Time-of-flight spectroscopy and the Disk Chopper Spectrometer

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NCNR Neutron Spectroscopy Tutorial
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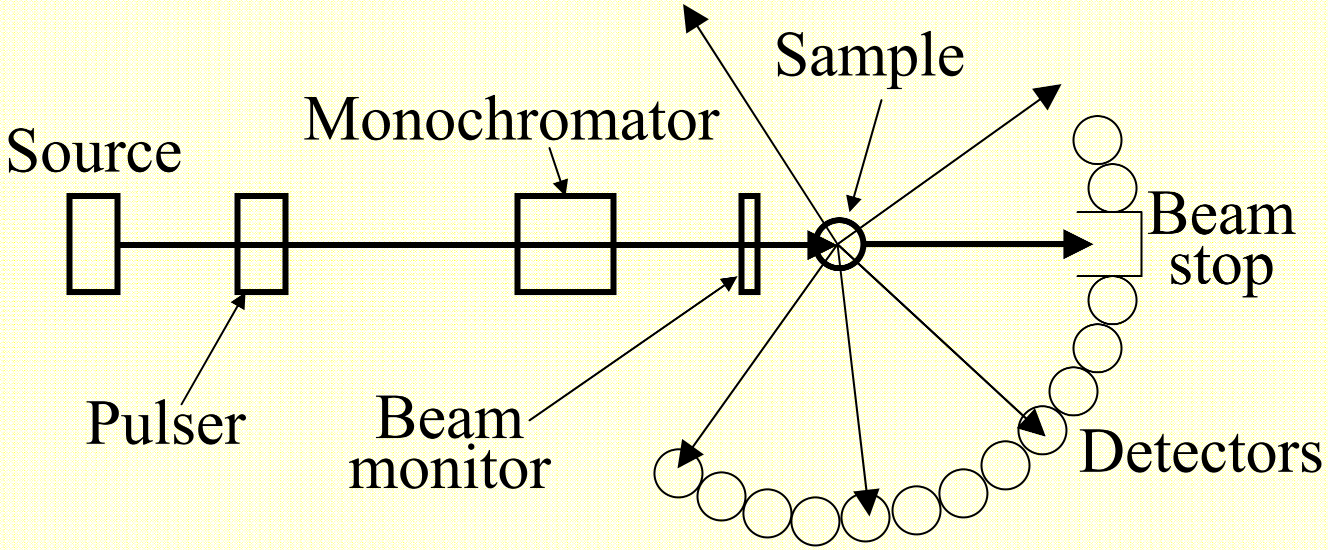
Time-of-flight spectroscopy



- Monochromatic bursts of neutrons strike the sample.
- Some of the neutrons are scattered.
- Some of the scattered neutrons are detected.
- The time between pulses, T, is divided into N time channels of width $\Delta = T/N$. (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.

How do we obtain S(Q,ω) from I(i,j)?

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

- 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
- 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

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

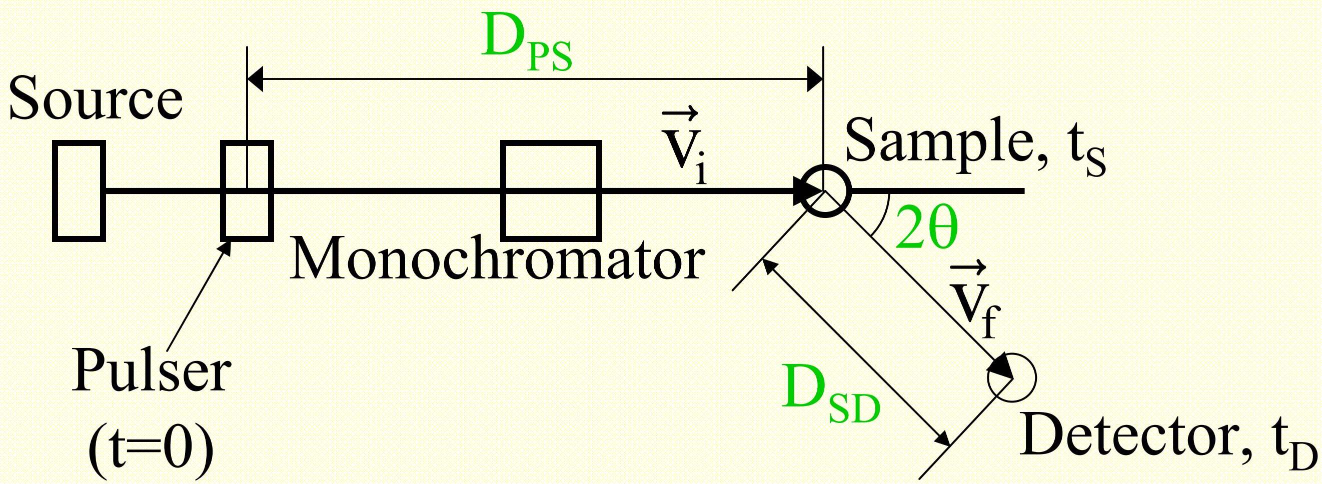
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{d^2\sigma}{d\Omega dt}\cdot\frac{dt}{dE_f}$$

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

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

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 $\vec{v}_f$.

