Time-of-flight spectroscopy and the Disk Chopper Spectrometer (DCS)

John R.D. Copley

Summer School on Methods and Applications of Cold and Thermal Neutron Spectroscopy

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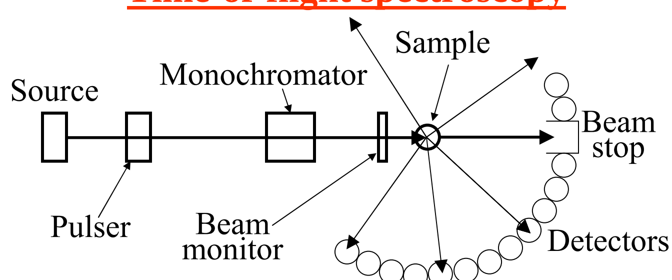
Time-of-flight spectroscopy



Neutrons from the source are pulsed and monochromated.
Monochromatic bursts of neutrons strike the sample.
Some of the neutrons are scattered.
Some of the scattered neutrons are counted in the detectors.
The time between pulses, T, is divided into N time channels of width $\Delta t = T/N$. (At the DCS, N=1000). Detector events are stored in a 2-d histogram **I(i,j)** [i labels the detector, j labels the time channel].

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How do we obtain S(Q,ω) from I(i,j)?

$$I(i,j) \Leftrightarrow I(2\theta,t) = N\Phi\left[\frac{d^2\sigma}{d\Omega dt}\right]\Delta\Omega\Delta t$$

- Raw data: $I(i,j)$
- $I(2\theta,t)$: Number of neutrons per second scattered at angle 2θ into solid angle $\Delta\Omega$, reaching detector within time interval $[t_D, t_D+\Delta t]$
- N: Number of atoms of sample in the beam
- Φ: Number of neutrons per second per unit area in the incident beam (incident flux)
- $\frac{d^2\sigma}{d\Omega dt}$: Double differential scattering cross section (w.r.t. time); depends on 2θ and t
- $\Delta\Omega$: Solid angle subtended by detector
- Δt: Width of time channel

To the extent that $\Delta\Omega$ and Δt are constants, $\frac{d^2\sigma}{d\Omega dt} \propto I(2\theta,t)$

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How do we obtain S(Q,ω) from I(i,j) (contd.)?

Double differential scattering cross section w.r.t. energy | Double differential scattering cross section w.r.t. time

$$E_f = \frac{1}{2}mv_f^2 = \frac{1}{2}m\frac{L_{SD}^2}{t_{SD}^2} \qquad \frac{d^2\sigma}{d\Omega dE_f} = \frac{d^2\sigma}{d\Omega dt}\cdot\frac{dt}{dE_f}$$

$$\left[\frac{d^2\sigma}{d\Omega dt} \propto I(2\theta,t)\right]$$ (from previous slide)

Since $E_f \propto \frac{1}{t_{SD}^2}$, $\frac{dE_f}{dt} \propto \frac{1}{t_{SD}^3}$, $\frac{dt}{dE_f} \propto t_{SD}^3$, and $\frac{d^2\sigma}{d\Omega dE_f} \propto I(2\theta,t)\,t_{SD}^3$.

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_S}{4\pi\hbar}\frac{k_f}{k_i}S(Q,\omega)$$

k_i is fixed and $k_f \propto \frac{1}{t_{SD}}$

$$\text{Hence } S(Q,\omega) \propto I(2\theta,t)\cdot t_{SD}^4$$

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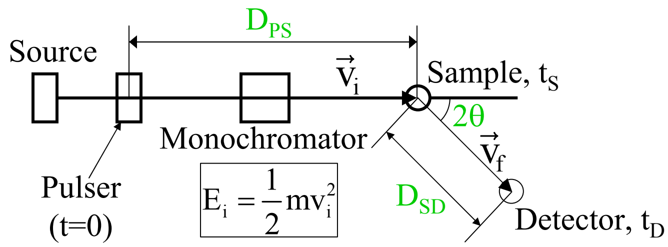
How do we obtain Q and ω?



Knowing D_{PS} and v_i, we obtain $t_S = D_{PS}/v_i$.

