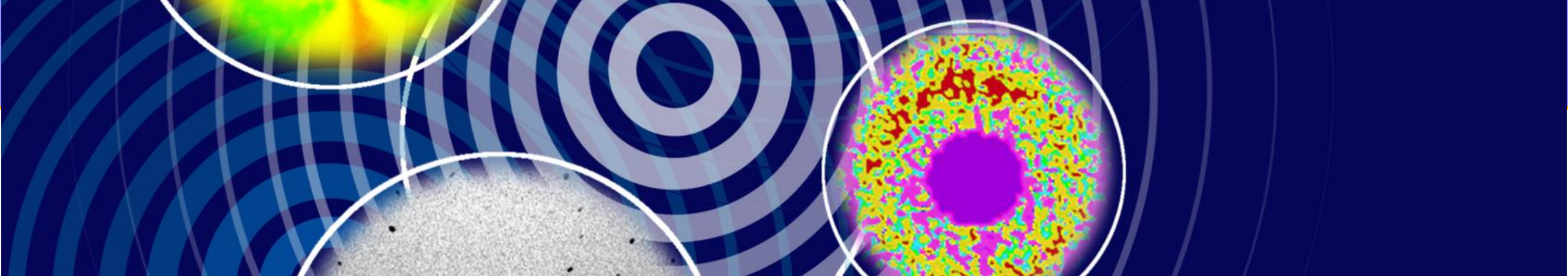


INTRODUCTION TO INELASTIC NEUTRON SCATTERING

Sylvain PETIT
Laboratoire Léon Brillouin
CEA – CNRS – Université Paris-Saclay
91190 Gif sur Yvette, France
sylvain.petit@cea.fr

Outline

1. Diffraction 
2. Can we learn more ? 
3. Cross sections 
4. In practice TOF 
5. In pratice TAS 
6. Polarization 
7. ESS and polychromatic pulses 
8. More … 
7. Tonight 

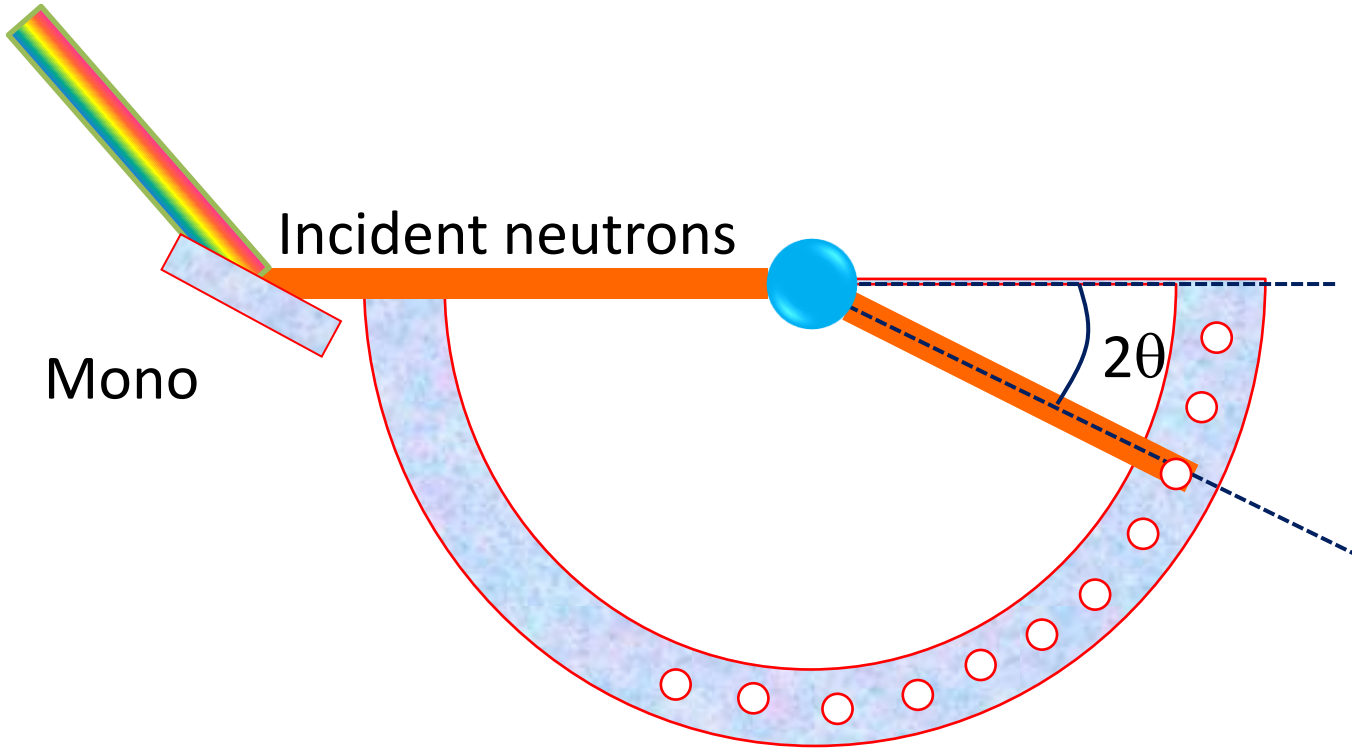
References

https://www.neutron-sciences.org/

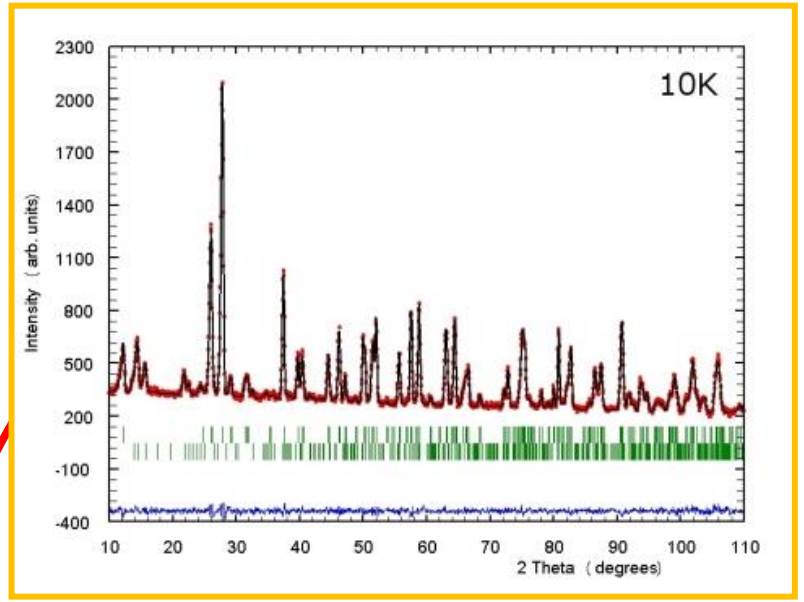
Articles by
Eric Ressouche, Mechthilde Enderle, Stéphane Raymond
And others …

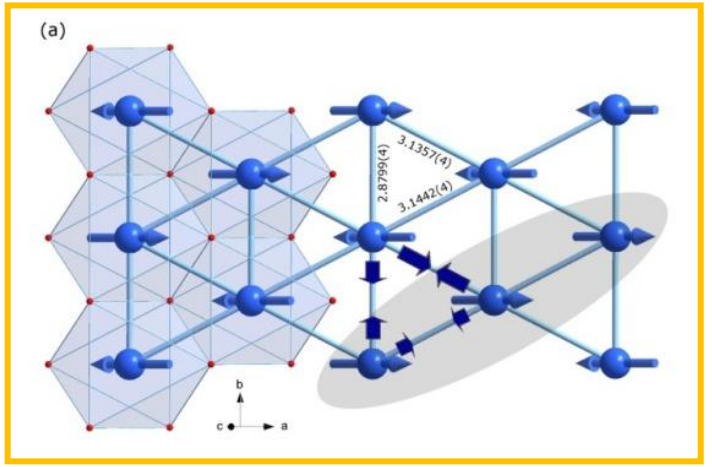
1. Diffraction

Diffraction



« simple » and robust





FUNDAMENTAL FORMULAS 1 & 2

$$F_N(\mathbf{Q}) = \sum_{\ell} b_\ell \; e^{i\mathbf{Q}\mathbf{r}_\ell} \; e^{-W_\ell}$$

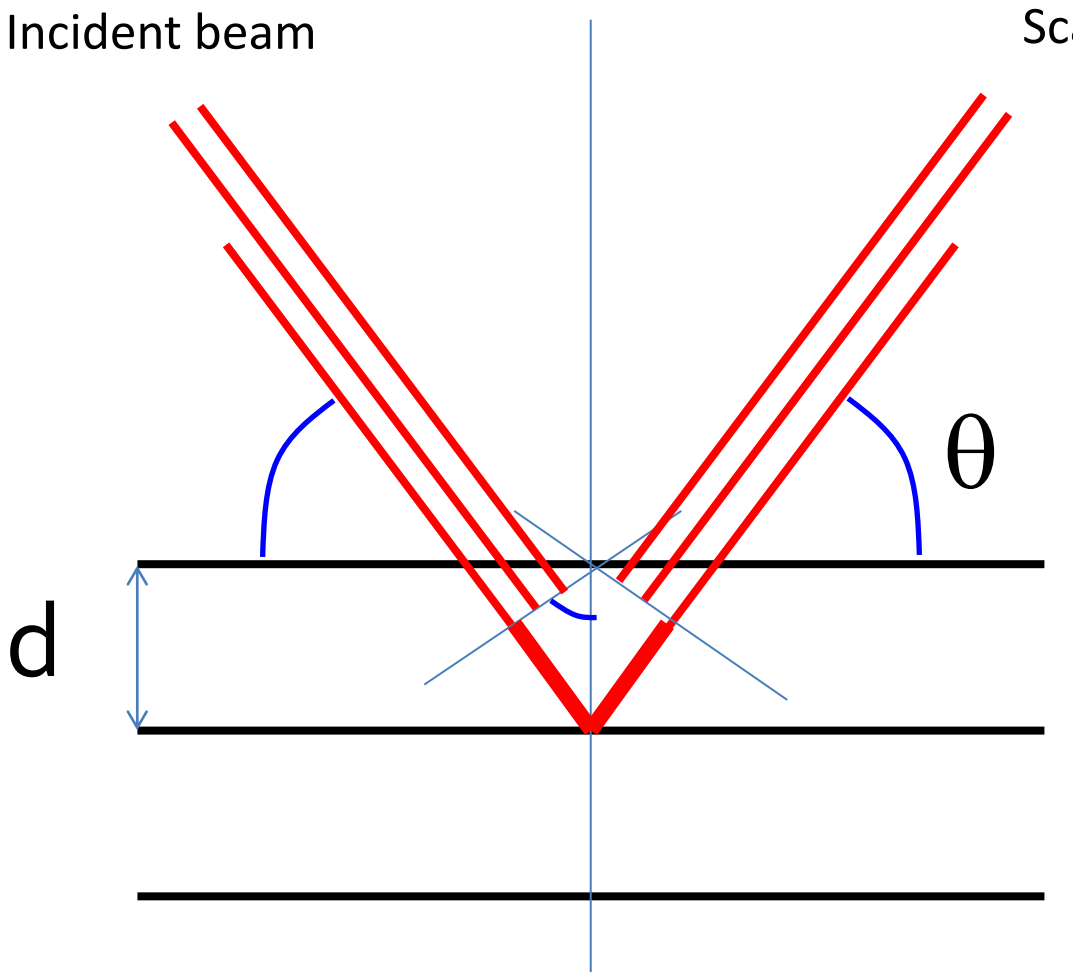
Strong interaction with nuclei

$$\mathbf{F}_M(\mathbf{Q}) = \sum_{\ell} \mathbf{S}_{\ell\perp} e^{i\mathbf{Q}\mathbf{r}_\ell} \; e^{-W_\ell}$$

The spin of the neutron interacts with the dipolar field created by the spin (and orbital motion) of unpaired electrons

2. Can we learn more ?

Can we learn more ?

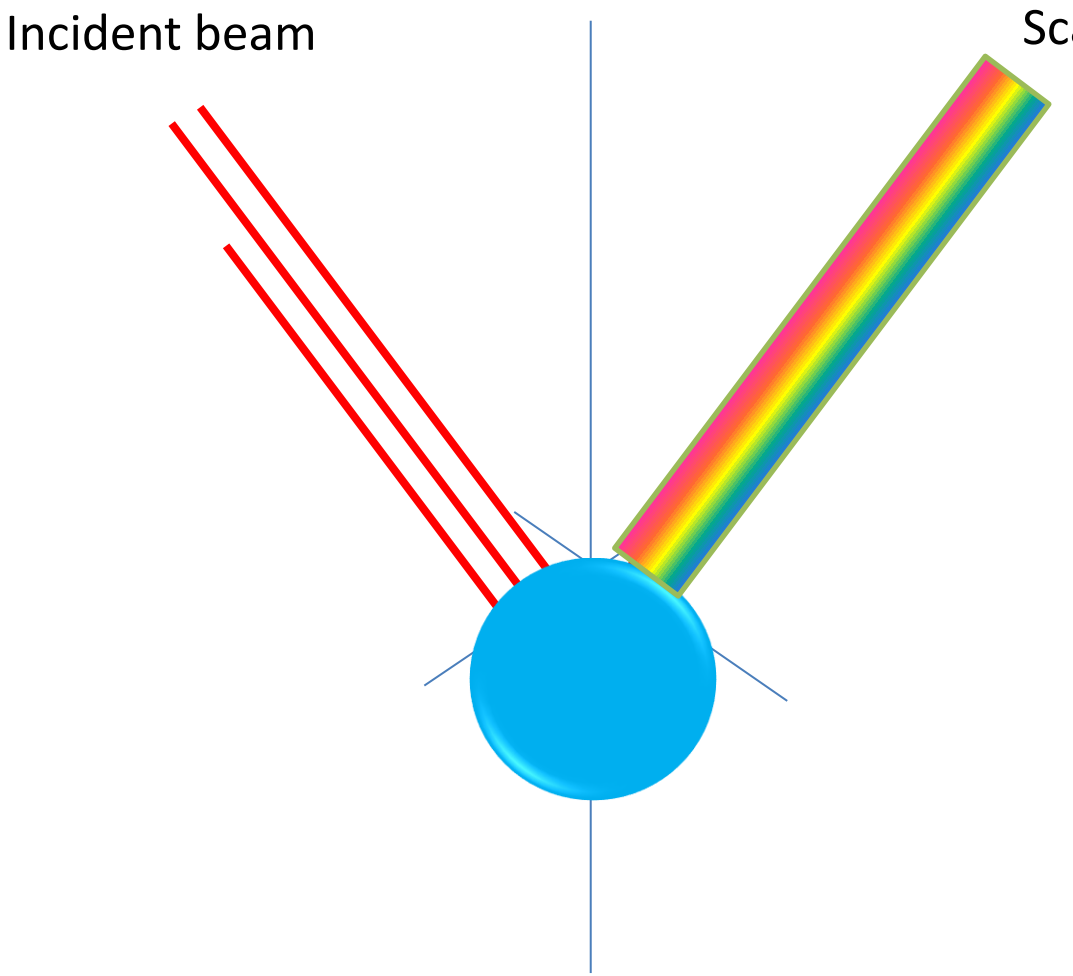


Bragg law

$$\lambda = 2d \sin\theta$$

Diffraction is an ***elastic*** process…

Can we learn more ?

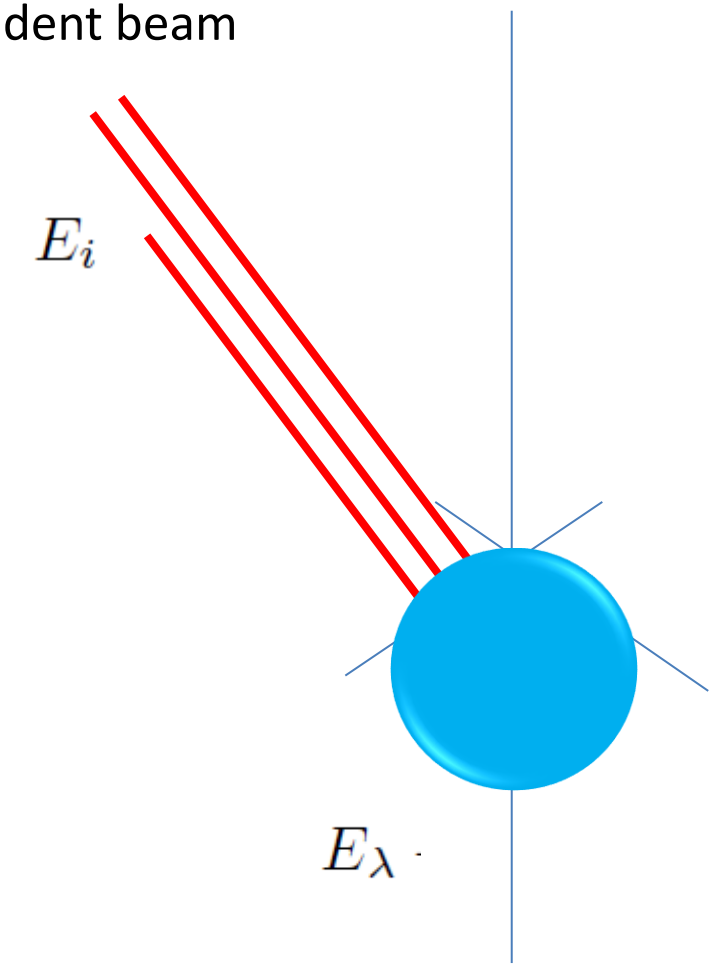


However …

Depending on the interaction with the sample, neutrons can gain or loose energy (hence rainbow colors)

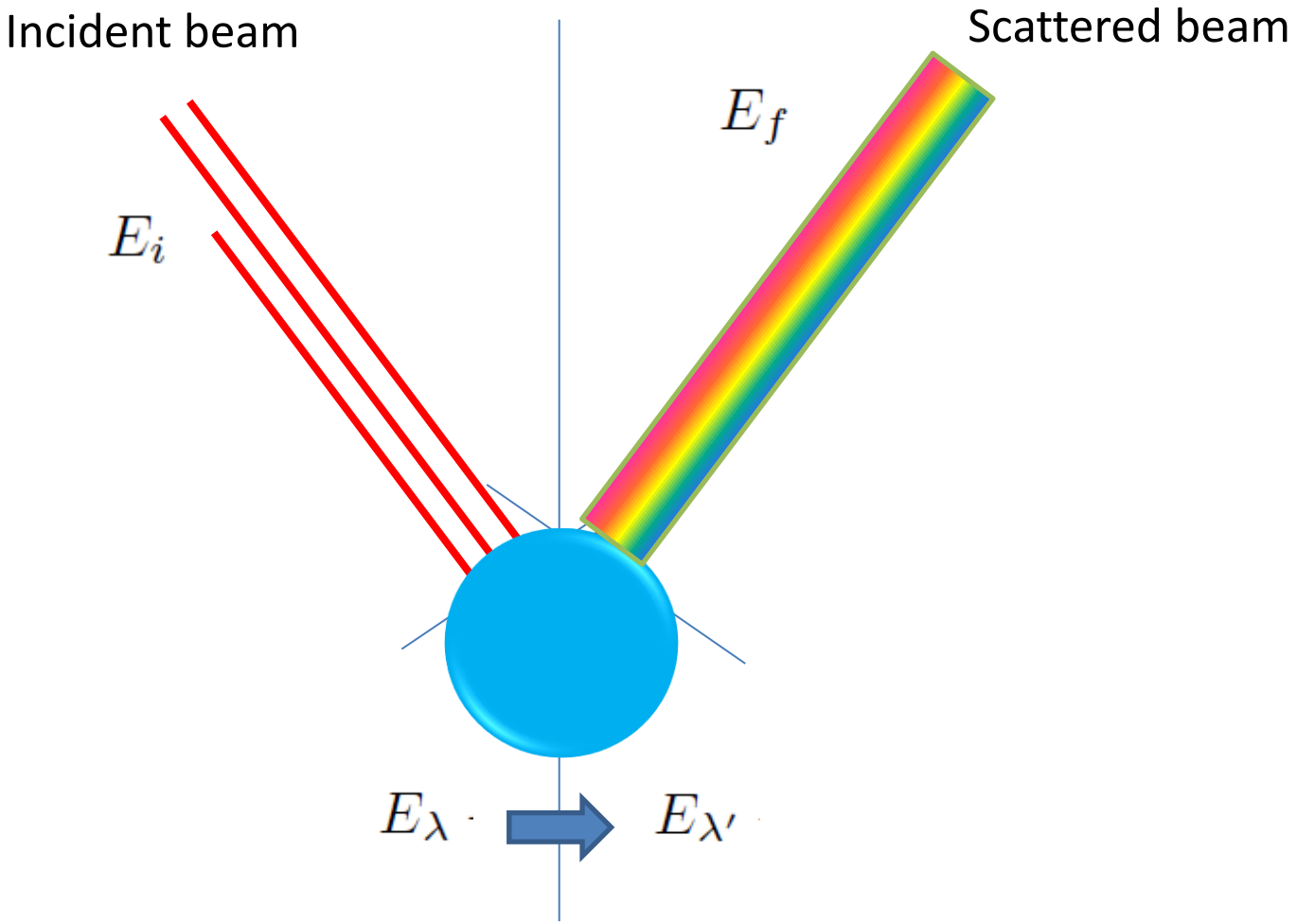
Can we learn more ?

Incident beam

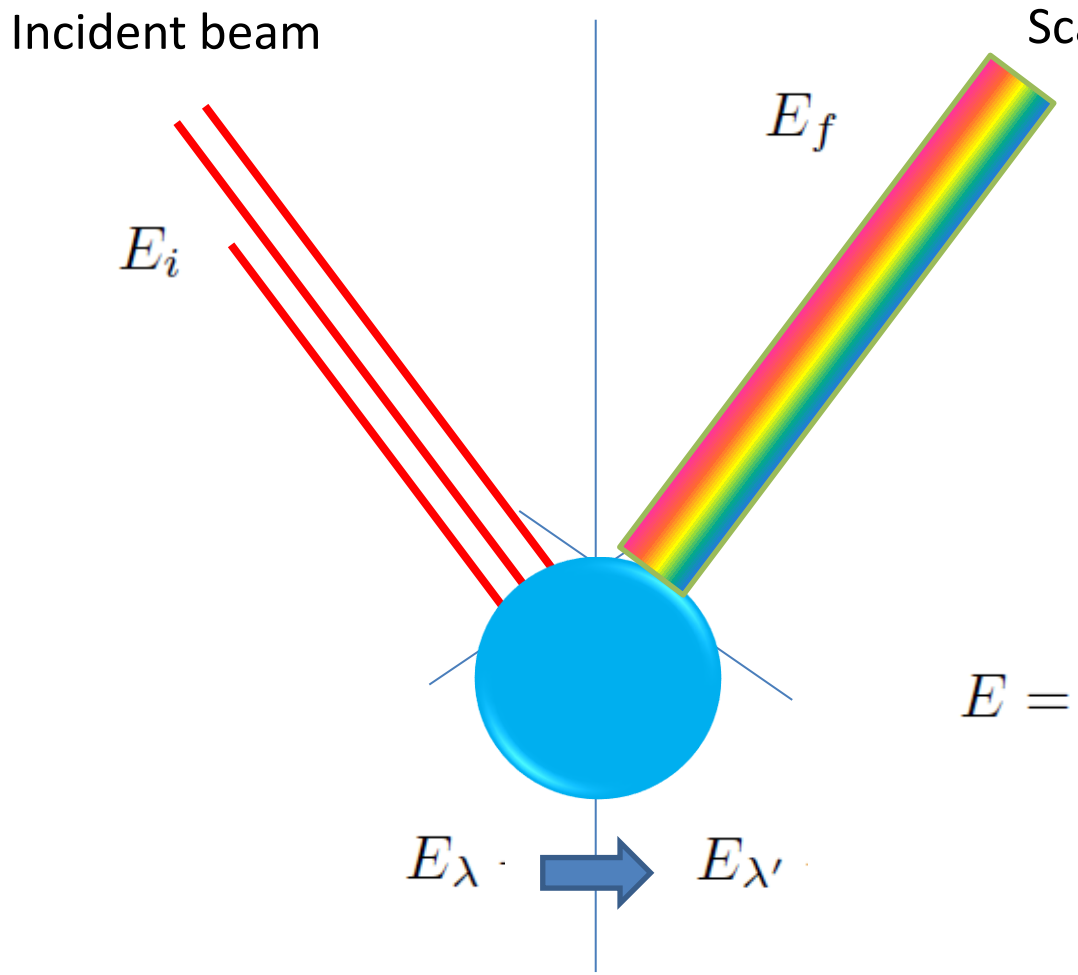


Scattered beam

Can we learn more ?



Can we learn more ?



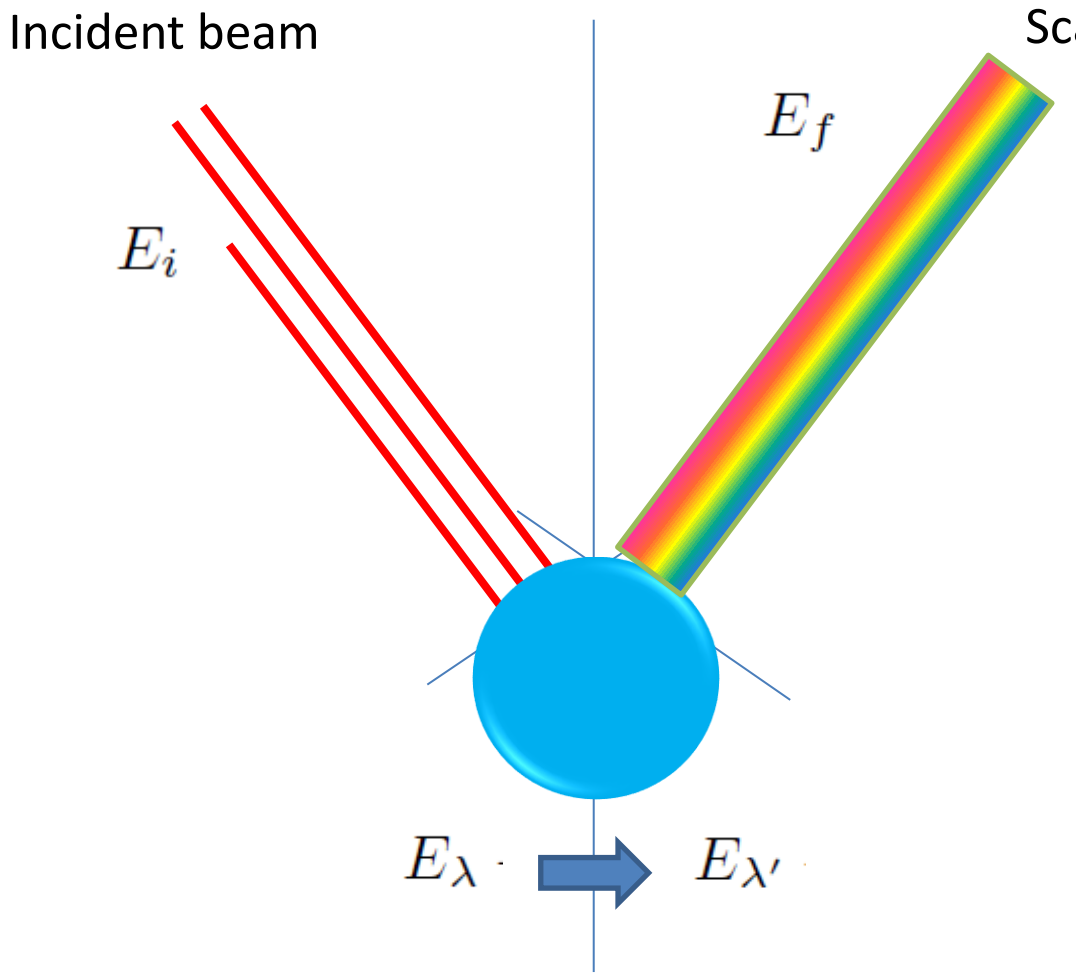
Energy is conserved

$$E_\lambda + E_i = E_{\lambda'} + E_f$$

Energy is transferred

$$E = \hbar\omega = E_i - E_f = E_{\lambda'} - E_\lambda$$

Can we learn more ?



