142,143}. Flipping ratios of the scattered beam above three are generally considered acceptable; below this value, experiments become extremely challenging or impractical.

Protein solutions

Proteins are large molecules composed of specific amino acid sequences folded into well-defined three-dimensional structures. Their biological function is closely linked to their dynamics, which span a wide range of motions, from large-scale domain rearrangements to localized diffusive, rotational and internal fluctuations, as well as low-frequency damped vibrations.

NSE data from protein solutions are most commonly analysed using a single-exponential decay of the ISF (Fig. 4). The relaxation rate is divided by Q^2 to obtain an effective diffusion coefficient $Deff(Q)$ (equation 25). In the dilute limit, $Deff(Q)$ is expected to be Q -independent and equal to the translational diffusion coefficient, expressed as $Deff(Q) = D$, corresponding to purely Fickian diffusion (equation 24), often matching values obtained from dynamic light scattering⁹⁵. Any Q dependence of $Deff(Q)$ reflects contributions from interparticle interactions, rotational motion and internal protein dynamics. Within the approximations underlying equations 12 and 19, and in the appropriate Q range and dilution, $Deff(Q)$ isolates these internal modes on top of single-particle diffusion.

Fig. 4

Protein dynamics in solution measured by NSE.

A, Normalized intermediate scattering function measured for mercuric ion reductase at a set of scattering wave vectors, Q , expressed in $\text{\AA}^{-1}$. Solid lines represent single exponential fits (equation 20). Data are shifted by a consecutive factor of 0.9 for clarity²⁴⁶. **B**, The effective diffusion coefficient $D_c(Q)$ ($Deff(Q)$ in equation 25) obtained by neutron spin echo (NSE) measurements as a function of Q for 10%, 17.5% and 25% mass-fraction lysozyme solutions at 25 °C (ref. 247). No internal dynamics is observed. **Ca**, Activation of domain motion in NHERF1 upon binding to the FERM domain. **Cb–Cd**, Experimental $Deff(Q)$ (equation 25) data for NHERF1-dFERM (open red squares) and NHERF1-hFERM (open blue squares) are compared with calculated rigid-body motions (parts **Cb** and **Cc**) and with calculations that include interdomain motions (part **Cd**). Solid red and blue squares indicate the diffusion coefficient measured by pulsed-field gradient NMR for NHERF1-dFERM and NHERF1-hFERM, respectively¹³⁴. $I(Q,t)/I(Q,0)$, normalized intermediate scattering function. Part **A** reprinted with permission from ref. 246, Elsevier. Part **B** reprinted with permission from ref. 247, IOP. Part **C** reprinted with permission from ref. 134, Elsevier.

These dynamic processes span multiple orders of magnitude in both space and time. NSE spectroscopy is a particularly powerful technique for the study of protein dynamics, with a unique sensitivity to slow, cooperative motions of protein domains. NSE covers a broad temporal window, from 1 picosecond to several hundred nanoseconds, and probes length scales extending up to the overall size of large proteins. As a result, the technique has been successfully applied to investigate a wide range of collective protein motions, including segmental flexibility in immunoglobulins^{144,145}, the influence of substrate binding on catalytic efficiency in enzymes^{146, 147–148}, domain–domain interactions underlying allosteric activation in signalling proteins^{134,135,149} and self-diffusion processes in protein solutions^{150,151}.

NSE studies have further demonstrated that protein conformational changes are governed not only by ligand binding but also by discrete thermal fluctuations, such that multiple conformational substates within an accessible energy range can be populated with significant probability. This behaviour is particularly evident in intrinsically disordered proteins, which lack a stable, well-defined three-dimensional fold and exhibit dynamical properties closely resembling those of conventional polymer chains^{152, 153–154}.

Biopharma

Monoclonal antibodies (mAbs) have revolutionized the pharmaceutical industry, particularly in the treatment of autoimmune disorders and cancer. These laboratory-engineered antibodies are designed to bind selectively to specific antigens, enabling precise therapeutic action. Prominent examples include rituximab for non-Hodgkin lymphoma, obinutuzumab for chronic lymphocytic leukaemia and follicular lymphoma, infliximab and adalimumab for inflammatory immune diseases, and trastuzumab for HER2+ breast cancer. More recently, mAbs such as casirivimab and imdevimab had a critical role in the treatment of COVID-19. Owing to their specificity and versatility, mAbs have become a cornerstone of modern medicine, with ongoing research expanding their therapeutic applications.