Knowing D_{SD}, t_S, and t_D, we obtain $v_f = D_{SD}/(t_D - t_S)$.

Knowing v_f, we obtain $E_f = \frac{1}{2} m v_i^2$.

$$\vec{k}_i = \frac{m\vec{v}_i}{\hbar}$$

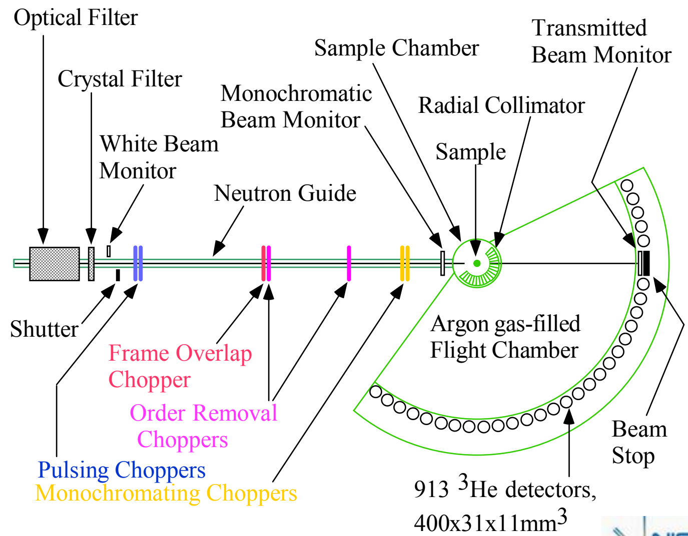
Hence $\hbar\omega = E_i - E_f$

and $\vec{Q} = \vec{k}_i - \vec{k}_f$

$$\vec{k}_f = \frac{m\vec{v}_f}{\hbar}$$

The Disk Chopper Spectrometer (DCS)

The Disk Chopper Spectrometer - schematic



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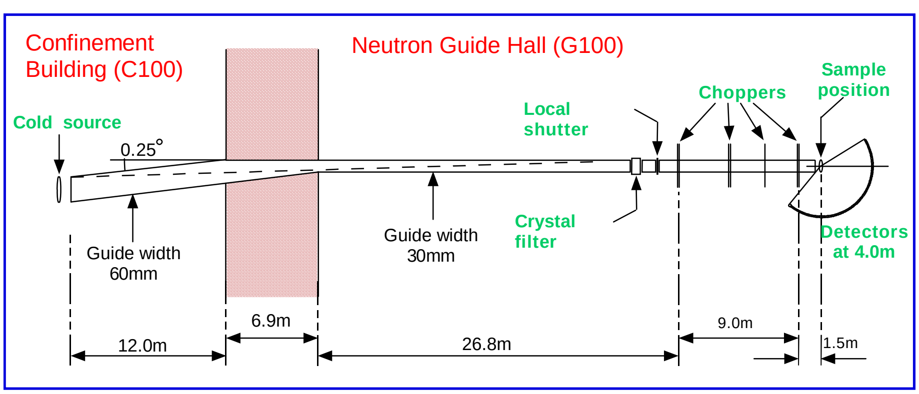
The Disk Chopper Spectrometer

Plan view



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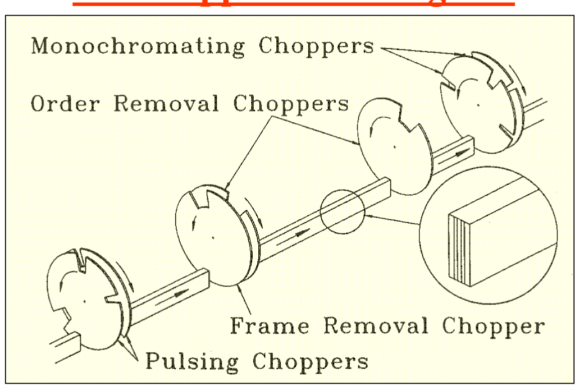
Neutron guides in the confinement building

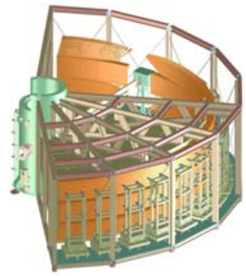
www.ncnr.nist.gov/expansion2/yqims2

The choppers and the guide



The *pulsing* and *monochromating* choppers are counter-rotating pairs, permitting a choice of pulse widths; they normally run at 20,000 rpm. The *order removal* choppers (also 20,000 rpm) remove contaminants. The *frame removal* chopper *alleviates* the problem of frame overlap. It runs at 20,000/m or 20,000(m-1)/m rpm; m is a small integer (typically m~λ/2).