Sample gains energy
(neutrons loose energy)

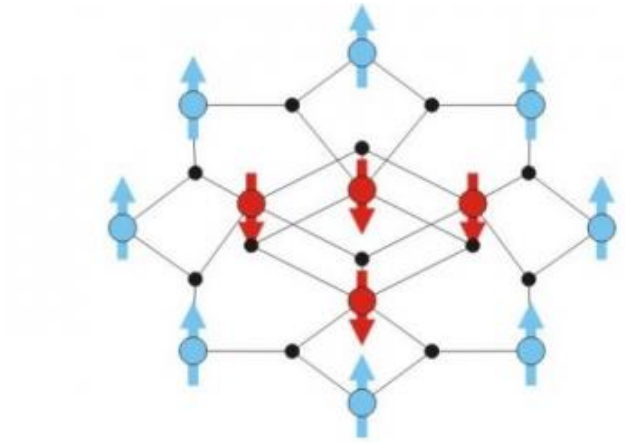
$$E = \hbar\omega \ > 0$$

Sample looses energy
(neutrons gain energy)

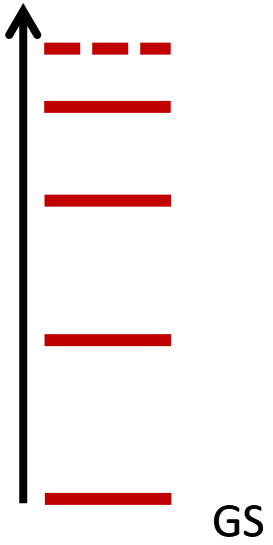
$$E = \hbar\omega \ < 0$$

Example 1 : Mn12-acetate

Mn12-acetate : a molecular nanomagnet



Each molecule is a quantum object characterized by a discrete spectrum



Mn^{3+} S = 2 Mn^{4+} S = 3/2 · O

- The ground state is actually a ferrimagnetic arrangement
- Possible magnetization reversal by thermal effects, but also by quantum effects

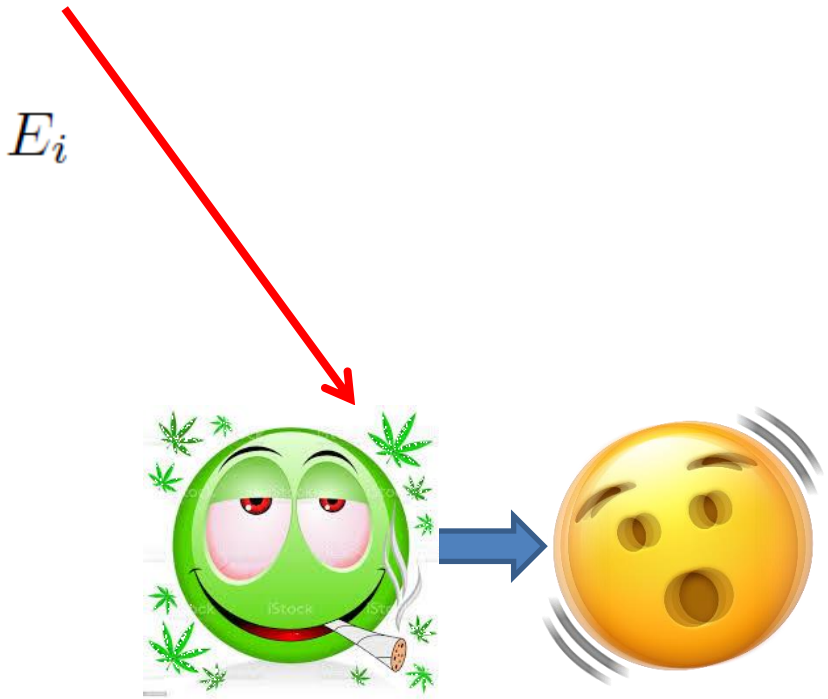
Example 1 : Mn12-acetate

T= 0 (in the ground state) :

E_i

Example 1 : Mn12-acetate

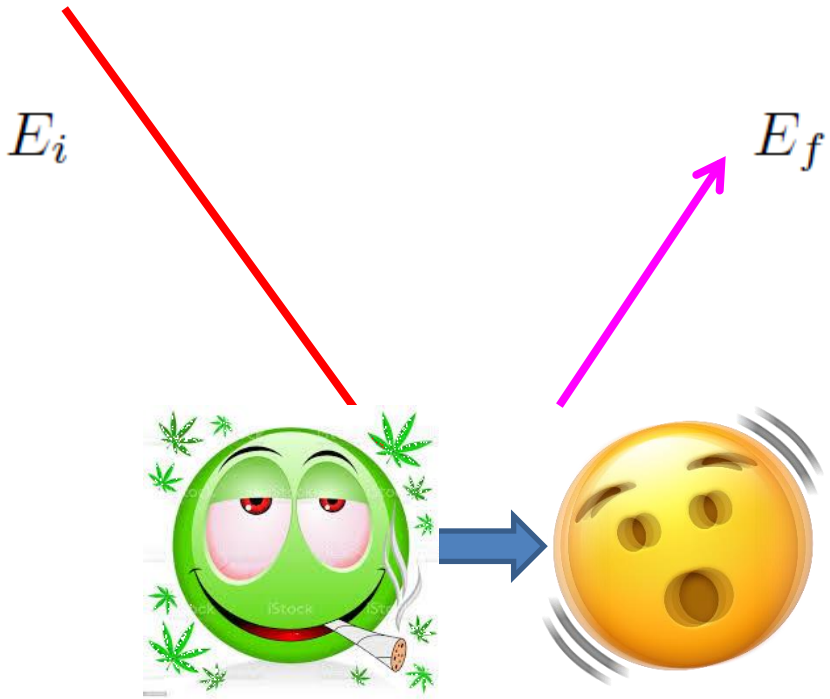
T= 0 (in the ground state) :



- Gets excited by populating an excited state with energy E

Example 1 : Mn12-acetate

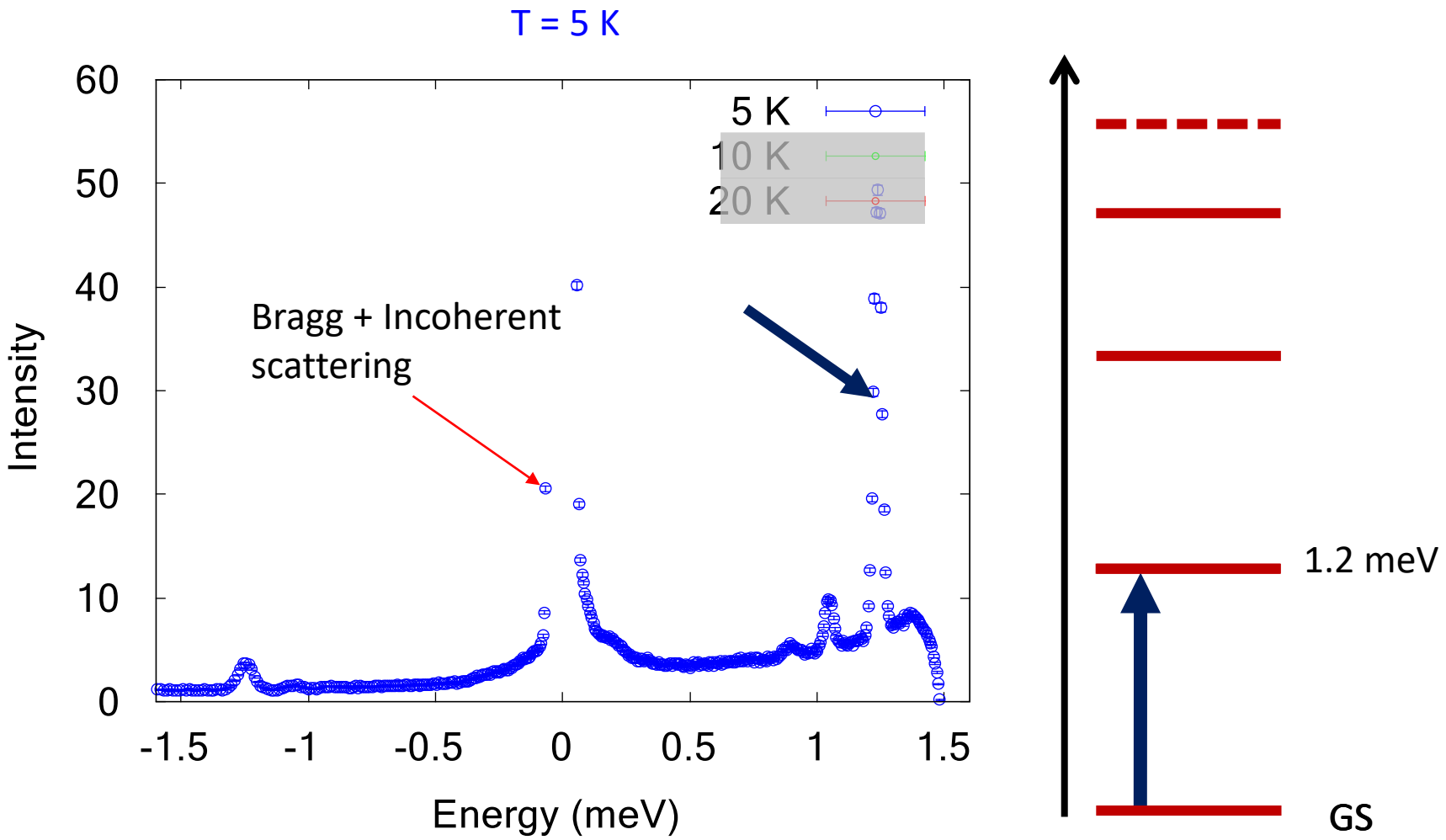
T= 0 (in the ground state) :



- Gets excited by populating an excited state with energy E
- The outgoing neutron has less energy

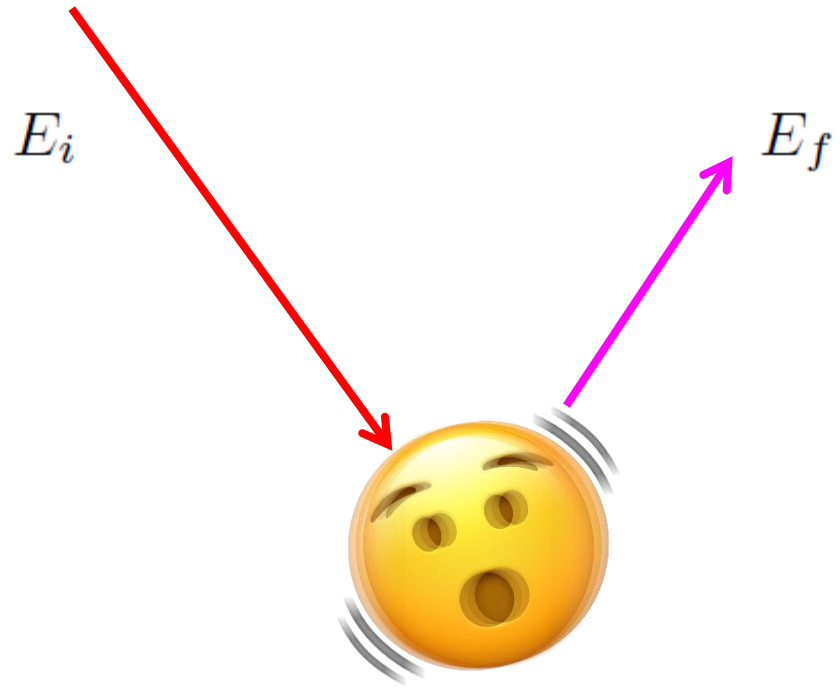
$$E = \hbar\omega = E_i - E_f$$

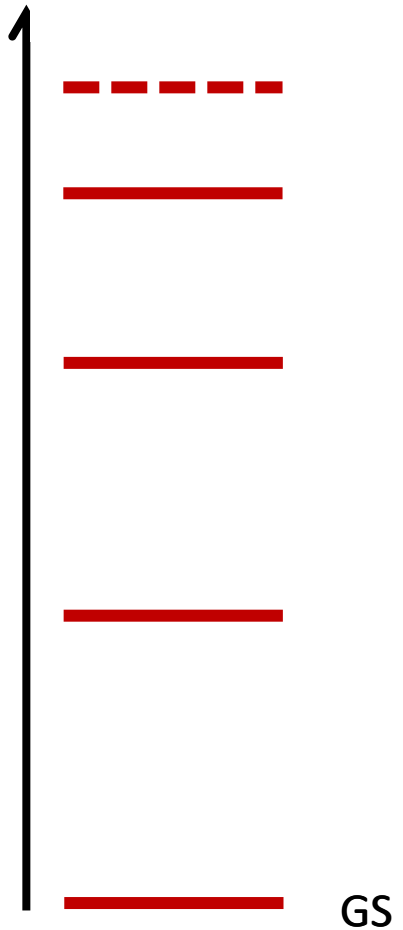
Example 1 : Mn12-acetate



Example 1 : Mn12-acetate

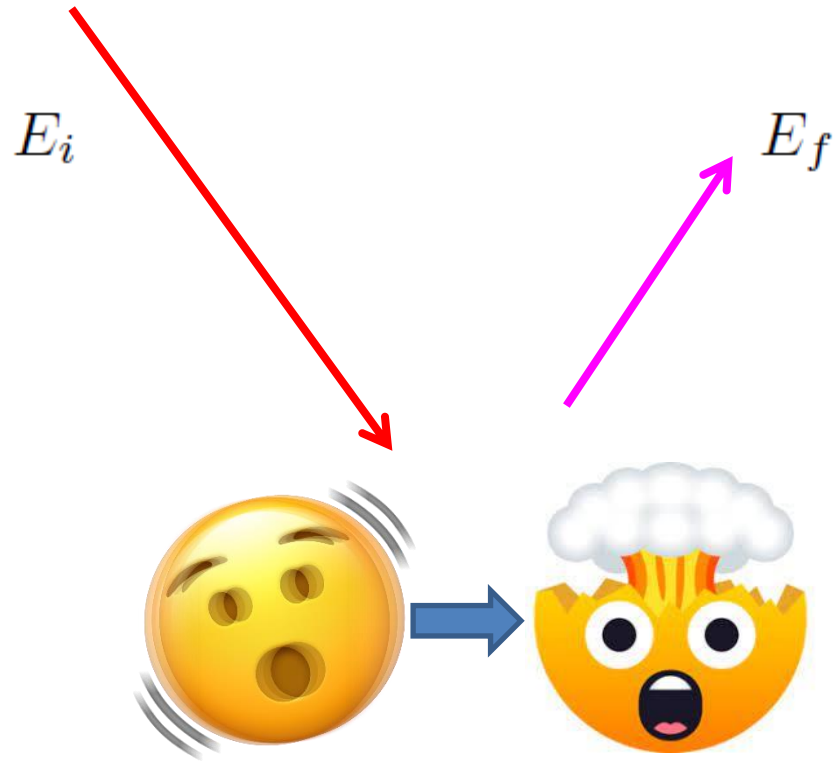
At finite T, excited states are populated up to Boltzmann factor $\frac{\exp -E_n/k_BT}{\sum_n \exp -E_n/k_BT}$

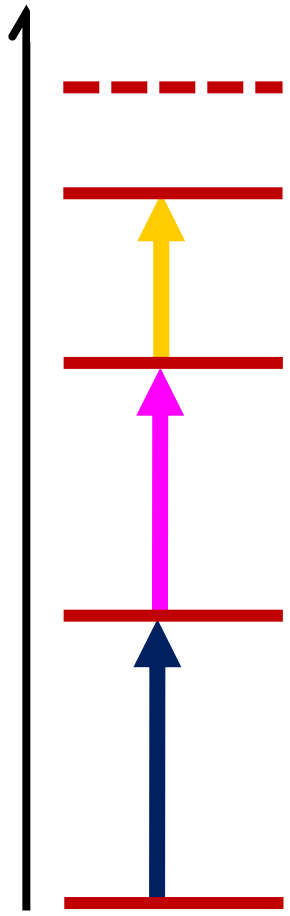




Example 1 : Mn12-acetate

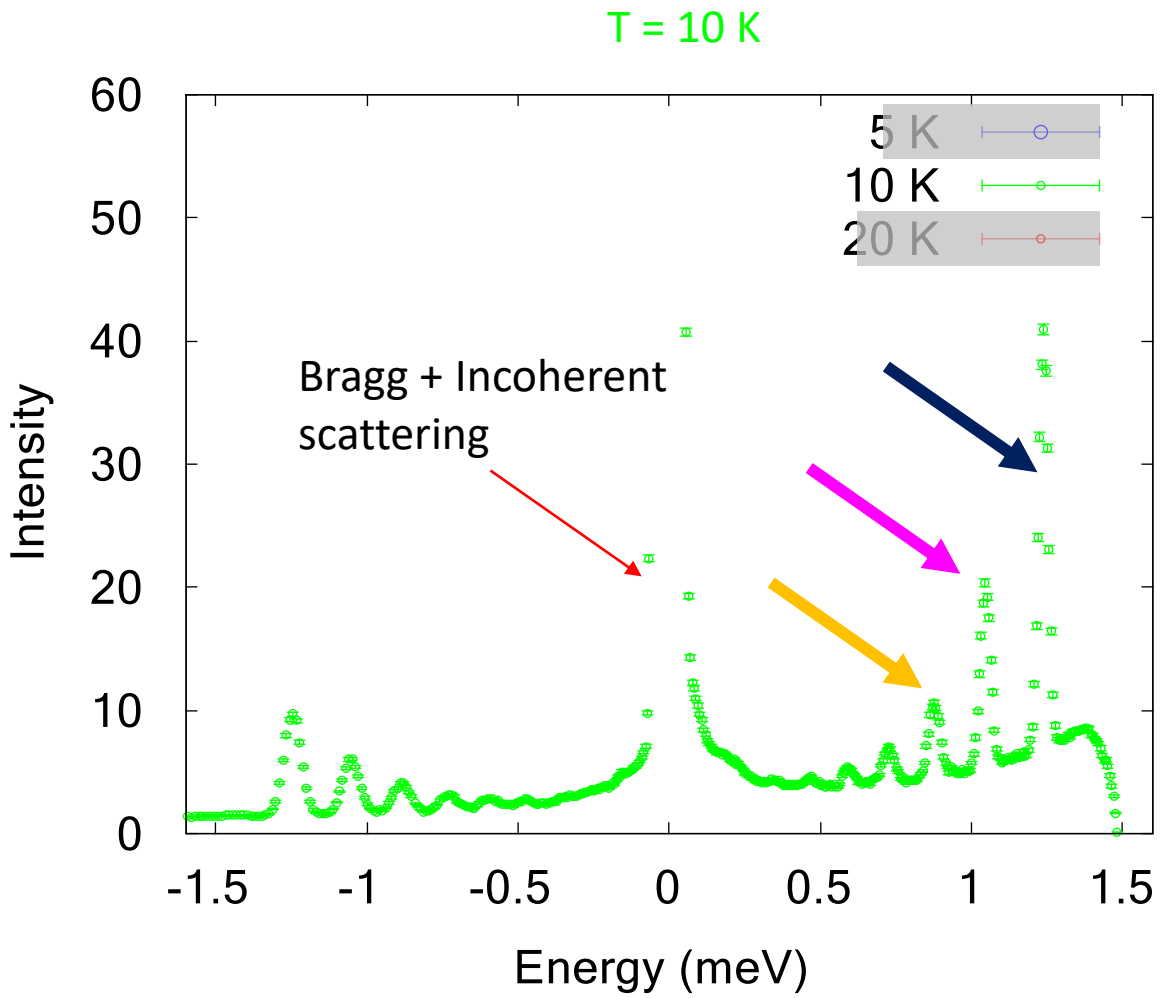
At finite T, excited states are populated up to Boltzmann factor $\frac{\exp -E_n/k_BT}{\sum_n \exp -E_n/k_BT}$

