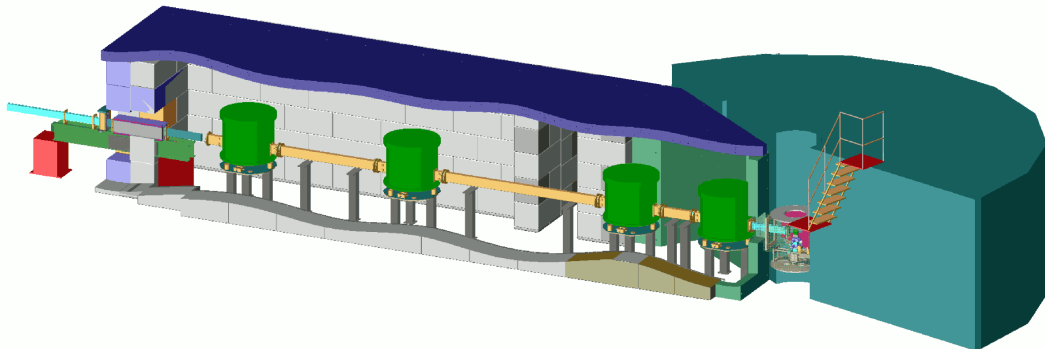# TOFTOF

Time-of-flight spectrometer

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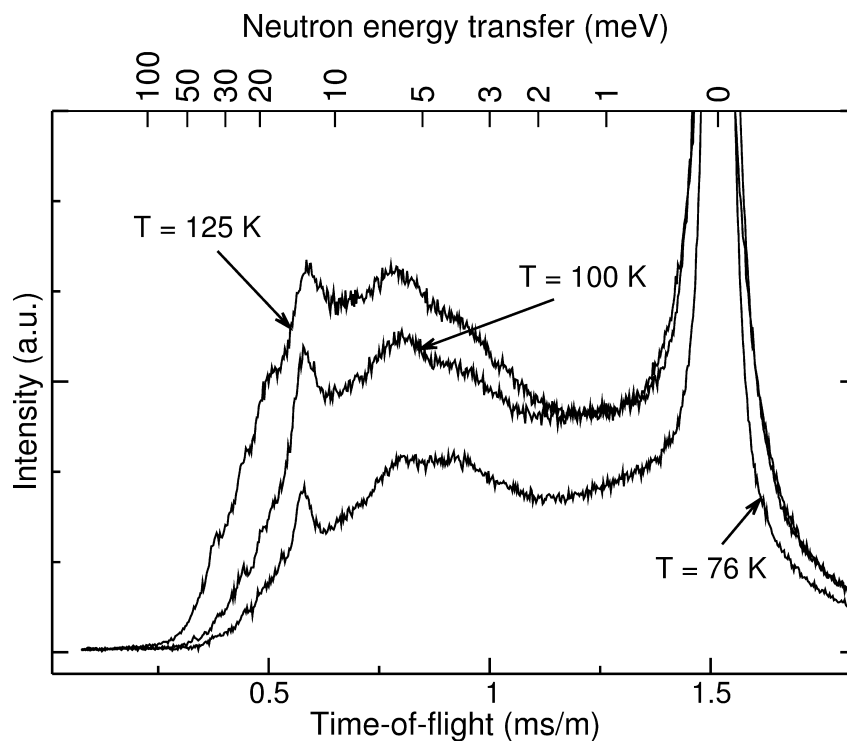
Contents

Fig. 1: Neutron time-of-flight spectrum of pentafluorotoluene, taken from [1]. Elastic scattering happens at energy transfer zero, quasielastic scattering in a region of approximately $0 \pm 1\,\text{meV}$, inelastic scattering at larger energy transfers.

Scattering experiments are carried out in order to obtain information about the structure and dynamics of the studied systems (e. g. crystals, liquids, nanoparticles). Optical microscopes are simpler to understand and operate but their resolution is limited by the wavelength of light. There are only few techniques which give access to the length scale of molecules and atoms. Of those, one of the most important is scattering which gives direct information on the disposition and motions of atoms weighted according to the scattering probability, or cross-section [3].

There are several kinds of scattering experiments, depending on the subject matter. In this experiment we want to introduce you to *quasielastic neutron scattering* (QENS). Quasielastic scattering is referring to a broadening of the elastic line in a spectrum. The extend of this broadening is approximately $1\,\text{meV}$. Whereas in inelastic scattering (which will not be further discussed in this experiment), discrete maxima or bands appear clearly separated from the elastic line. While one can gain information about the structure or periodic motions (i. e. phonons) of the sample using *diffraction* or *inelastic scattering*, respectively, it is possible to analyse non-periodic motions (e. g. diffusion) with quasielastic scattering.

