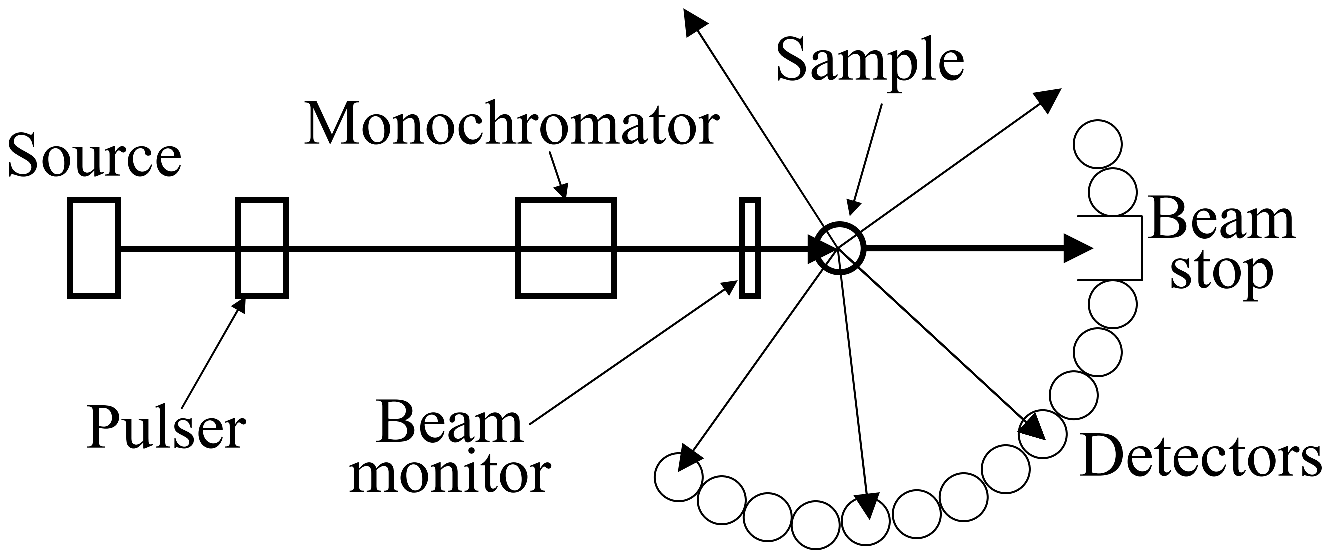
Time-of-flight spectroscopy and the Disk Chopper Spectrometer

NCNR Spectroscopy Summer School
June 22-26, 2009

Time-of-flight spectroscopy



- 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 Δ=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], relative to the minimum time "tsd-min", i.e. $t_{SD}(\min)+j\Delta$.

How do we obtain $S(Q,\omega)$ from $I(i,j)$?

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

Number of atoms illuminated

Solid angle subtended by detector

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

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)

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

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

$$E_f = \frac{m}{2}\frac{L_{SD}^2}{t_{SD}^2}$$

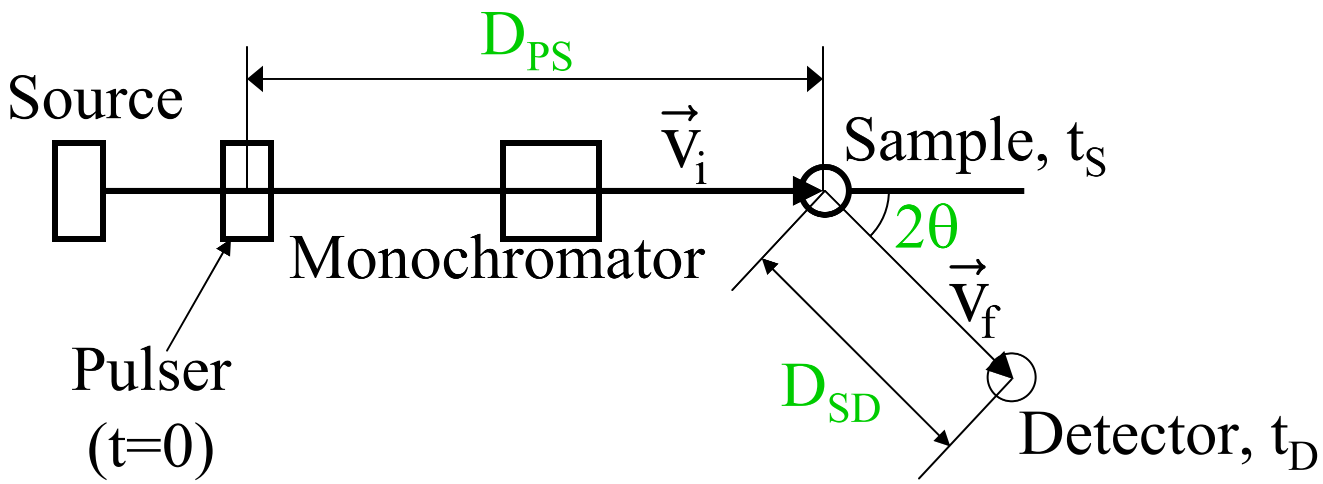
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{d^2\sigma}{d\Omega dt} \cdot \frac{dt}{dE_f}$$

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

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_S}{4\pi\hbar}\frac{k_f}{k_i} S(Q,\omega) \text{ and } k_f \propto t_{SD}^{-1}$$

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

How do we obtain Q and ω?