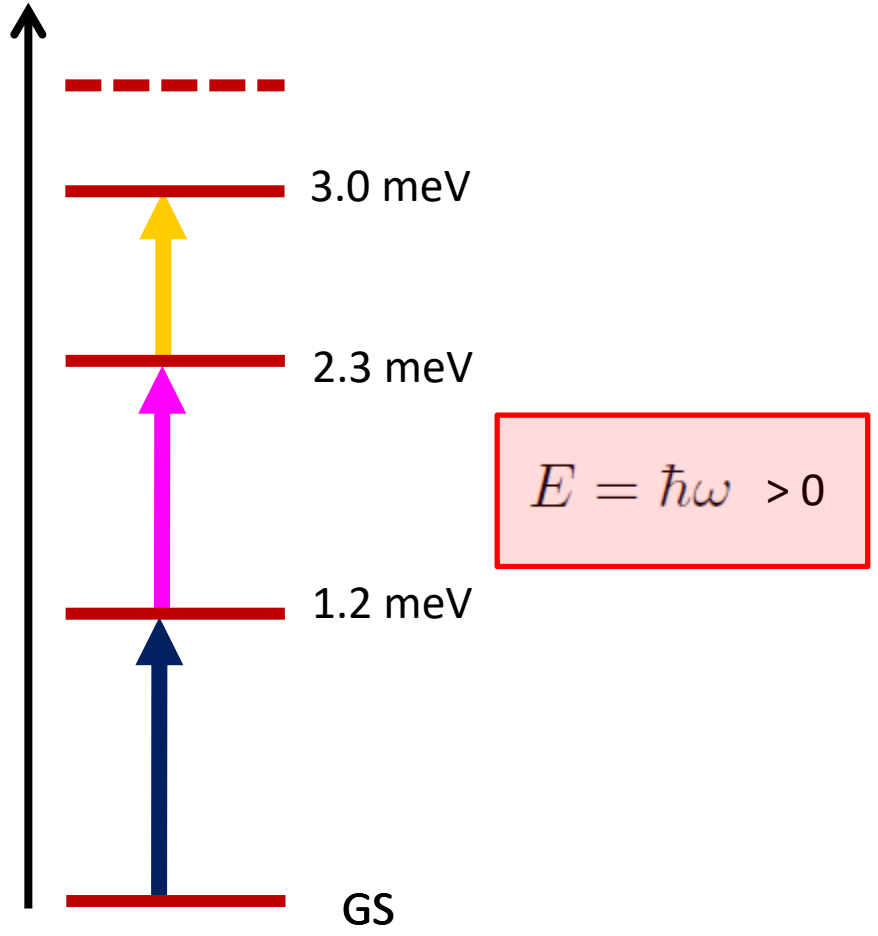




$E = \hbar\omega > 0$

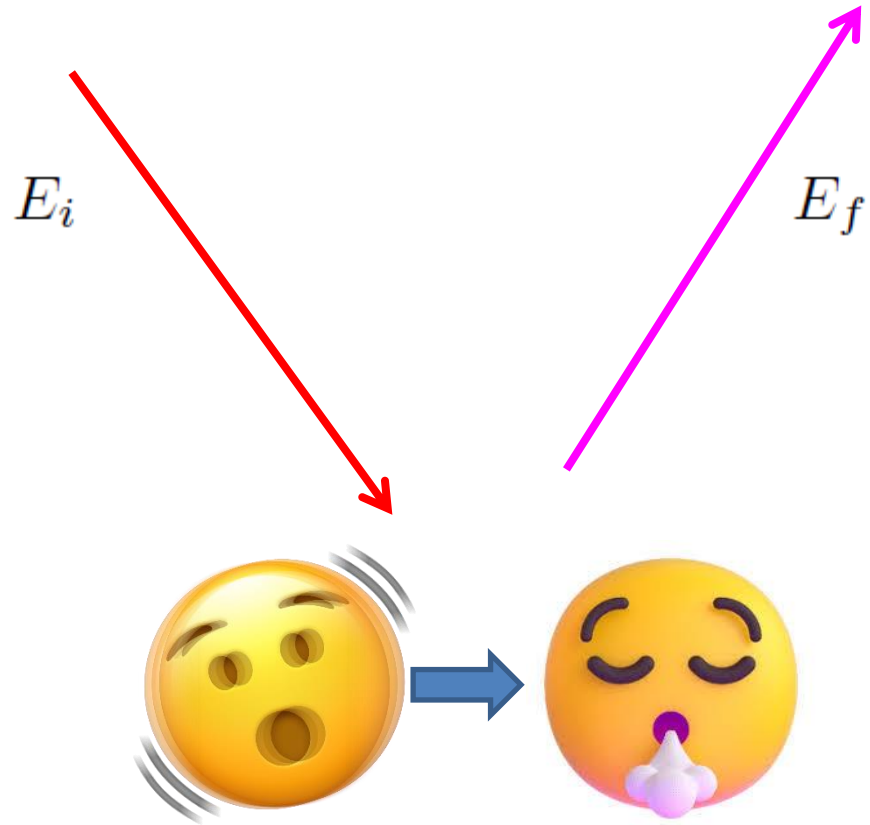
Example 1 : Mn12-acetate

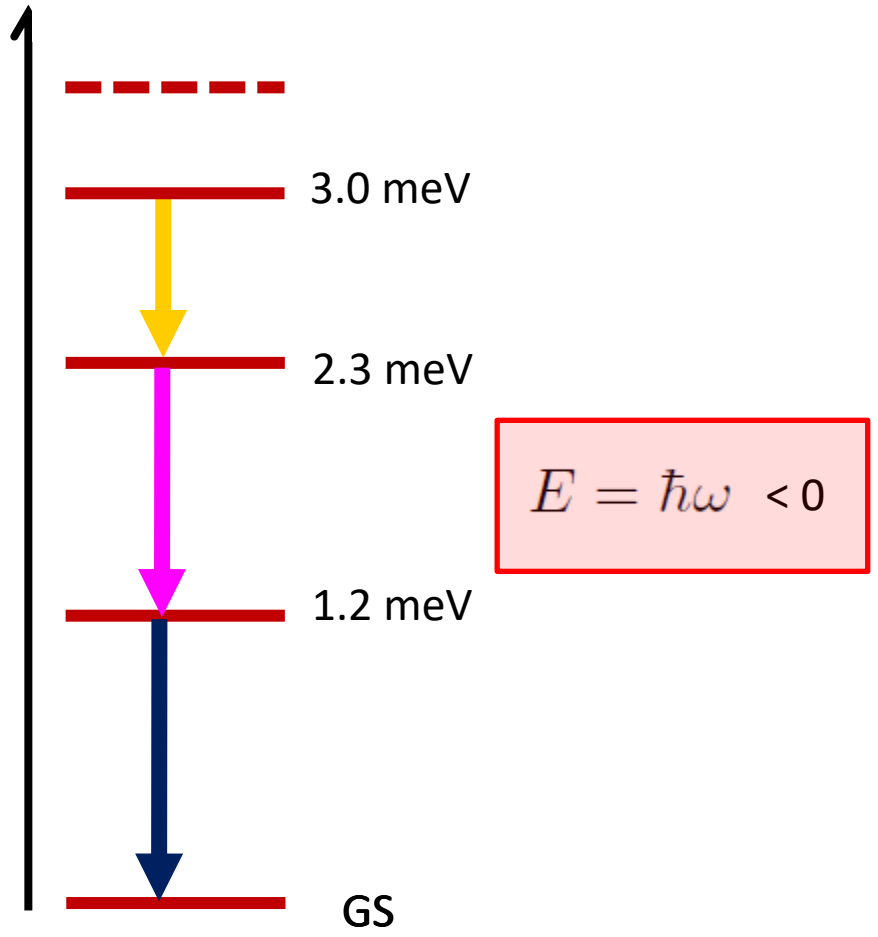




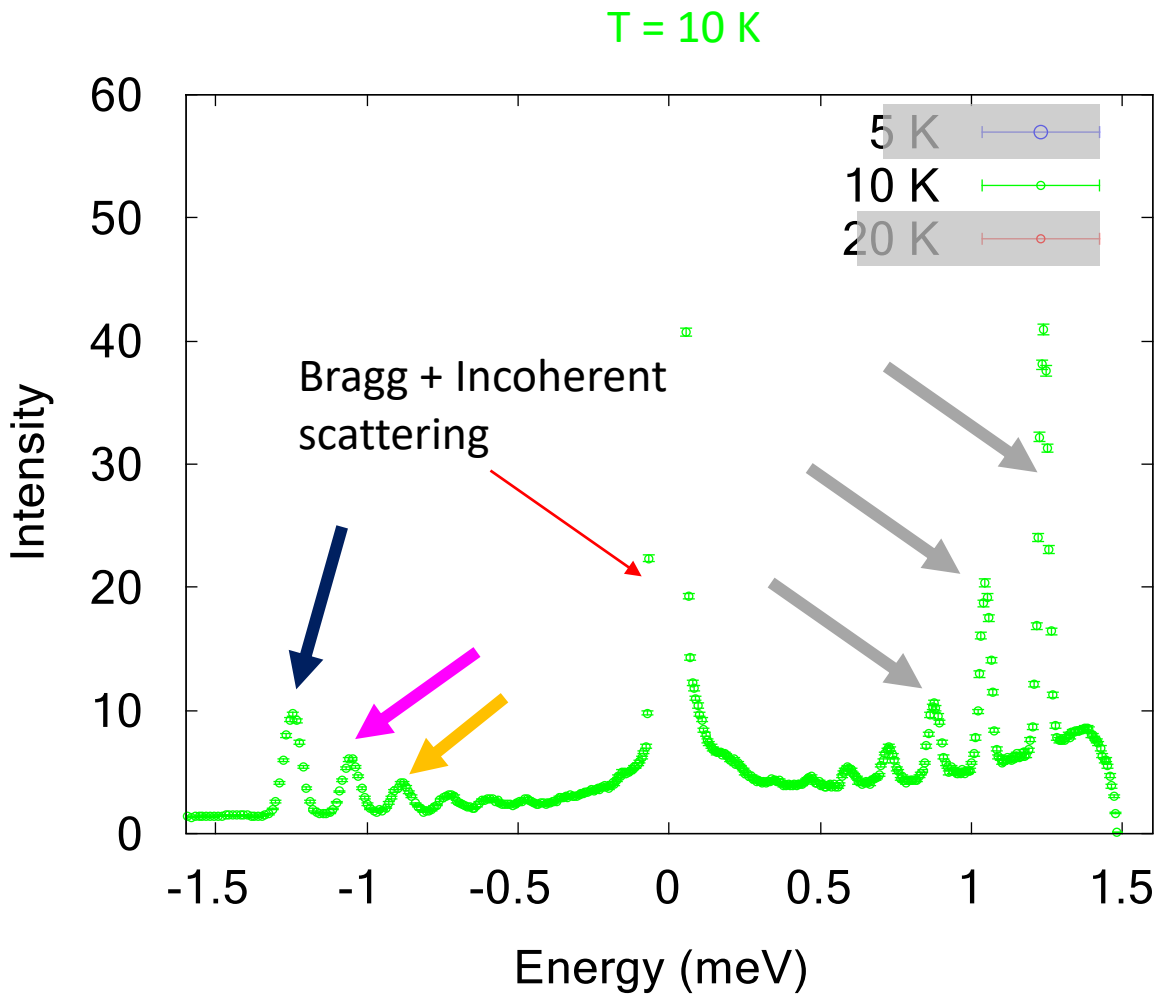
Example 1 : Mn12-acetate

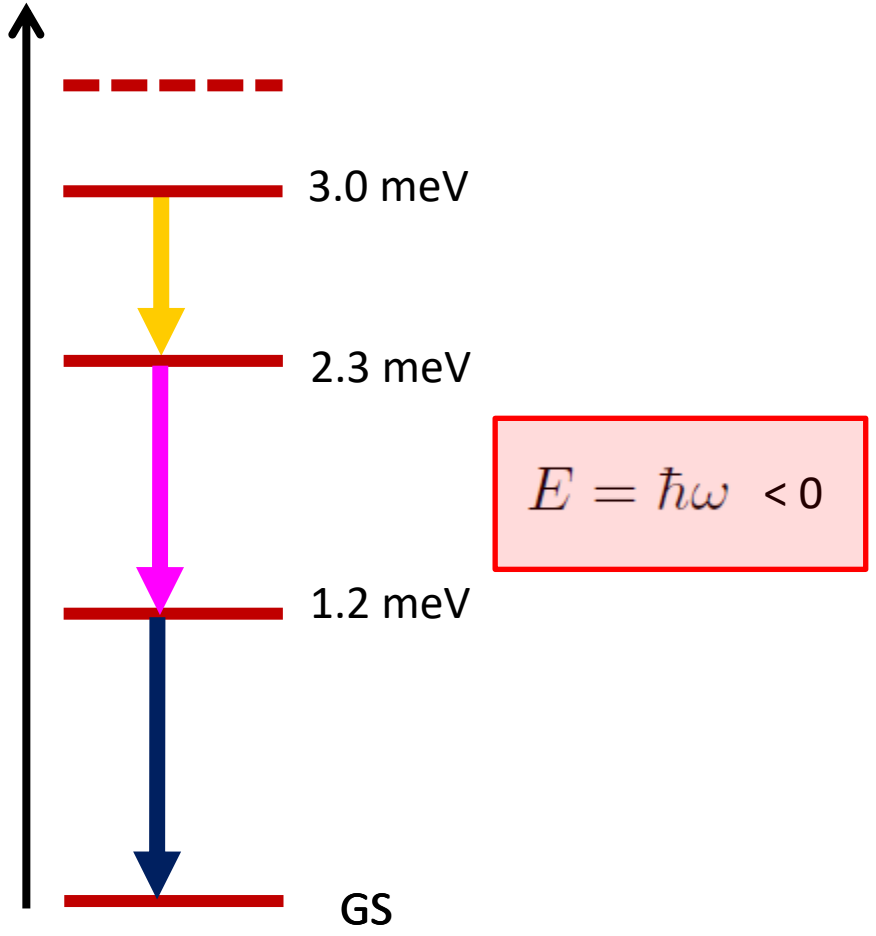
At finite T, excited states are populated up to Boltzmann factor $\frac{\exp -E_n/k_BT}{\sum_n \exp -E_n/k_BT}$



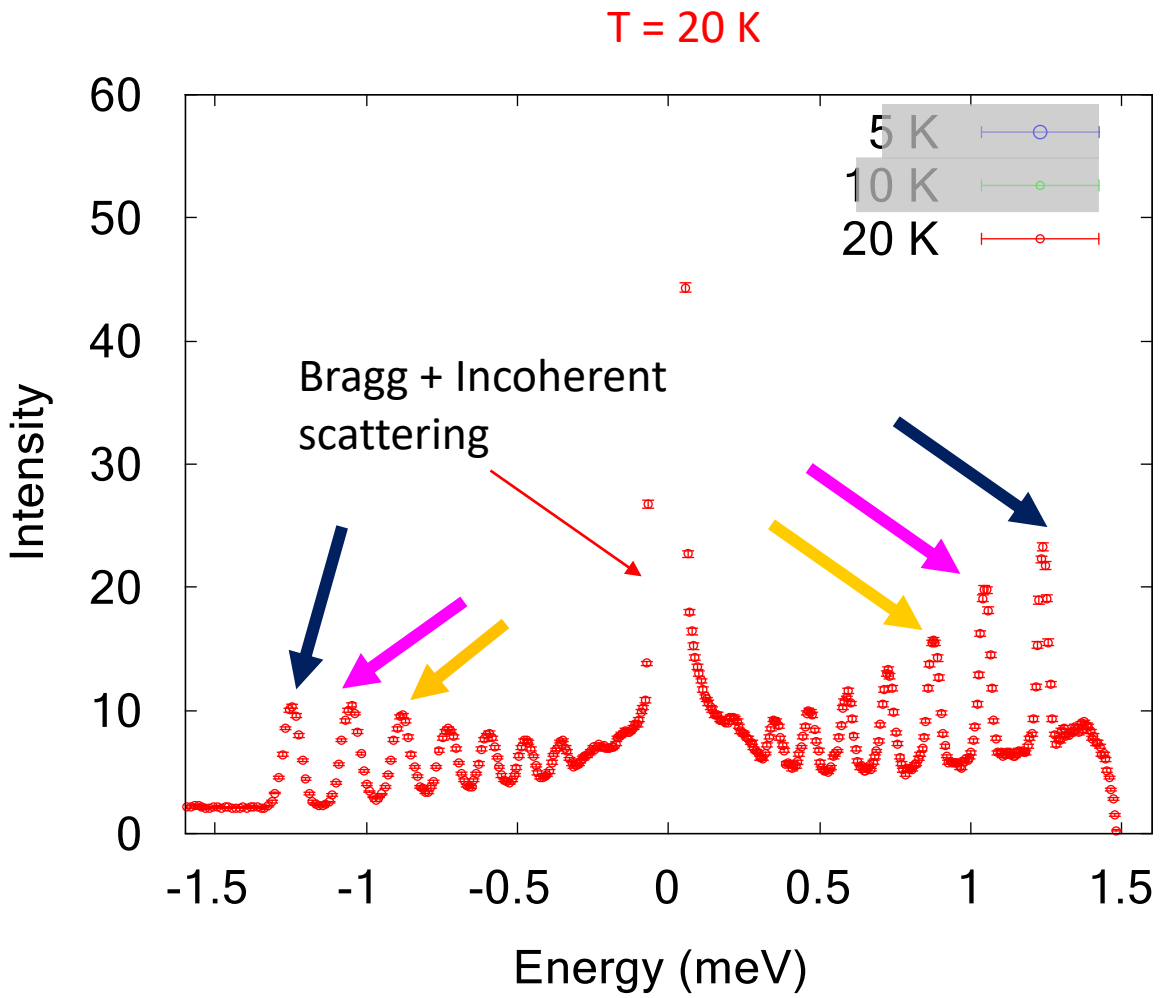


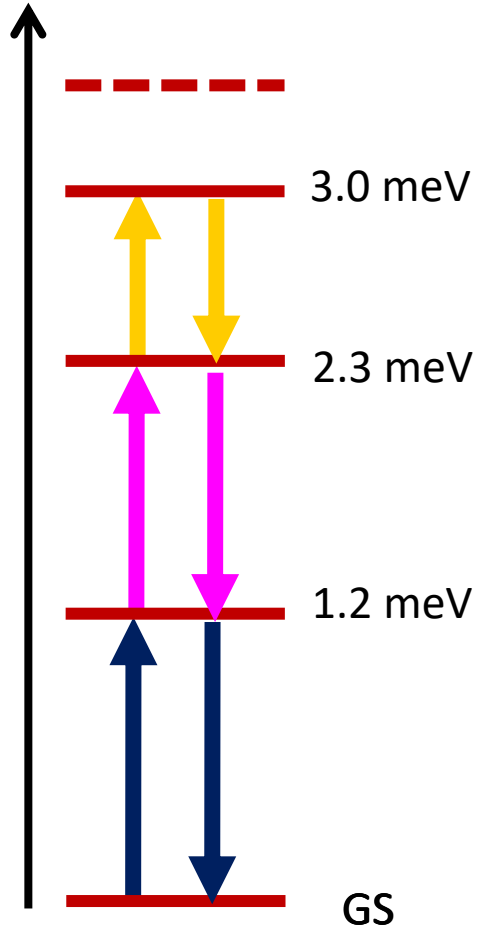
Example 1 : Mn12-acetate





Example 1 : Mn12-acetate



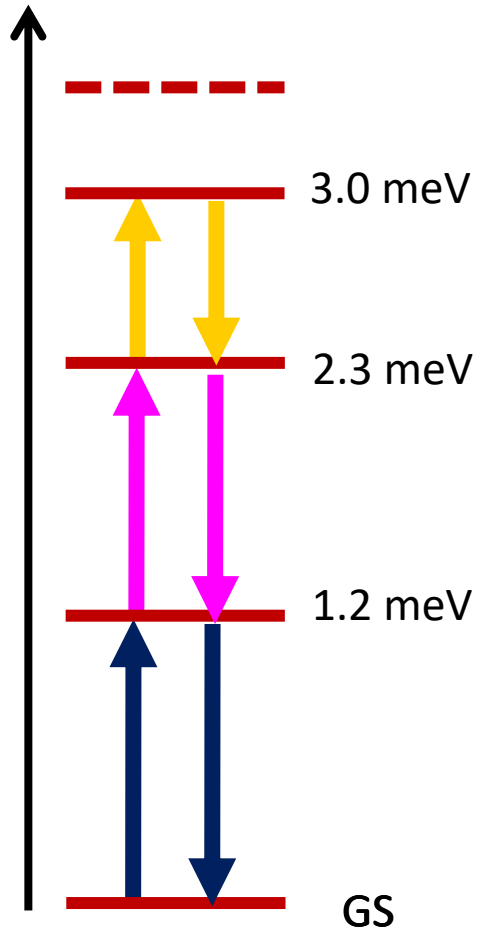


Example 1 : Mn12-acetate

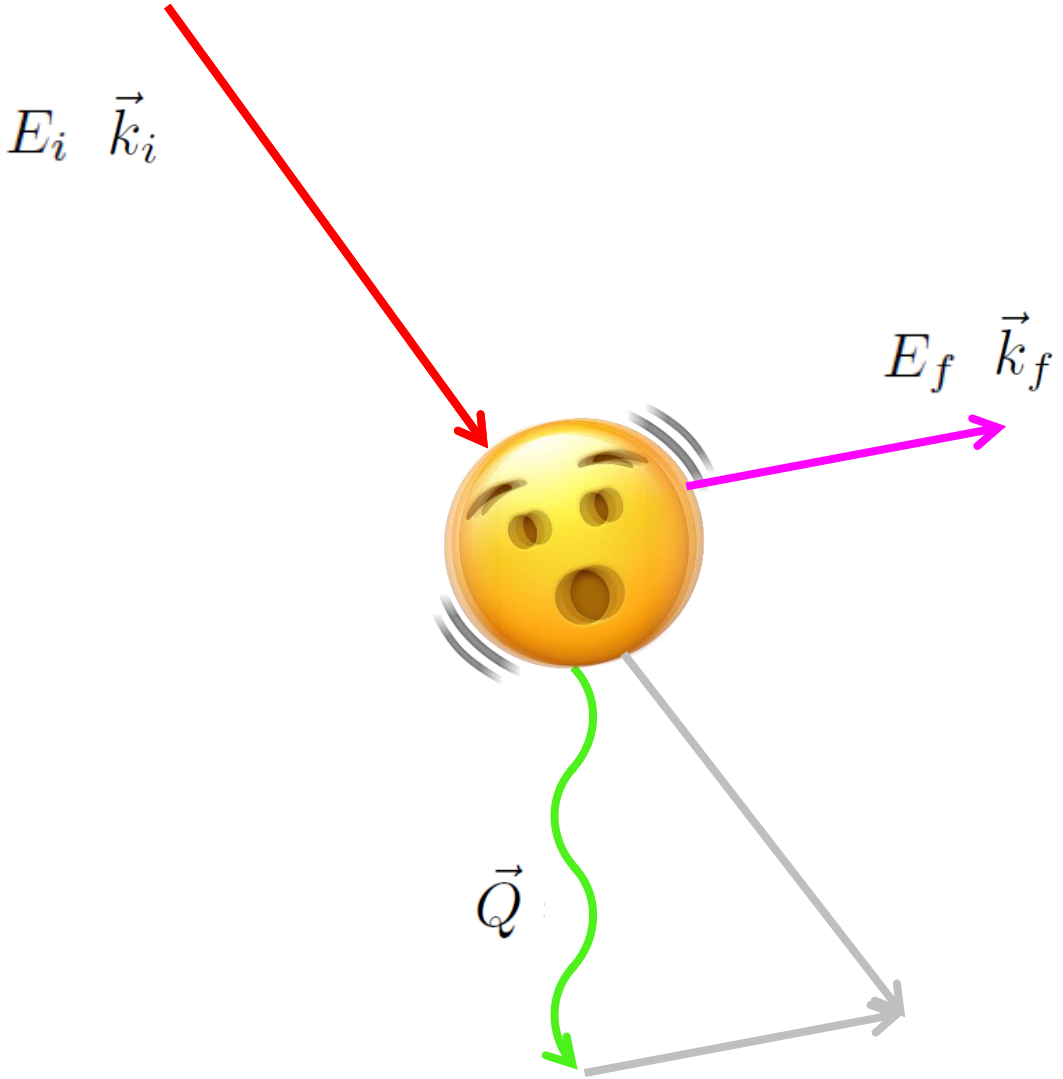
Neutrons induce transitions from a given quantum state to another:

- The energy of such a transition is the energy difference between two quantum levels
- With increasing T, more and more levels get populated, hence more and more transitions become visible.

$$\frac{\exp -E_n/k_BT}{\sum_n \exp -E_n/k_BT}$$



Example 2 : Phonons

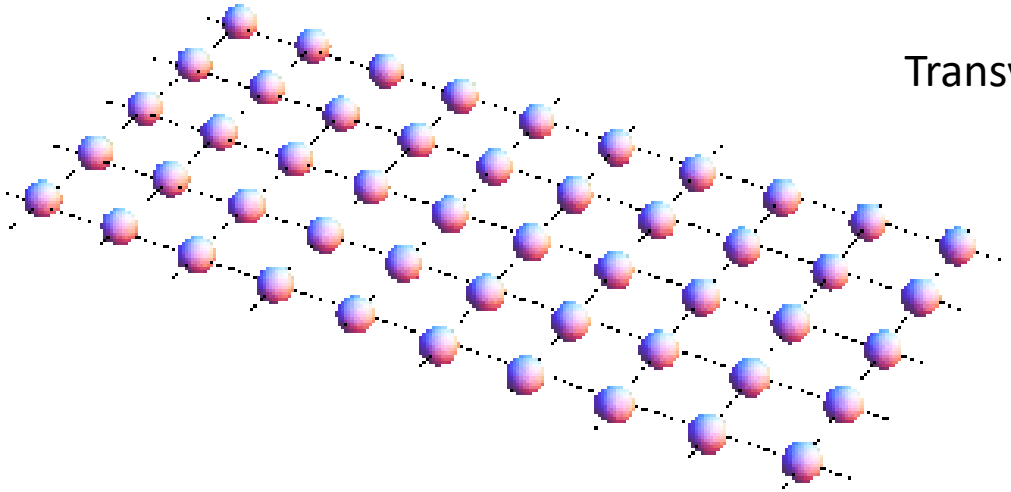


- Gets excited by creating a phonon with energy E and momentum Q

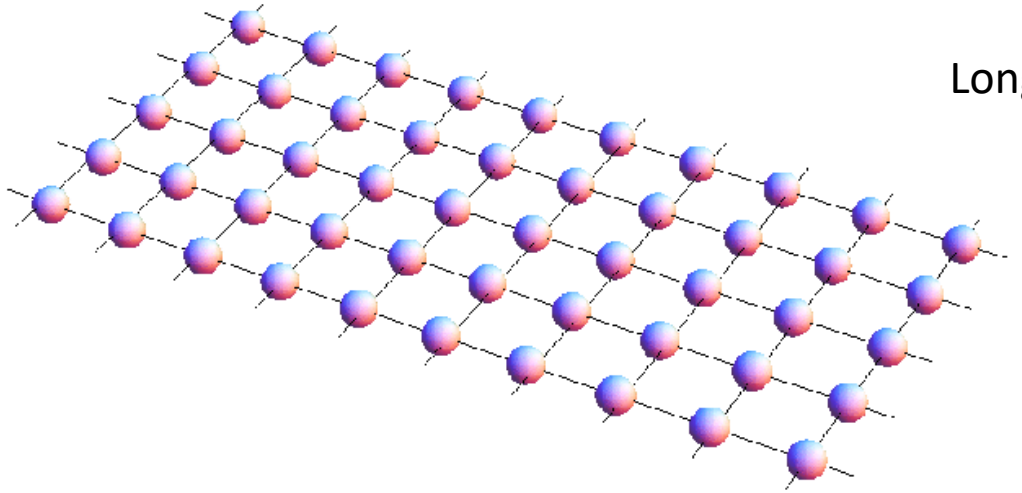
$$E = \hbar\omega = E_i - E_f$$

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

Example 2 : Phonons



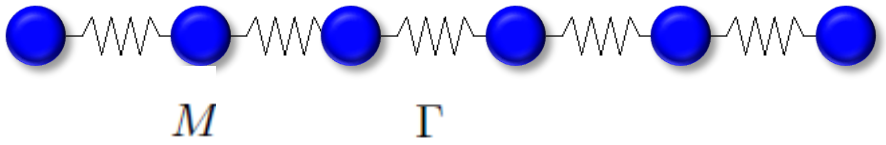
Transverse



Longitudinal

Example 2 : Phonons

Monoatomic chain



$$M\frac{d^2}{dt^2}u_m = \Gamma\ (u_{m+1} + u_{m-1} - 2u_m)$$

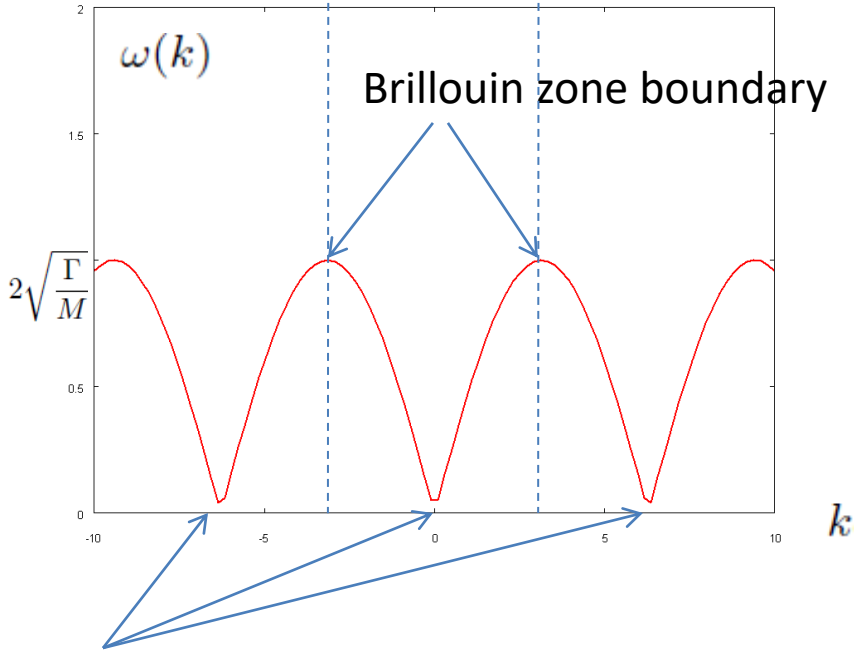
Force constant between atoms

Fourier Transfrom

$$-M\omega^2 = \Gamma\ \left(e^{ika} + e^{-ika} - 2\right)$$

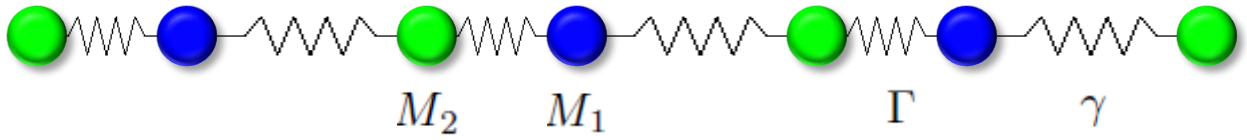
$$\omega(k) = 2\sqrt{\frac{\Gamma}{M}}\sin\frac{ka}{2}$$

Dispersion relation



Example 2 : Phonons

Di-atomic chain



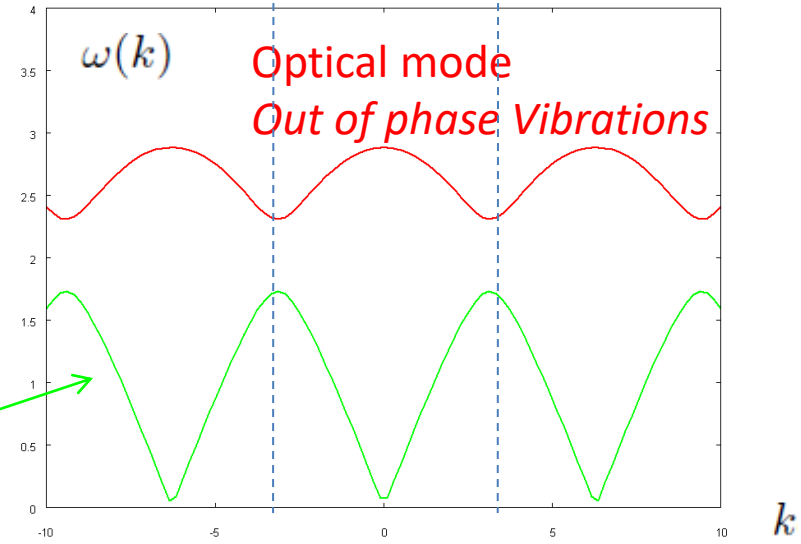
$$M_1 \frac{d^2}{dt^2} u_{m,1} = \Gamma\ (u_{m,2} - u_{m,1}) + \gamma\,(u_{m-1,2} - u_{m,1})$$

$$M_2 \frac{d^2}{dt^2} u_{m,2} = \Gamma\ (u_{m,1} - u_{m,2}) + \gamma\,(u_{m+1,1} - u_{m,2})$$