Prior to the experiment, you should read and understand these instructions you won't have much time to do so during the experiment. You should also work out the question section. In the following discussion we will follow the path of the neutrons from the source over the sample to the detector. Then theory of scattering will be introduced, so that one can understand which information can be obtained from the scattered neutrons. Thereon the specific experiment will be explained.

To carry out the experiment you should bring: this introduction; your answers to the ques-

tions; paper and a pen. After having started the measurement of the reference sample, we will show you the spectrometer TOFTOF. Afterwards we will prepare a sample, which we then will measure. Finally, we will evaluate the data together.

1 Basics

1.1 The neutron source FRM II

In general there are two techniques produce neutrons for a scattering experiment – spallation and nuclear fission. During spallation, huge nuclei (e. g. lead) are bombarded with protons, subsequently split and, among others, emit neutrons. The FRM II is a nuclear reactor optimized for use as a neutron source. Here, ^{235}U captures a thermal neutron and thereby becomes unstable. The nucleus fissures and, among others, emits three fast neutrons.

These fast neutrons must be slowed down (moderated) to thermal energies, that is room temperature, in order to initiate a new fission. One neutron is needed for the fission, while the others will be used for the neutron scattering experiments. The moderation occurs in D_2O of about 300 K which encloses the core.

In order to further slow down the neutrons, and thereby match their energies to the ones of atomic motions, a tank containing liquid D_2 at 25 K is located close to the fuel element. From this *cold source* several neutron guides lead the neutrons to the instruments. Inside these guides, the neutrons are transported by total reflection at the inner walls. The time of flight spectrometer TOFTOF is located at the end of neutron guide 2a in the neutron guide hall.

1.2 The time-of-flight spectrometer TOFTOF

Cold neutrons move with a velocity of several hundred m/s. Hence one can determine the kinetic energy of the neutrons comfortably by a time of flight (TOF) measurement along a certain distance. If one sets the initial energy of the neutrons before the scattering event to a well-known value and measures the final energy (or velocity) after the scattering process, the energy transfer can be determined. Since the position of the detectors is fixed, the scattering angle is also known.

During time of flight spectroscopy the energy transfer is measured by a time of flight measurement of the neutrons. The advantage of the time of flight technique is that a huge range of momentum and energy transfer can be captured simultaneously.

TOFTOF is a multi chopper time of flight spectrometer with direct geometry [4]. This means that all neutrons have (more or less) the same energy before interacting with the sample. After being scattered by the sample, the energy transfer can be determined. Both, the tuning of the energy of the incident neutrons (their wavelength) and the determination of the energy of the scattered neutrons is done by time of flight.

The neutrons are directed to the spectrometer through a neutron guide, which has a supermirror coating. The end of the guide is double focusing.
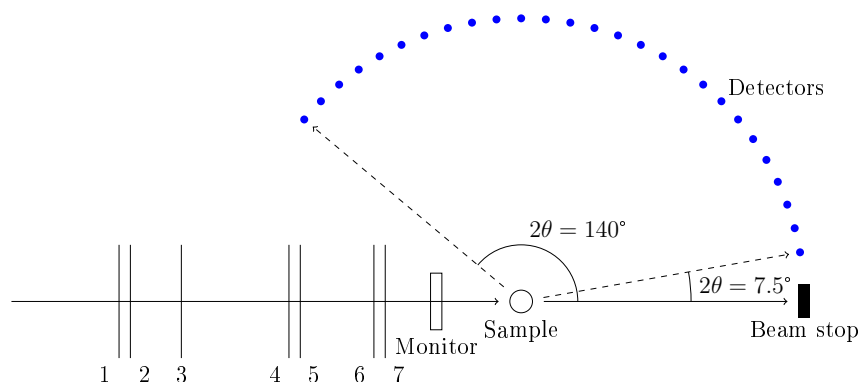
Fig. 2: Schematic drawing of TOFTOF. Following the neutron guide, first are paired choppers 1 & 2 which work together with 6 & 7 as velocity selector. Choppers 3 & 4 remove higher orders, 5 is the frame overlap chopper. The time needed for the neutrons to get from the sample to the detectors encodes their energy.

The primary spectrometer consists of seven rotating chopper discs which are placed in evacuated vessels (colored green on the cover page). The discs are made of carbon fiber composites and are coated with neutron-absorbing boron. On opposing sides, slits have been manufactured into the discs through which neutrons can pass. The first and last pair of choppers rotate in opposite direction each.

The incoming white neutron beam is pulsed by the first pair of choppers (choppers 1 and 2, pulsing choppers). This pulse still consists of neutrons with all velocities (or wavelength). Thus the pulse spreads along the way to the last chopper pair. These last two choppers (choppers 6 and 7, monochromating choppers) select a narrow range of wavelengths out of the pulse. The third and fourth chopper filter out higher orders (higher order removal choppers).