In dilute aqueous solutions, mAbs exist as dispersed monomers. As concentration increases, however, they tend to self-associate into clusters of preferred size and ordering. The characteristic cluster size often remains consistent over a broad concentration range¹⁵⁵. Therapeutic formulations frequently involve highly concentrated mAb

solutions, which can exhibit dramatically increased viscosity. This high viscosity poses a major challenge for formulation, injectability and delivery, particularly for subcutaneous administration.

By combining NSE spectroscopy with SANS and small-angle X-ray scattering (SAXS) and molecular simulations, it has been possible to directly observe the transition from monomeric to clustered states in mAb solutions as a function of concentration. One representative study demonstrated that cluster formation is directly responsible for the undesirable viscosity increase and that these clusters resemble micelle-like assemblies¹⁵⁵. This work further highlights the role of excluded-volume interactions in controlling viscosity, suggesting that rational modification of antibody primary structure could provide a pathway to engineer improved solutions.

A complementary study on IgG1-based mAbs investigated the structural and dynamic origins of viscosity changes under various physiochemical conditions such as pH, ionic strength and salt composition¹⁵⁶. In the presence of a specific salt, reversible and long-lived dimer formation was observed even in dilute solutions, with dimers adopting an elongated conformation. At higher concentrations, these dimers interact to form loosely bound, transient clusters, producing a hierarchical aggregation process that leads to pronounced viscosity enhancement. Similar behaviour across multiple mAbs systems suggests that reversible dimer formation may be a common feature of high-viscosity formulations. Notably, even subtle changes in the amino acid sequence were found to induce large variations in viscosity at elevated concentrations, underscoring the sensitivity of macroscopic solution properties to microscopic protein structure. These insights are highly relevant for the manufacturability, delivery, stability and therapeutic delivery of mAbs.

Polymers

One of the most successful application areas of NSE spectroscopy is the study of polymer dynamics, both in the bulk and in solution. Although this section provides a general overview, comprehensive treatments of NSE applications to polymer systems can be found elsewhere¹¹⁸. In general, NSE studies of polymers focus on systems in macroscopic equilibrium and are typically conducted in the small-angle scattering regime.

In the bulk polymer systems, NSE probes nanoscopic dynamics that is directly relevant to macroscopic rheological behaviour, whereas in solutions it provides access to both transport and local dynamics. Covering relaxation times between tens of picoseconds to hundreds of nanoseconds and length scales from nanometres to tens of nanometres, NSE uniquely bridges the gap between local segmental motion and global chain dynamics. When combined with complementary techniques such as rheology, dielectric spectroscopy and SANS, NSE enables a comprehensive and multiscale characterization of polymer motions.

A key advantage of neutron scattering lies in its sensitivity to light elements and the possibility of isotopic substitution. In homopolymers, introducing small fractions (10–20%) of hydrogenated chains into a deuterated matrix isolates the signal of individual chains, enabling the study of single-chain conformation by SANS and confirmation of Flory's random-coil model^{157,158}. Applying the same isotopic contrast scheme in NSE allows access to single-chain dynamics and has provided decisive experimental validation of de Gennes's reptation model^{159, 160–161}, first demonstrated by Wischniewski and co-workers¹⁶². This approach has since been extended to composites and confined systems^{132,162, 163–164}, in which contrast matching can isolate the polymer signal within complex environments.

For polymers with complex architectures — including diblock copolymers and bottlebrushes — selective deuteration permits component-specific dynamic analysis^{140,141,165}. In solution, contrast is achieved through deuterated solvents, while incoherent background from hydrogenated components must be minimized. Prior SANS characterization is essential to ensure proper sample preparation, sufficient intensity, dominance of coherent scattering and a clear understanding of which molecular entities contribute to the NSE signal.