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

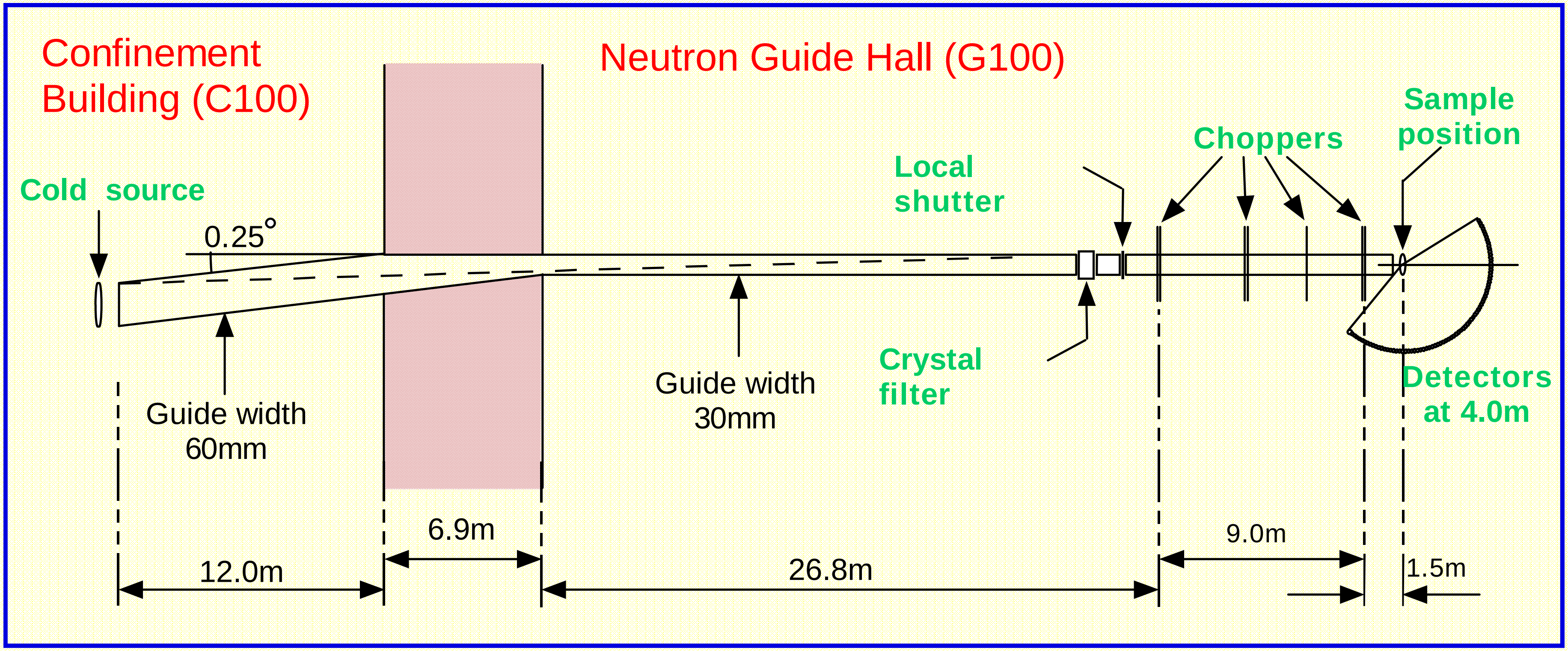
Hence $\hbar\omega = E_i - E_f$

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

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