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

Knowing D_{SD}, t_S, t_D, and 2θ, we obtain $\vec{v}_f$.

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

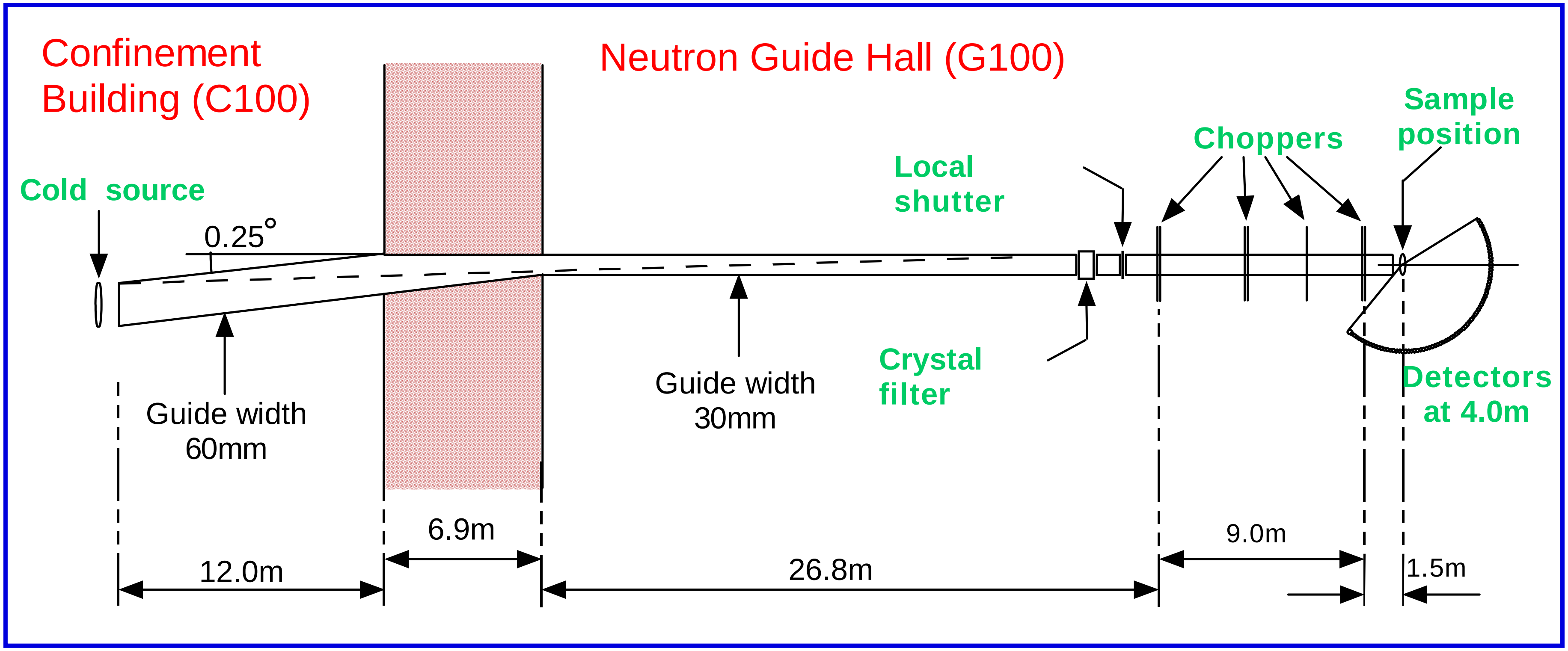
Hence $\hbar\omega = E_i - E_f$

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

$$E = \frac{1}{2}mv^2$$

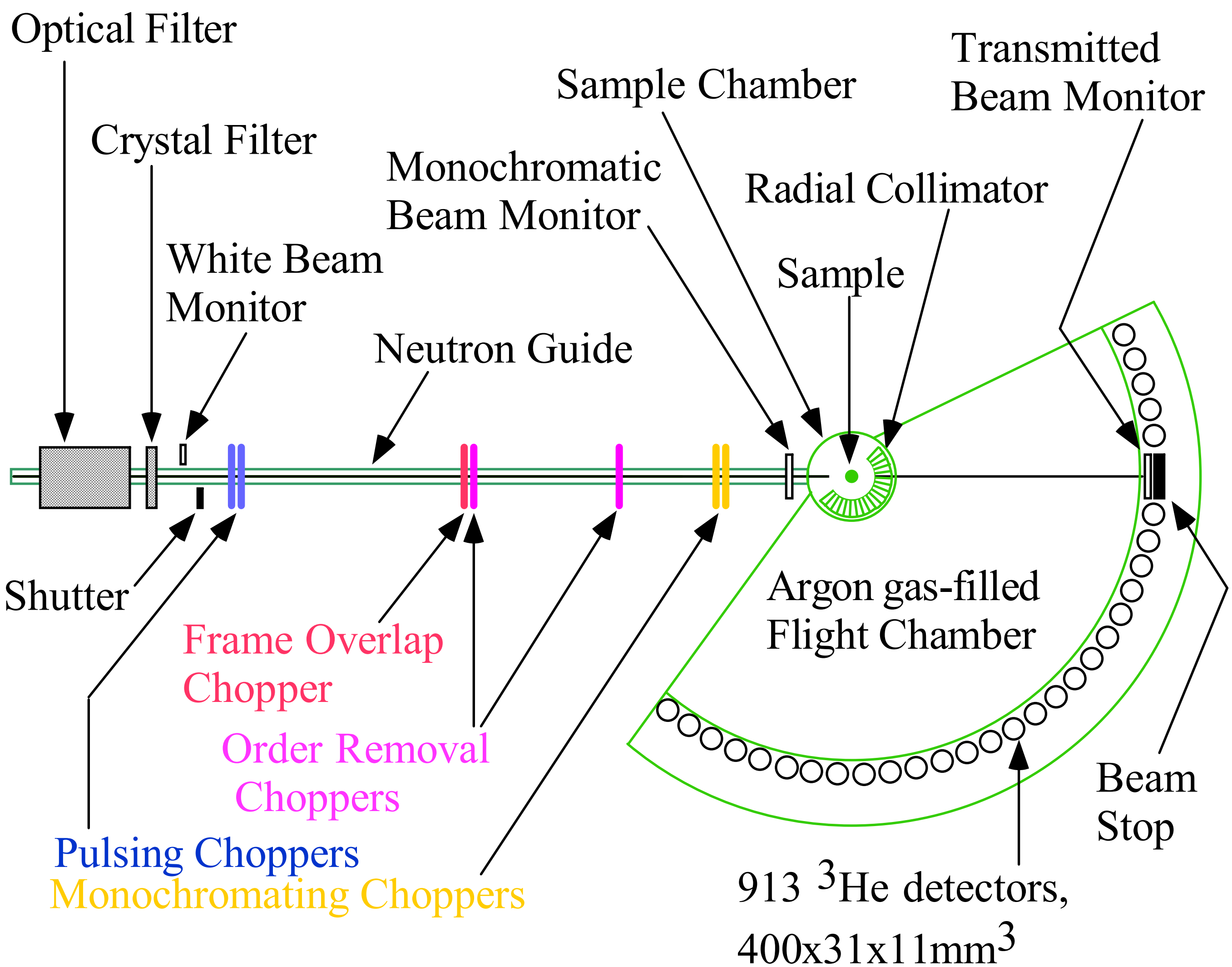
The Disk Chopper Spectrometer

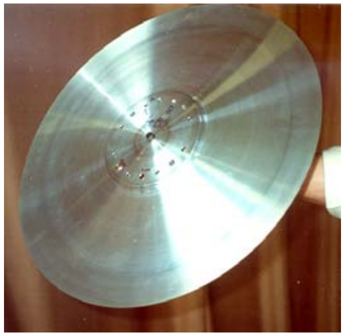
Plan view



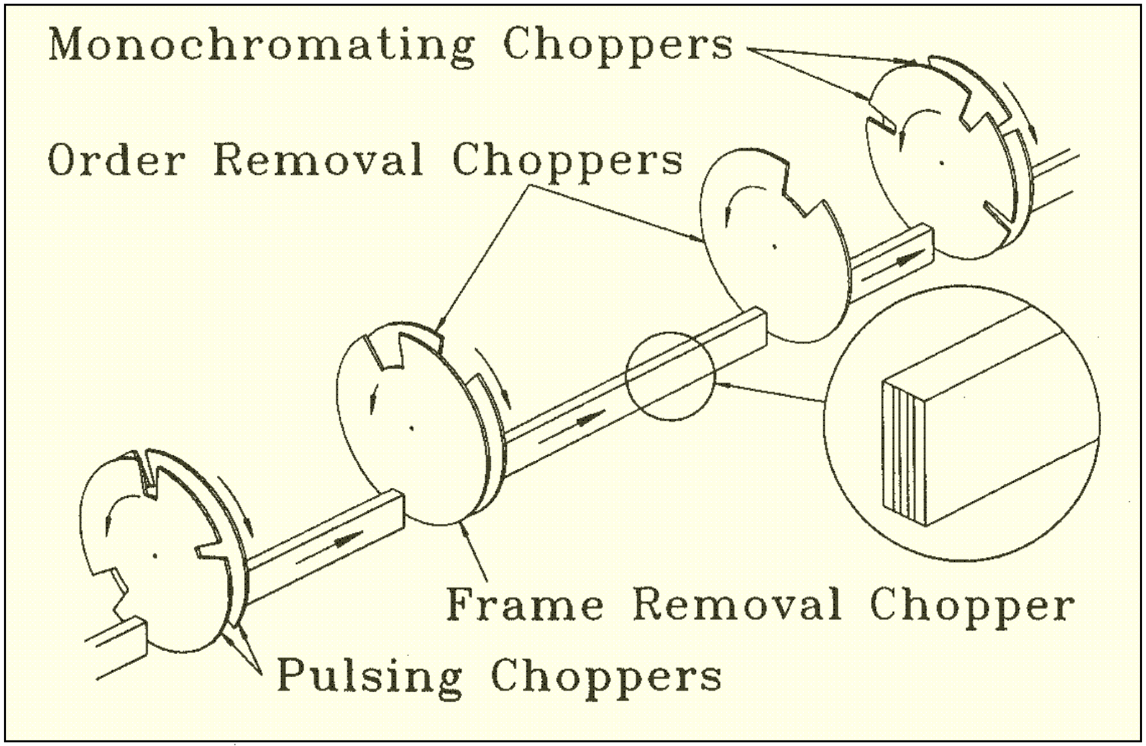
The Disk Chopper Spectrometer

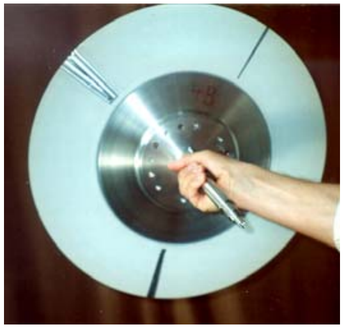
Schematic





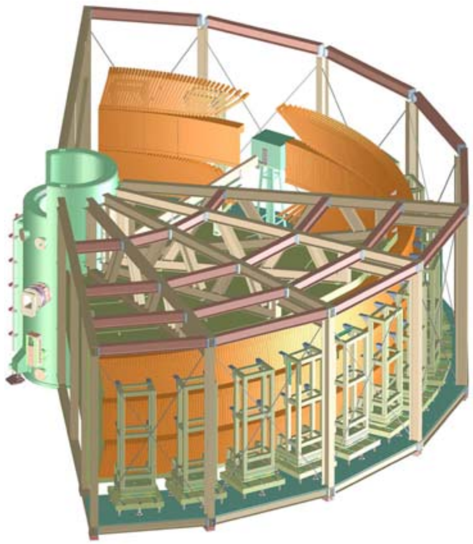