Theoretical descriptions of polymer dynamics are commonly based on the bead-spring model, a coarse-grained representation in which polymer chains are described as Gaussian chains of beads connected by entropic springs. Each segment experiences both entropic restoring forces and stochastic forces, leading to a Langevin equation that is solved using normal-mode analysis. Using the Gaussian approximation (Supplementary Note 3), the single-chain ISF is obtained by treating each segment as a scattering centre with no internal structure (equation 26).

For unentangled polymer melts, chain dynamics is accurately described using the Rouse model^{118,166} (Fig. 5a). NSE experiments have shown that the relaxation of internal chain modes follows a Q^{-2} scaling and that the dynamic structure factor exhibits a stretched exponential decay, consistent with Rouse predictions^{162,167,168}.

Fig. 5

Single-chain polymer dynamics.

a, Single-chain dynamics measured by neutron spin echo of a polyethylene oxide sample with $M_w = 2.1 \text{ kg mol}^{-1}$ at $T = 413 \text{ K}$. Symbols represent data collected at various values for the magnitude of the scattering vector, Q , and the solid lines represent a global fit to all Q values using the Rouse model (equation 26). **b**, Single-chain dynamics measured by neutron spin echo of a polyethylene oxide sample with $M_w = 81 \text{ kg mol}^{-1}$ at $T = 400 \text{ K}$. Symbols represent data collected at various Q values, and solid lines represent a global fit to all Q values using the reptation model (equation 27). The data were fitted over the time range $t > 10 \text{ ns}$ and subsequently extrapolated to $t = 0$ (ref. 168). $S(Q,t)/S(Q,0)$, normalized intermediate scattering function. Reprinted with permission from ref. 168, ACS.

At sufficiently high molecular weight, polymer dynamics becomes dominated by entanglements, leading to reptation-like motion within tube-like constraints formed by surrounding chains (Fig. 5b). NSE measurements provide direct experimental evidence for the slowing down of chain motion relative to Rouse behaviour^{132,159,160,163}, as well as for additional processes such as contour length fluctuations¹⁶⁹ and constraint release¹⁷⁰.

In polymer blends and block copolymers, segmental dynamics is influenced by dynamical heterogeneity, microphase separation and interfacial effects. Selective isotopic labelling enables isolation of individual components, revealing substantial deviations from the dynamics of pure homopolymers. NSE has been used to quantify this heterogeneity by comparing the measured $F(Q,t)/F(Q,0)$ with the appropriate reference system^{171, 172–173}.

Microphase separation in block copolymers, caused by thermodynamic instability between chemically distinct blocks, results in well-defined nanostructured domains such as lamellae, cylinders and spheres, whose chain dynamics can be probed using NSE. Notably, NSE spectroscopy has probed the chain junction dynamics of lamellar diblock copolymer melts at the order–disorder transition temperature via selective hydrogen labelling of the junction point in deuterated diblock copolymers¹⁷⁴. A dynamic response of one order of magnitude faster than expected for Rouse dynamics was observed, driven by tension at interfacial walls near the order–disorder transition temperature^{174,175}. In ethylene oxide strand of polystyrene-block-poly(ethylene oxide) mixed with lithium bis(trifluoromethanesulfonyl)imide salt¹⁴⁰, increasing salt concentration was shown to increase monomeric friction increases with a concomitant decrease in tube diameter. This increase in monomeric friction is the same as in the homopolymer¹⁷⁶, whereas the decrease in tube diameter indicates temporary Li^+ ion-coordinated crosslinks between neighbouring chains.

Many materials rely on complex polymeric architectures, such as polymeric gels with chemically or physically crosslinked strands^{177,178}, microgels^{179, 180–181} or polymeric micelles formed by diblock copolymers with a rigid core and hairy corona¹⁸². Although SANS provides structural information such as correlation lengths, NSE adds crucial insight into molecular dynamics in these soft, disordered environments^{183,184}. Frozen inhomogeneities with minimal dynamics are revealed by a plateau in the normalized ISF¹⁷⁸. In dynamic systems, analysis of $F(Q,t)$ may require development of new models. Chain fluctuations are limited by crosslinking and the presence of charges¹⁸⁵, leading to modified Zimm dynamics. Advanced models that explicitly sum fluctuation modes account for constraints such as restricted mode types or altered internal relaxation due to friction, and are applicable to various systems, including polyelectrolyte solutions¹⁸⁶ and intrinsically disordered proteins^{179, 180, 181–182,187}.