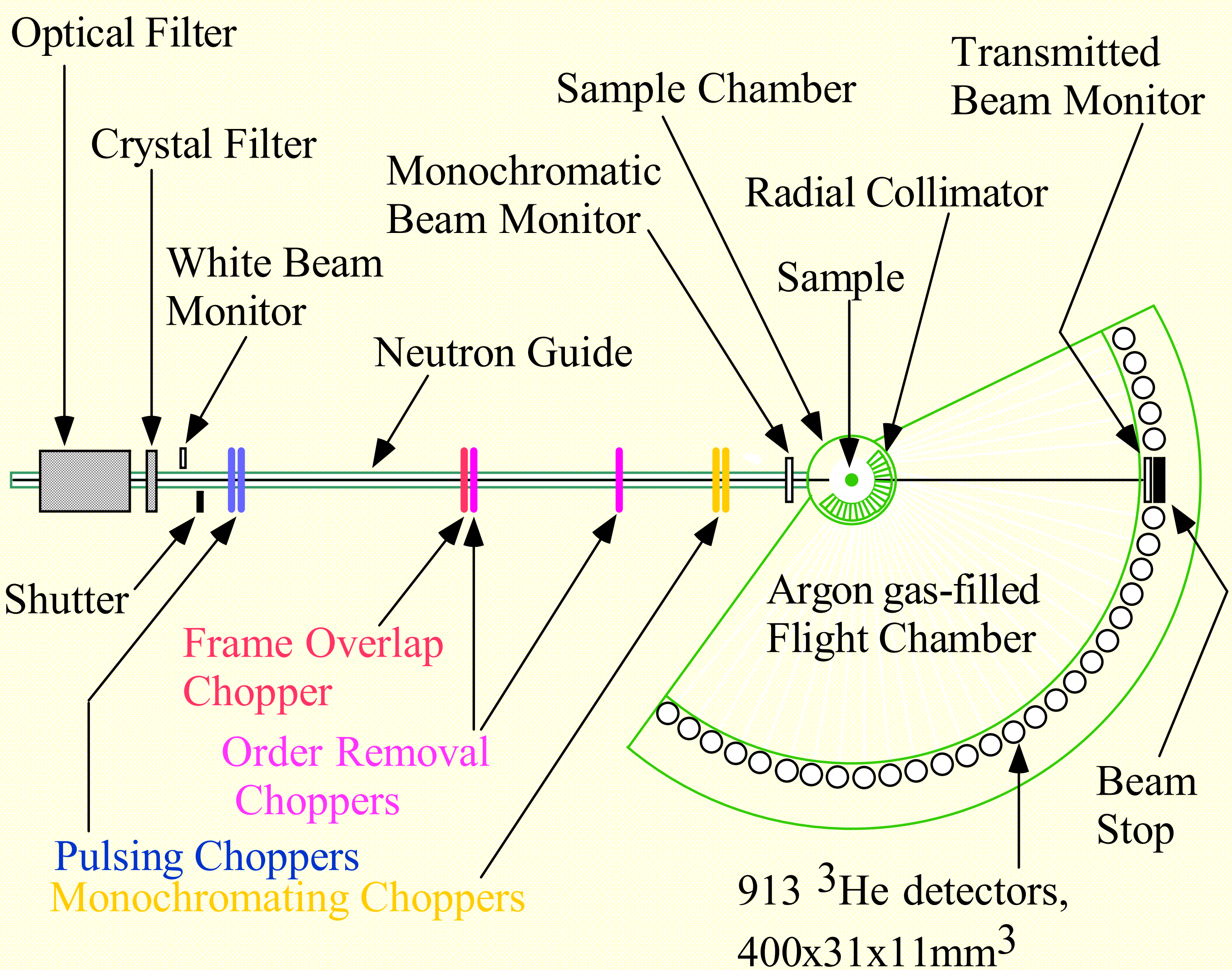
The Disk Chopper Spectrometer

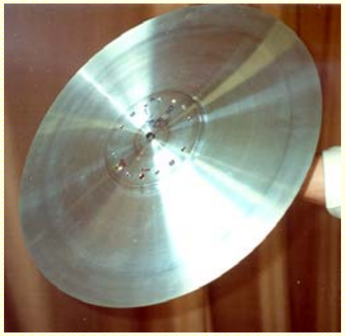
Plan view (to scale)



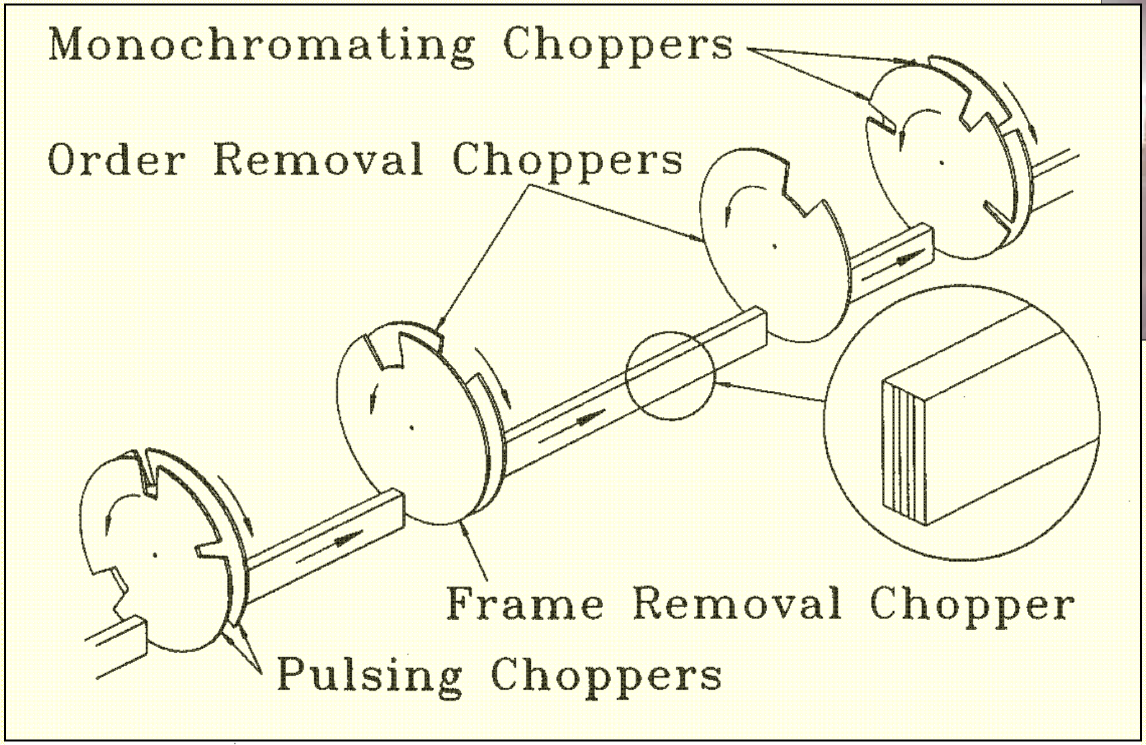
The Disk Chopper Spectrometer

Schematic (not to scale)