The fifth chopper is the frame overlap chopper. After the scattering process some neutrons fly towards the detectors, where they will be registered as a function of arrival time. It is essential that all scattered neutrons of one pulse are detected before the neutrons from the next pulse arrive. The overlap of slow neutrons from a pulse with fast neutrons of the following pulse inside the secondary spectrometer is called frame overlap. The frame-overlap-chopper blocks out several pulses, in order to avoid such an overlap.

The energy resolution (i.e. the width of the elastic line) is mainly determined by the chosen wavelength and the length of the neutron pulse that impinges on the sample. A good energy resolution can be achieved with a high rotational speed of the chopper discs (up to 22000 revolutions/minute). The energy resolution of the spectrometer can be changed continuously in the range from roughly $5\,\mu$eV to $5\,$meV (Fig. 3). By defining the energy uncertainty one can modify the time of observation in the range from roughly 1 ps to 1 ns.

The intensity of the incident neutron beam is recorded with a monitor, which is located between the primary spectrometer and the sample. An ionization chamber is used as a monitor, filled with fissile matter (^{235}U). The incoming neutrons trigger a fission and the high-energy nuclear fission products generate a clear voltage pulse, due to their high ionization density.

After passing the monitor, the neutrons hit the sample. Most of the neutrons are transmitted and are captured in the beamstop, but about 10 % of the neutrons are scattered in all possible directions. The neutrons that are scattered in the direction of the detector enter the flight chamber,
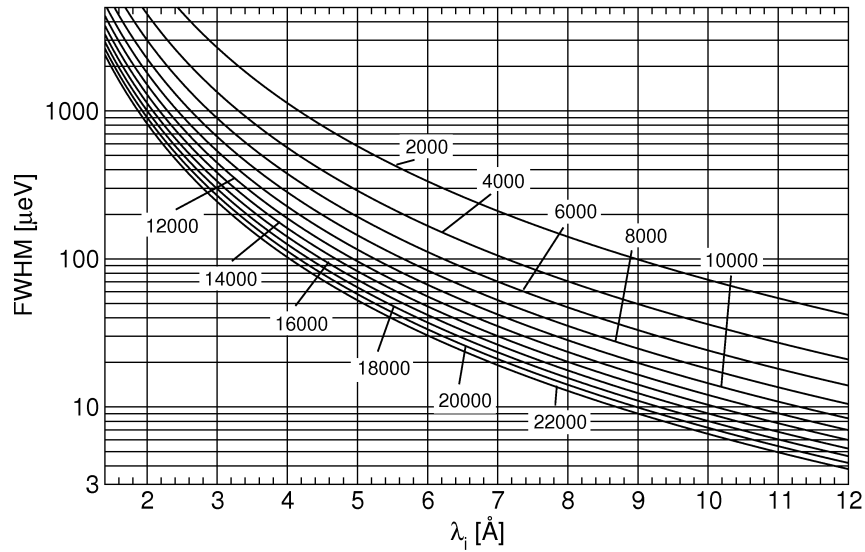
Fig. 3: Calculated energy resolution of the TOFTOF spectrometer shown for several chopper rotation speeds as function of the initial neutron wavelength. The chopper rotation speeds are given in rounds per minute (rpm) [4].

which occupies the space between the sample and detectors. The chamber is filled with argon in order to avoid unwanted scattering with air molecules.

Altogether 1000 ^{3}He-detectors (40 cm long and 3 cm in diameter) are placed tangential to the Debye-Scherrer-circle and also tangential to an imaginary spherical surface with a radius of 4 m around the position of the sample. Thus the flightpath from the sample to the detectors is 4 m long. The scattering angle 2θ covers a region from 7.5° to 140°. The detection of the scattered neutrons inside the ^{3}He-detectors occurs via a (n,p)-reaction. Hereby the neutrons are registered and tagged with a time stamp. The amount of detected neutrons is saved in time of flight bins for each detector in raw data files.

2 Theory

2.1 Cross sections

The probability that a neutron is scattered by a nucleus is denoted by the scattering cross section σ. It depends on:

1. the element

2. the isotope

3. the relative spin orientation of neutron and nucleus

Imagine a single crystal. The scattering cross section of every nucleus i can be decomposed into $\overline{\sigma} \pm \Delta\sigma_i$ where $\overline{\sigma}$ is the average over the whole crystal. This averaged part of the scattering cross section is called the *coherent scattering cross section*: scattered neutrons which can be

nuclide / element	σ_{coh} (barn)	σ_{inc} (barn)	σ_{abs} (barn)
^{1}H	1.758	80.27	0.3326
^{2}H	5.592	2.05	0.0005
H	1.760	80.26	0.3326
C	5.551	0.001	0.0035
N	11.01	0.5	11.51
O	4.232	0.001	0.0002
F	4.017	0.001	0.0096
Al	1.495	0.01	0.231
P	3.307	0.005	0.172
V	0.02	5.08	5.08

Table 1: Coherent and incoherent scattering cross sections as well as absorption cross sections of some selected nuclei or elements in their natural isotope composition, 1 barn = $100\,\mathrm{fm}^2$. Source: [3].

described by this part of the scattering cross section "see" a regular lattice and interfere to a regular scattering pattern.