One-component nanocomposites, such as polymer melts with chains grafted to silica nanoparticles, exhibit altered Rouse spectra owing to anchoring of one chain end^{188,189}. Across these systems, Q dependence and curve shape reveal key structural and dynamic molecular details. Combining NSE with backscattering and ToF

spectroscopy allows coherent and incoherent contributions to be resolved, even in complex systems such as rubbers¹⁹⁰.

Membranes

NSE is used to study the dynamics of amphiphilic membranes in solution. Such systems form monolayers or bilayers that separate hydrophilic and hydrophobic domains, and exhibit hierarchical structures spanning length scales from a few nanometres (bilayer thickness) to hundreds or thousands of nanometres (vesicles, lamellae or sponge phases). Prior SANS measurement is essential to determine structural length scales and interparticle interactions.

Membrane systems are typically prepared in deuterated solvents to maximize **neutron** contrast; moreover, selective deuteration allows specific components to be emphasized. For example, in oil–water microemulsions, contrast choices can isolate either domain mobility or membrane dynamics. Incoherent scattering from hydrogenated components must be carefully considered in all cases. NSE is particularly well-suited to probing translational diffusion, shape fluctuations and membrane undulations over timescales from picoseconds to microseconds.

In spherical microemulsions, membrane shape fluctuations — arising from bending moduli on the order of thermal energy^{191,192} — are enhanced near the form factor minimum^{138,193}. Although spherical micelles display only translational diffusion within the typical NSE time and Q range¹⁹⁴, worm-like micelles exhibit polymer-like bending fluctuations^{195, 196, 197–198}. When a membrane-like structure can be identified, for example, for bicontinuous microemulsions or large vesicles, the theoretical description developed by Zilman and Granek (equation 28) for two-dimensional membranes can be applied. It was first validated by dynamic light scattering¹⁹⁹ and subsequently by NSE²⁰⁰. The Zilman and Granek model has since become a standard framework for extracting membrane bending moduli from NSE data (κ NSE)^{138,193,201, 202, 203, 204, 205–206}.

Given the biological importance of lipid membranes, NSE studies increasingly focus on unilamellar vesicles. Because vesicles are large relative to the Q range, their undulations can be treated as those of a flat membrane²⁰⁷ in the limit of (in which R is the mean radius of the vesicles), and the dynamics due to membrane undulations can be modelled using a simple stretched exponential (equations 28 and 29). However, finite bilayer thickness introduces effects that need to be accounted to reconcile bending moduli obtained by NSE with those obtained by other methods^{208, 209–210}. For sufficiently high Q , (typically $Q > 0.05 \text{ \AA}^{-1}$) can be identified with the unrelaxed bending rigidity (refs. 208,209). In the framework of the polymer brush model²¹¹, is related to the relaxed, equilibrium, bending rigidity (equation 30). Additionally, overall vesicle translational diffusion dynamics needs to be taken into account by simple multiplication of a Fickian diffusion term (equation 24). With modern NSE spectrometers, confinement effects imposed by vesicle curvature have become observable, including restrictions on undulation wavelengths and sensitivity to membrane viscosity for small vesicles^{19,212,213}. When the vesicles do not satisfy the limit, the expression found in Granek et al.²¹² should be applied.

In addition to long-range undulations, deuterating the hydrophobic component NSE can detect membrane thickness fluctuations in both surfactant and lipid membranes^{137,139,214} (Fig. 6). These fluctuations, visible in the region of the membrane form factor minimum, can be modelled using (equation 32). Theoretical work by Bingham et al. attributes these fluctuations to membrane compressibility with viscous damping²¹⁵, in agreement with NSE observations^{137,139,214,216,217}.