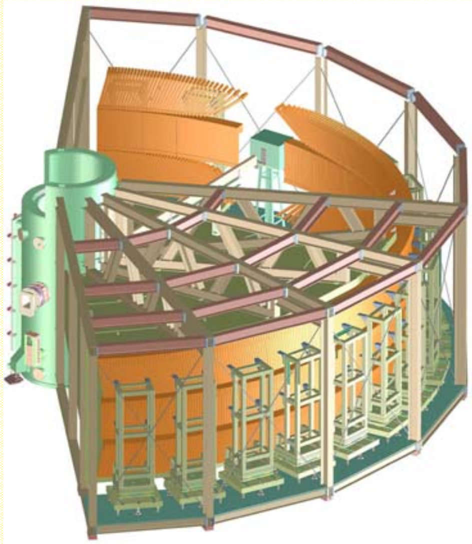


The choppers and the guide



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.

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.

What can one study using the DCS?

Single particle and/or collective motions in all sorts of materials

such as metals, insulators, semiconductors, glasses, magnetic materials, heavy fermions, superconductors, solid and liquid helium, plastic crystals, molecular solids, liquid metals, molten salts, biomolecules, water in confined geometries, polymer systems, micelles, microemulsions, etc., etc.,

under all sorts of conditions

such as (at the NCNR) T ≈50 mK to ≈1900K, P to ≈1.0 GPa, B to ≈11.5T, also strong electric fields, controlled humidity, etc., etc.,

provided that

- the length and time scales (Q and ω ranges) are consistent with instrument capabilities
- the scattering (and absorption) cross sections are acceptable
- the quantity of material is acceptable

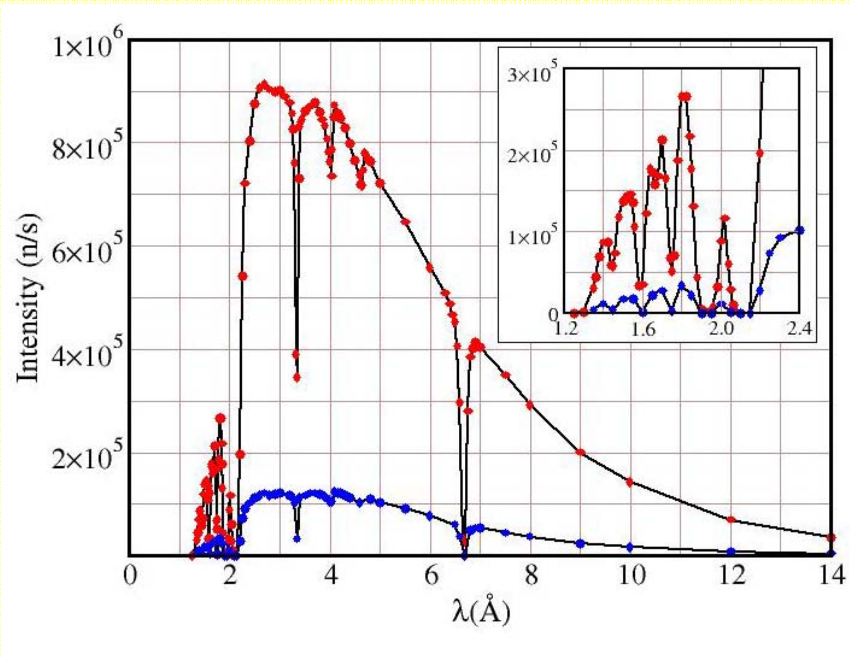
See the NCNR annual reports for examples.

http://www.ncnr.nist.gov/AnnualReport/

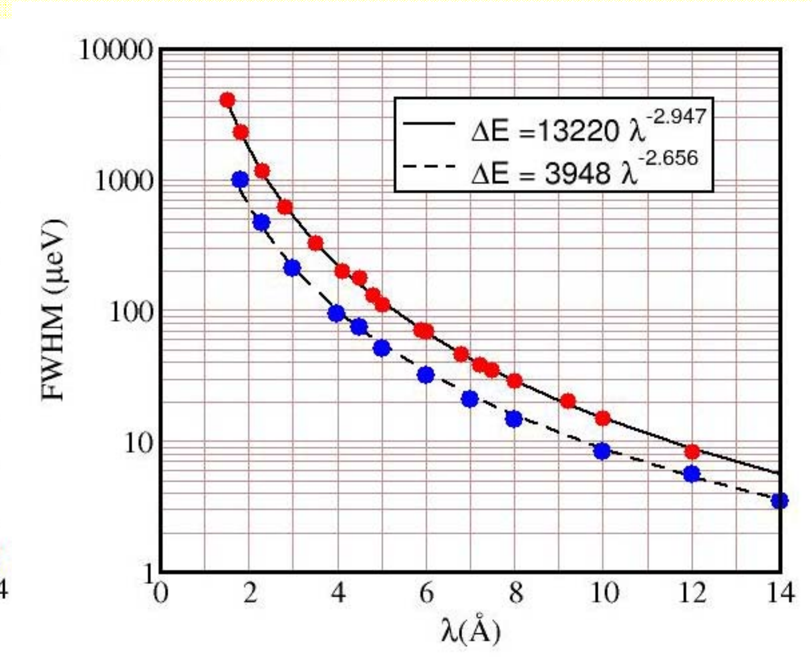
Considerations when running an experiment: choice of wavelength, chopper speeds, and resolution mode

