Questions:

high resolution spectrometers

Student's Name:

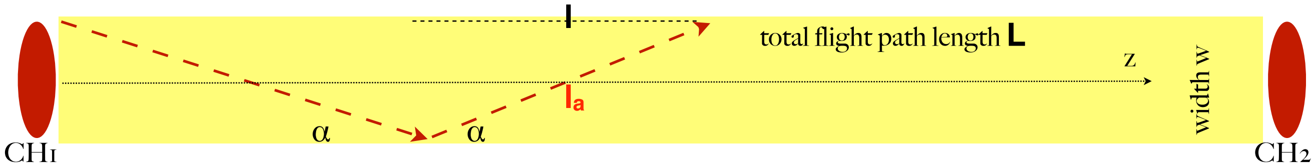
Course Name

The aim of this question is to get a feeling for the energy resolution of different spectrometer types: time-of-flight (TOF), backscattering (BS) and spin echo (NSE) spectrometers.

All the following calculations will be considered for a **neutron wavelength of λ=6.3 Å**. Planck's constant is h=6.6225 10^{-34} Js, sometimes usefully expressed as h=4.136 μeV ns. Neutron mass m_n=1.675 10^{-27} kg.

Calculate the neutron speed v_n in [m/s] and the neutron energy in μeV. v_n=630 m/s; En= 2080 μeV.

TOF:



All contributions to the energy resolution in time-of-flight can be formulated as time uncertainty Δt/t. We consider only the primary spectrometer (before sample) and aim for an energy resolution better than 1μeV.

Show first that Δ/E=2Δt/t (express E as fct. of v and assume Δs =0): **E=**________and with Δs=0:
ΔE=_________, which results in **ΔE/E**=-_______.

Several contributions add to the neutron flight time uncertainty Δt. To simplify, let's consider a chopper spectrometer with flight path L between two choppers as sketched in the figure and let's first look at neutrons flying parallel to z. **Calculate the flight time along path L**: T_0~ ______ s. If we want to get an **energy resolution of 1μeV, this corresponds to ΔE/E** ~ ________for 6.3Å neutrons. This can give us an idea for the **maximum allowed flight time difference along L: ΔE/E_0*T_0/2 ~** ____________μsec

For the reflected neutrons estimate the max. flight path differences in a super-mirror guide with m=2 coating and width w. The critical angle α (maximal reflection angle = half divergence) in such a guide is **α ~ 0.1° m λ =** _____°. **Estimate the flight path difference** with respect to neutrons which fly parallel. One way is to show that **ΔL/L = (1/cos α)-1** and thus the resulting **ΔL/L=**_________ = Δt/t and therefore **ΔE/E~** _________. **l =** _______; **l_a =** ______; **l/l_a** = ___________ independent of w; **ΔL = n*(l_a-l) =** _____________ and thus ΔL/L = (1/cos α)-1. We see that this contribution is not critical.

Another contribution is the **chopper opening time** which leads to a **spread in neutron velocity** and thus to flight time differences dt. In order to reach similar **Δt/t = Δv/v** as above one needs fast rotating choppers delivering short pulses. If ch1 releases at t=0 an arbitrarily sharp pulse of white beam, then the ch2-delay T corresponding to v_0 and the ch2-opening time determines Δv/v. We want again **1μeV energy resolution** and the corresponding **Δv/v_0=Δt/T=**________. The **chopper opening time must then be t_{ch2} < 1/2*(1μeV/E_0)*L/v_0 =** ______**[s/m] *L [s].** Δt_{ch2} = β/360./freq, where β is the chopper window opening and β/360 is the duty cycle. We see that this condition is easier fulfilled by increasing the flight path (or by decreasing v_n which we have fixed), by increasing the chopper frequency or by narrowing the chopper window (intensity loss). Choosing a **duty cycle of 0.01** one needs a very long **flight path** between ch1 and ch2 of **L=100m** and a high **chopper frequency of** ____**Hz =** _____ **rpm to reach 1μeV energy resolution**. The condition becomes more restrictive if we consider the finite opening time of the first chopper as well.

Finally, we mention that all the contributions in the primary and secondary spectrometer have to be added, e.g. quadratically:Δt/t = sqrt[$(\Delta t_1/t_1)^2$+$(\Delta t_2/t_2)^2$+.......]. Additional choppers are usually needed to avoid frame overlap and harmonics, which reduces the intensity further. To achieve a 1μeV energy resolution by TOF is technically demanding (choppers), expensive (guides) and low in flux. Thus TOF-chopper-instruments have typically energy resolutions >10μeV. ex.: IN5 at 6.3Å has roughly 40μeV energy resolution.

Increasing C helps but reduces the maximum Q. **Calculate the elastic Q for 3Å, 6Å and 15Å neutrons, assuming a maximum scattering angle of 140°:** Q = ________________ = ____ , ______ and _________.