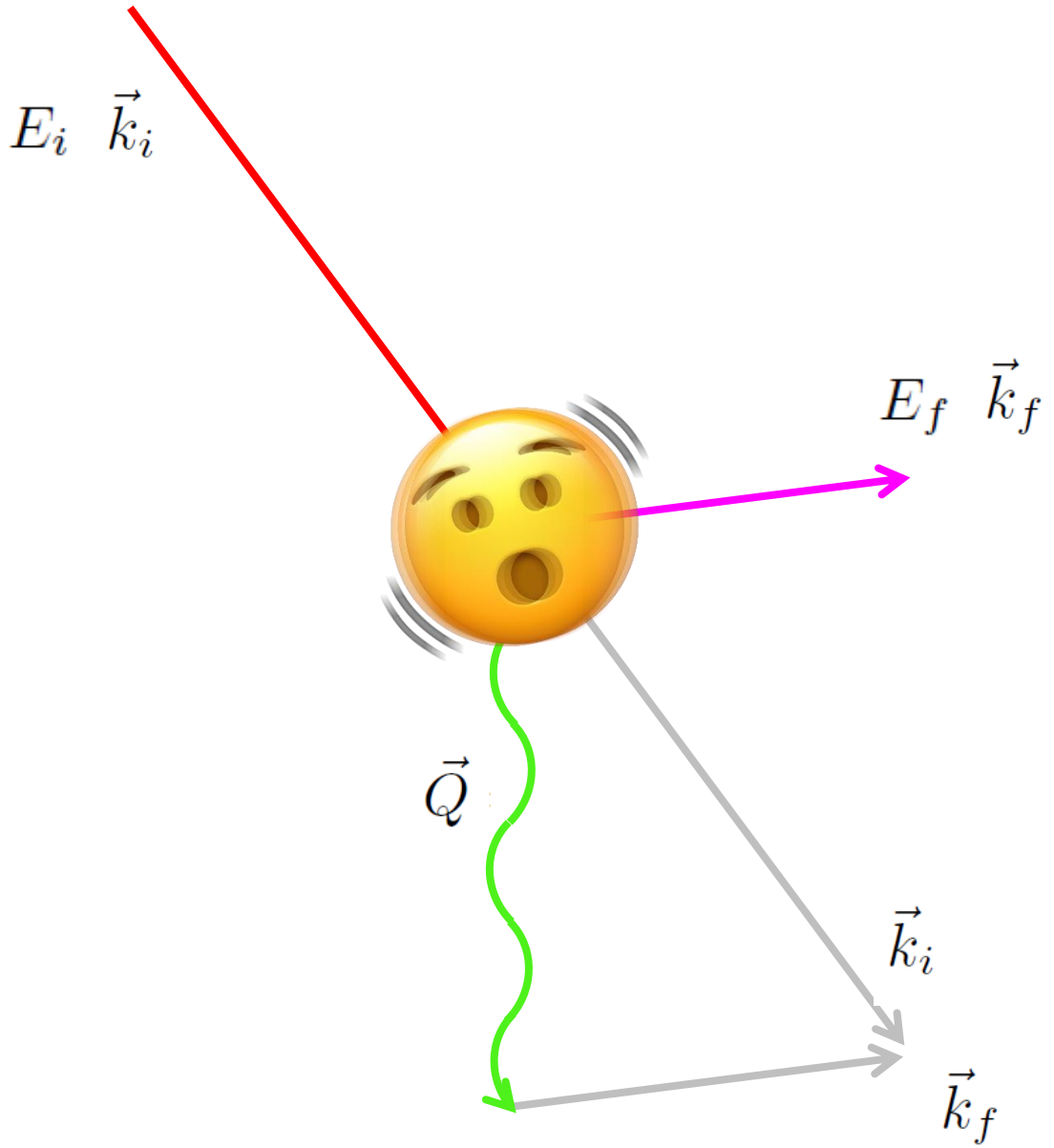
Force constants between atoms

Fourier transform: for each k, eigenvalue problem

$$\begin{pmatrix} \omega^2 - \frac{\Gamma+\gamma}{M_1} & \frac{\Gamma+\gamma e^{-ika}}{\sqrt{M_1 M_2}} \\ \frac{\Gamma+\gamma e^{ika}}{\sqrt{M_1 M_2}} & \omega^2 - \frac{\Gamma+\gamma}{M_2} \end{pmatrix} \begin{pmatrix} \sqrt{M_1}u_1 \\ \sqrt{M_2}u_2 \end{pmatrix} = 0$$

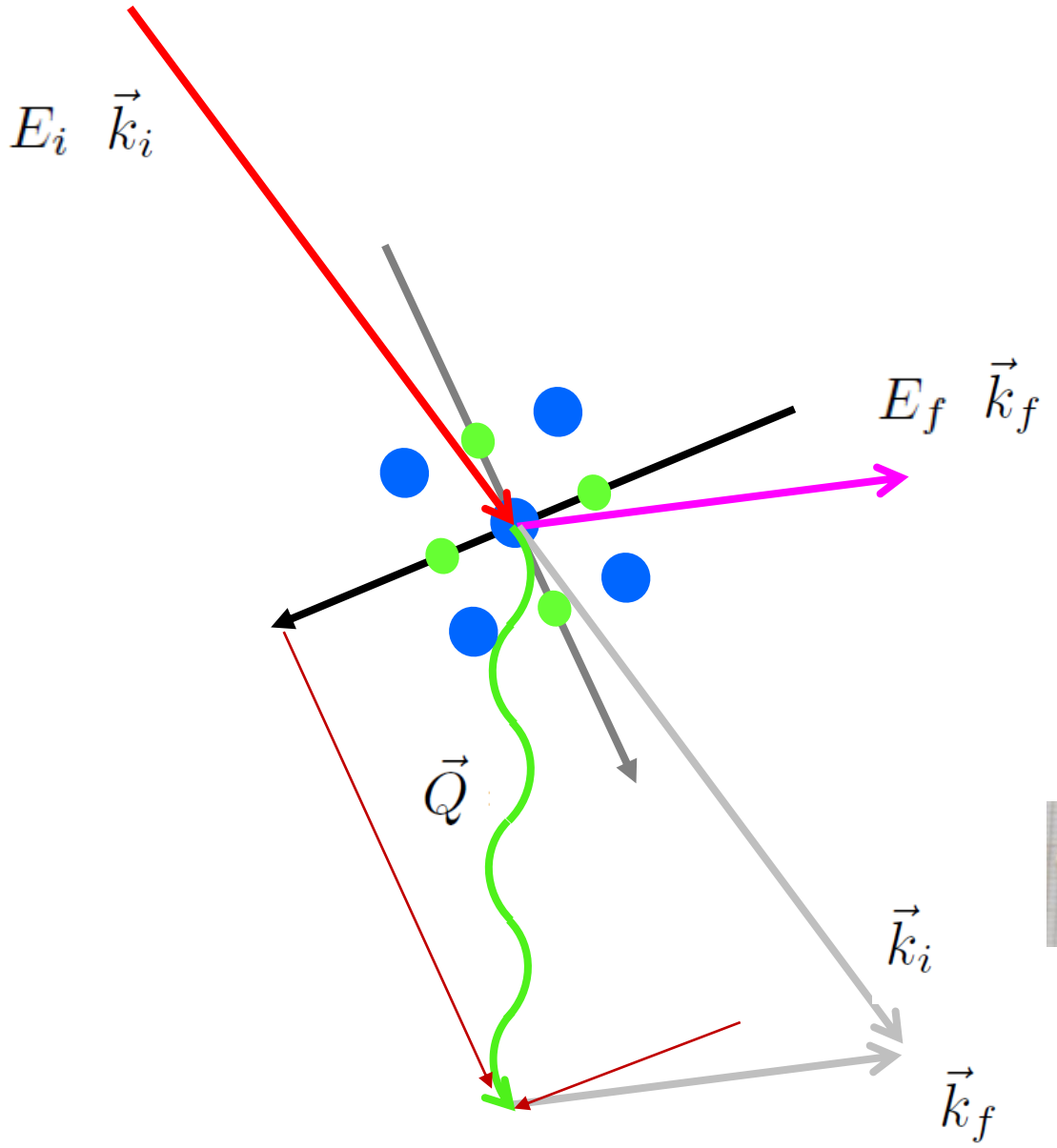


Single crystal

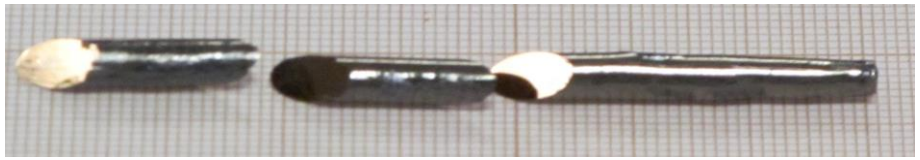


- Gets excited by creating an excitation with energy E and momentum Q
- Q is a vector
- single crystal sample

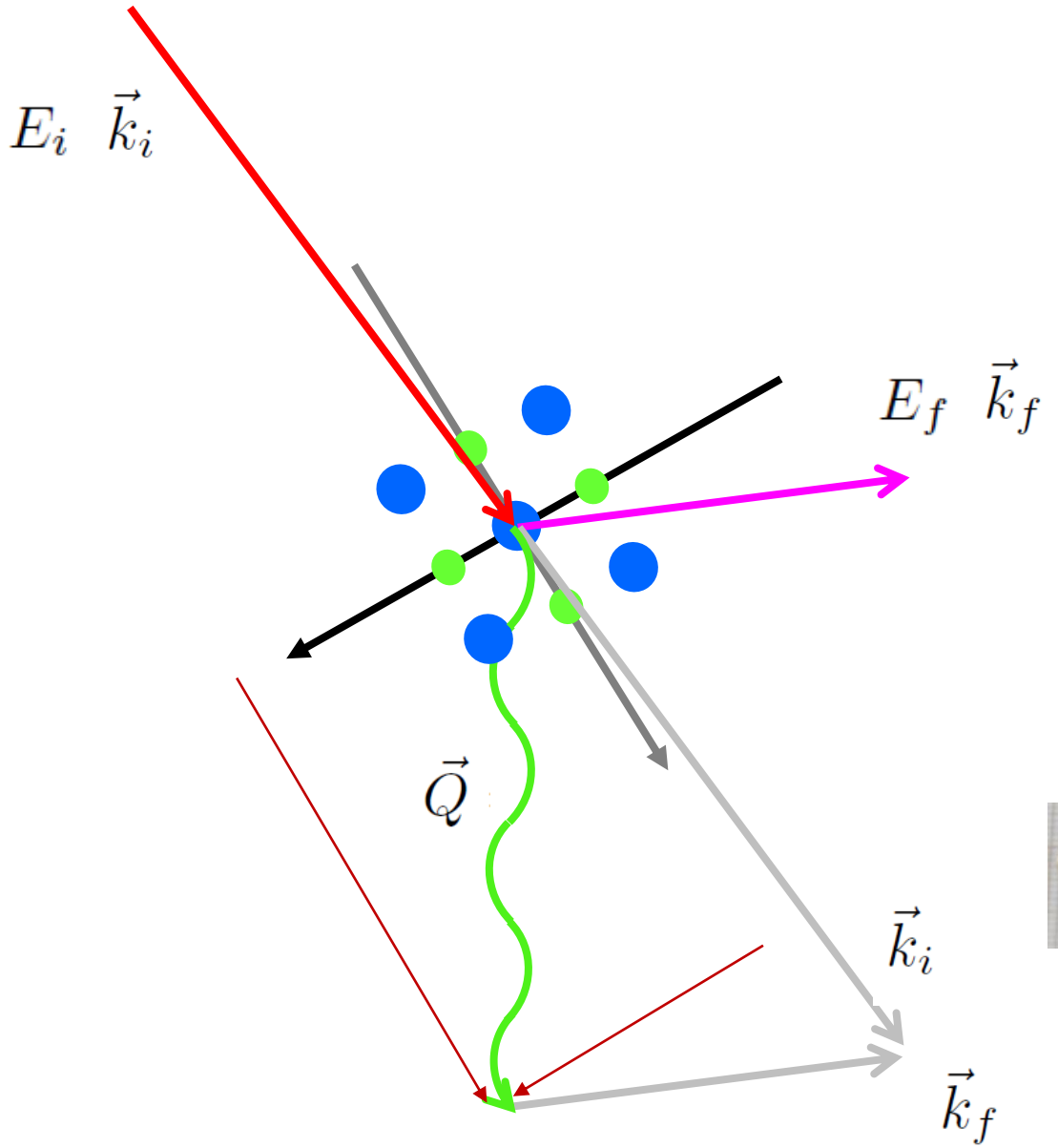
Single crystal



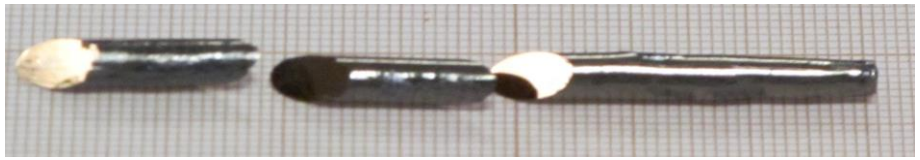
- Gets excited by creating an excitation with energy E and momentum Q
- Q is a vector
- single crystal sample



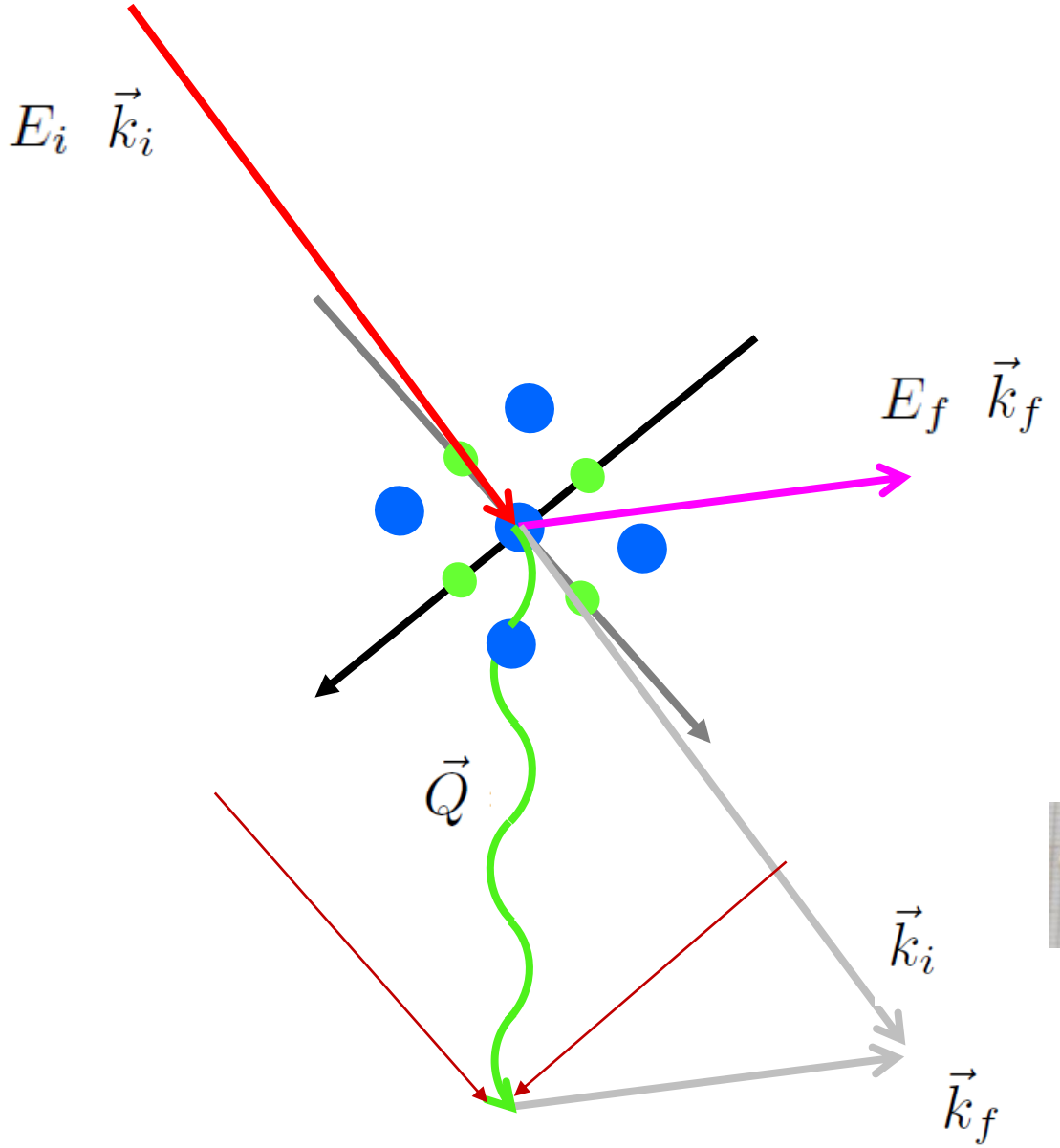
Single crystal



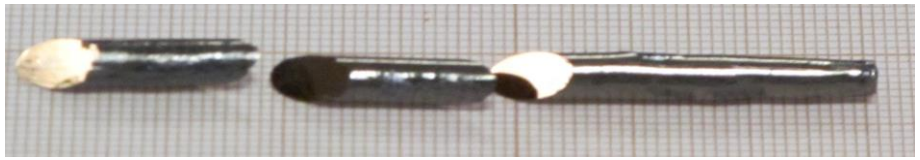
- Rotate the sample to select the components of Q with respect to the sample's lattice



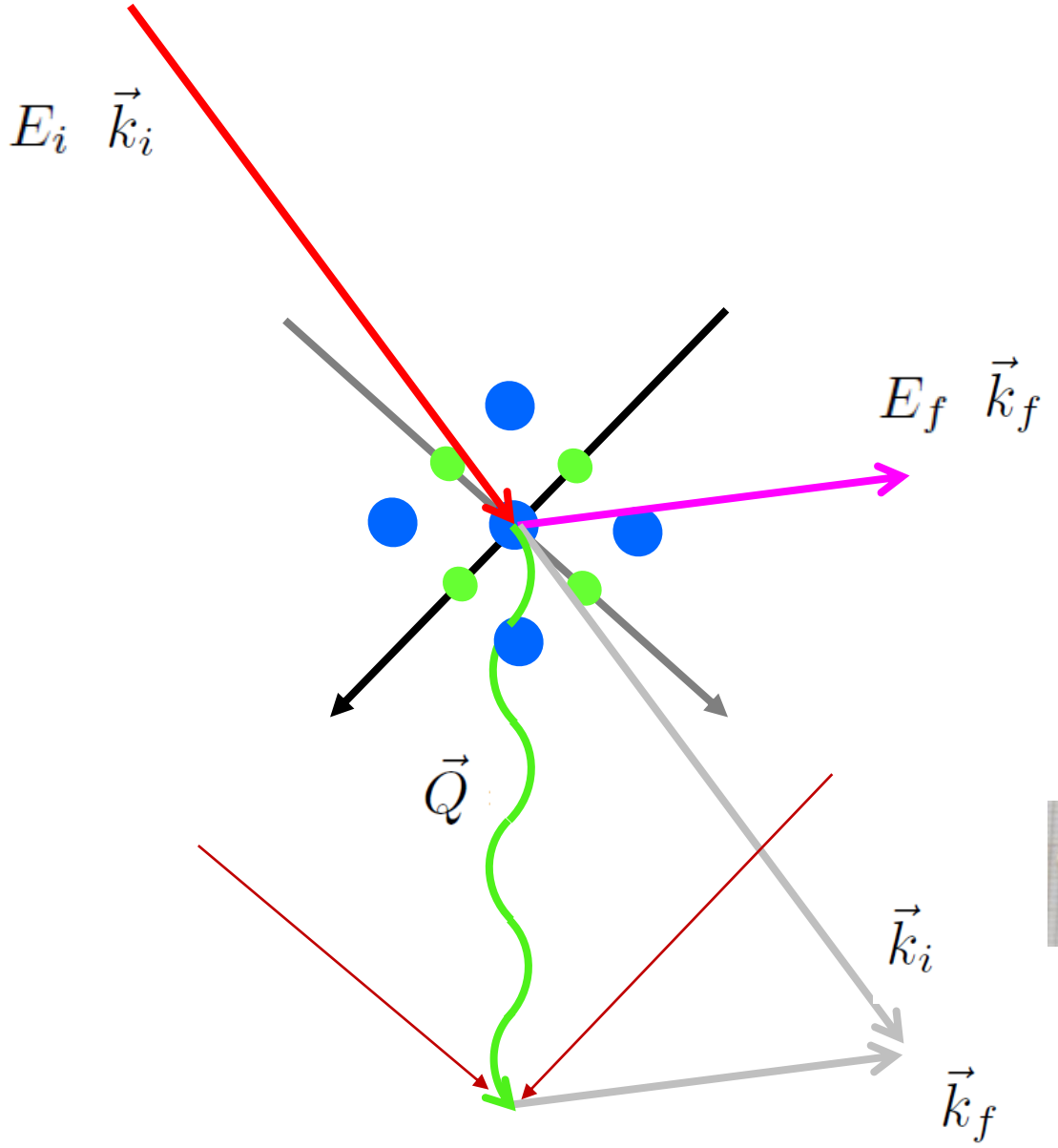
Single crystal



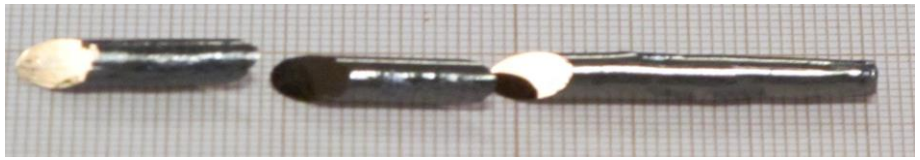
- Rotate the sample to select the components of Q with respect to the sample's lattice



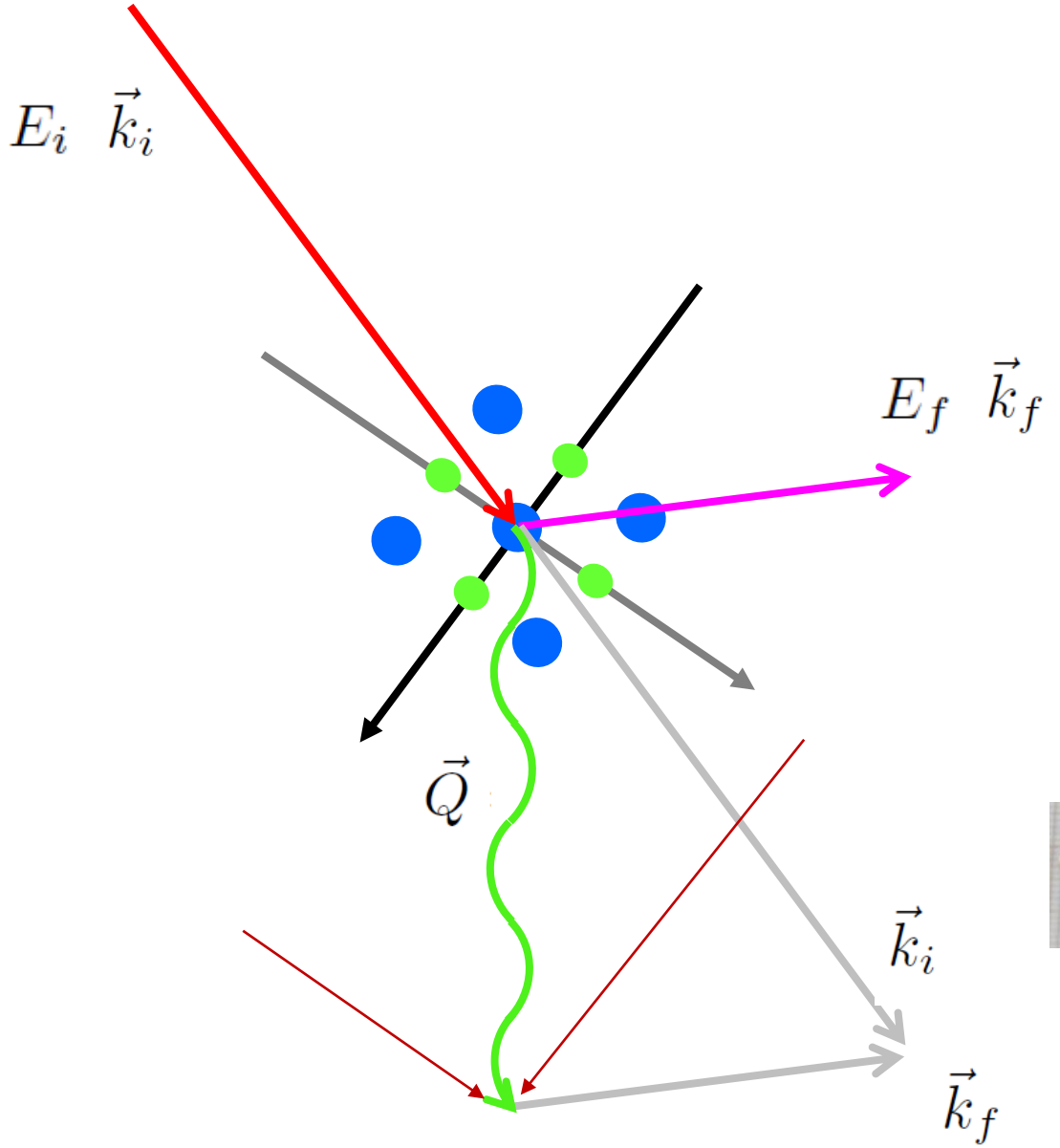
Single crystal



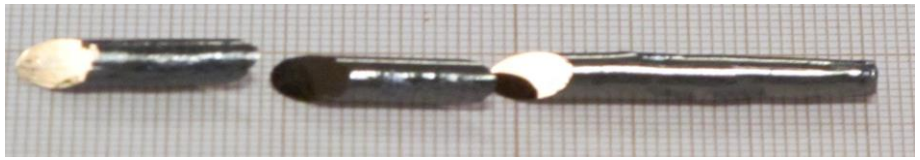
- Rotate the sample to select the components of Q with respect to the sample's lattice