Considerations when running an experiment

Intensity at sample I(E)



Resolution width ΔE



Quantities that can be varied/chosen:

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

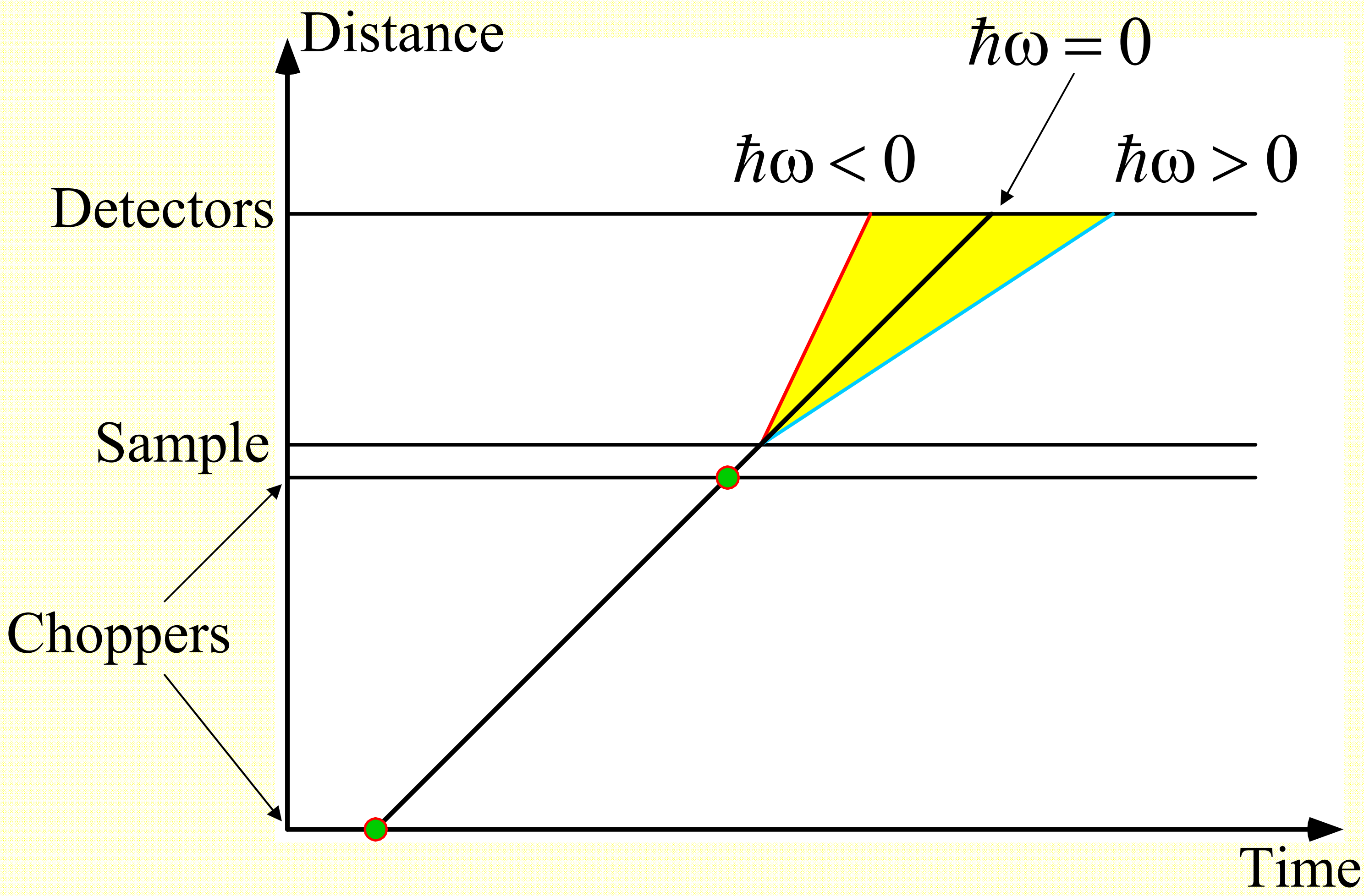
- $I(E) \propto T^2/T_S = T / m$
- $\Delta E \propto T$
- $\hbar\omega$ range increases with m (frame overlap less of a problem)