Fig. 6

Membrane bending and thickness fluctuations in lipid membranes.

a, Normalized intermediate scattering (ISF) function measured using **neutron spin echo** of unilamellar vesicles of dipalmitoyl phosphocholine vesicles at 50 °C. Fits are to the Zilman and Granek model (equation 28). **b**, Relaxation rate (Γ) divided by Q^3 for distearoyl phosphocholine (DSPC) vesicles. Fits are to equation 32. Inset: normalized ISF plotted against the rescaled variable $t^{2/3}/Q^2$ (ref. 139) (equation 31). $I(Q,t)/I(Q,0)$, normalized ISF; Q , magnitude of the scattering vector. Reprinted with permission from ref. 139, APS.

Beyond elastic properties, NSE now provides access to membrane viscosity^{19,105,212,213,216,217}, which is important for understanding molecular transport and permeation in biological membranes.

Grazing incidence NSE of membranes

A specialized application of NSE involves grazing incidence conditions, in which scattering occurs via an evanescent wave that probes sample dynamics close to a flat, rigid interface^{218, 219–220}. Analogous to grazing incidence SANS for structural studies, grazing incidence NSE is used to probe interfacial dynamics, including membrane fluctuations of lamellar microemulsions under the constraint of a rigid wall²¹⁸, or polymer fluctuations of microgel particles²²¹ or brushes²²² fixed at the interface^{218, 219–220}.

The sample environment is similar to that used in neutron reflectometry, typically consisting of a thick silicon block with a liquid reservoir. A highly collimated neutron beam enters the silicon block and undergoes total reflection at the silicon–sample interface. Only the evanescent wave penetrates the sample and contributes to the scattering signal. By tuning the wavelength and incident angle, the penetration depth of the evanescent wave can be controlled, allowing selective probing of near-interface regions.

Confinement by rigid interface may substantially modify membrane undulation spectra or polymer dynamics at the interface^{218,223}. Because the probed volume is extremely small (on the order of tens of nanometres), the scattered intensity is correspondingly weak. Neutron optical elements such as resonators or waveguide structures coated onto the silicon surface can enhance interfacial intensity²²⁴. At pulsed neutron sources, neutron prisms combined with broad wavelength bands have been used to obtain uniform penetration depths across the full pulse²²⁵.

Reproducibility and data deposition

Calibrations

NSE measurements are self-contained and auto-calibrated (equations 7 and 8). The echo signal is divided by the polarization measured during the experiment through the up and down measurements, as well as by the instrumental resolution, which is systematically measured using standard elastic scatterers such as carbon powder or Ti₂O₈Zr. Hence, $F(Q,tF)$ is always normalized, which eliminates or minimizes effects due to imperfections of the instruments components, such as detector efficiency, finite incoming beam polarization and flipper efficiency, among others.

The wavenumber Q and Fourier time tF both depend on wavelength (equation 4). Given that neutron beams used for NSE have a broad wavelength distribution, the largest uncertainty in the independent variables Q and tF arises from the wavelength distribution; other sources of error, such as the scattering angle and the field integral, are substantially smaller. As a result, ISF curves from all instruments can be compared without further calibration, in that there is no need to carry reference samples from one instrument to another.

Although NSE is a powerful tool covering a unique region of (Q, t) space, it is an intensity-limited technique, and because of the small number of instruments available worldwide, it is often difficult to acquire beamtime to reproduce results. Facilities routinely calibrate their instruments to ensure correct operation, but to gain additional confidence in experimental data, results are often compared with those from other techniques such as SANS, neutron backscattering, bulk susceptibility or dynamic light scattering, in which at least partial overlap exists in the accessible phase space.

Distortions

NSE data can be very noisy if the contrast conditions are not chosen properly. NSE is more sensitive than other neutron spectroscopies to the simultaneous presence of both coherent and incoherent scattering, because these contributions tend to cancel each other (equation 9). On one hand, this characteristic can degrade the NSE signal; on the other, it reduces the risk of misinterpreting the results. The experiment must be carefully prepared, taking

into account prior information on the static structure factor. Once the experiment begins, the probed Q range must be selected with care, considering the polarization of the scattered beam.