The flight chamber and detectors



The flight chamber is argon-filled to reduce scattering of neutrons traveling the 4 m distance from sample to detectors.
There are 913 detectors in 3 banks, from -30º to +140º.

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Why do we need all those choppers?

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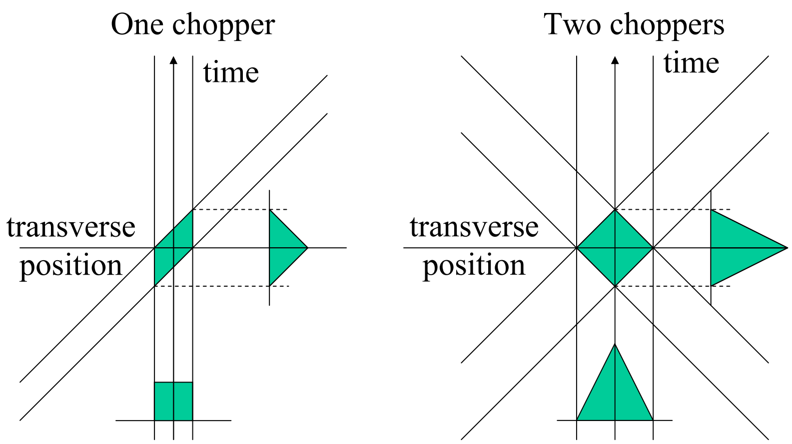
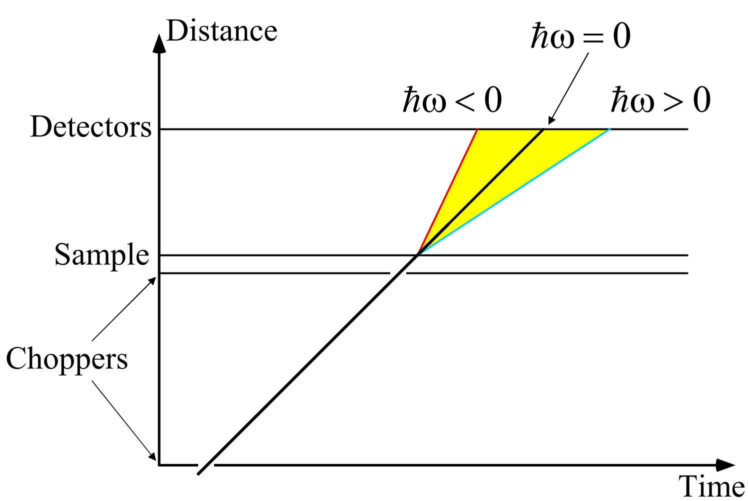
Counter-rotating choppers

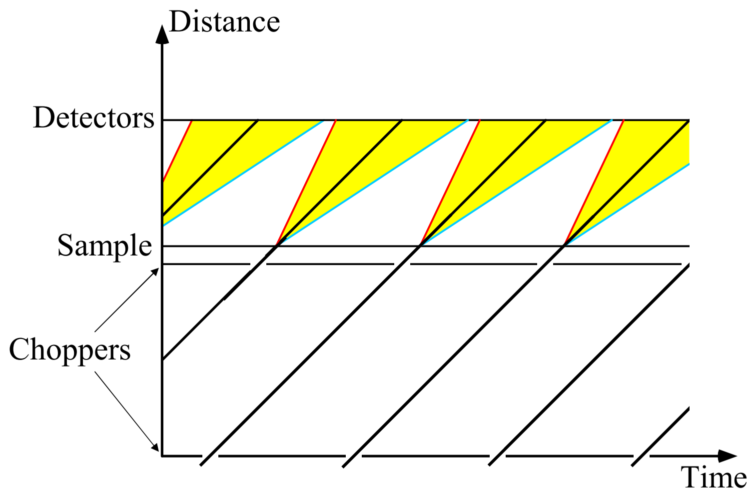


With two choppers and the same resolution width, we get twice the intensity.