Choice of chopper slot widths W

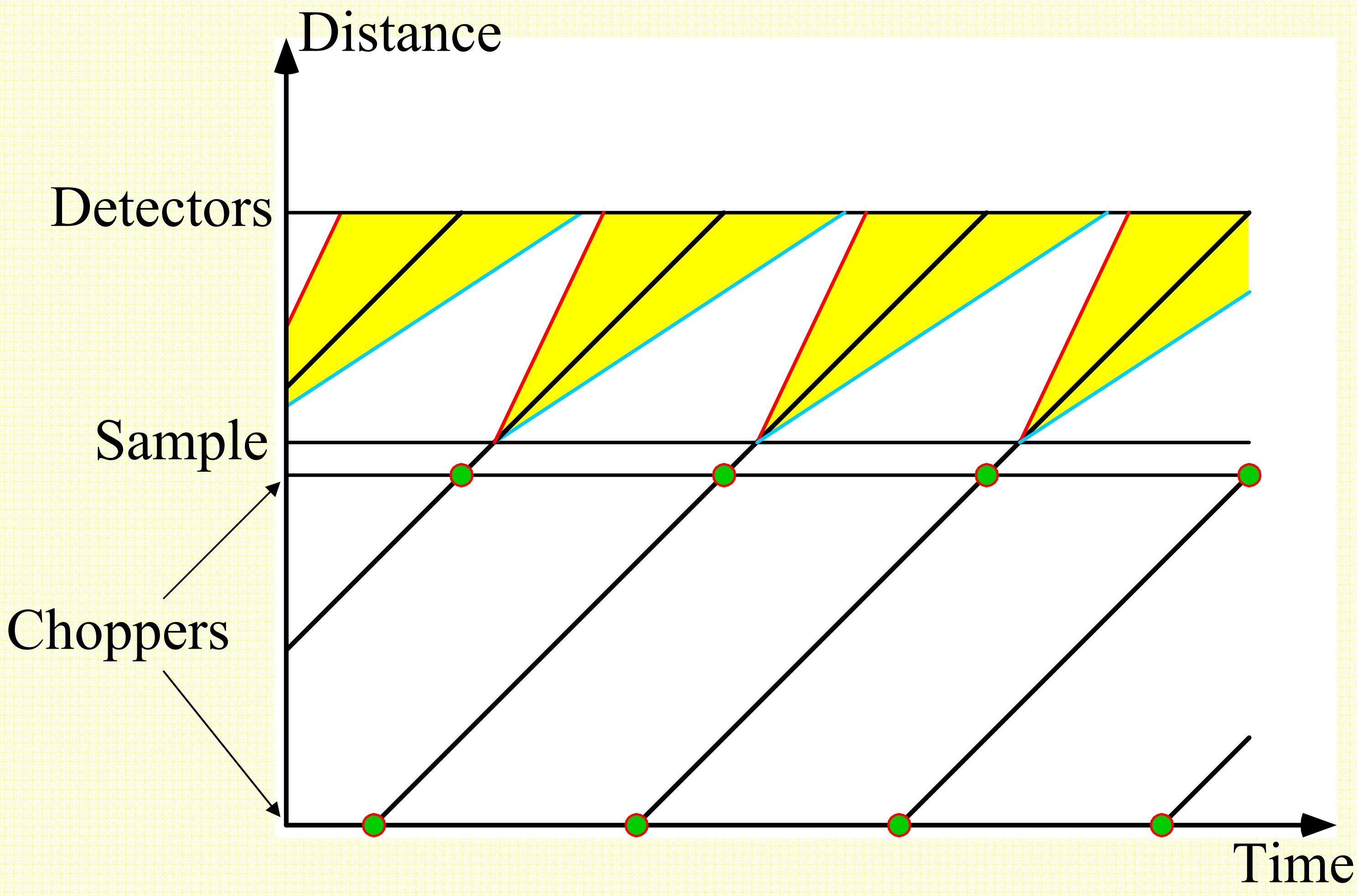
- I(E) varies roughly as W^3
- ΔE varies roughly as W