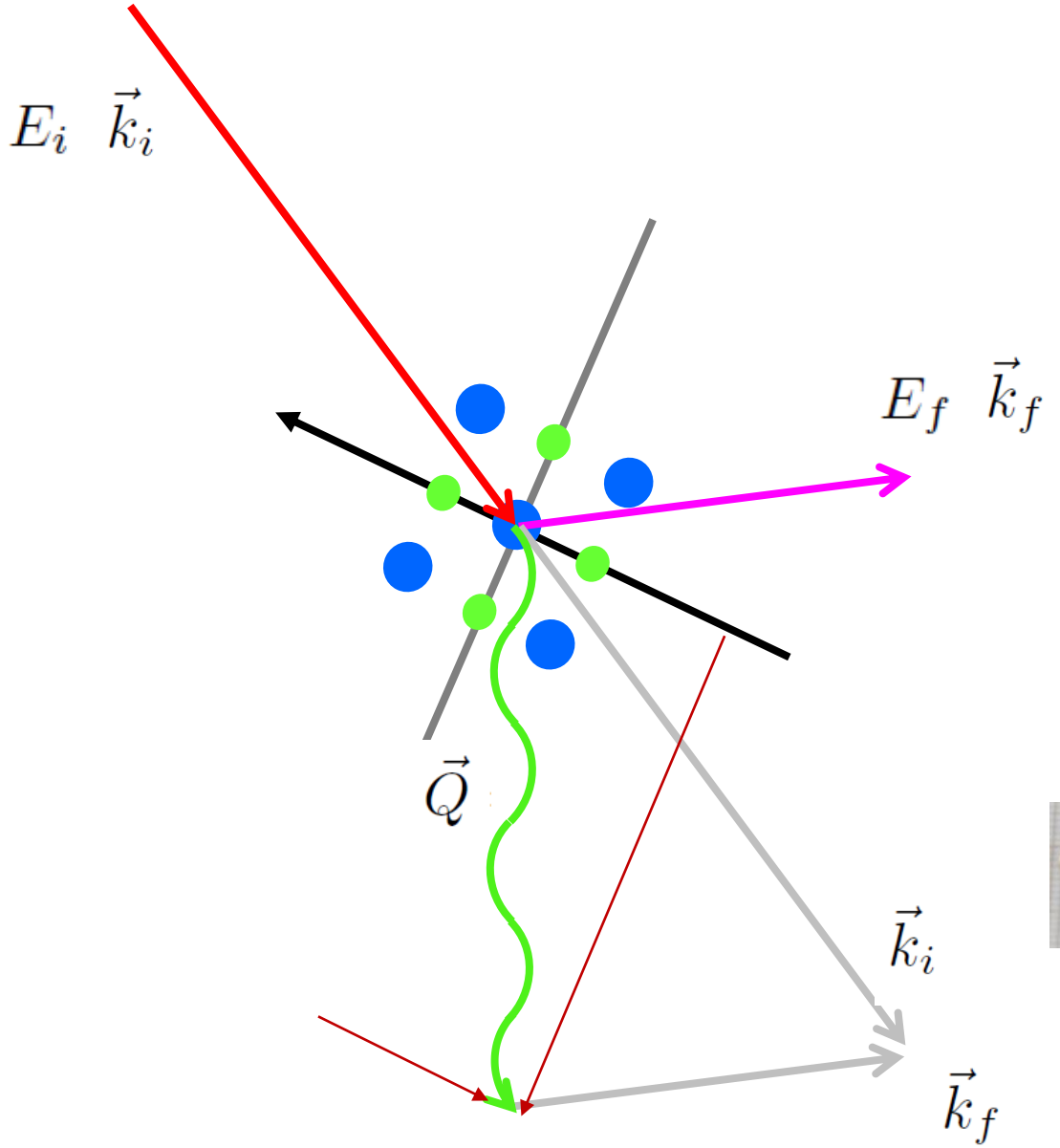
Single crystal



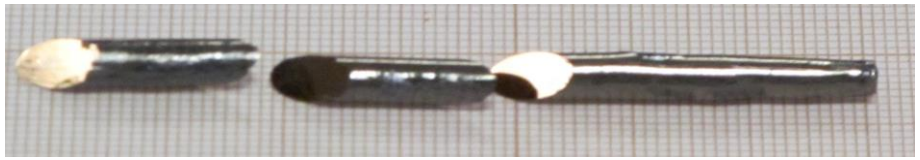
- Rotate the sample to select the components of Q with respect to the sample's lattice



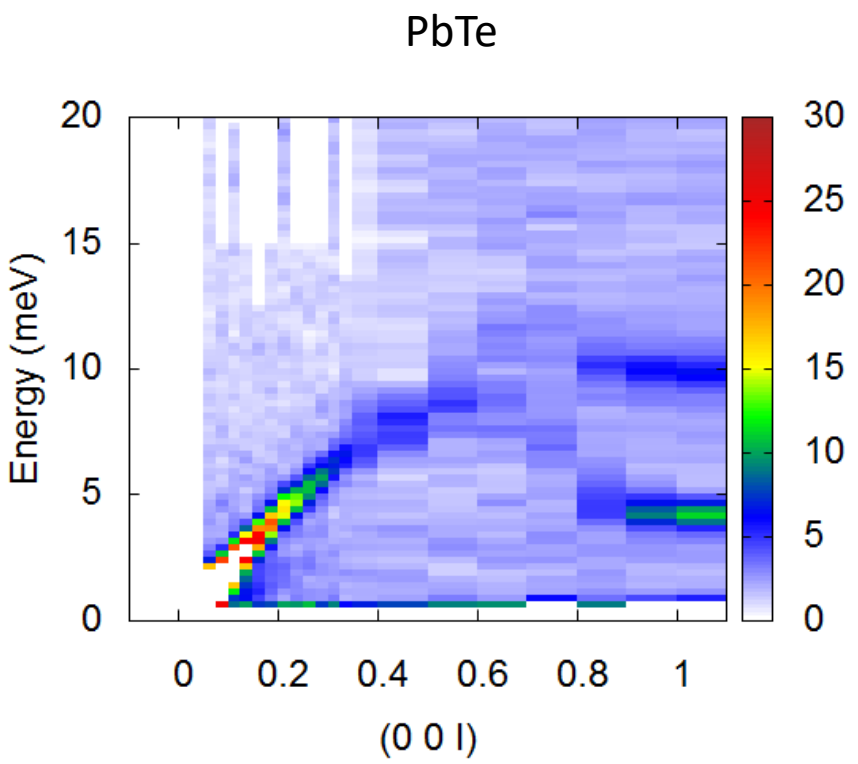
Single crystal



- Rotate the sample to select the components of Q with respect to the sample's lattice



Phonons

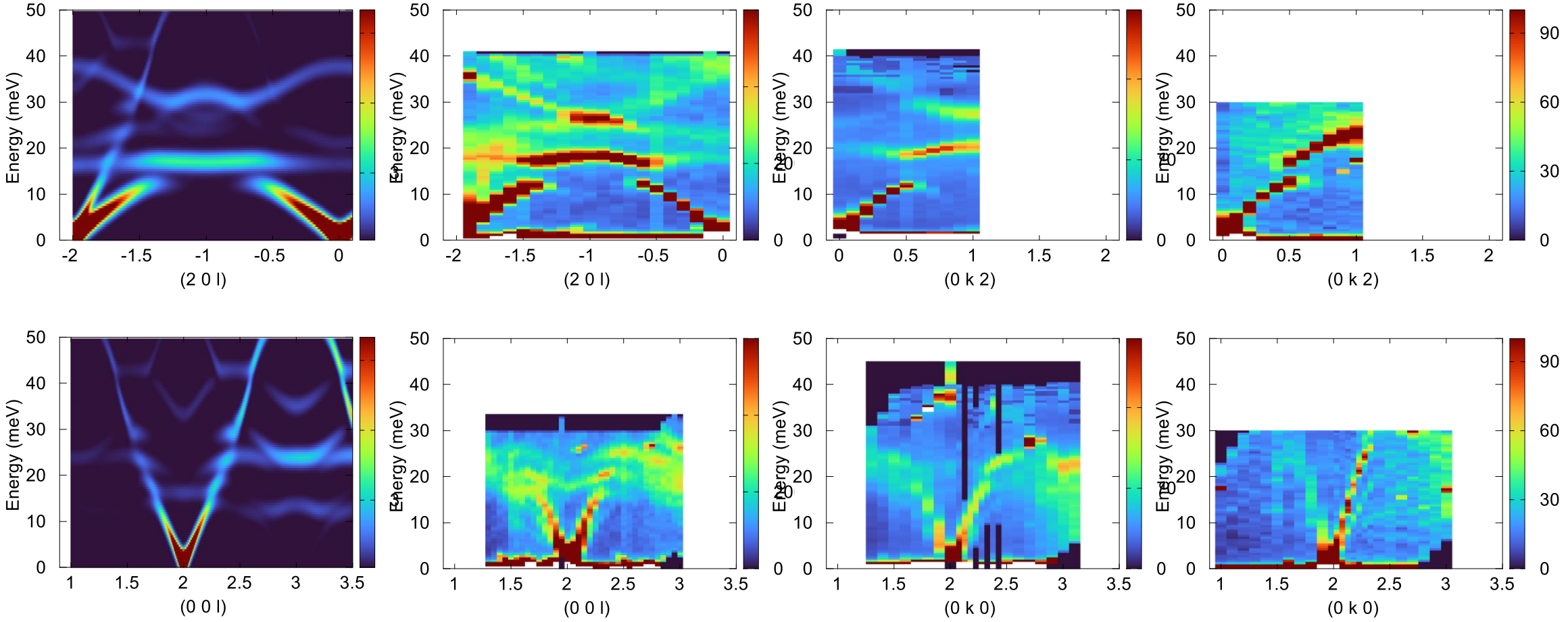


Direct observation of the phonon dispersion in (Q,ω) space !!

Q is a vector

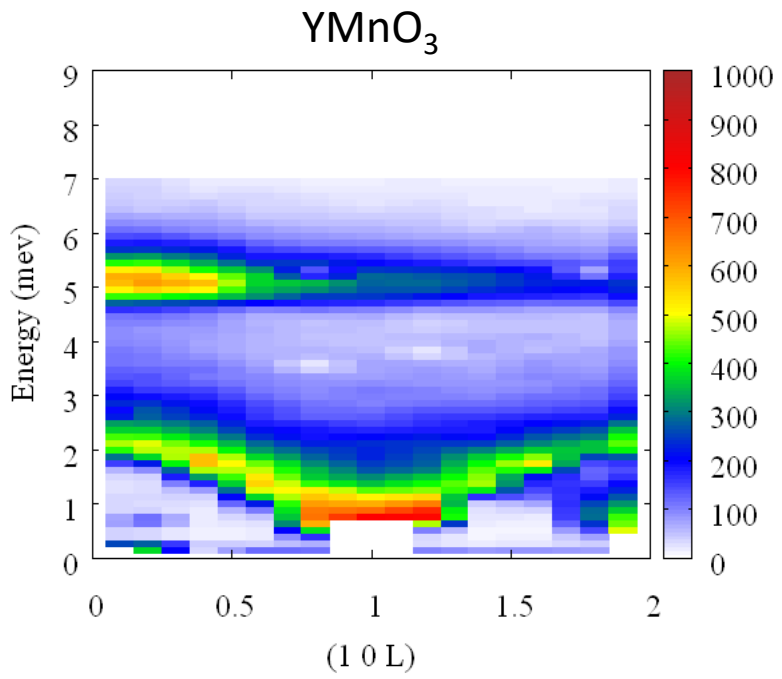
Phonons

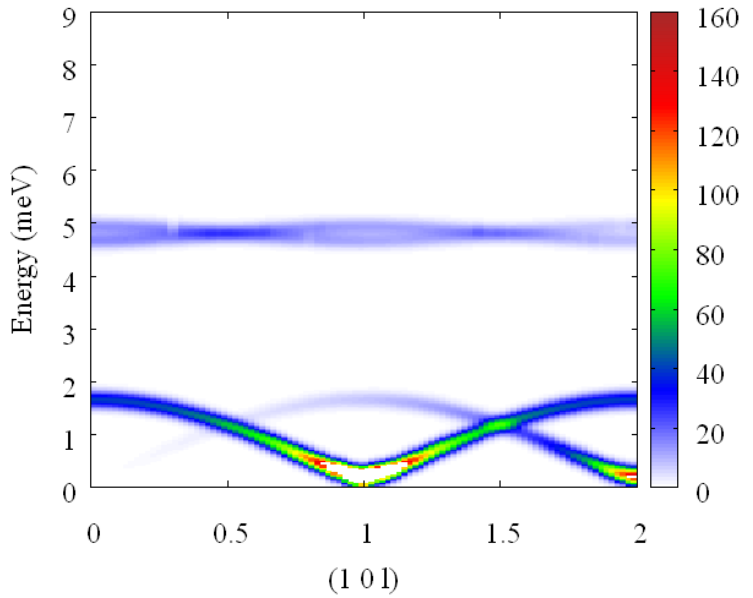
$SrCuO_2$, Sr_2CuO_3, Ca_2CuO_3

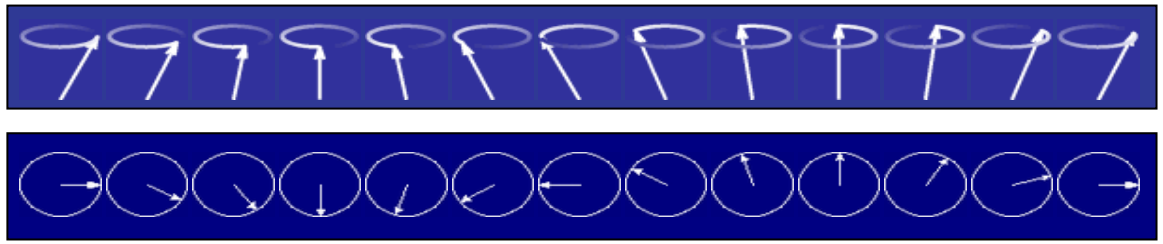


Compare to DFT calculations and study the structure of materials

Spin waves







Direct observation of the spin wave dispersion in (Q,ω) space !!

Determine magnetic exchange and anisotropies

3. Cross sections

Phonons

Inelastic scattering by phonons

$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{k_f}{k_i} \sum_s |F_s(Q=\tau+k)|^2 \ \{(1+n(\omega))\ \delta(\omega-\omega_{k,s}) + n(\omega)\ \delta(\omega+\omega_{k,s})\}$$

Creation

Annihilation

- Phonons are bosons
- « detailed balance »
- Dynamical structure factor

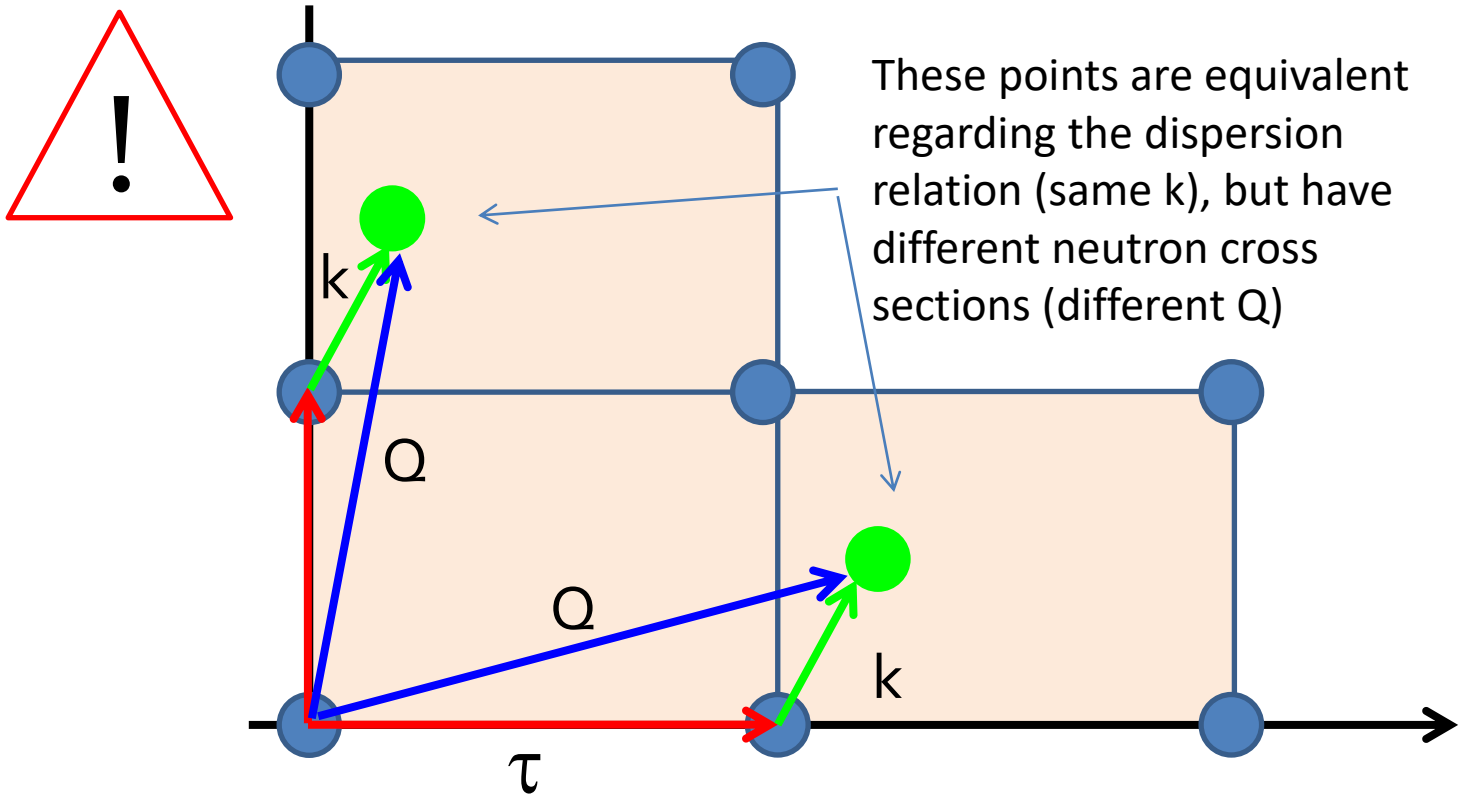
Bose-Einstein

$$n(\omega_{Q,s}) = \frac{1}{e^{\frac{\hbar\omega_{Q,s}}{k_B T}} - 1}$$

$$F_s(Q=\tau+k) = \sum_\ell b_\ell\ e^{i\vec{Q}.\vec{r}_\ell}\ e^{-W_\ell}\ \frac{1}{\sqrt{M_\ell\ \omega_{k,s}}}\ (\vec{Q}.\vec{e}^{\,(s)}_{k,\ell})$$

$\omega(k)$ is periodic. It suffices to study it in a single Brillouin zone

$$F_s(Q = \tau + k) = \sum_\ell b_\ell \; e^{i\vec{Q}.\vec{r}_\ell} \; e^{-W_\ell} \; \frac{1}{\sqrt{M_\ell \; \omega_{k,s}}} \; (\vec{Q}.\vec{e}_{k,\ell}^{\,(s)})$$

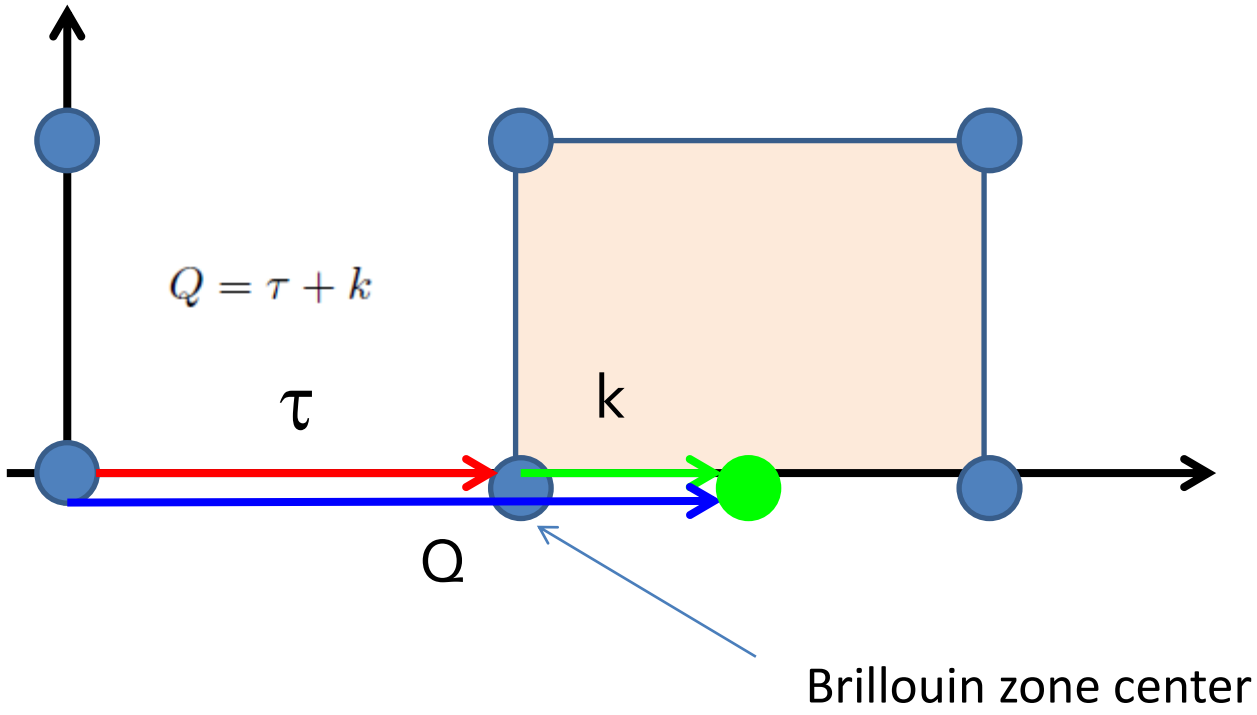


These points are equivalent regarding the dispersion relation (same k), but have different neutron cross sections (different Q)

τ = Brillouin zone node = Bragg peak position

k = wavevector within the Brillouin zone

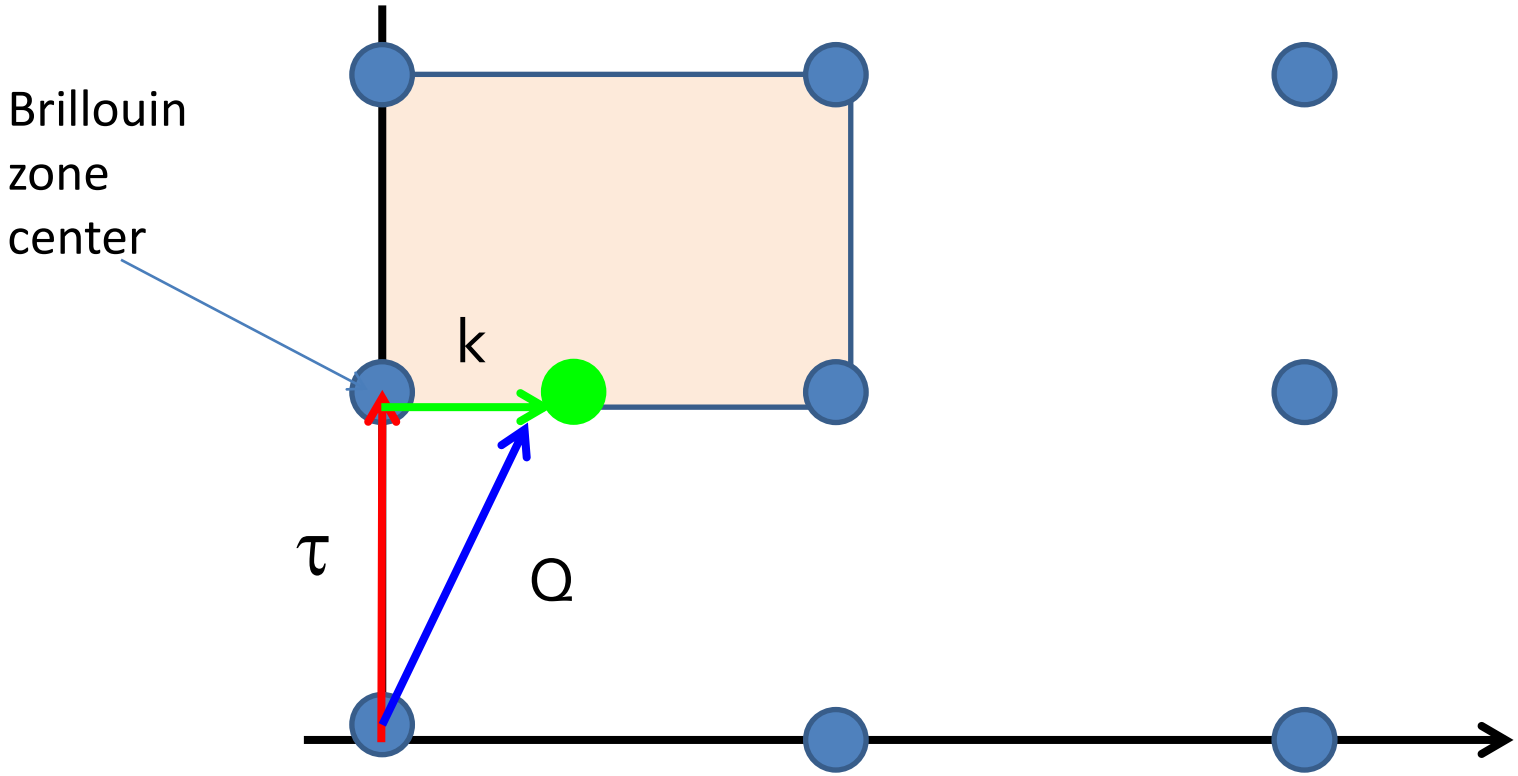
$$F_s(Q = \tau + k) = \sum_{\ell} b_\ell \; e^{i\vec{Q}.\vec{r}_\ell} \; e^{-W_\ell} \; \frac{1}{\sqrt{M_\ell \; \omega_{k,s}}} \; (\vec{Q}.\vec{e}^{\,(s)}_{k,\ell})$$



Longitudinal phonon propagating along x :

Phonons

$$F_s(Q = \tau + k) = \sum_\ell b_\ell \; e^{i\vec{Q}.\vec{r}_\ell} \; e^{-W_\ell} \; \frac{1}{\sqrt{M_\ell \; \omega_{k,s}}} \; (\vec{Q}.\vec{e}^{\,(s)}_{k,\ell})$$



Transverse phonon propagating along x

Spin waves

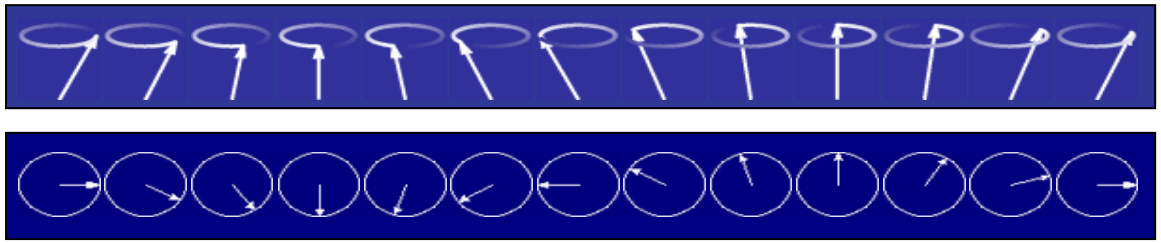
Inelastic scattering by spin waves

$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \sum_s A_s \left[(1+n(\omega_{Q,s}))\ \delta(\omega-\omega_{Q,s}) + n(\omega_{Q,s})\ \delta(\omega+\omega_{Q,s})\right]$$

Creation

Annihilation

- Spin waves are bosons
- « detailed balance »

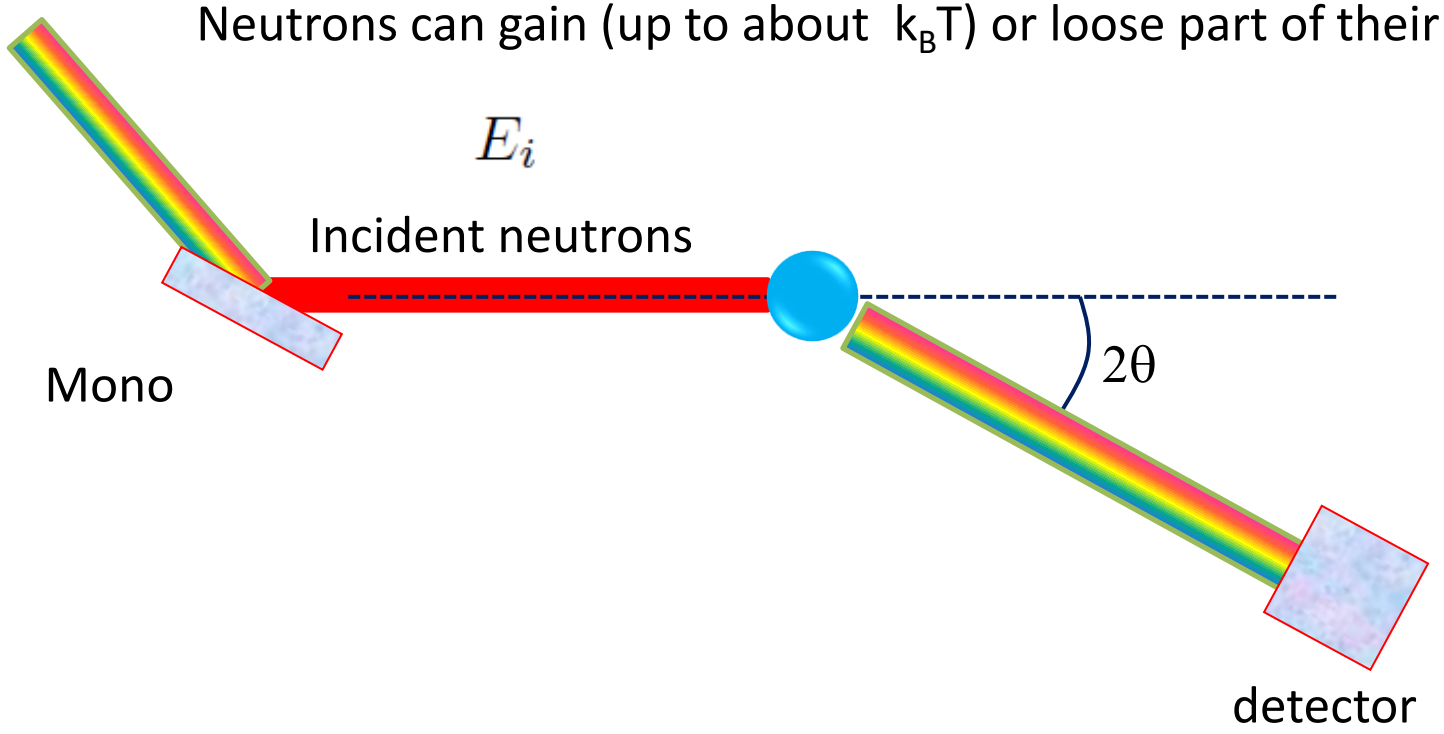


How to perform INS ?