In contrast, the $\Delta\sigma$ are distributed randomly throughout the crystal and the scattering of the neutrons which can be described by the $\Delta\sigma$ does not interfere to a special pattern. This effect is attributed to an artificial quantity, the *incoherent scattering cross section*.

The proton (^{1}H) has the biggest incoherent cross section of all nuclei we study normally (about 80 barn, cf. Tab. 1). For practical purposes, the big difference between the incoherent scattering cross section of the proton and the deuteron (^{2}H) is of enormous importance. Using isotope exchange, i. e. (partial) deuteration of molecules, specific parts of the sample can be masked.

Vanadium scatters at the employed wavelengths also mainly incoherently although not as strong as the proton.

2.2 Principle of a scattering experiment

At a scattering experiment, two important values are recorded (cf. Fig. 4):

- The scattering vector $\mathbf{Q}$ is defined as the difference between the wave vector $\mathbf{k}_f$ of the scattered wave (f as "final") and the wave vektor $\mathbf{k}_i$ of the incident wave (i as "initial"). The momentum gained or lost during the scattering process can be calculated by

$$\Delta\mathbf{p} = \hbar\mathbf{Q} = \hbar(\mathbf{k}_f - \mathbf{k}_i)\,. \tag{1}$$

However, the momentum transfer is commonly not noted. Instead, the scattering vector is commonly stated in units of inverse Ångstrom.

- The energy transfer ΔE is defined as the energy of the neutron after E_f and before E_i the
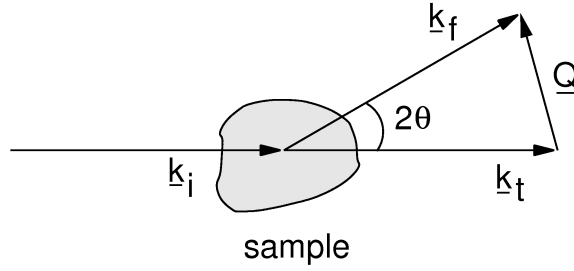
Fig. 4: Schematic representation of a scattering experiment. $\mathbf{k}_{i,f,t}$ are the wave vectors of the initial (incoming), final (scattered) and transmitted neutrons, respectively. $\mathbf{Q}$ is the scattering vector.

scattering process:

$$\Delta E = \hbar\omega = \hbar(\omega_f - \omega_i) = \frac{\hbar^2(|\mathbf{k}_f|^2 - |\mathbf{k}_i|^2)}{2m_n} \ . \tag{2}$$

The energy transfer is measured in meV. Often, ω is written incorrectly instead of $\hbar\omega$.

The absolute value of the wave vectors $\mathbf{k}$ is defined as $|\mathbf{k}| = 2\pi/\lambda$, with an refractive index $n \approx 1$ (which is a very good approximation for neutrons). However, the scattering vector cannot be measured directly, only the wave vector of the incident and scattered neutrons. Using the law of cosine one obtains a general equation for converting k_i and k_f to Q:

$$|\mathbf{Q}|^2 = |\mathbf{k}_i|^2 + |\mathbf{k}_f|^2 - 2|\mathbf{k}_i||\mathbf{k}_f|\cos(2\theta) \ . \tag{3}$$

In the case of elastic scattering, the energy transfer is zero. Hence $|\mathbf{k}_i| = |\mathbf{k}_f|$ simplifies the equation to

$$Q = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right) \tag{4}$$

where $Q = |\mathbf{Q}|$. Roughly speaking a distance d in direct space corresponds to a Q value

$$Q = \frac{2\pi}{d} \ . \tag{5}$$

Therefore one can extract information about the physical configuration of the nuclei in the sample by analyzing the intensity of the elastic scattering as a function of Q (the diffractogram), cf. Fig. 6. Furthermore the intensity at a certain value of Q as a function of energy (a spectrum) provides information about the motion of the nuclei (see Fig. 6).

