Time-of-flight measurements using the Disk Chopper Spectrometer

- Useful relationships among λ, k, v, τ, E.
- How do we obtain (Q,ω) from $(2\theta,t)$: $S(Q,\omega)$ from $I(2\theta,t)$?
- How do we determine values of t for each time channel?
- How do we decide what wavelength to use?
- Time-distance diagrams
- What are contaminant wavelengths and how do we remove them?
- What is frame overlap and how do we avoid it?
- Container scattering and background corrections
- Normalization and detector efficiency corrections

Useful relationships

$$k = 2\pi/\lambda$$
$$mv = h/\lambda$$
$$\tau = 1/v$$

$$E = \tfrac{1}{2}mv^2 = \frac{\hbar^2 k^2}{2m}$$

$$\tau[\mu s/mm] \approx \frac{\lambda[Å]}{4}$$

$$E[meV] \approx \frac{82}{(\lambda[Å])^2}$$

An example

If $\lambda = 4$ Å (= 0.4 nm),

$k \approx 1.57$ Å^{-1}

$v \approx 0.99$ mm/µs

$\tau \approx 1.01$ µs/mm

$E \approx 5.1$ meV

How do we obtain Q and ω given 2θ and t?

We know λ_i, hence v_i, $\boxed{\vec{k}_i}$, and $\boxed{E_i}$.

Given $t\,(\equiv t_{SD})$ and 2θ, and knowing D_{SD}, we obtain v_f, $\boxed{\vec{k}_f}$ and $\boxed{E_f}$.

$$\boxed{\begin{aligned} \hbar\omega &= E_i - E_f \\ \vec{Q} &= \vec{k}_i - \vec{k}_f \end{aligned}}$$

$$\left(\begin{array}{l} D_{SD} \text{ is the distance from sample to detector} \\ t_{SD} \text{ is the time-of-flight from sample to detector} \end{array} \right)$$

How do we obtain S(Q,ω) from I(2θ,t)? (part 1)

Number of neutrons per second scattered at angle 2θ into solid angle ΔΩ, reaching detector within time interval $[t_D, t_D+\Delta t]$

Number of atoms illuminated

Solid angle subtended by detector

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

Width of time channel

Number of neutrons per second per unit area in the incident beam (incident flux)

Double differential scattering cross section (w.r.t. time)

$\boxed{\text{To the extent that } \Delta\Omega \text{ and } \Delta t \text{ (and N and } \Phi\text{) are constants, } \dfrac{d^2\sigma}{d\Omega dt} \propto I(2\theta, t)}$

How do we obtain S(Q,ω) from I(2θ,t)? (part 2)

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

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

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{d^2\sigma}{d\Omega dt}\cdot\frac{dt}{dE_f}$$

Since $E_f \propto 1/t^2, \frac{dE_f}{dt} \propto \frac{1}{t^3}$; hence $\frac{d^2\sigma}{d\Omega dE_f} \propto \frac{d^2\sigma}{d\Omega dt}t^3$.

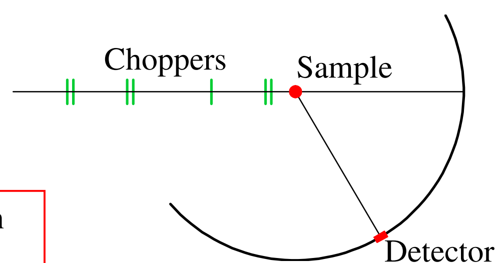
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_B}{4\pi\hbar}\frac{k_f}{k_i}S(Q,\omega)$$

Scattering function

$$\boxed{\text{Thus } S(Q,\omega) \propto I(2\theta,t)\cdot t^4}$$

How do we determine values of t for each time channel?

Knowing when the choppers were open, and all required distances, we know when neutrons reach the sample (t_S).



We define a delay time Δ (known as "tsd-min"). The time channel counter is reset at all times $t_S+\Delta$.

The time between pulses at the sample is T. The time channel width is $\delta t = 0.001\Delta$.

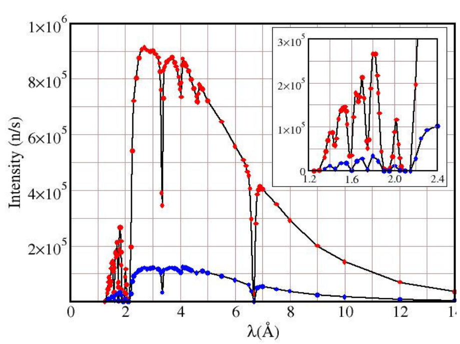
The k'th time channel (k=1,1000) corresponds to sample-to-detector times of flight from $t = \Delta+(k-1)\delta t$ to $t = \Delta+k\delta t$.

How do we decide what wavelength to use?