Time-distance diagrams

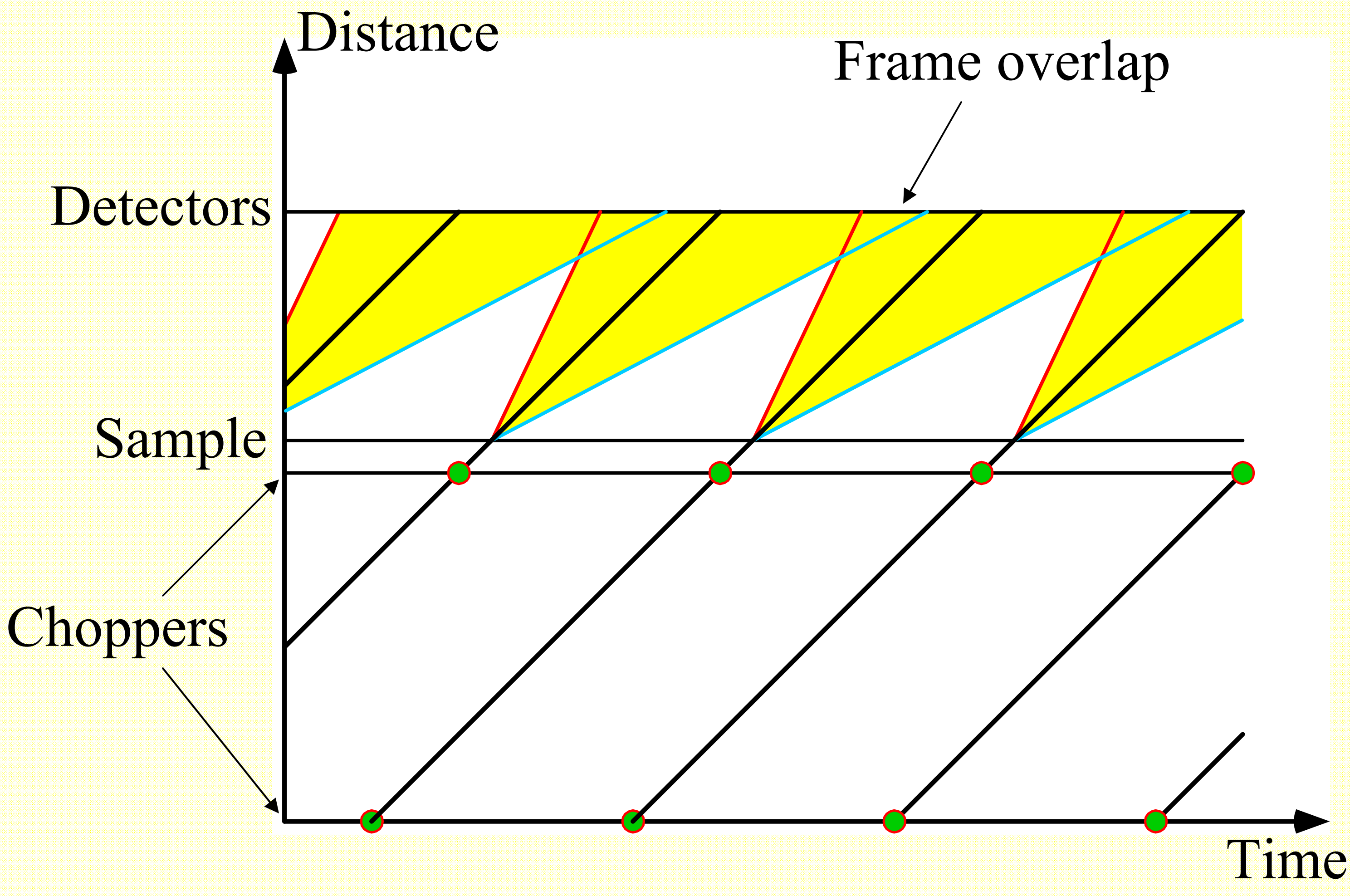
Time-distance diagrams - single pulse



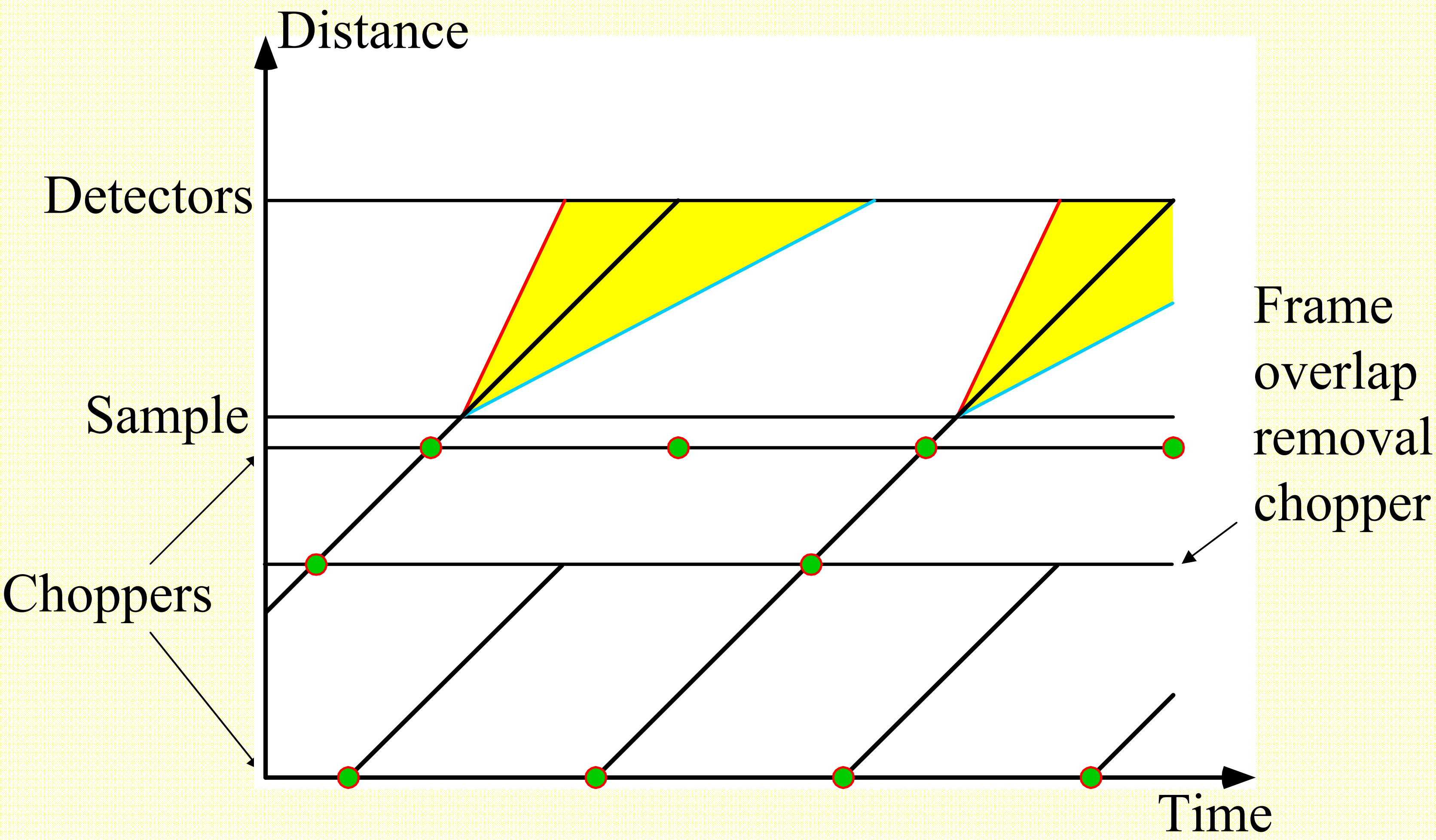
Time-distance diagrams - multiple pulses