The choppers and the guide





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 remove contaminants (also 20,000 rpm). The *frame removal* chopper *alleviates* the problem of frame overlap; it runs at 20,000/m or 20,000(m-1)/m rpm, where 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.

Corrections for the container and background, and data normalization

Container scattering and background corrections

SC: sample plus container

C: container only

B: background

V: vanadium

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

f(2θ): "self-shielding factor"

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

Normalization and detector efficiency corrections

IN THEORY

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

IN PRACTICE

Beam monitor counts/efficiency → C_S^{BM}

Detector efficiency → η^D

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

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

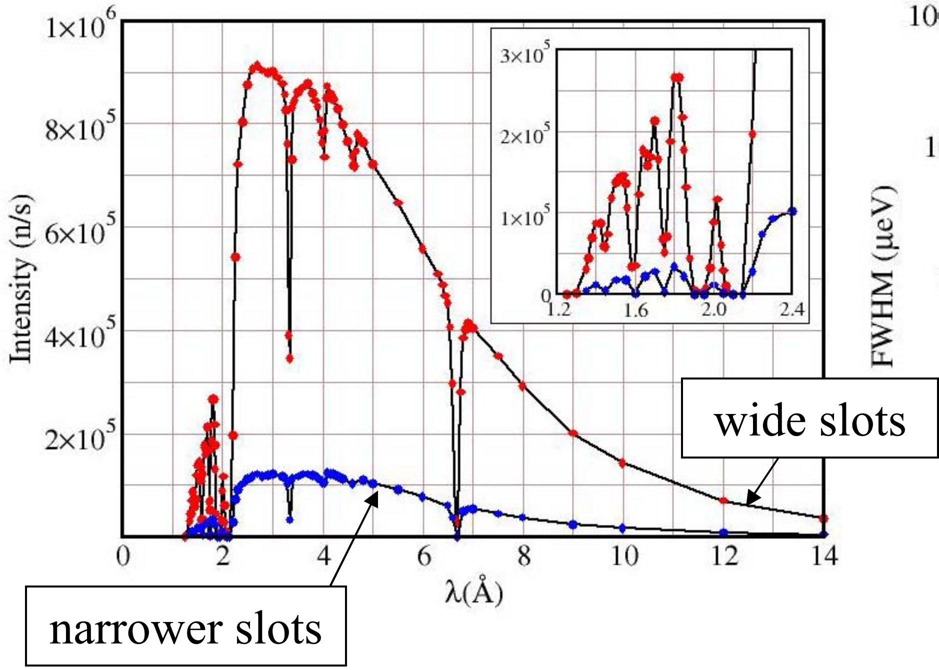
HENCE

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

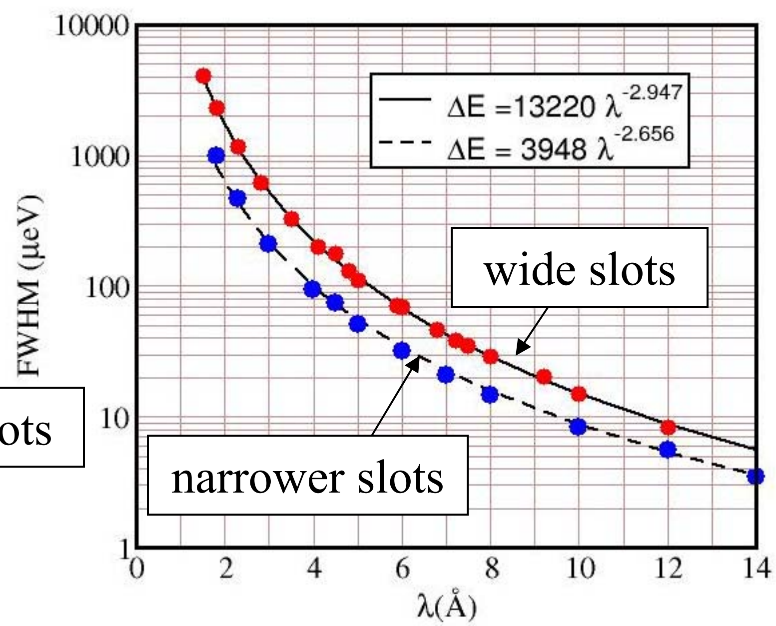
Considerations when running an experiment: choices of wavelength, chopper speeds, and resolution mode