2.3 Correlation & scattering functions

The position and the motions of the nuclei in any system can be described using correlation functions. It can be shown that these correlation functions are what is measured with scattering methods.
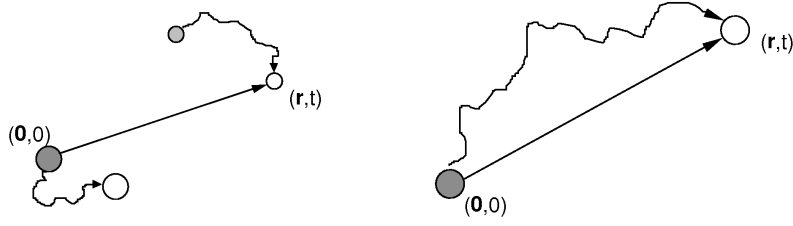
Fig. 5: Left: Pair correlation, right: self correlation. In the case of pair correlation, the second particle may be a different one than the first one but it doesn't have to.

The *pair correlation function* $G_{\text{pair}}(\mathbf{r}, t)$ gives the probability to find a particle j at time t at the place $\mathbf{r}$ if this or another particle i was at time $t = 0$ at the origin $\mathbf{r} = \mathbf{0}$, as shown in Fig. 5. The pair correlation function is

$$G_{\text{pair}}(\mathbf{r}, t) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \int \langle \delta\{\tilde{\mathbf{r}} - \mathbf{R}_i(0)\} \cdot \delta\{\tilde{\mathbf{r}} + \mathbf{r} - \mathbf{R}_j(t)\}\rangle \, \mathrm{d}\tilde{\mathbf{r}} \,, \tag{6}$$

with the number of particles N, an integration variable $\tilde{\mathbf{r}}$ and the place $\mathbf{R}_j(t)$ of particle j at time t. The angle brackets $\langle\rangle$ denote an ensemble average.

The *self correlation function* or *auto correlation function* $G_{\text{self}}(\mathbf{r}, t)$ gives the probability to find one particle at time t at place $\mathbf{r}$ if this very particle was at time $t = 0$ at the place $\mathbf{r} = \mathbf{0}$, see again Fig. 5. It is defined as

$$G_{\text{self}}(\mathbf{r}, t) = \frac{1}{N} \sum_{i=1}^{N} \int \langle \delta\{\tilde{\mathbf{r}} - \mathbf{R}_i(0)\} \cdot \delta\{\tilde{\mathbf{r}} + \mathbf{r} - \mathbf{R}_i(t)\}\rangle \, \mathrm{d}\tilde{\mathbf{r}} \,. \tag{7}$$

In the following, we will assume that the samples are powder samples or liquids (i. e. not single crystals) and will therefore use the absolute value of $\mathbf{r}$, r, instead of the vector.

It is possible to calculate the pair and self correlation function from the scattered intensities. Roughly, the calculation is as follows:

From the intensity of the scattered neutrons measured as function of momentum and energy change, one obtains the *double differential scattering cross section* which can be seen as the sum of a coherent and an incoherent part:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'} = \frac{k_f}{k_i} \frac{N}{4\pi} \left(\sigma_{\text{coh}} S_{\text{coh}}(Q, \omega) + \sigma_{\text{inc}} S_{\text{inc}}(Q, \omega) \right) \,. \tag{8}$$

It denotes the probability that a neutron is scattered into the solid angle $\mathrm{d}\Omega$ with an energy change $\mathrm{d}E'$. N is the number of scattering nuclei and $S(Q, \omega)$ is called the *scattering function*.

The Fourier transform in time and space of the coherent scattering function $S_{\text{coh}}(Q, \omega)$ is nothing but the pair correlation function $G_{\text{pair}}(r, t)$ and the Fourier transform in time and space of $S_{\text{inc}}(Q, \omega)$ is the self correlation function $G_{\text{self}}(r, t)$.

Three functions are important:

1. the *correlation function* $G(r,t)$

2. the *intermediate scattering function* $I(Q,t)$ which is the Fourier transform (from r to Q) of $G(r,t)$

3. the *scattering function* $S(Q,\omega)$ which is the Fourier transform (from t to ω) of $I(Q,t)$

All of them exist in two versions, considering pairs of particles (pair correlation function) or only one particle (self correlation function).

For the intermediate scattering function $I(\mathbf{Q},t)$ one can obtain further expressions – for a pair correlation

$$I_{\text{coh}}(\mathbf{Q},t) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \left\langle \mathrm{e}^{-\mathrm{i}\mathbf{Q}\mathbf{R}_i(0)} \mathrm{e}^{\mathrm{i}\mathbf{Q}\mathbf{R}_j(t)} \right\rangle \tag{9}$$

and for the self correlation function

$$I_{\text{inc}}(\mathbf{Q},t) = \frac{1}{N} \sum_{i=1}^{N} \left\langle \mathrm{e}^{-\mathrm{i}\mathbf{Q}\mathbf{R}_i(0)} \mathrm{e}^{\mathrm{i}\mathbf{Q}\mathbf{R}_i(t)} \right\rangle \ . \tag{10}$$

At neutron spin echo spectrometers, the intermediate scattering function is measured – all other neutron scattering spectrometers, including TOFTOF, measure the scattering function.