BS:

reactor backscattering spectrometers are based on perfect crystal optics. High energy resolution is achieved by choosing Bragg angles Θ as close as possible to 90°. Two major terms determine then the energy resolution: the spread in lattice spacing Δd/d of the monochromator and the angular deviation ε from backscattering direction (the latter includes the beam divergence α if considered as ε = α/2).

Write down the **Bragg equation** (neglecting higher orders): ______________ or equivalently using k=2π/λ and τ = 2π/d (reciprocal lattice vector of the Bragg reflection): ____________.

Deduce the wavelength resolution Δλ/λ by differentiating: **Δλ** =___________ + ____________ and thus **Δλ/λ =** _____________ +______________ , or equivalently: **Δk=**______________________________ and thus **Δk/k=** _________________. The energy resolution is given by two terms. The first one, Δd/d =Δτ/τ , can be calculated by the dynamical scattering theory as $\Delta\tau/\tau = h^2/m\ 4\ F_\tau\ N_c$, where F_τ is the structure factor of the reflection used and N_c the number density of atoms in the unit cell. The second one, the **angular deviation,** can for Θ ≈ 90° be expanded in powers of Θ and contributes approximately as Δλ/λ**~$\Delta\Theta^2/4$** (ΔΘ in radian).

Calculate now the contribution to the energy resolution of both terms for a perfect crystal Si(111) monochromator (6.271Å, but approximate by 6.3Å as above).

With $F_{\tau=(111)}$ and N_c for Si(111) the **extinction contribution for Si(111) in backscattering** is $\Delta d/d=1.86\ 10^{-5}$ and thus **ΔE/E=**___________ and **ΔE=**_______μeV.

Estimate the energy resolution contribution due to **deviation from backscattering:**

- given by a sample diameter of 4cm in 2m distance from the analyser. ΔE/E=_______, **ΔE=**_____μeV

- given by this sample at 1m distance: ΔE/E=_____, **ΔE=**_____μeV

- **given by a detector being placed near backscattering,** a **sample - analyser distance of 1m** and the distance sample center - **detector center = 10cm below the scattering plane**; the focus of the analyser sphere is placed in the middle between sample and detector: **ΔE/E=** _______. **ΔE=**______μeV

These examples shows that for small enough deviations from BS energy resolutions of <1μeV are easily achievable. Comparing this to TOF contributions above, it becomes clear that for a spallation source backscattering instrument, which combines TOF in the primary spectrometer with near-BS in the secondary spectrometer, it is very difficult to achieve sub-μeV resolution. The SNS BS instrument with 80m flight path has for example an energy resolution for Si(111) of 2.5μeV.

NSE

(question formulated together with Peter Fouquet): in neutron spin echo one uses the neutron spin which undergoes precessions in a magnetic field B. The precession angle ϕ after a path length l depends on the field integral, given by $\phi = \gamma * B * l / v_n$ (gyromagnetic ratio of the neutron, v_n=neutron speed). For a polychromatic beam the precession angles of the neutron spins will be very different depending on the neutron speed and thus a previously polarised beam becomes depolarised. The trick is then to send the neutrons after the sample through a field with opposite sign and with the same field integral. Therefore, for elastic scattering, the precessions are “turned backwards”, again depending on the neutron velocity, and the full polarisation is recovered. This allows to use a wide wavelength band (different incident neutron speed) and therefore a high intensity which is ‘decoupled’ from the energy resolution.

In order to estimate a typically achievable energy resolution, we can calculate the longest time which is easily accessible in NSE. The NSE time is given by: $\mathbf{t_{NSE} = \hbar\, \gamma\, Bl / (m_n\, v_n^3)}$ thus it is proportional to the largest achievable field integral B*l, which we take as 0.25 [T*m].

Calculate the longest NSE time t_{NSE} for λ=6.3Å neutrons (use v_n calculated above), knowing that $\gamma = 1.832\ 10^8$ [T^{-1} s^{-1}] , $\hbar = 1.054*10^{-34}$Js; and $m_n = 1.675*10^{-27}$ kg: **t_{NSE} = ______ ns. Convert this time into an energy** by multiplying its reciprocal value with h=4.136 μeV ns; we get: **E_{NSE}= ________ μeV**.

For comparing measurements in time and in energy one often refers to Fourier-transformation which relates e.g. the characteristic relaxation time τ of an exponential relaxation in time to the width of a Lorentzian function in energy by τ=1/ω. In spite the fact that the relaxation time is usually smaller than the longest NSE time, converting the corresponding energy resolution by this relation gives: **E_τ = _________ μeV** . Because of $\tau < t_{NSE}$ and also because energy spectrometers can usually resolve better than the HWHM, the comparable resolution energy lies somewhere in between the two values calculated.

Note that the **longest NSE time depends on wavelength λ as t_{NSE}~**_____. Thus the resolution improves fast for increasing λ, but like calculated for the other spectrometers above, the maximum Q is reduced.