Considerations when running an experiment

Intensity at sample I(E)



Resolution width ΔE



<u>Quantities that can be varied or chosen:</u>

Chopper period T*

Wavelength λ

* Normally T=3000μs

Chopper slot widths W

"Speed ratio denominator" $m=T_S/T$

(T_S is period at sample)

Considerations when running an experiment

Choice of wavelength λ

- 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)

Choice of chopper period T and/or speed ratio denominator m

- $I(E) \propto T^2/T_S = T/m$ (since $T_S = mT$)
- $\Delta E \propto T$
- $\hbar\omega$ range increases with m (frame overlap becomes less of a problem)

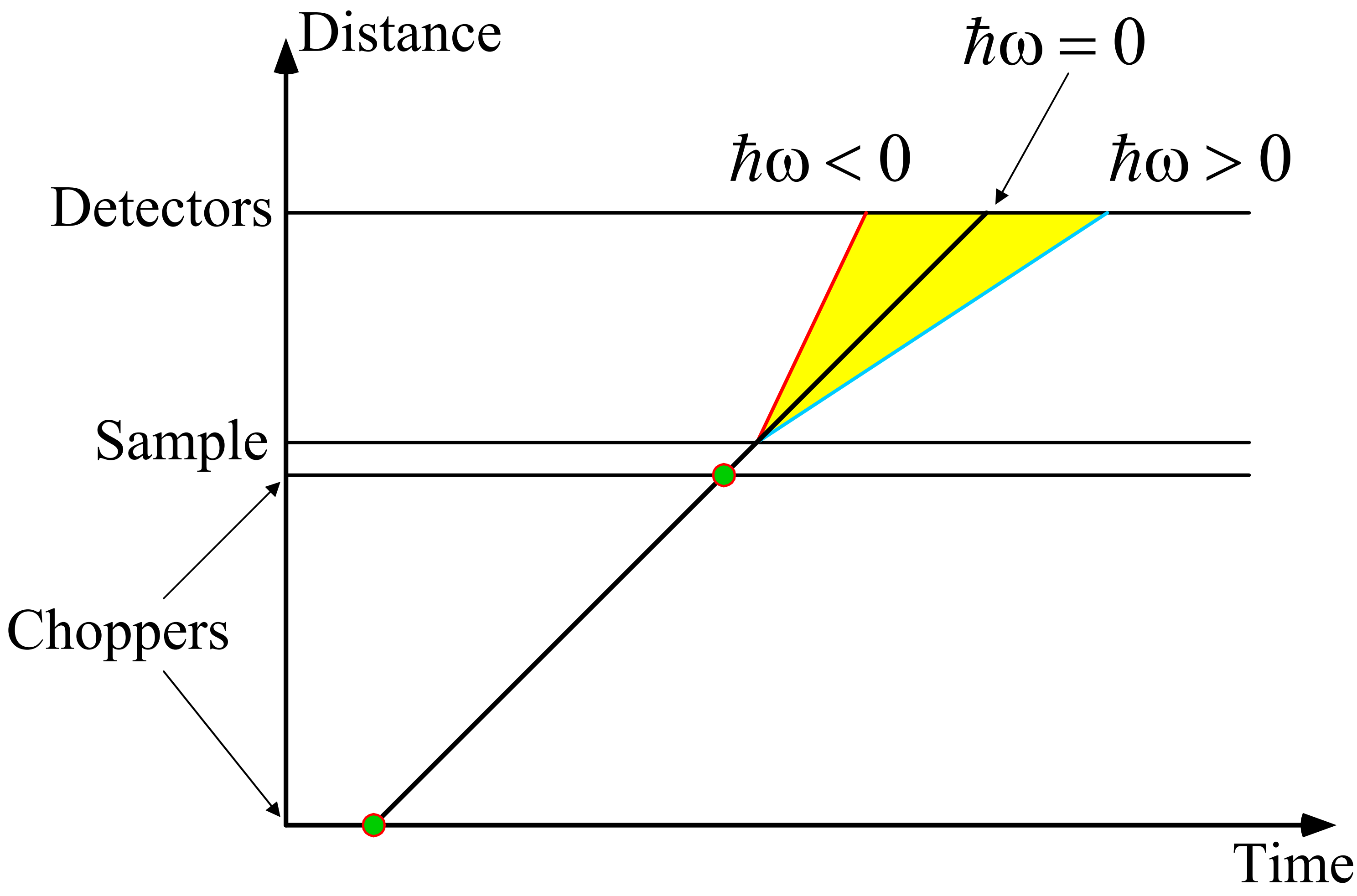
Choice of chopper slot widths W

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

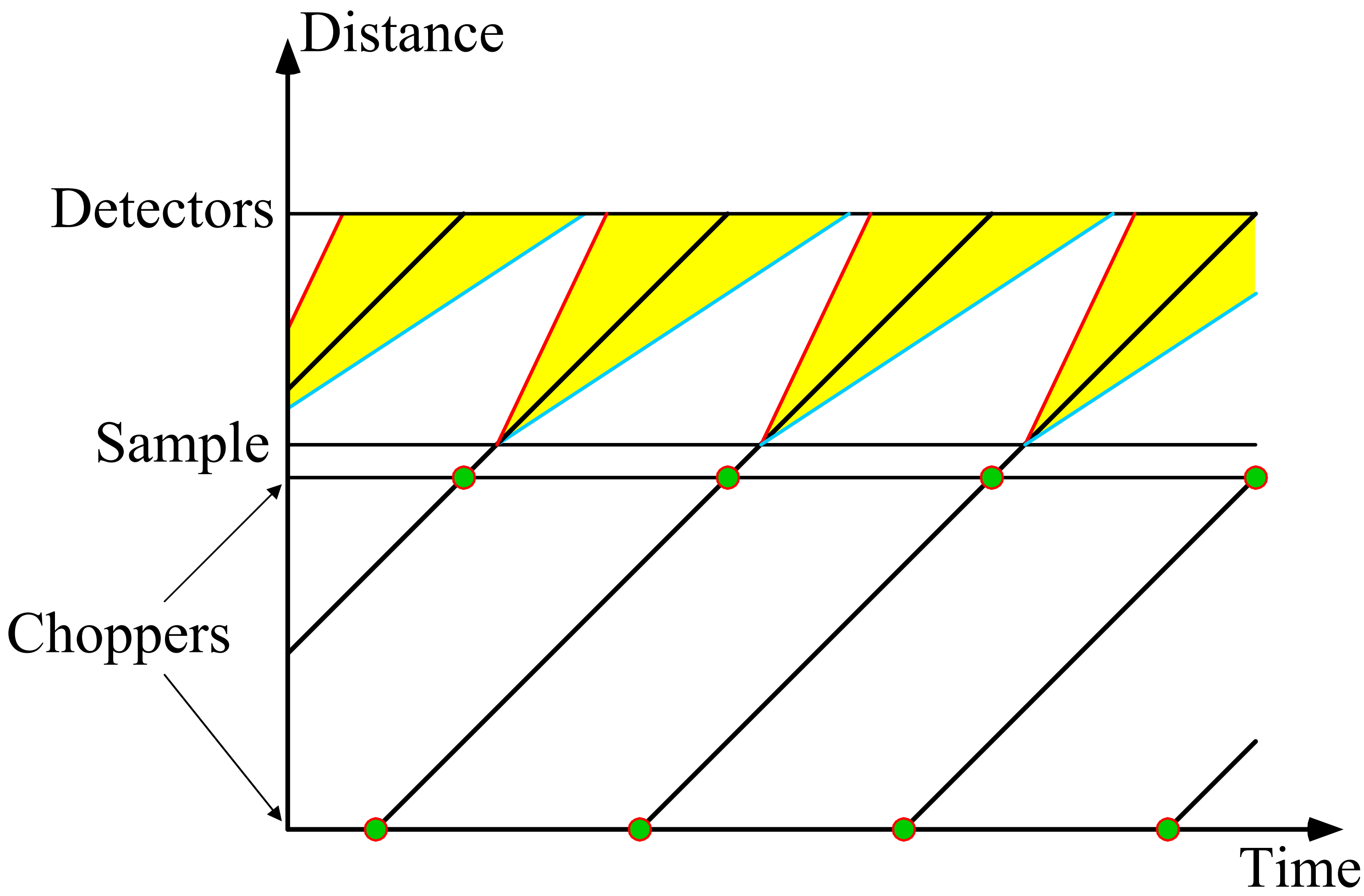
Why do we need all those choppers?