Time-distance diagrams - single pulse



Time-distance diagrams - multiple pulses



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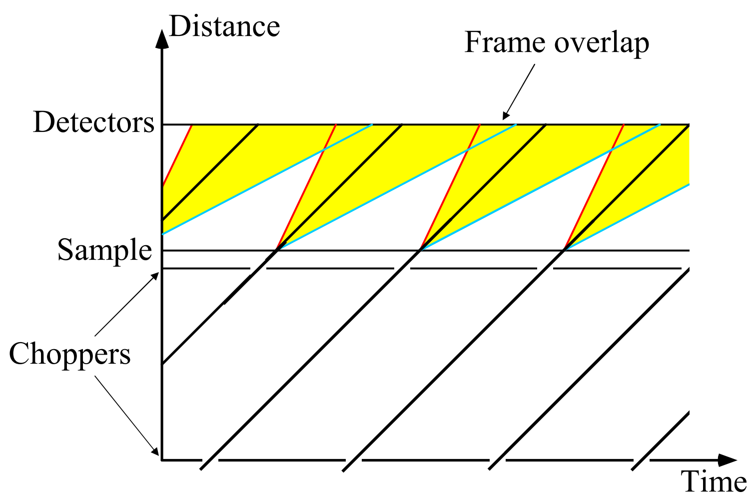
Frame overlap



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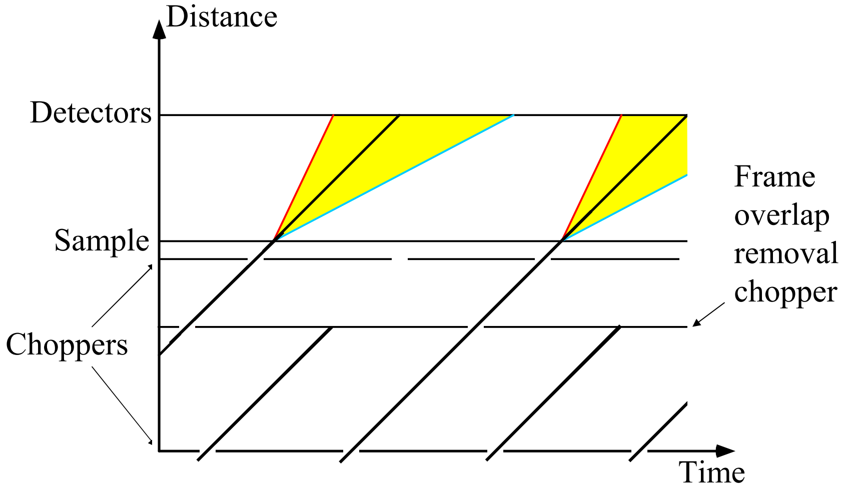
Removal of frame overlap



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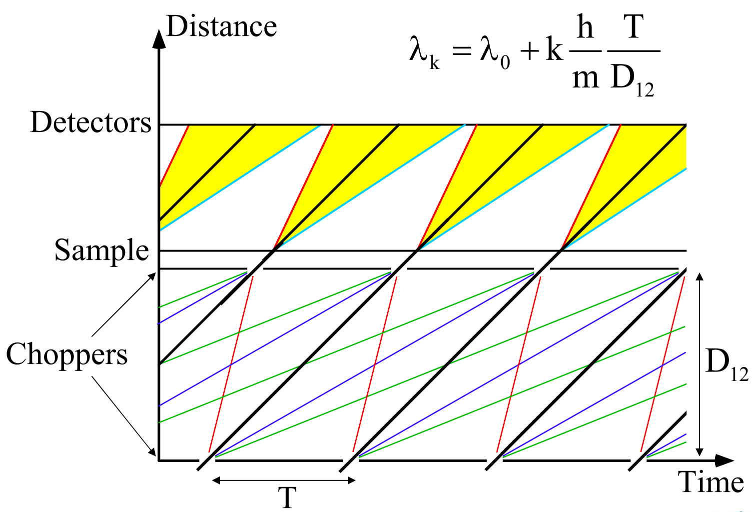
What are "contaminant" wavelengths ("orders")?