What is frame overlap?

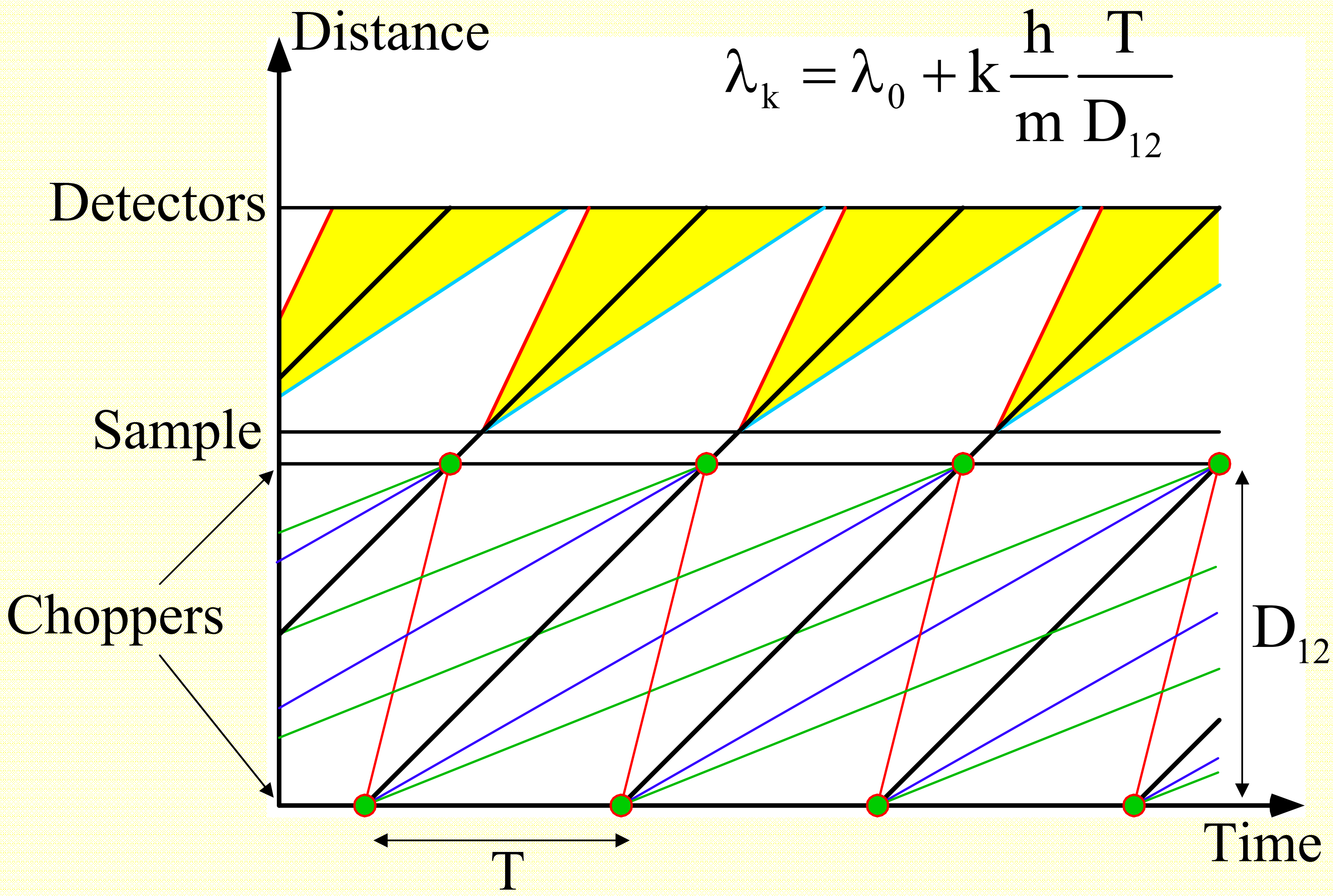


“Removal” of frame overlap



What are contaminant wavelengths ("orders")?

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



Removal of contaminant wavelengths