As for all neutron scattering methods, multiple scattering can distort the NSE results. For typical samples, the transmission is easily kept above 90%, and multiple scattering is assumed to be negligible compared with other uncertainties. However, for each experiment, the acceptable level of multiple scattering should be evaluated.

The instrumental resolution of NSE is sensitive to the neutron path. The reference sample used to experimentally measure the resolution should mimic the shape of the sample as closely as possible. For this reason, the same sample cooled to a very low temperature is sometimes used as a resolution measurement.

Because the incoming wavelength distribution in NSE is broad, the Q resolution is comparable with $\Delta\lambda/\lambda$. This is usually appropriate for most applications of NSE, such as amorphous samples or diffuse magnetic scattering. However, the broad wavelength spread can cause problems in particular cases; for example, a Bragg peak from a polycrystalline material is smeared in Q , corrupting a wide Q range. This issue is minimized in ToF-NSE because the wavelength resolution is much better. Moreover, as tF depends on λ^3 , a $\Delta\lambda/\lambda$ of $\approx 15\%$ results in $\Delta tF/tF \approx 45\%$. This is usually not a problem because NSE results are typically exponentially decaying functions of time, but may become relevant in some cases⁷¹.

Data deposition

NSE data are always measured at neutron source facilities, which are publicly funded institutions. Raw data and metadata are stored according to each facility's rules. At the moment, there is no push towards a common NeXuS data format across instruments. Most facilities use an open-data policy model such as the ILL data policy²²⁶. After a measurement, those conducting the research have exclusive access to the data, and, after an embargo period (which differs between facilities), the data become open-access according to the FAIR (findable, accessible, interoperable and reusable) principles. Most facilities also allow data collection under proprietary rules.

Currently, each instrument has its own data acquisition strategy, raw data format and data reduction software. Interoperability is only achieved on the level of reduced data.

There are no databases for NSE spectra, because only few instruments exist. Moreover, differences in data formats between instruments would make the creation of a useful NSE-specific database rather difficult.

Limitations and optimizations

Limitations

The intensity of NSE has made dramatic progress since the early days, and it remains the only technique that provides nanoelectronvolt energy resolution. Nevertheless, typical counting times limit the applicability of the techniques to relatively large sample quantities that are stable over hours, and they severely restrict the possibility of performing parametric and in situ studies. In this sense, the main limitation of NSE is the slow rate of data acquisition. This limitation is compounded by the scarce availability of instruments. The slow data acquisition rate is common to all neutron scattering methods, and neutron spectrometers in general, owing to the low incoming beam flux even at the most intense neutron sources. The neutron beam flux on an NSE spectrometer ($\approx 10^8$ n cm⁻² s⁻¹) is order of magnitudes smaller than fluxes available using visible or X-ray photons. Typically, NSE experiments are carried out on carefully selected samples to investigate scientific questions that cannot be otherwise addressed.

Compared with other neutron spectroscopy methods, NSE also suffers from intrinsic limitations in detector coverage. This has been effectively managed by selecting NSE applications for which the relevant information is concentrated in a narrow Q range, such as single-chain polymer dynamics or bending fluctuations of phospholipid membranes. Recently, WASP demonstrated the possibility of substantially increasing detector coverage, thereby opening up new frontiers for NSE. However, the longest Fourier time achievable on WASP is not as long as on

Neutron spin echo spectroscopy

other NSE instruments, and its vertical angular coverage is only about 2° , whereas other QENS spectrometers have detector coverage of the order of up to three steradian.

NSE is almost exclusively a QENS method, best suited for probing relaxation processes that produce a broadening of the elastic line. By contrast, studies of inelastic features very close to the elastic line are extremely challenging and performed only rarely^{40,71}. This difficulty stems from the broad incoming wavelength distribution. In general, a different set-up^{5,6} or a dedicated instrument^{14,227,228} would be required to measure the narrow linewidths of inelastic peaks.