Time-distance diagrams

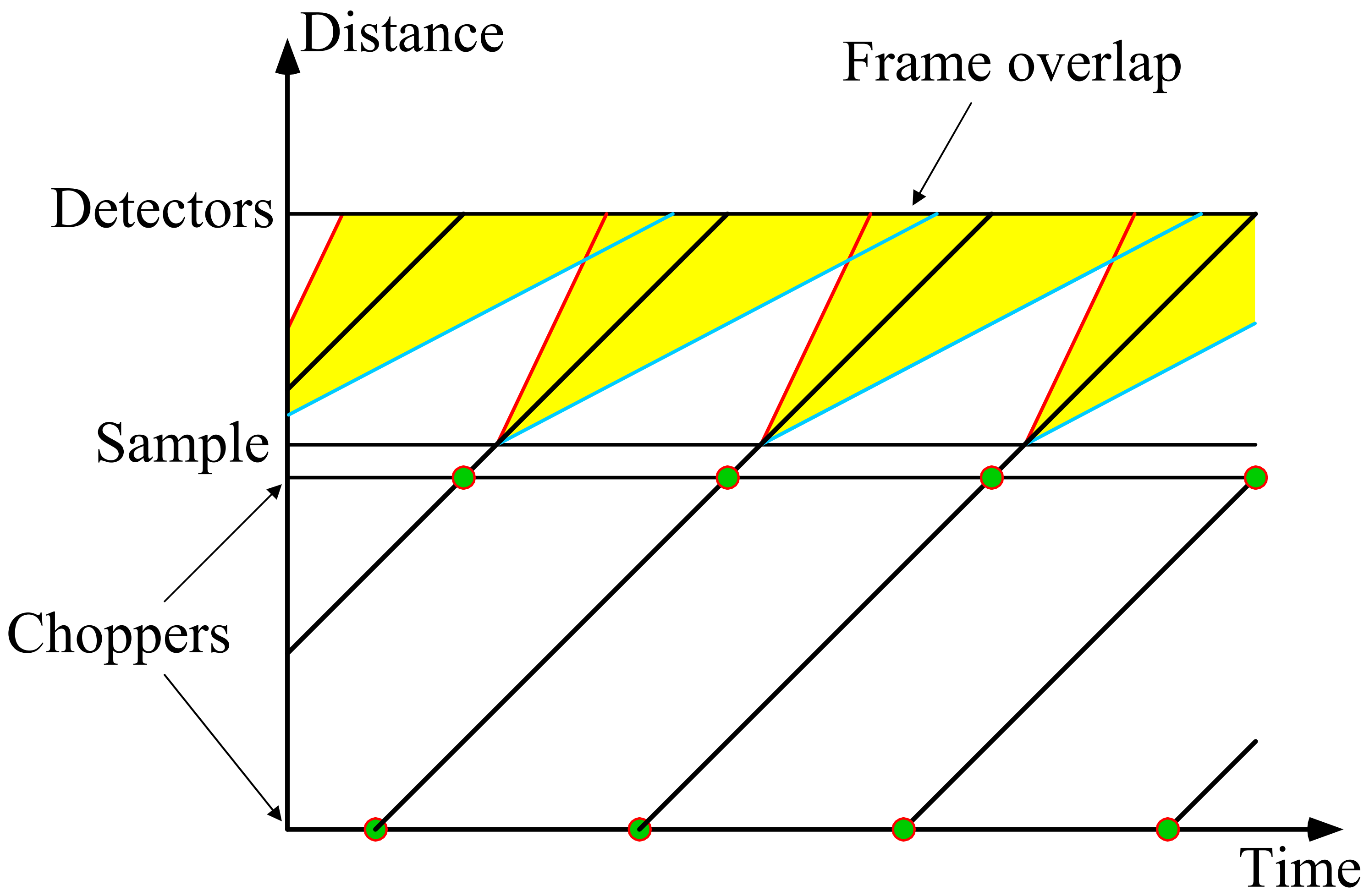
Time-distance diagrams - single pulse



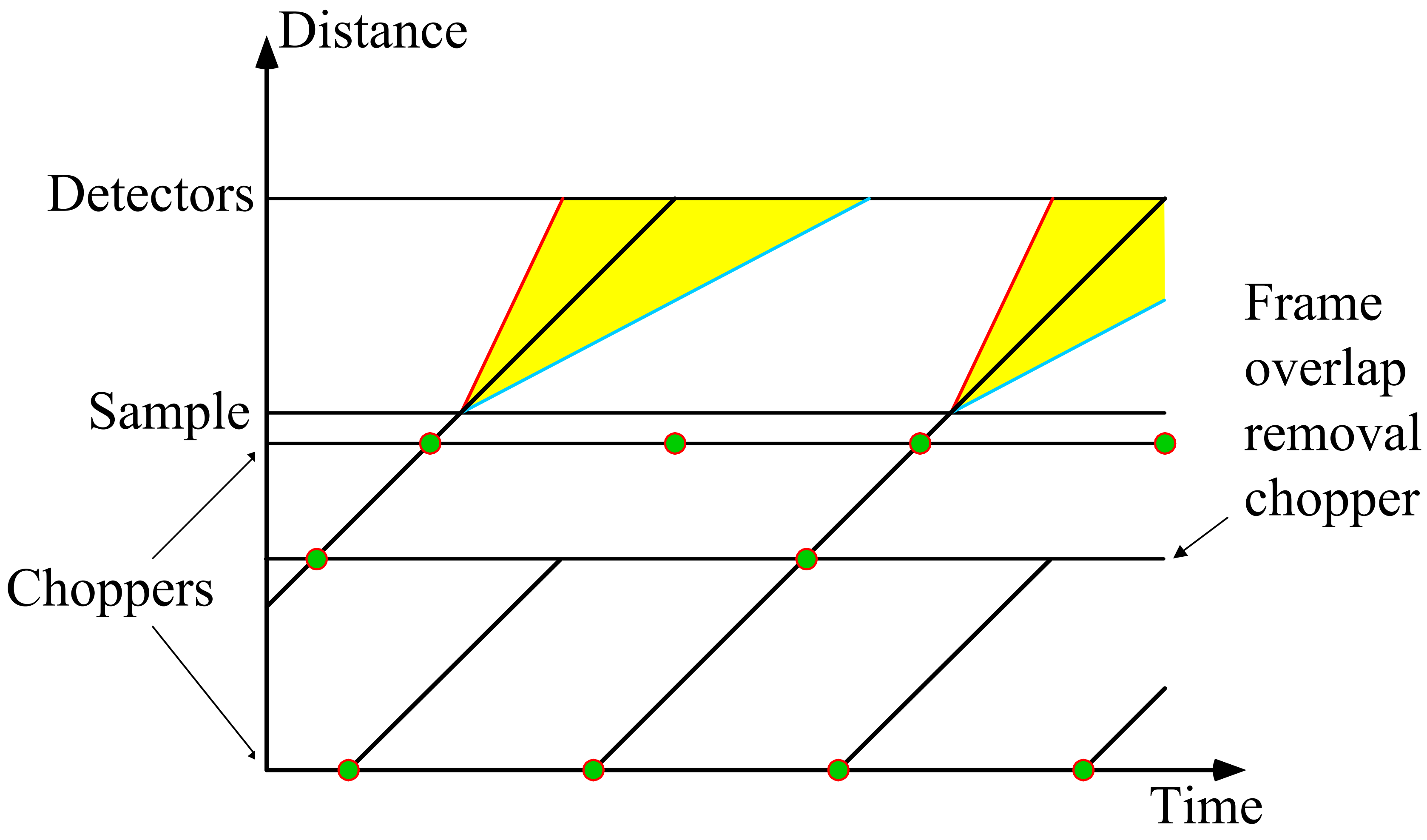
Time-distance diagrams - multiple pulses