4. TOF

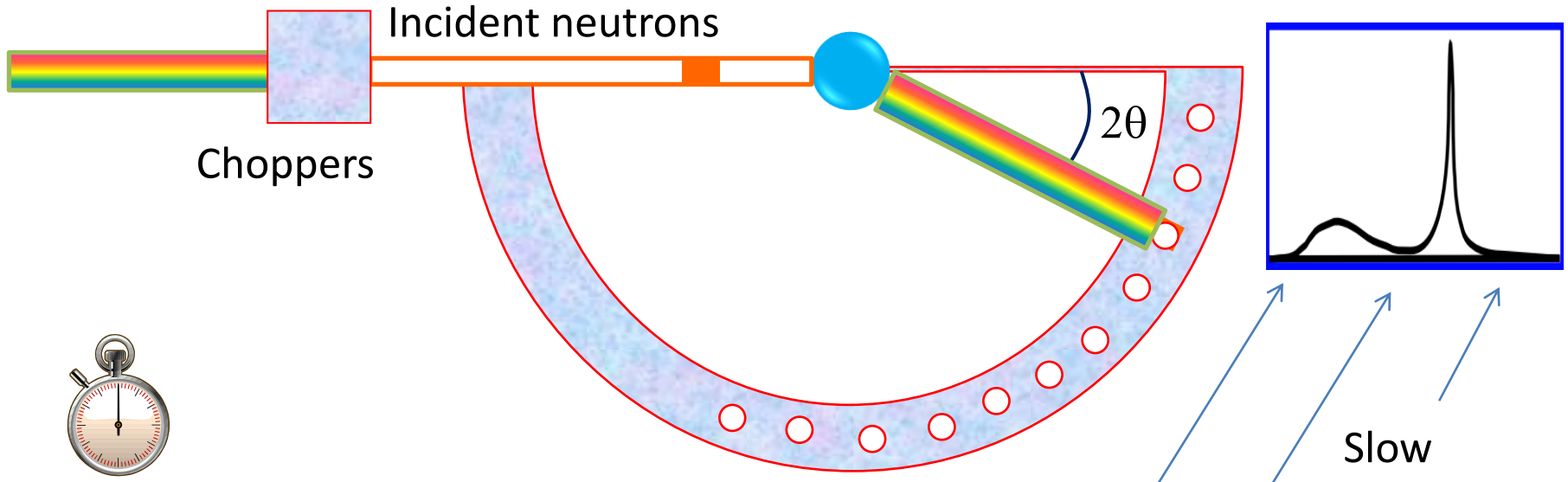
How to perform INS ?

Neutrons can gain (up to about k_BT) or loose part of their energy (up to E_i)



How to determine E_f ?

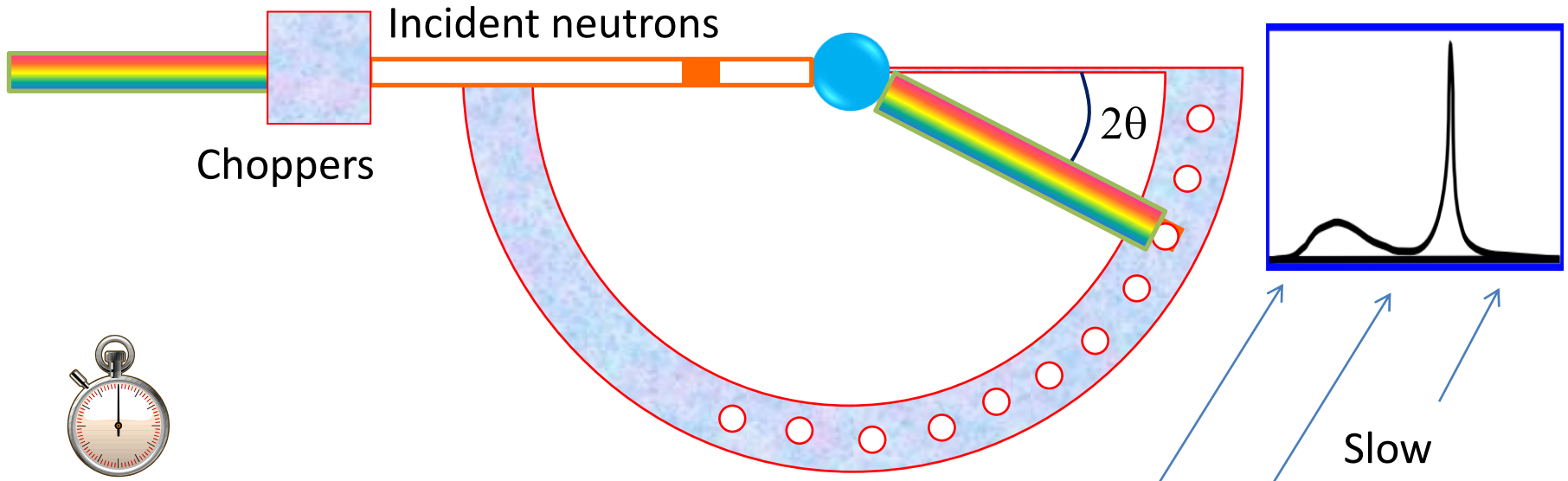
TOF



Select the final energy by time of flight over a distance d

$$t = \frac{d}{\sqrt{2E_f/m_n}}$$

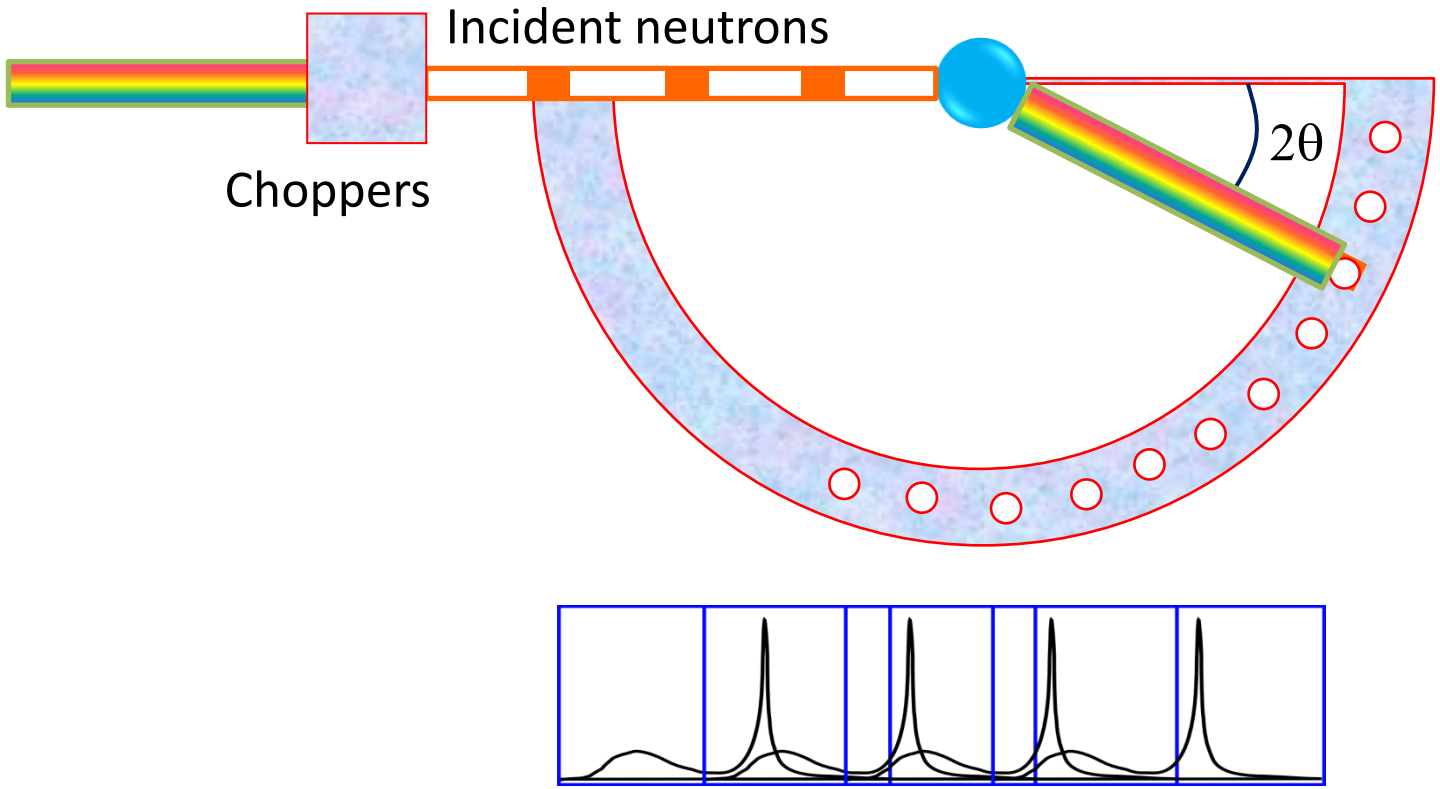
GREAT !! Meaures all 2θs (hence |Q|) at the same time



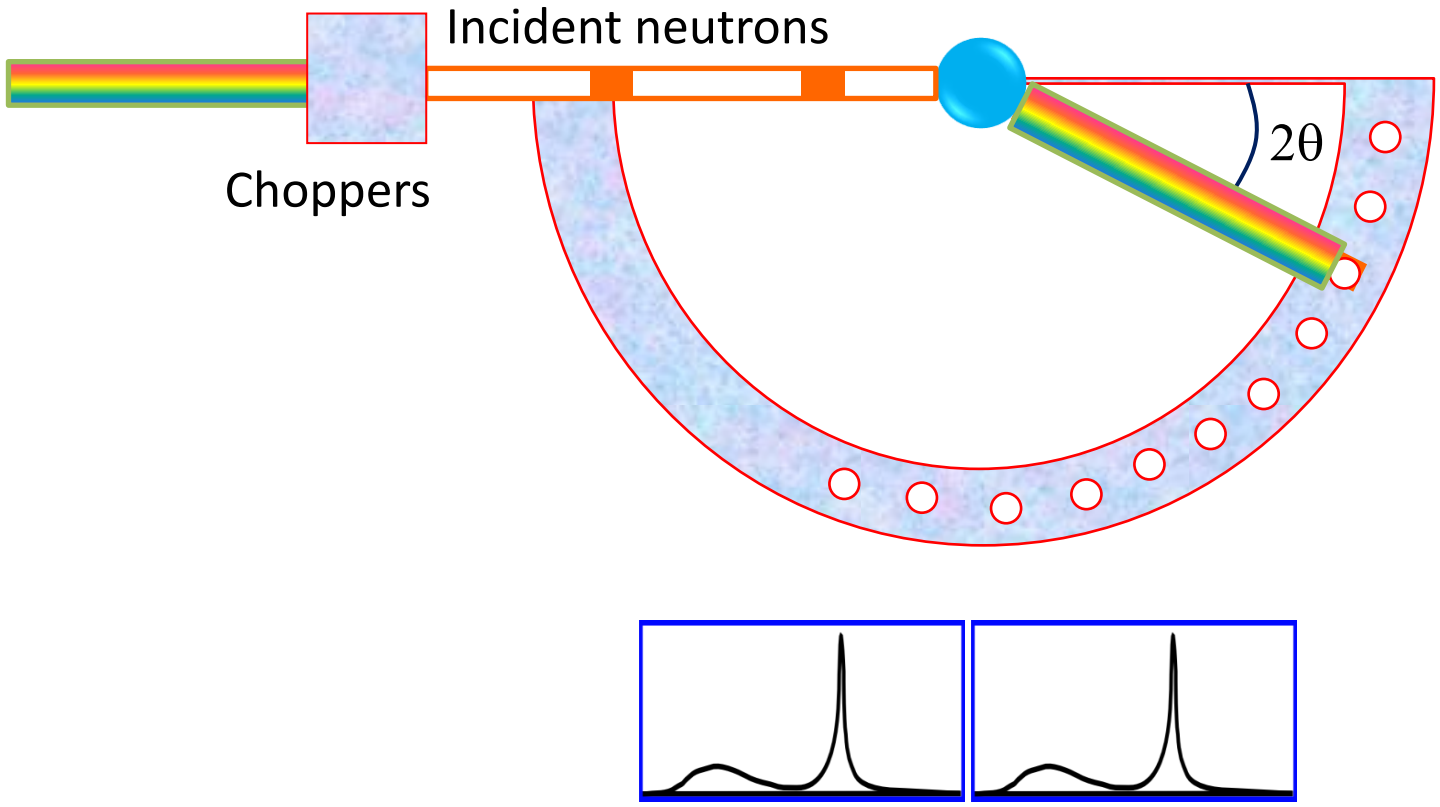
Select the final energy by time to travel a distance d

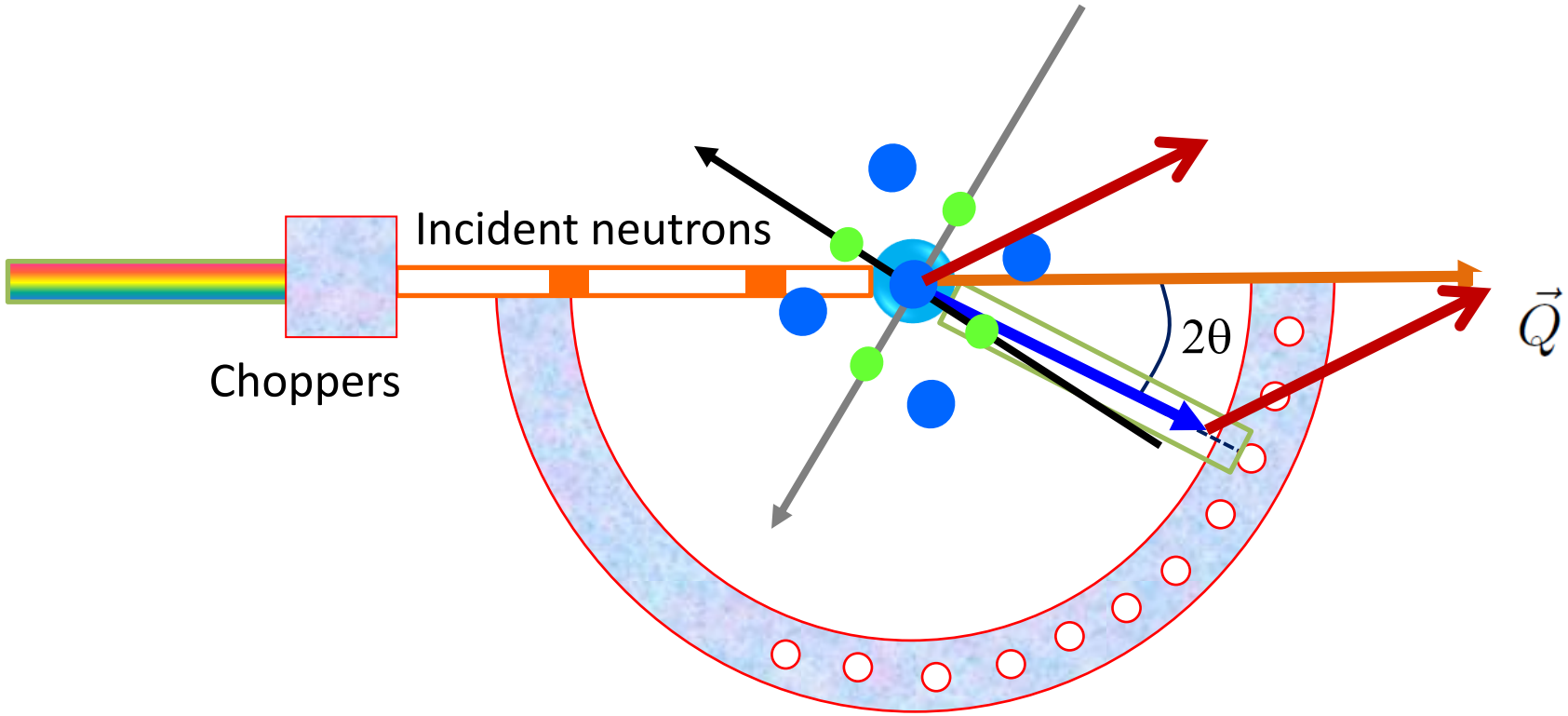
$$t = \frac{d}{\sqrt{2E_f/m_n}}$$

BUT Frame overlap …

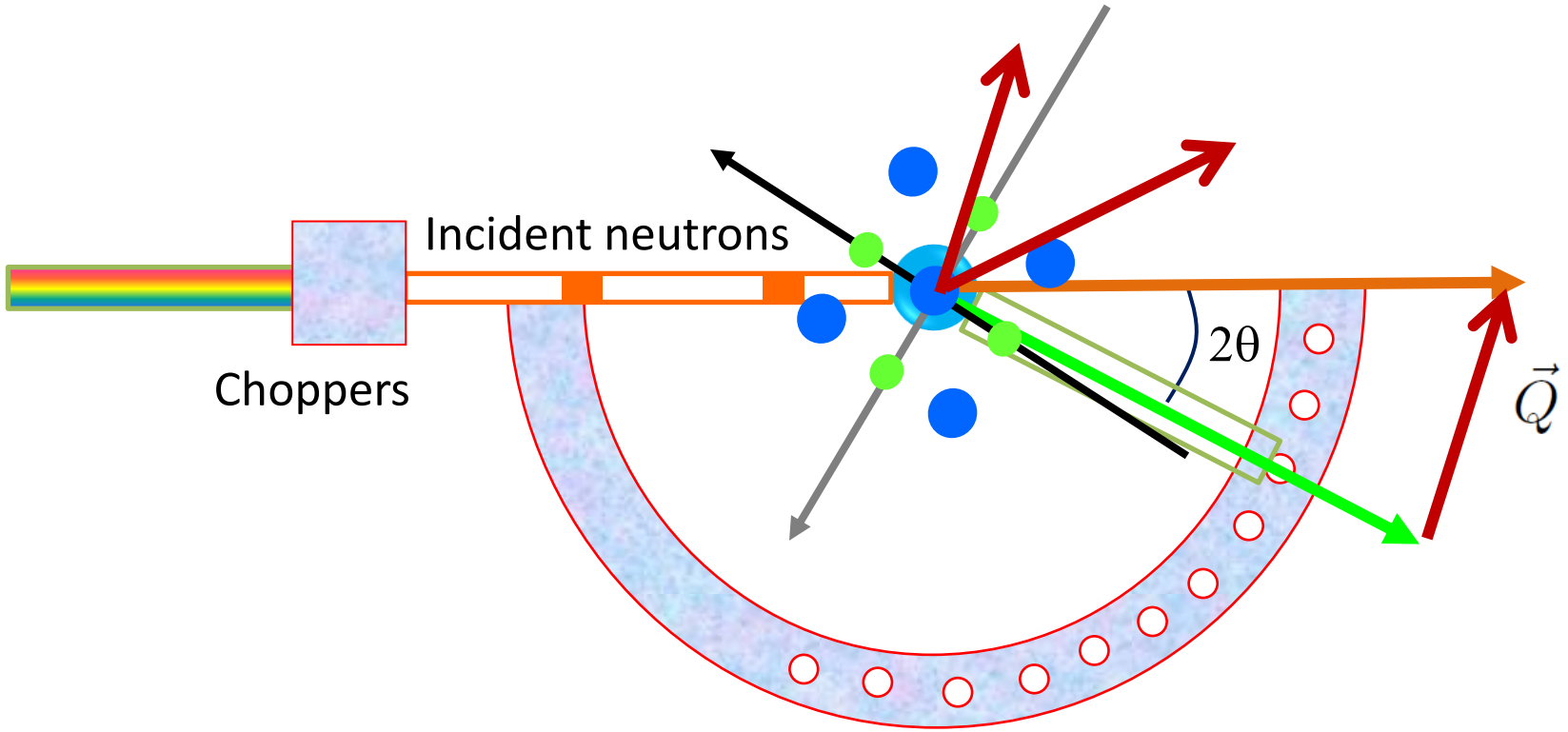


BUT Frame overlap, chop the beam (reduce the flux)



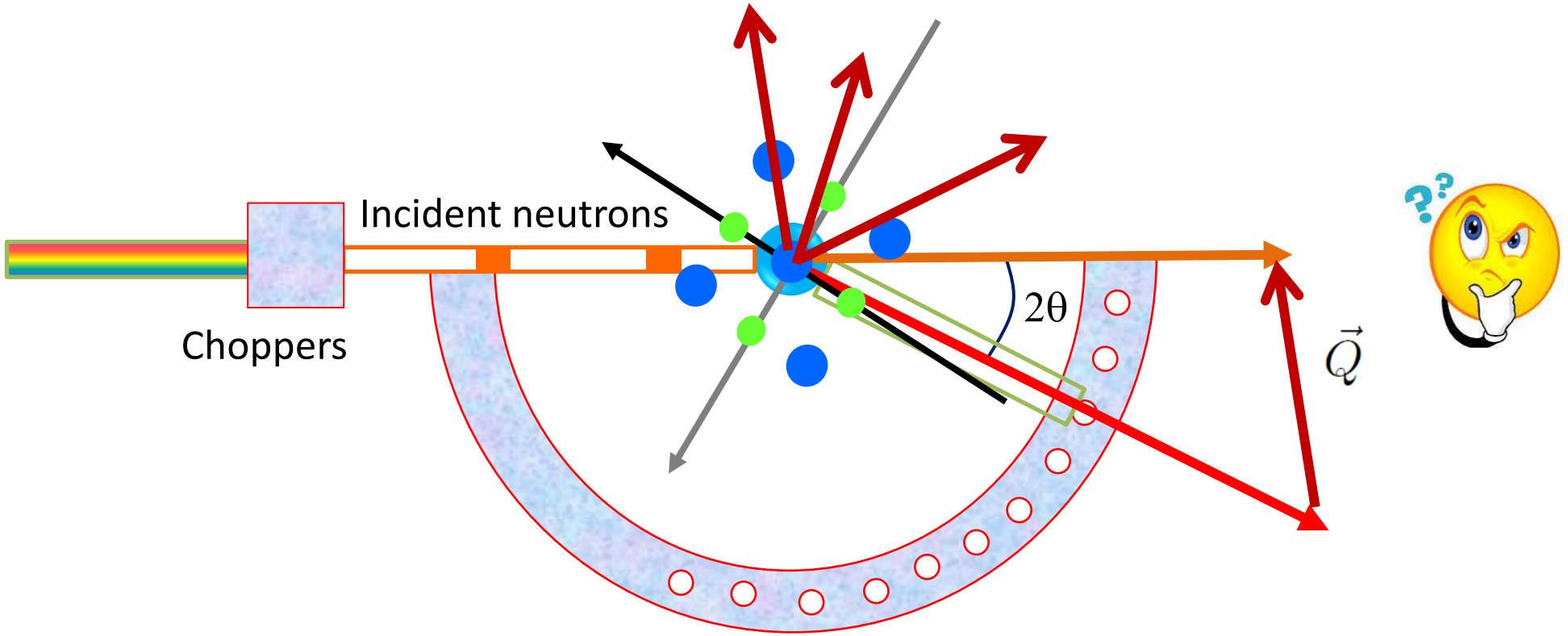


Sample rotation : for a given 2θ, at time t (hence given final energy), the scattering is due to different Qs (modulus and components)



Sample rotation : for a given 2θ, at time t (hence given final energy), the scattering is due to different Qs (modulus and components)