At TOFTOF, we mainly probe the non-periodic motions in disorded materials, for instance diffusion processes in liquids. If a scatterer performs several motions simultaneously (but independently from each other), the resulting incoherent scattering function is a convolution in energy space of the single scattering functions, for example

$$S_{\text{total}}(Q,\omega) = S_{\text{diffusion}}(Q,\omega) \otimes S_{\text{internal motion}}(Q,\omega) \ . \tag{11}$$

As a convolution corresponds to a multiplication after Fourier transform, one can also write

$$I_{\text{total}}(Q,t) = I_{\text{diffusion}}(Q,t) \cdot I_{\text{internal motion}}(Q,t) \ . \tag{12}$$

If two scatterers perform two motions independently from each other and both cause incoherent scattering, the recorded total incoherent scattering function is simply the sum of the two scattering functions, for example

$$S_{\text{total}}(Q,\omega) = S_{\text{solute}}(Q,\omega) + S_{\text{solvent}}(Q,\omega) \ , \tag{13}$$

which is also a sum after Fourier transform to the intermediate scattering function.

This decomposition of the scattering functions into parts is *very* important.

Due to the limited number of supporting points it is not possible to obtain the correlation function by numerical Fourier transform of the measured scattering function. Therefore, one proceeds the other way round: After inventing a plausible correlation function, one performs a Fourier transform of this theoretical function to a scattering function and checks if this can describe the data.

The hereby obtained theoretical scattering function $S_{\text{theor}}(Q,\omega)$ is fitted to the measured scattering function $S_{\text{meas}}(Q,\omega)$ after convolving the theoretical scattering function with the measured instrumental resolution. The instrumental resolution is often determined using a vanadium sample which is an elastic, incoherent scatterer.

3   Experiment

3.1   The system

In this experiment we will study the diffusive motions of molecules, e.g. *n*-alkanes or salt solutions. By analyzing this system we want to learn more about the mechanism of molecular self-diffusion, i.e. internal motions of the molecules and long-range diffusion processes.

3.2   Modelling the motions

Molecules in general are by far too complex to come up with a scattering function which describes all the motions correctly. Therefore, very simplified models are used. Assuming that the molecule itself is rigid and moves as a whole, one obtains the scattering function

$$S_{\text{diffusion}}(Q, \omega) = \frac{1}{\pi} \frac{|\Gamma_d(Q)|}{\omega^2 + \Gamma_d(Q)^2} \; , \tag{14}$$

a Lorentzian with a Q-dependent width $|\Gamma_d(Q)|$. If the diffusion follows exactly Fick's law, one obtains

$$|\Gamma_d(Q)| = D \cdot Q^2 \tag{15}$$

with the diffusion coefficient D which is normally given in m^2/s.

Deviations from this ideal $\propto Q^2$ law indicate that the observed process is not ideal Fickian diffusion. A constant (too large) value of Γ_d at small Q can be a sign of *confinement*: the molecule cannot escape from a cage formed by the neighbouring molecules. If the width Γ_d goes towards a constant value at large Q, this can be a sign of *jump diffusion* which should rather be named *stop-and-go diffusion*: the molecule sits for some time at a certain place, then diffuses for a while, gets trapped again, ...

Try to fit the data with one Lorentzian. If this model does not describe the data satisfactorily, the assumption of a rigid molecule was probably not justified. The scattering function for a localized motion can be written as:

$$S_{\text{intern}}(Q, \omega) = A_0(Q) \cdot \delta(\omega) + (1 - A_0(Q)) \cdot \frac{1}{\pi} \frac{|\Gamma_i|}{\omega^2 + \Gamma_i^2} \; , \tag{16}$$

that is the sum of a delta-function and a Lorentzian (confer also figure 6). $|\Gamma_i|$ gives the frequency of the motion, $A_0(Q)$ is called the *elastic incoherent structure factor* (EISF) and it gives information on the long time average position of the scatterer, in first approximation the size of the localized motion.

As we assume that the molecule performs a local motion and long-range diffusion simultaneously but independently from each other, we have to convolve the two functions with each other. The result is the sum of two Lorentzians:

$$S(Q, \omega) = F(Q) \cdot \left\{ \frac{A_0(Q)}{\pi} \frac{|\Gamma_d(Q)|}{\omega^2 + \Gamma_d(Q)^2} + \frac{1 - A_0(Q)}{\pi} \frac{|\Gamma_d(Q)| + |\Gamma_i|}{\omega^2 + (|\Gamma_d(Q)| + |\Gamma_i|)^2} \right\} \; . \tag{17}$$

3.3 The experiment itself

We might either produce a sample together or fill an existing sample into the aluminium hollow cylindrical container or a flat aluminium container. This sample is then measured at TOFTOF, additionally a vanadium standard and the empty aluminum container will be measured. The length and number of measurements will have to be adjusted to the available time, it will be necessary to use some measurements of the preceding groups.