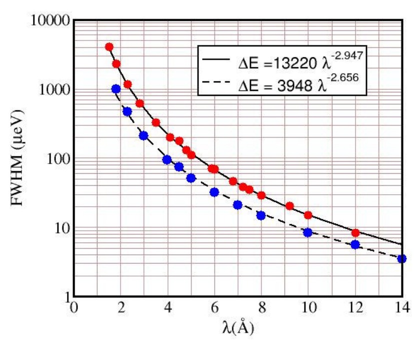
- Intensity I(λ) is highly structured at short λ.
  At long λ, I(λ) drops ~50% for every 2Å.
- Energy resolution varies roughly as $1/\lambda^3$.
- Q range and Q resolution vary as 1/λ.
- Bragg peaks can be troublesome at short λ.

Dependence of intensity and resolution on wavelength

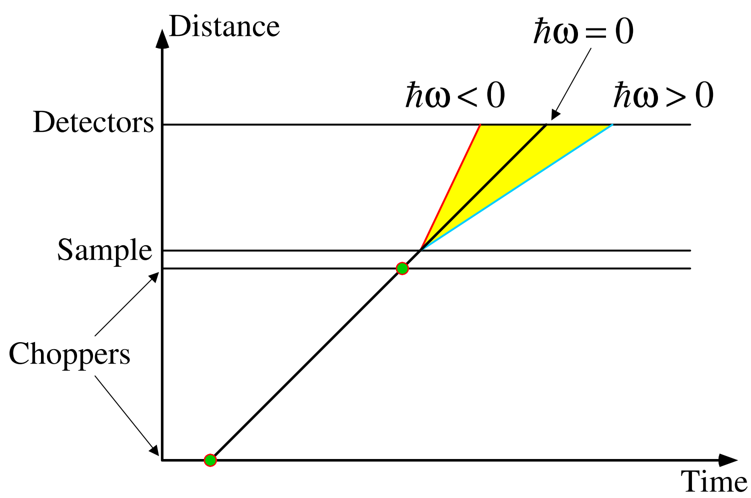
I(E)



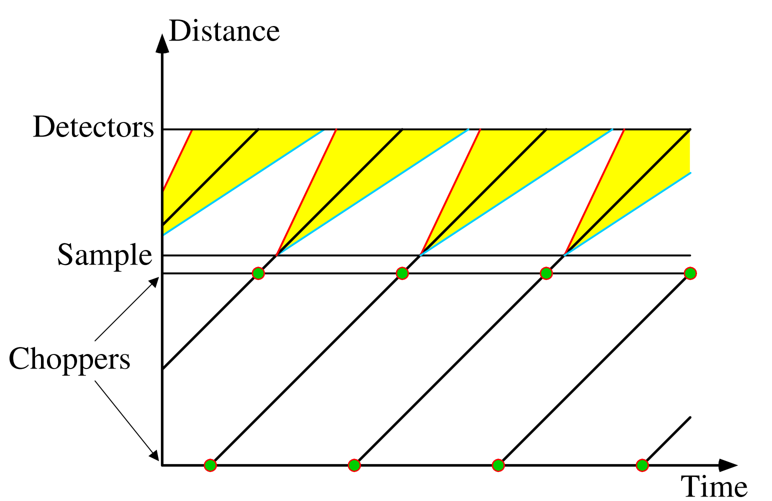
ΔE



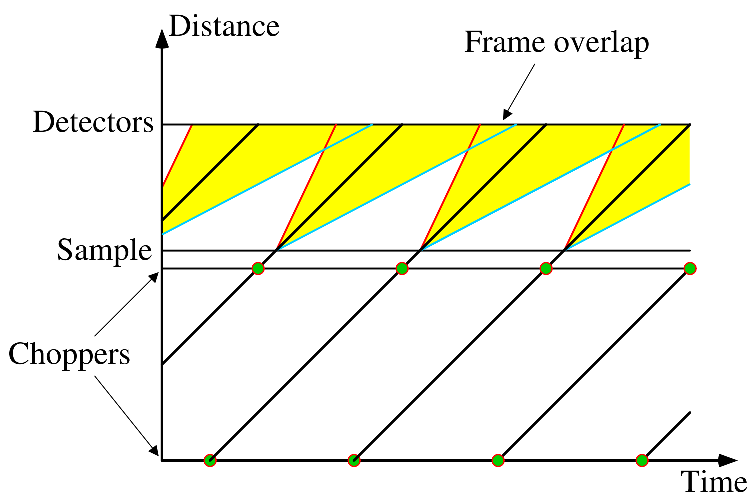
Time-distance diagrams - single pulse



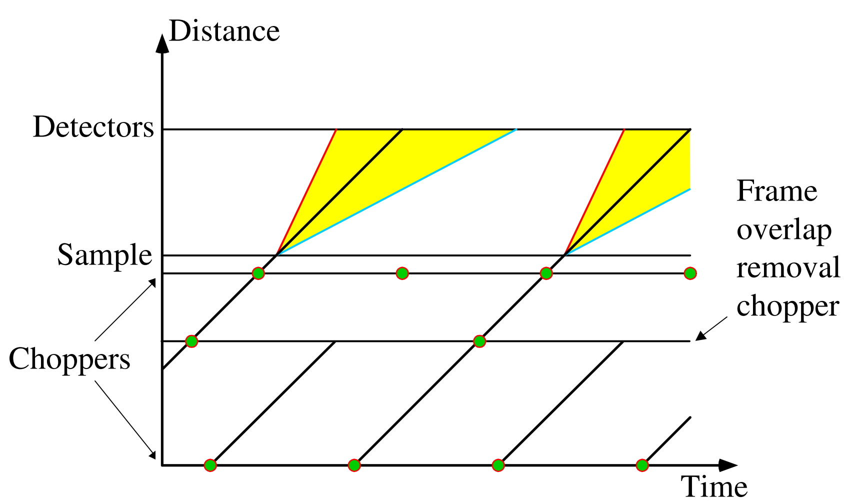
Time-distance diagrams - multiple pulses



What is frame overlap?