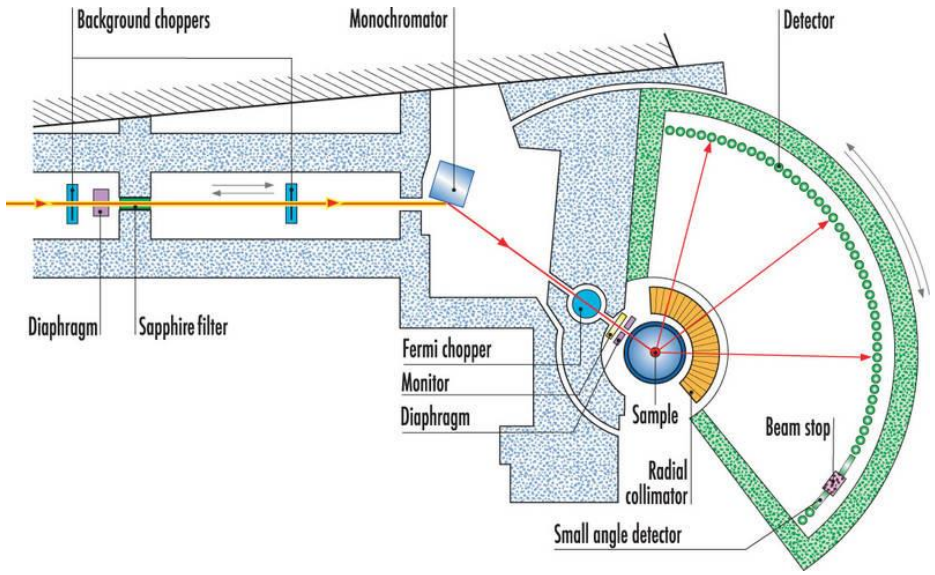
TOF

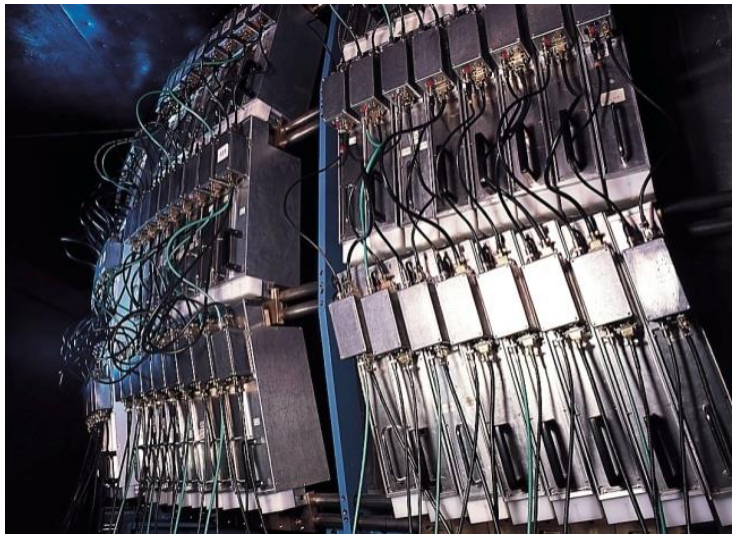


Sample rotation : for a given 2θ, different (Qs, E_f) are probed, as a function of time of flight: it is **necessary to repeat for a number of orientations of the sample**

TOF

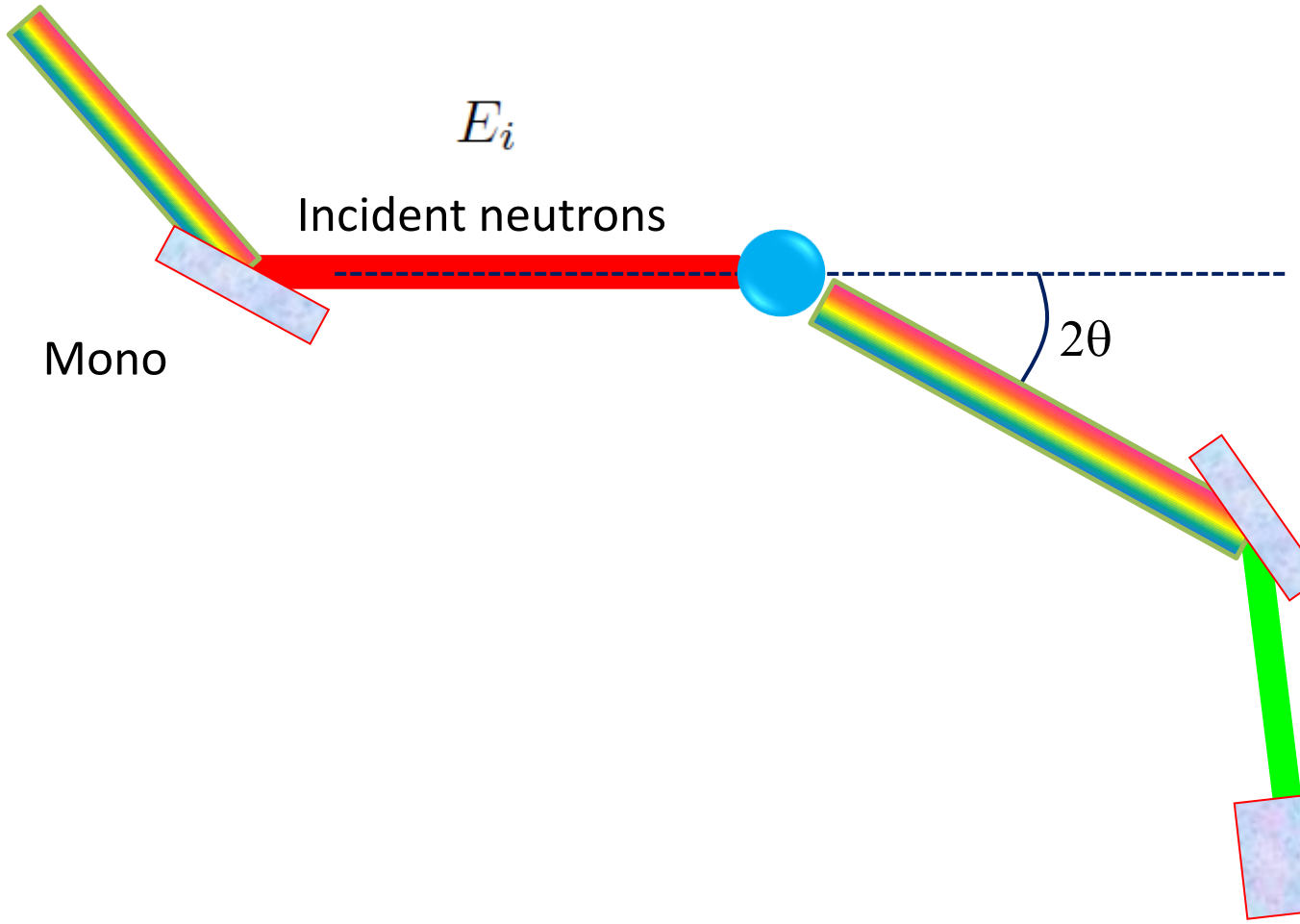
Time of flight spectrometer
IN4, IN5, IN6-Sharp @ ILL
FOCUS @ PSI
…