You will do all sample changes in the presence of a tutor who explains the procedure in detail.

3.4 Data reduction

The instrument saves the number of counts as a function of scattering angle and time-of-flight, $N(2\theta, \text{tof})$. The next step is the data reduction which applies several corrections and transforms to get rid of many instrument-specific properties of the data and convert them to a scattering function $S(Q, \omega)$.

Data reduction (and later on also data evaluation) is done using the program Mantid Workbench [5]. On the Desktop lauch the icon `Mantid Workbench`. Mantid Workbench is used in many large scale facilities and it includes a variety of instrument routines, including a TOFTOF data reduction routine. A detailed description of how to launch and run the routine is available at the instrument.

Mantid Workbench is structured in *workspaces*. A workspace contains all necessary data like the time of flight/energy transfer of the neutron, its 2θ/Q - values and the intensity. It also contains so called metadata, i.e. information about the measurement settings or sample conditions (e.g. temperature). Any operation on the data takes as an input a workspace and the output is stored in another workspace.

Raw data files that have been measured under the same conditions (e.g. temperature) can be added and treated as one data set. This will be done in the loading routine. After reading the data files, the raw data $N(2\theta, \text{tof})$ are normalized to the incoming neutron flux. The empty can measurement is subtracted from the data and the sensitivity of each detector is calibrated using the vanadium standard measurement. As vanadium is an incoherent scatterer, it should scatter the same intensity in all directions. The only effect which causes deviations from an isotropic scattering is the Debye-Waller-factor (DWF) which is well-known and can be corrected. This is followed by the calculation of the energy transfer from the time-of-flight so that one obtains $S(2\theta, \omega)$.

The next step is to calculate the momentum transfer Q from the scattering angle 2θ and the energy transfer ω using equation (3). During this step, we obtain about 1000 spectra with relatively low statistics each and a varying value of Q as the energy transfer varies. To get a better statistics and to have spectra which have the same Q for all values of energy transfer, the 1000 spectra are grouped into about n spectra of constant ΔQ in the same routine. The binning parameters can be set in TOFTOF data reduction routine.
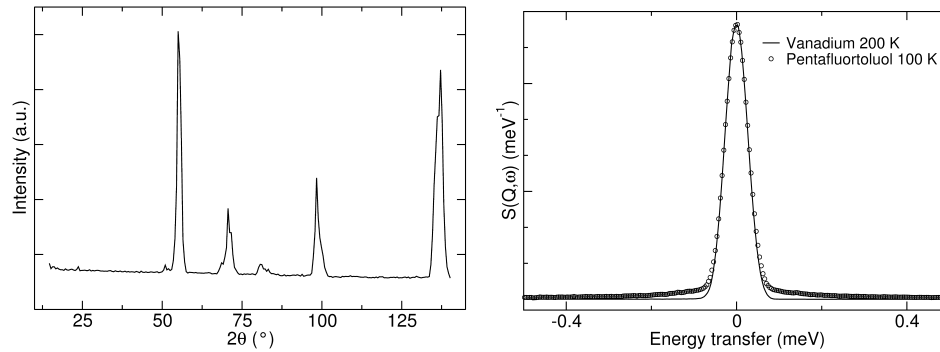
Fig. 6: Left: Neutron diffraction patterns of solid pentafluortoluene at $100\,\mathrm{K}$ ($\lambda_i = 6\,\text{Å}$), taken from [1]. If the scattering vector is a reciprocal lattice vector, the positive interference of neutron waves yields a maximum in the scattered intensity. The sharp features in the diffraction pattern indicate an ordered lattice. Right: The spectra $S(Q, \omega)$ of pentafluortoluene ($\circ$) and vanadium (–) at a momentum transfer of $Q = 1.1\,\text{Å}^{-1}$, cf. also [1]. The solid sample shows only an internal motion, can therefore be described by equation 16.

3.5   Data evaluation

For a quantitative analysis, fit the spectra with the functions given in section 3.2. For this purpose, a fit-routine in Mantid Workbench can be used. For the fit, the binned data sets of $S(Q, \omega)$ for both the sample and the vanadium resolution measurement are required since the theoretical functions have to be convolved with the experimental resolution. Both data sets will have been created during the data reduction routine. Plot the data set you want to fit, and evoke the Fit Function Routine (for a single spectra) in Mantid Workbench. Using the *Add Function* command, you can build the appropriate fit function, e.g.

$$S(Q, \omega) = Convolution\left[Resolution; (DeltaFunction + Lorentzian)\right] + Linear Background$$
$$(18)$$

The *Multi data set fitting* interface can be used to do a (sequential) fit for all Q-values in the data set. Judge the fit quality by the reduced χ^2 and by visually inspecting the fits together with the data. Plot the obtained parameters for the width, Γ, as function of Q^2 and determine the diffusion coefficient.