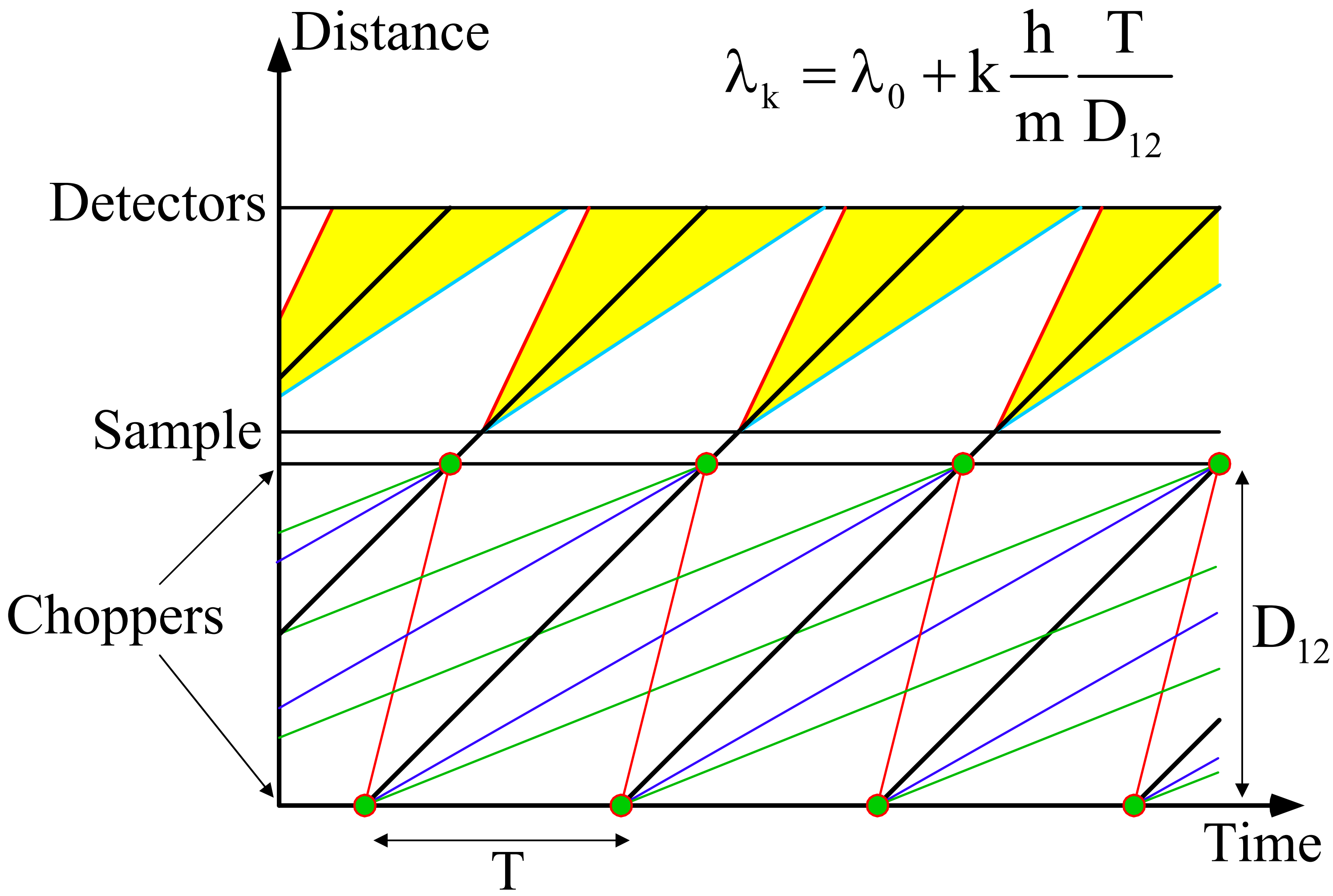
What is frame overlap?



“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