Another limitation of NSE arises from its nature as a Fourier transform technique, which imposes constraints on the signal-to-noise ratio. Here we define the signal-to-noise ratio as the ratio between the quasielastic or inelastic feature of interest and the total scattering intensity. In this definition, the signal-to-noise ratio in an NSE experiment corresponds to the ratio between the echo amplitude and echo average. On other neutron spectrometers, the signal-to-noise ratio is given by the height of the elastic line compared with the background. Values of the order of 104 can be achieved on backscattering or ToF spectrometers. On NSE, typical signal-to-noise values are better than 101. This figure of merit can only be improved slowly, following the square root of the counting time.

Finally, the applicability of NSE is limited by the presence of Bragg peaks. Because of the broad incoming wavelength range, Bragg scattering can distort the wavelength distribution, creating artefacts in the NSE signal. This problem can be mitigated using ToF-NSE.

Optimizations

NSE instruments are optimized for the characteristics of their neutron source. The most eloquent example is the SNS-NSE, the only ToF-NSE instrument, which exists due to the pulsed nature of the SNS. Instruments are also optimized to serve the user community within the ecosystem of other spectrometers at each facility. Therefore, IN15 and WASP have complementary characteristics.

The main figures of merit of NSE are its dynamic range — particularly the maximum accessible tF — and its data acquisition rate, with the two typically being inversely related. WASP represents a new and important development, providing a good dynamic window, access to slower dynamics than other neutron spectrometers and angular coverage more than ten times larger than on other NSE spectrometers. However, to fully take advantage of these characteristics, experimental design must match instrument capabilities.

NSE experiments, like any experiment, must be carefully prepared. For nuclear scattering, either coherent or incoherent scattering must dominate; isotopic substitution, particularly deuteration, is therefore a critical tool. The deuteration scheme must be appropriate for the scientific objective. For magnetic scattering experiments, the fraction of magnetic scattering must be sufficient not to be obscured by nuclear scattering (which constitutes the background as the echo average). Having a sufficient sample quantity, typically 1 g, is also essential to complete measurements within the allocated time. Finally, the system dynamics must match the dynamic range of the instrument. For these reasons, an NSE experiment often requires preparatory measurements using other techniques — often SANS (preferable to SAXS, although SAXS may suffice), polarized neutron diffraction, backscattering or ToF spectroscopy.

Outlook

Since its inception, NSE has evolved alongside advances in neutron technology, including improved neutron guides, velocity selectors, polarizers and analysers. These developments have increased neutron flux at long wavelengths and enabled access to longer Fourier times while maintaining reasonable counting times. Instrument flexibility has also improved, allowing more efficient and optimized data collection.

The use of NSE has also expanded through the development of new ideas and concepts, such as extended angular coverage implemented in instruments such as IN11C, SPAN and WASP. Regardless of the instrument geometry, beam correction elements remain essential. Finite beam size leads to variations in neutron path lengths, whereas magnetic field inhomogeneities arise from Maxwell's equations. Correction elements have reduced

inhomogeneities by a factor larger than 100 (refs. 23,229), and optimized magnetic field designs have decreased required corrections by a factor of three compared with simple solenoids^{41,42}.

Further progress is likely possible, although no immediate breakthrough is currently in view. This does not imply that NSE is no longer needed. If we restrict ourselves to diffusive processes, for which the inverse relaxation time follows an approximate DQ^2 dependence, the time-length scale diagram shows that NSE covers roughly eight orders of magnitude in diffusion coefficient D (Fig. 1a). It is therefore reasonable to expect that many open questions remain within this range, and that new ones will continue to emerge.

The adoption of machine learning and other artificial intelligence-based approaches could improve the efficiency of data acquisition, analysis and interpretation²³⁰. However, possibly because NSE is a low-throughput technique, no such implementations for data analysis have yet been reported, to the best of our knowledge.

Progress does not solely rely on improved instrumentation. Equally important is the ability to interpret higher-quality data and extract maximal information. At present, we are only beginning to fully take advantage of the opportunities offered by the improvements in instrumentation over the past decade. For example, membrane systems have been widely studied since the introduction of the Zilman–Granek stretched exponential model¹⁹⁷, and many such systems have been investigated using NSE. However, results have often remained semi-quantitative. Only with the current generation of NSE spectrometers has it become possible to develop complex models²¹² that enable full quantitative analysis of NSE data¹⁹. It is likely that this is not the end point of NSE data interpretation, as additional factors — such as membrane viscosity²¹³, tension, tilt²³¹ and intermonolayer friction — affect dynamics within the accessible NSE time window. Given that membrane dynamics extend beyond NSE-accessible timescales, the emergence of MHz XPCS instruments²³² offer the possibility of combining NSE and XPCS to obtain a comprehensive picture of membrane dynamics. This combined approach could enable the study of more complex and practically relevant systems.