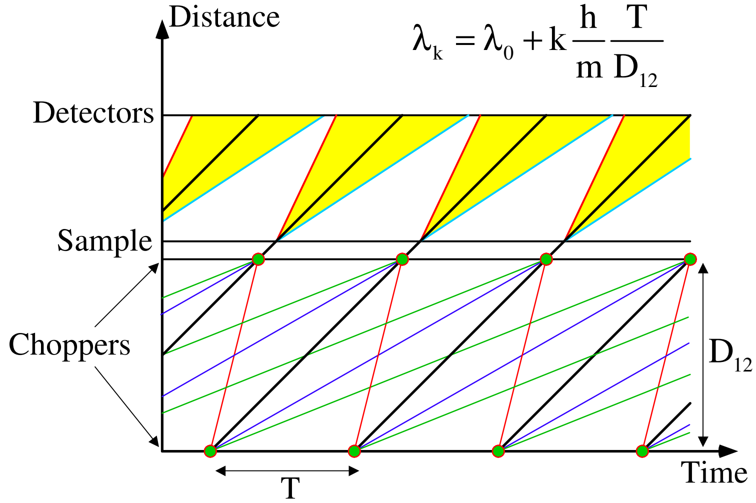


“Removal” of frame overlap

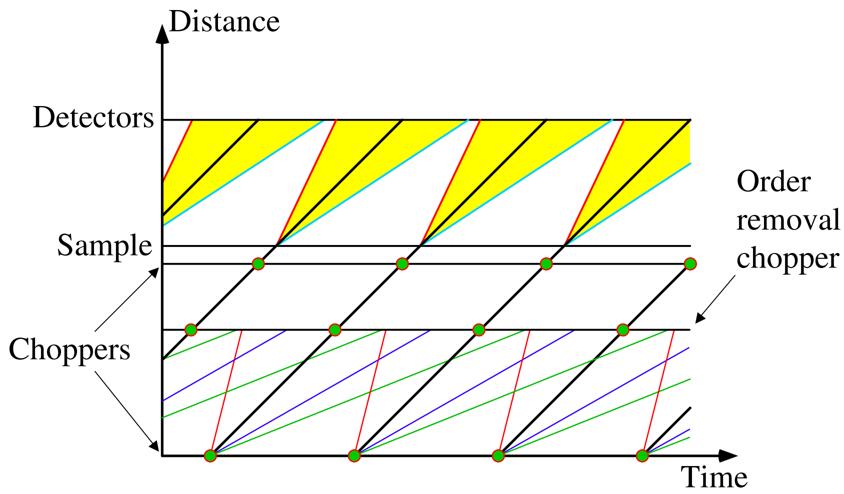


What are contaminant wavelengths ("orders")?

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



Removal of contaminant wavelengths



Container scattering and background corrections

$$C_S(2\theta,t) = \left[C_{SC}^{meas}(2\theta,t) - C_B^{meas}(2\theta)\right] - f(2\theta)\cdot\left[C_C^{meas}(2\theta,t) - C_B^{meas}(2\theta)\right]$$

$$C_V(2\theta,t) = C_V^{meas}(2\theta,t) - C_B^{meas}(2\theta)$$

SC: sample plus container

B: background

C: container only

V: vanadium

$f(2\theta)$: "self-shielding factor"

Normalization and detector efficiency corrections

Idealized count-rate

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

Total counts

Beam monitor counts/efficiency

Detector efficiency

$$C_S(2\theta,t) = N_S\cdot\frac{C_S^{BM}}{\eta^{BM}}\cdot\frac{1}{A_S}\cdot\left[\frac{d^2\sigma}{d\Omega dt}\right]_S \Delta\Omega\Delta t\cdot\eta^D(2\theta)$$

$$C_V(2\theta,t) = N_V\cdot\frac{C_V^{BM}}{\eta^{BM}}\cdot\frac{1}{A_V}\cdot\left[\frac{d^2\sigma}{d\Omega dt}\right]_V \Delta\Omega\Delta t\cdot\eta^D(2\theta)$$

Hence

$$\left[d^2\sigma/d\Omega dt\right]_S = \frac{C_S(2\theta,t)}{C_V(2\theta,t)}\left\{\frac{N_V}{N_S}\cdot\frac{C_V^{BM}}{C_S^{BM}}\cdot\frac{A_S}{A_V}\right\}\left[d^2\sigma/d\Omega dt\right]_V$$