If you measured the sample at different temperatures, repeat the procedure for all of them.

4   Questions to be answered *before* the experiment

1. Do you expect the vanadium sample to be activated by the neutron beam? What about the aluminium container with the real sample? (2 min)

2. The vanadium standard sample at TOFTOF is a hollow cylinder with an outer diameter of 22.5 mm and a height of 65 mm. The wall thickness is 0.6 mm. Which fraction of the neutrons that hit the vanadium will be scattered? How big is the transmission?

3. Why do the samples measured at TOFTOF mostly have a transmission of about 90 %? How can the transmission be adjusted? (3 min)

4. The substance to be measured is filled in a gap between the inner and the outer cylinder of the sample container. The inner diameter of the outer cylinder is always 22.5 mm, the inner cylinder can be chosen to have either 22.1 mm or 22.3 mm outer diameter. The height of the cylinders is 65 mm. How large is the sample volume for the two different inner cylinders? Which inner cylinder would you use? (5 min)

5. Please note where this handout could need improvement. (5 min)

5   Questions to be answered *during* the experiment

1. When measuring water-based samples, H_2O is most often replaced by D_2O when the water is not the subject of the study. Why? The signal of the solvent has to be subtracted in both cases! (2 min)

2. Why is the sample container made of aluminum? (2 min)

3. The Vanadium standard sample at TOFTOF (hollow cylinder, 2 cm outer diameter, 0.6 mm thickness) is a "7% scatterer", meaning that it transmits 93% of the neutrons. In the moment, TOFTOF has 1000 neutron detectors with an active area of 40x3 cm each in 4 m distance from the sample. Estimate the efficiency of the monitor detector using the *Monitor rate* and *Signal Rate* given by the control program. (5 min)

4. To calculate the energy of neutrons in meV with a well-known wavelength given in Å, one can use a formula

$$E \approx \frac{a}{\lambda^2} \, . \tag{19}$$

Determine a numerical value for a. How big is the initial energy E_i of the neutrons in the current experiment? (5 min)

5. What is the maximal energy transfer from the neutron to the sample? (1 min)

6. What is the maximal energy transfer from the sample to the neutron? (1 min)

7. Draw at least six scattering triangles (as shown in Fig. 4) for these points in the dynamical range:

   • Elastic scattering with a scattering angle of 7.5°; with a scattering angle of 140° (the first & last detector at TOFTOF)
   • Same scattering angles with neutron energy gain
   • Same scattering angles with neutron energy loss

   (6 min)

8. Locate those points in this dynamic range plot and determine which area in this plot is accessible in the current scattering experiment. (5 min)
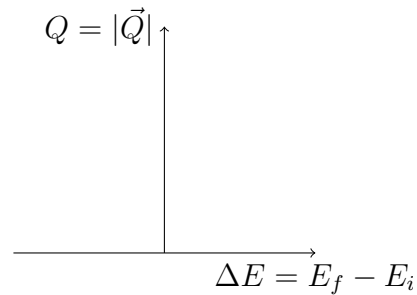
$$Q = |\vec{Q}|$$

$$\Delta E = E_f - E_i$$

Fig. 7: Dynamic range plot.

9. How can you distinguish coherent and incoherent scattering in the diffraction pattern? Which information can you extract from the spectra when they are caused by coherent or incoherent scattering, respectively? (2 min)

10. Why do we measure Vanadium? (three reasons; for one it is important that Vanadium scatters neutrons incoherently, for two it is important that the Vanadium signal does not have a quasielastic broadening) (6 min)

11. Assume that the scatterers in your sample are partially trapped. They diffuse inside a "cage" until they find a hole through which they can escape. How do the intermediate scattering function $I(Q,t)$ and the scattering function $S(Q,\omega)$ look like? (5 min)

6   Constants

$$m_n = 1.675 \cdot 10^{-27} \, \text{kg} \tag{20}$$

$$h = 6.626 \cdot 10^{-34} \, \text{J} \cdot \text{s} = 4.136 \cdot 10^{-15} \, \text{eV} \cdot \text{s} \tag{21}$$

$$\hbar = 1.055 \cdot 10^{-34} \, \text{J} \cdot \text{s} = 6.582 \cdot 10^{-16} \, \text{eV} \cdot \text{s} \tag{22}$$

$$e = 1.602 \cdot 10^{-19} \, \text{C} \tag{23}$$

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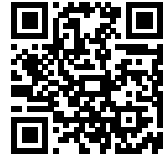
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