$$\lambda_k = \lambda_0 + k \frac{h}{m} \frac{T}{D_{12}}$$



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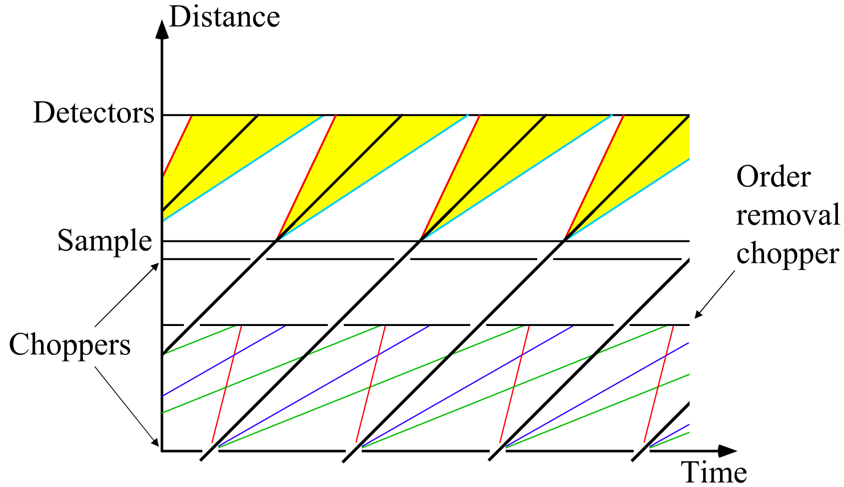
Removal of “contaminant” wavelengths



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Considerations when running an experiment:
1. Wavelength
2. Chopper speeds/periods
3. Widths of slots

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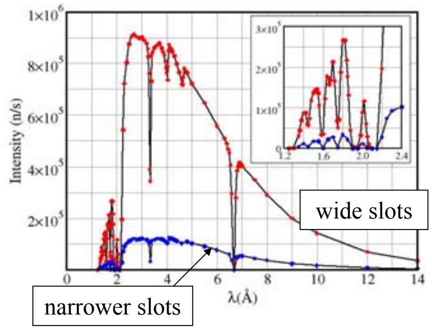
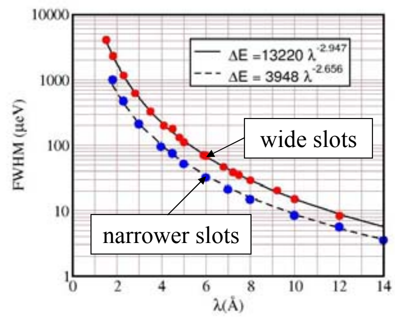
Choice of wavelength λ

Intensity at sample I(E)



Resolution width ΔE



- I(E) peaks around 2.5-4.5Å; at long λ, I(E) drops ≈ 50% for every 2Å.
- Energy resolution width ΔE varies roughly as $1/\lambda^3$
- Q range and Q resolution $\propto 1/\lambda$
- Bragg peaks can be troublesome at short λ (4.8Å is a popular choice)

Choices of chopper periods and slot widths

Chopper master period T, and period at sample T_S.

- Minimum T is 3000μs (corresponds to maximum speed 20,000 rpm)
- Resolution width $\Delta E \propto T$
- The intensity in a single pulse is $I_P(E) \propto T^2$
- The frequency of pulses at the sample is $1/T_S$
- Thus the intensity $I(E) \propto T^2/T_S = T/m$,

  where $m = T_S/T$ is known as the "speed ratio denominator"
- $\hbar\omega$ range increases with m (frame overlap becomes less of a problem)

Slot widths W

- I(E) varies roughly as W^3
- ΔE varies roughly as W