A similar perspective applies to intrinsically disordered proteins, for which suitable models have only been developed and tested over the past decade^{152,187}. In the near future, such models are expected to be increasingly applied to biologically relevant systems²³³.

The application of NSE to biologically relevant systems is currently limited by two main bottlenecks. First, NSE instrument scientists are typically not experts in biology, while relatively few biologists are fully aware of NSE's capabilities. This article contributes to bridging that gap.

The second limitation concerns sample requirements and stability. A new NSE spectrometer at the European Spallation Source could substantially improve this situation. Owing to its long pulse structure and compact cold source, such an instrument could measure a sample over the entire relevant Q range using a single configuration, whereas reactor-based instruments typically require three to four configurations. A wide simultaneous Q range may also facilitate kinetic measurements. Additionally, the compact cold source could deliver comparable neutron flux onto smaller sample volumes, thereby enabling experiments on reduced sample sizes. Similarly, the planned EXPANSE spectrometer²³⁴ at the Second Target Station is designed for small samples and broad Q coverage, taking advantage of the short pulse and high brilliance of the source.

As measurements on smaller sample volumes become feasible, and with advances in the production of lipid nanodiscs²³⁵ — including deuterated variants — it may become possible to study membrane protein dynamics and their coupling to membrane behaviour. The resulting data will likely be highly complex, potentially exceeding the capabilities of purely analytical models. Although still underutilized, molecular dynamics simulations can directly compute $F(Q,t)$, and their accessible timescales are reasonably well-matched to those probed by NSE²³⁶.

Another comparatively modest technical improvement that could enable new science is the development of improved high-temperature sample environments. Despite technical challenges, the ability to routinely reach temperatures of 700 K or 800 K would open opportunities to study high-temperature diffusion phenomena in materials science^{72,73,237}. This is particularly valuable because NSE bridges molecular and macroscopic length scales, which are directly relevant to the performance of functional materials such as batteries and hydrogen storage systems.

New opportunities are afforded by WASP, which enables the study of weakly scattering samples on the mesoscale and allows simultaneous investigation of coherent and incoherent dynamics within the same system. These capabilities are only beginning to be explored¹⁰⁸. The mesoscale uniquely accessible by NSE fills the gap between molecular and macroscopic regimes. As a result, NSE is well-positioned to contribute to understanding how macroscopic properties emerge from molecular building blocks, thereby supporting the rational design of materials^{86,87,100,238}.

In this short Primer, we have focused on mainstream applications of NSE. However, this should not discourage exploration of more unconventional applications or novel NSE variants, as has been successfully demonstrated in the past^{40,239, 240–241}.

Notes

Supplementary information The online version contains supplementary material available at <https://doi.org/10.1038/s43586-026-00508-0>. **Disclaimer** Certain trade names and company products are identified in order to provide specific information regarding experimental procedures. In no case does this imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the products are the optimal tool for the stated purpose. **Publisher's note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations. **Related links** **ILL data policy:** <https://www.ill.eu/for-ill-users/user-guide/after-your-experiment/data-management> **IN15:** <https://www.ill.eu/for-ill-users/instruments/instruments-list/in15/description/instrument-layout> **iNSE:** <https://www.issp.u-tokyo.ac.jp/labs/neutron/inst/NSE/en/> **J-NSE Phoenix:** <https://mlz-garching.de/j-nse> **SNS-NSE:** <https://neutrons.ornl.gov/nse> **vNSE:** <https://www.nist.gov/ncnr/chtrns-nse-neutron-spin-echo-spectrometer> **WASP:** <https://www.ill.eu/for-all-users/instruments/instruments-list/wasp/description/instrument-layout>

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