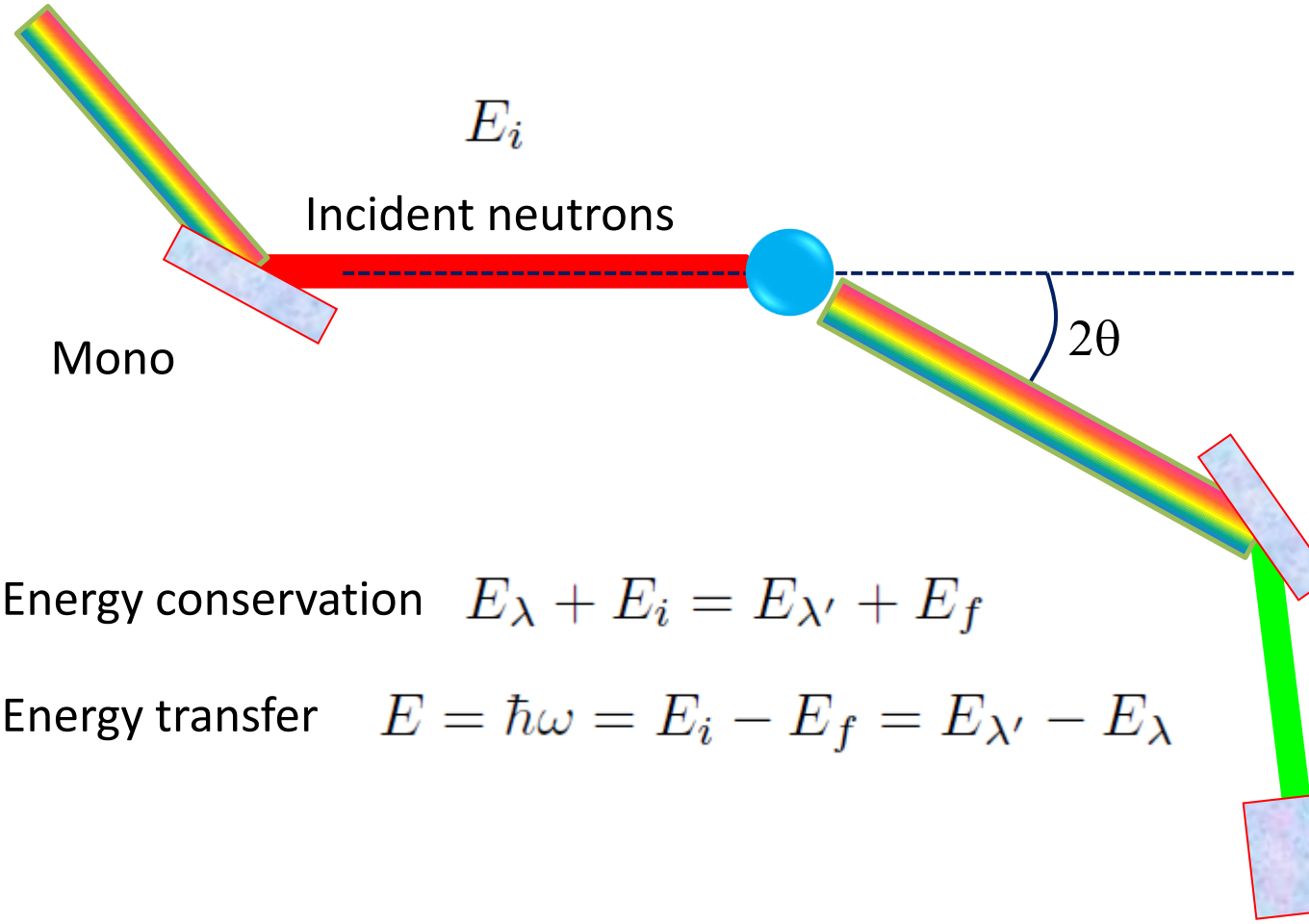
5. TAS

TAS



Selects a unique final energy in the scattered beam

TAS

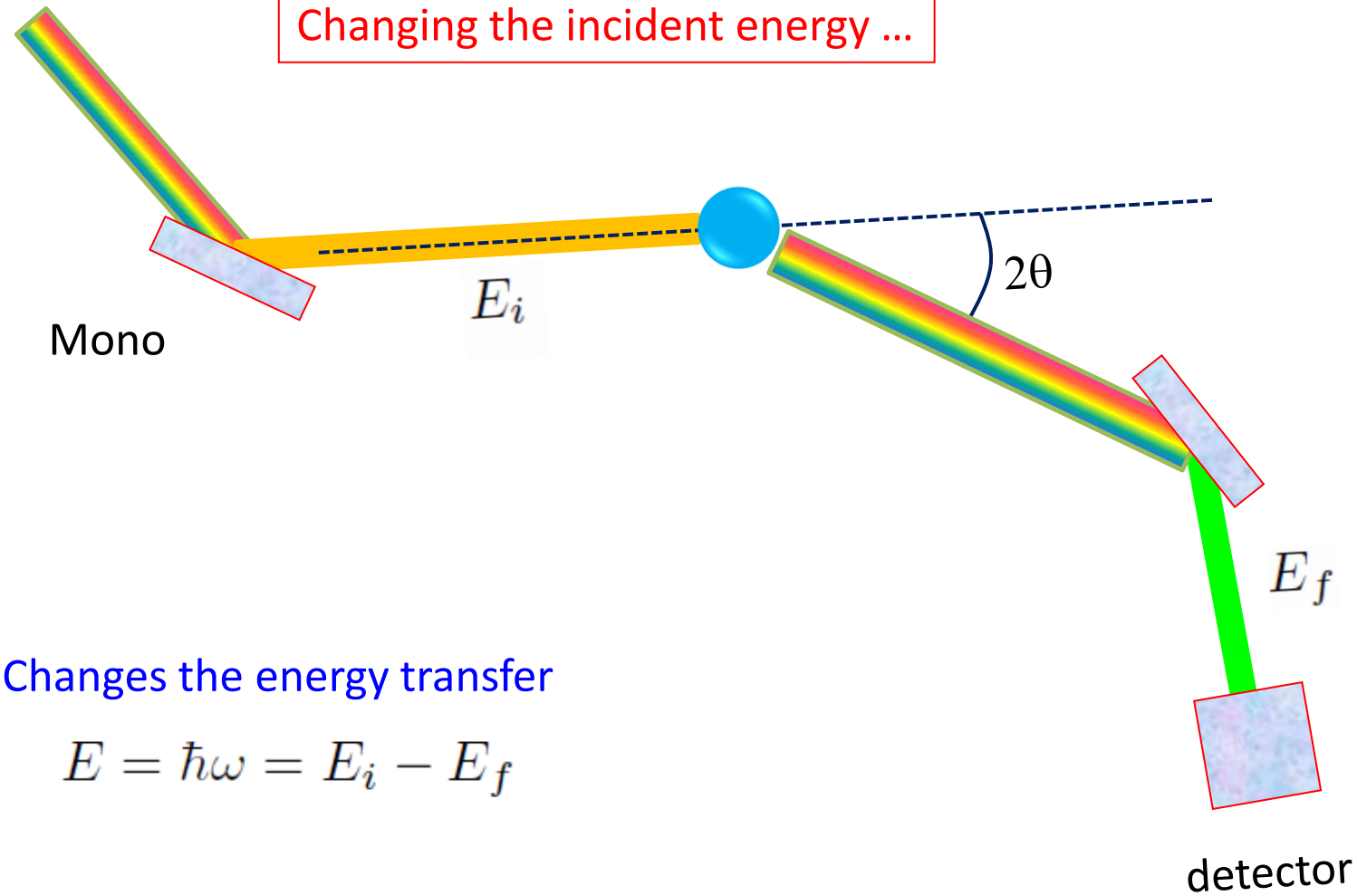


Selects a unique final energy in the scattered beam

Energy conservation $E_\lambda + E_i = E_{\lambda'} + E_f$

Energy transfer $E = \hbar\omega = E_i - E_f = E_{\lambda'} - E_\lambda$

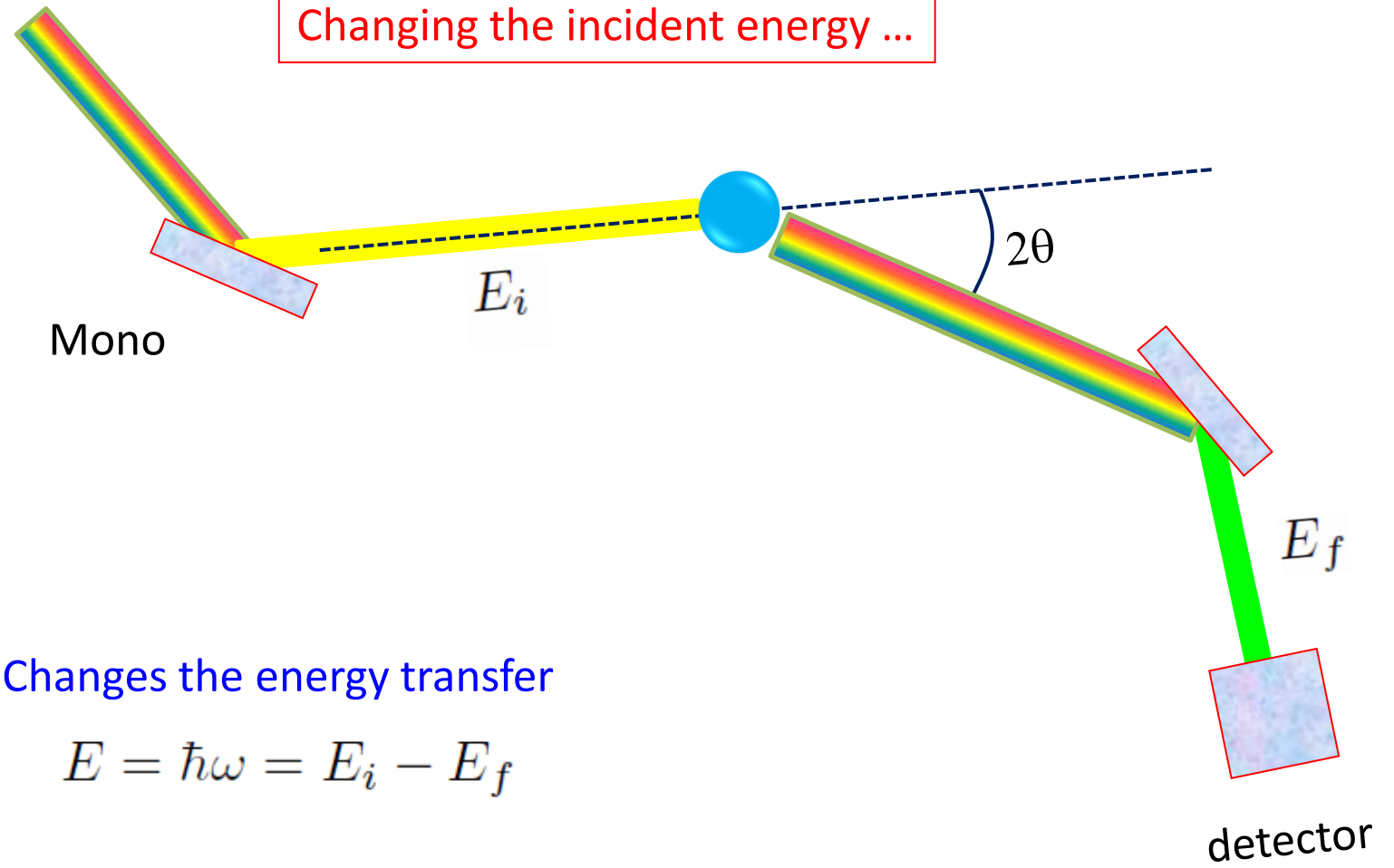
Changing the incident energy …



Changes the energy transfer

$$E = \hbar\omega = E_i - E_f$$

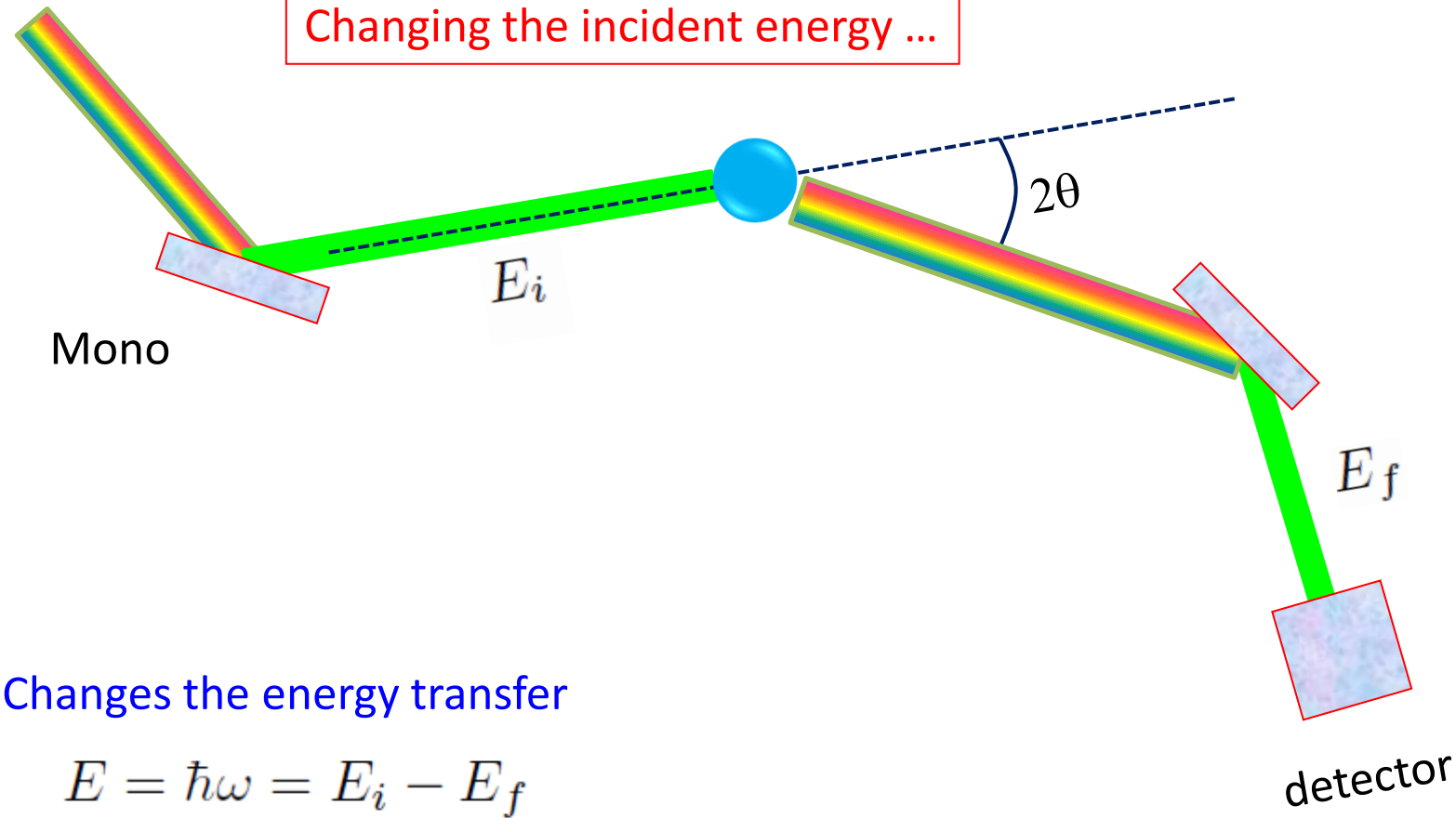
Changing the incident energy …



Changes the energy transfer

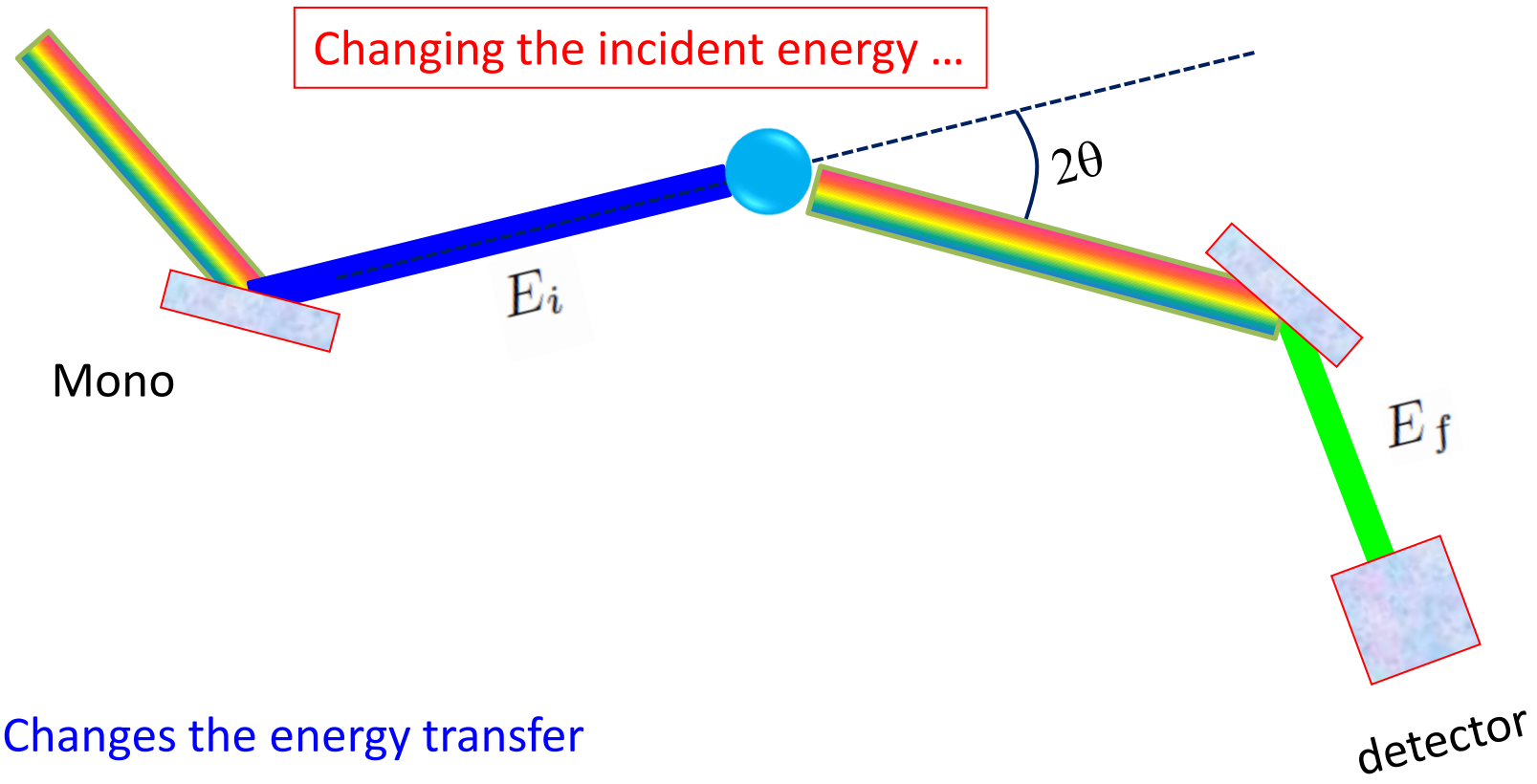
$$E = \hbar\omega = E_i - E_f$$

Changing the incident energy …



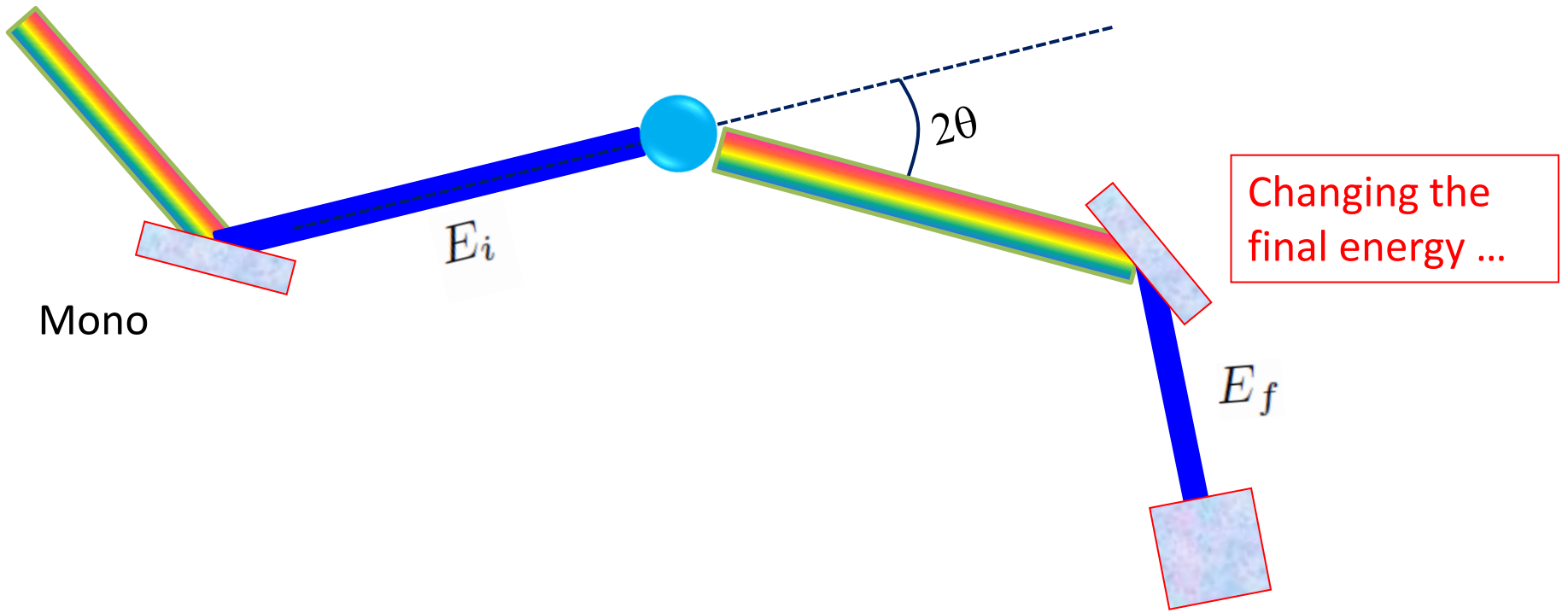
Changes the energy transfer

$$E = \hbar\omega = E_i - E_f$$



Changes the energy transfer

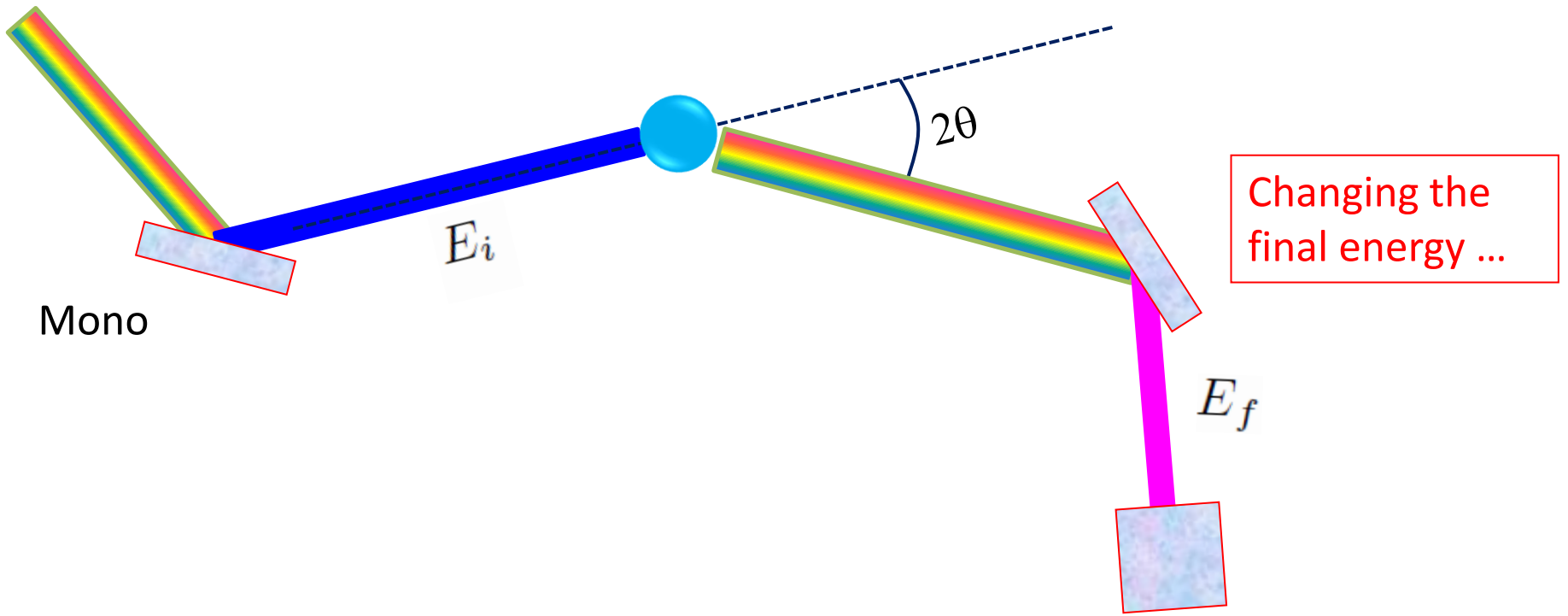
$$E = \hbar\omega = E_i - E_f$$



Changing the final energy …

Changes also the energy transfer

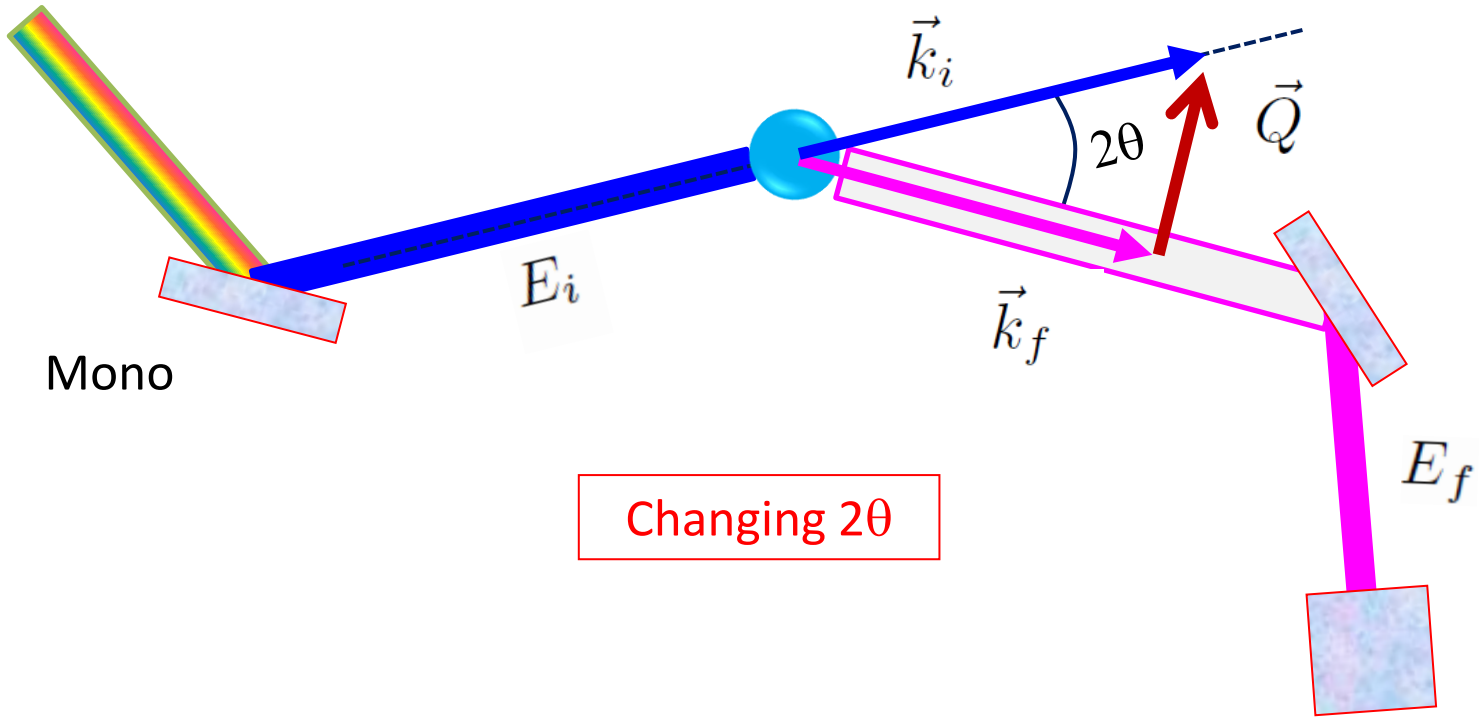
$$E = \hbar\omega = E_i - E_f$$



Changing the final energy …

Changes also the energy transfer

$$E = \hbar\omega = E_i - E_f$$

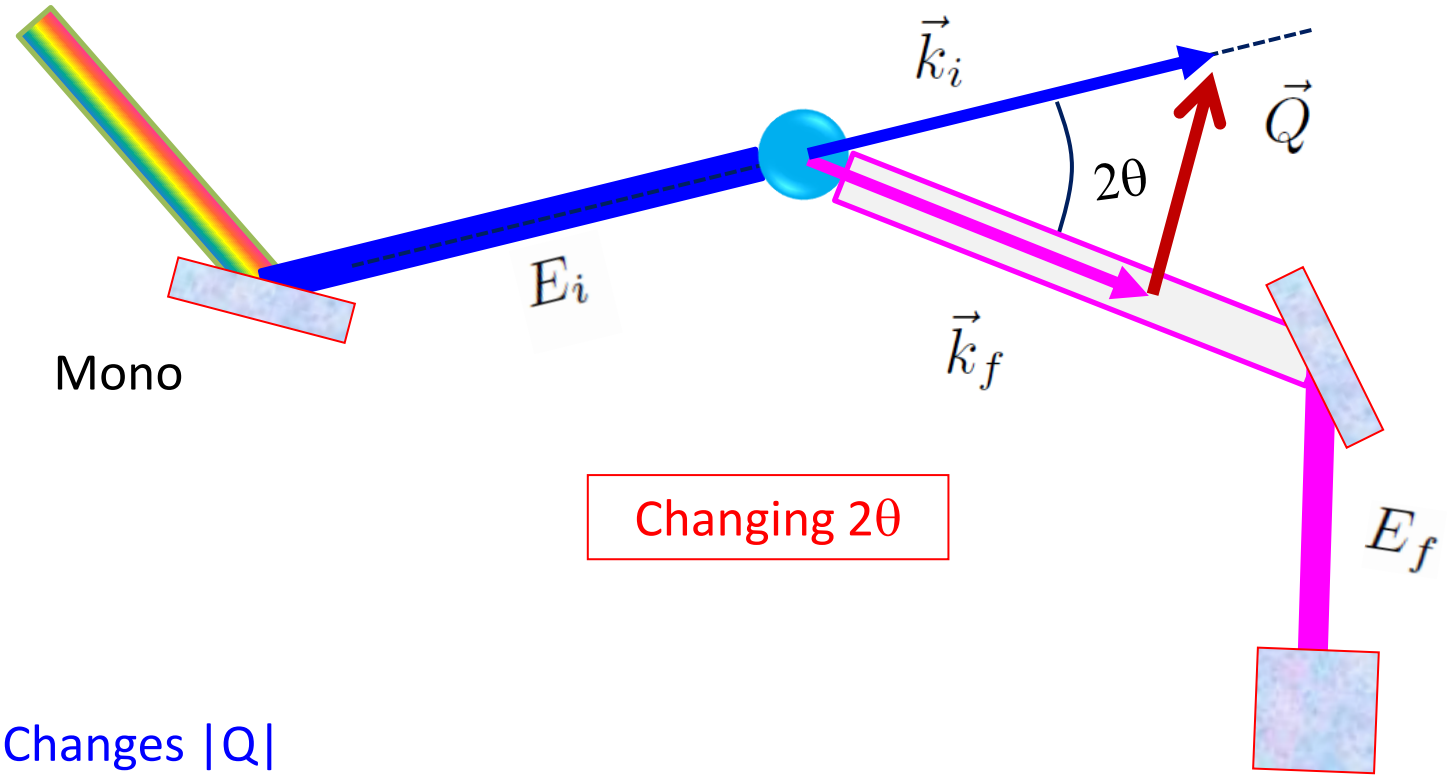


Changing 2θ

Changes |Q|

Scattered wavevector $\vec{Q} = \vec{k}_i - \vec{k}_f$

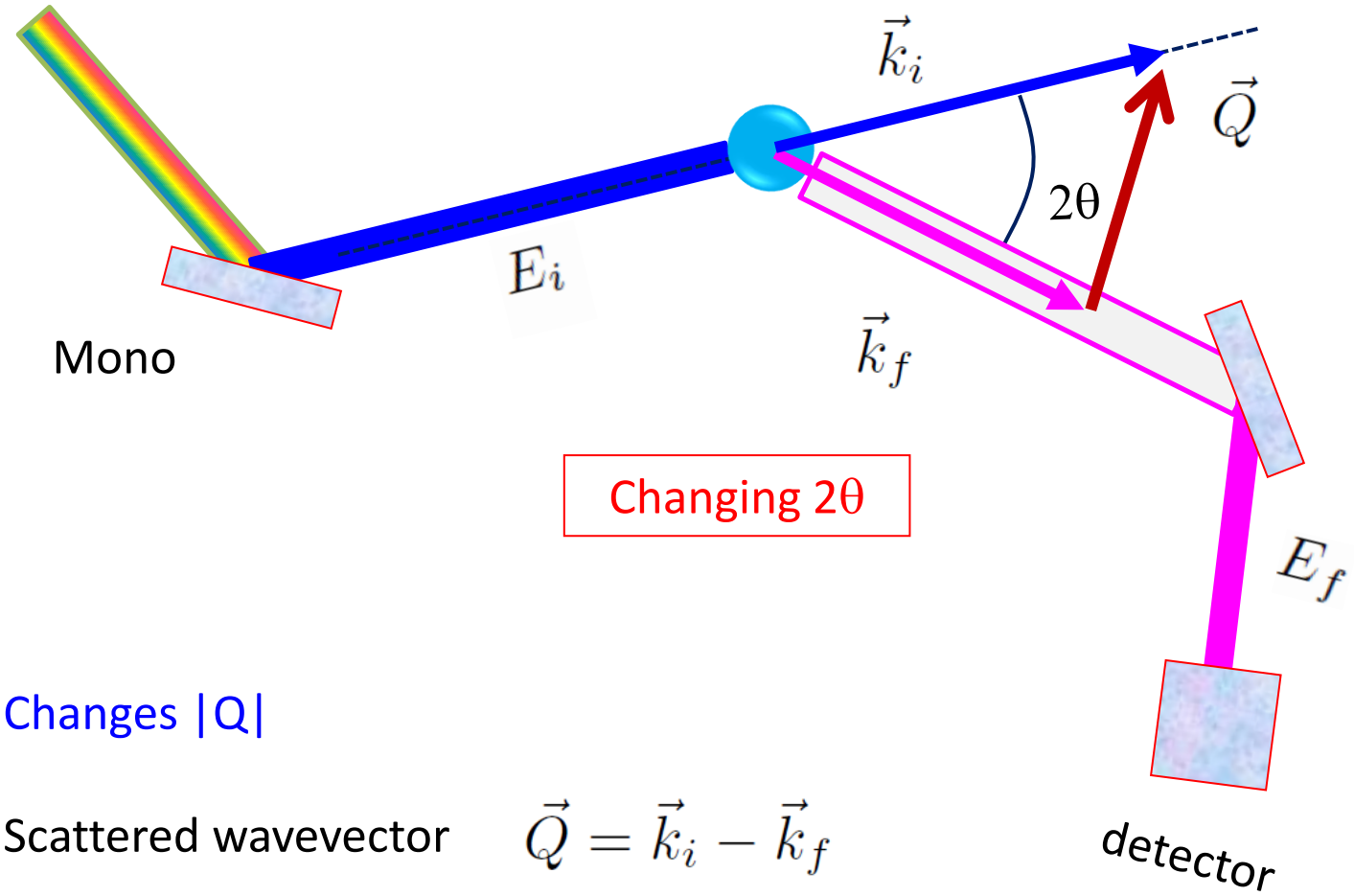
$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$



Changes |Q|

Scattered wavevector $\vec{Q} = \vec{k}_i - \vec{k}_f$

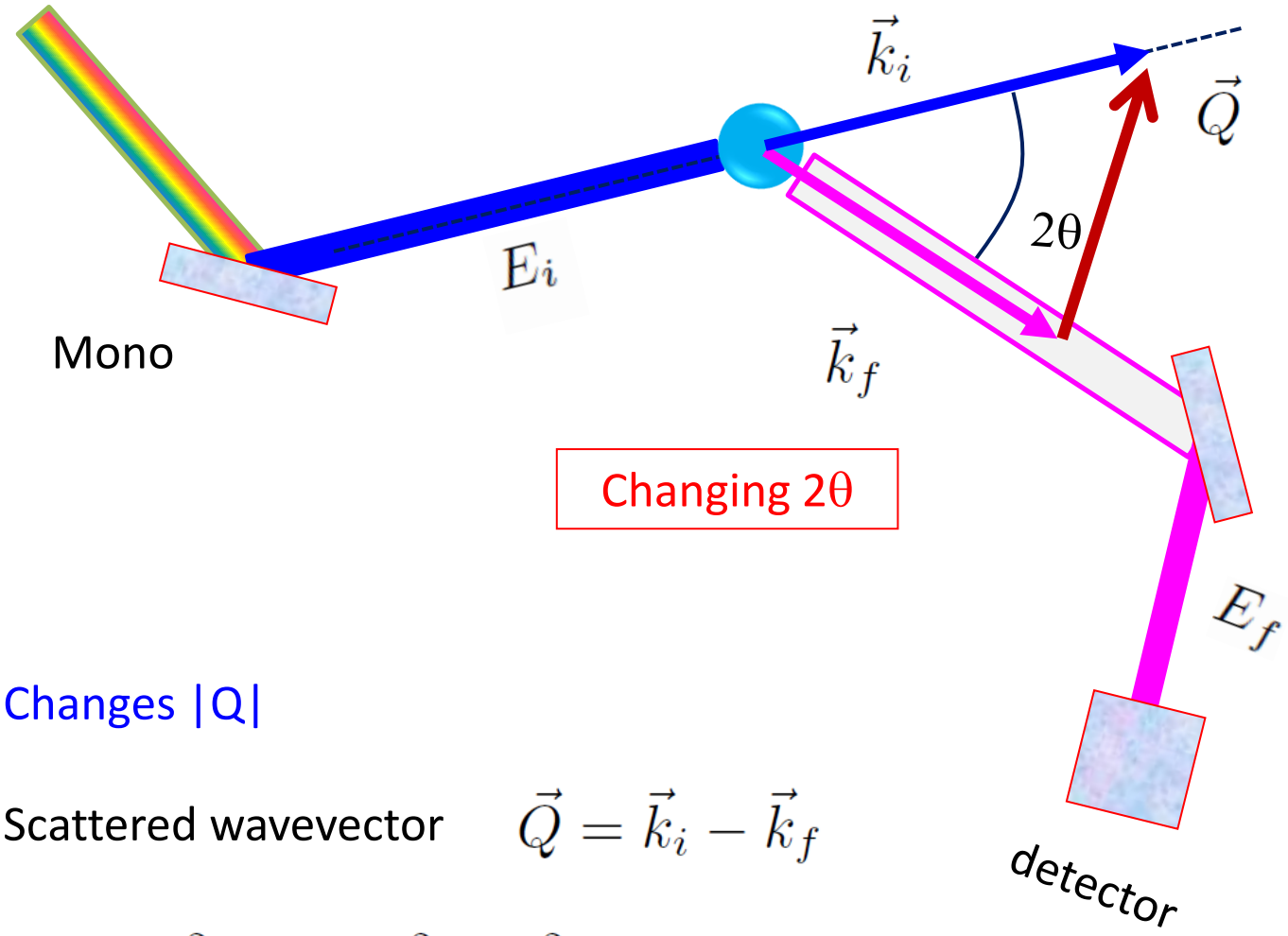
$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$



Changes |Q|

Scattered wavevector $\vec{Q} = \vec{k}_i - \vec{k}_f$

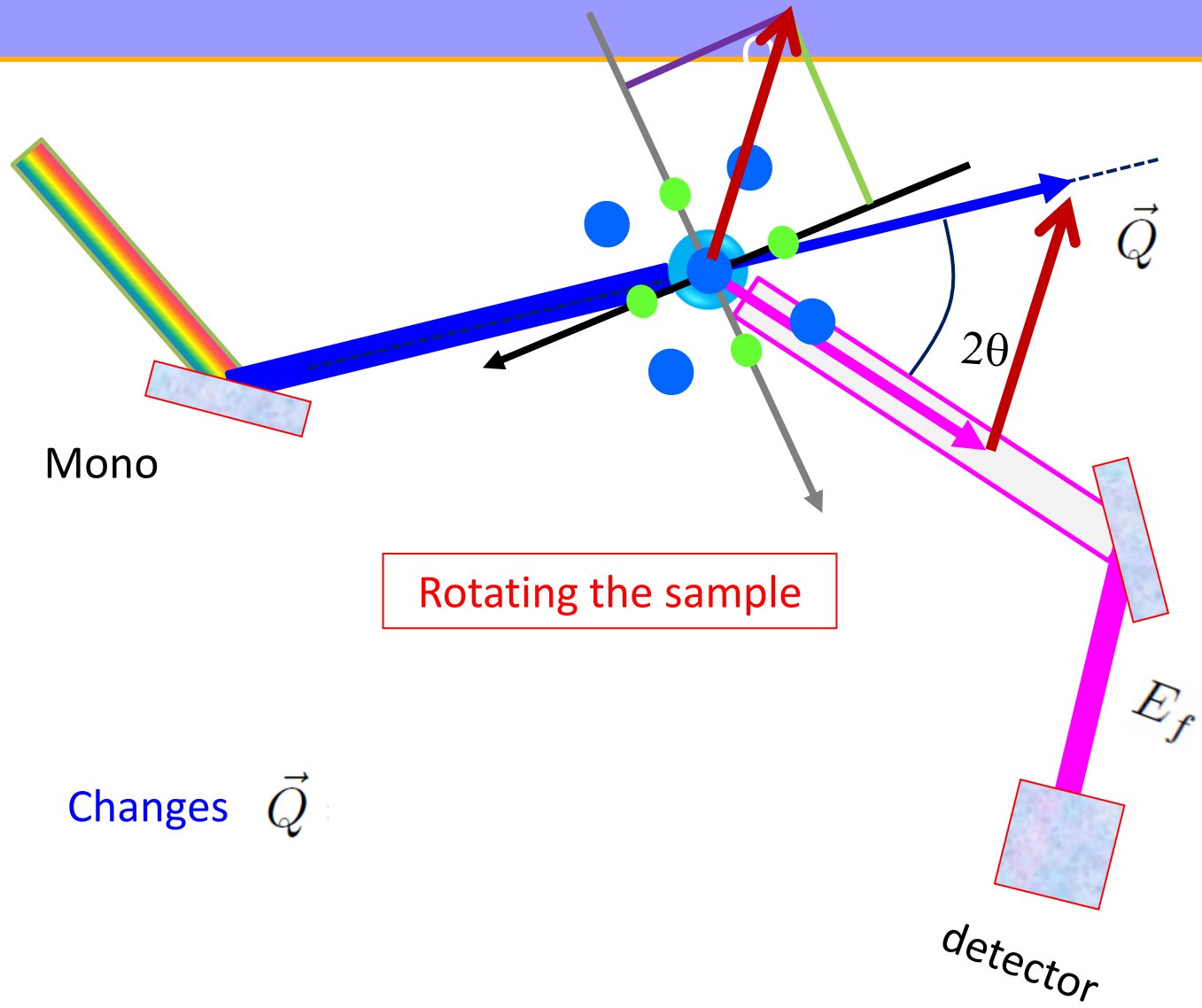
$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$



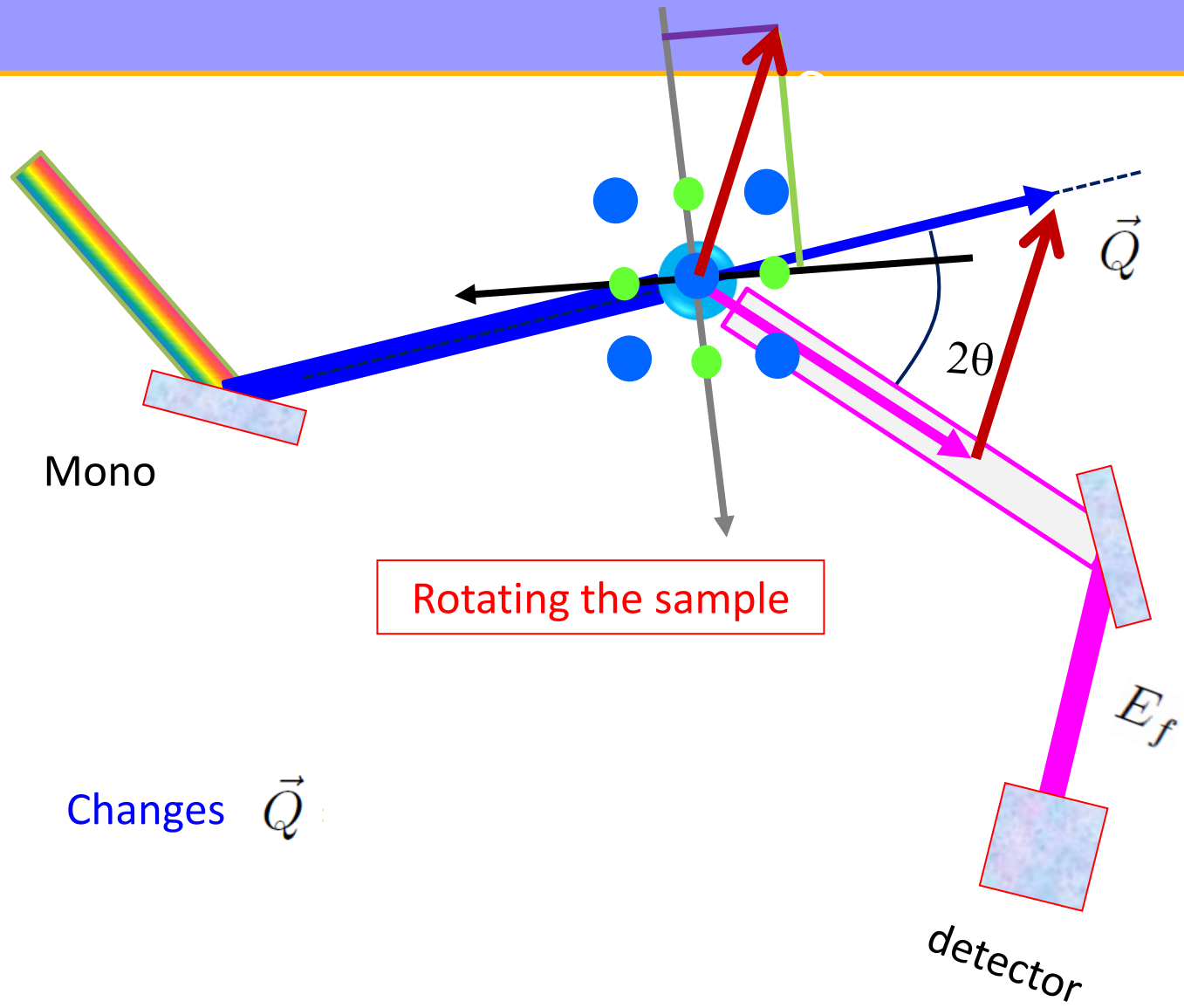
Changes |Q|

Scattered wavevector $\vec{Q} = \vec{k}_i - \vec{k}_f$

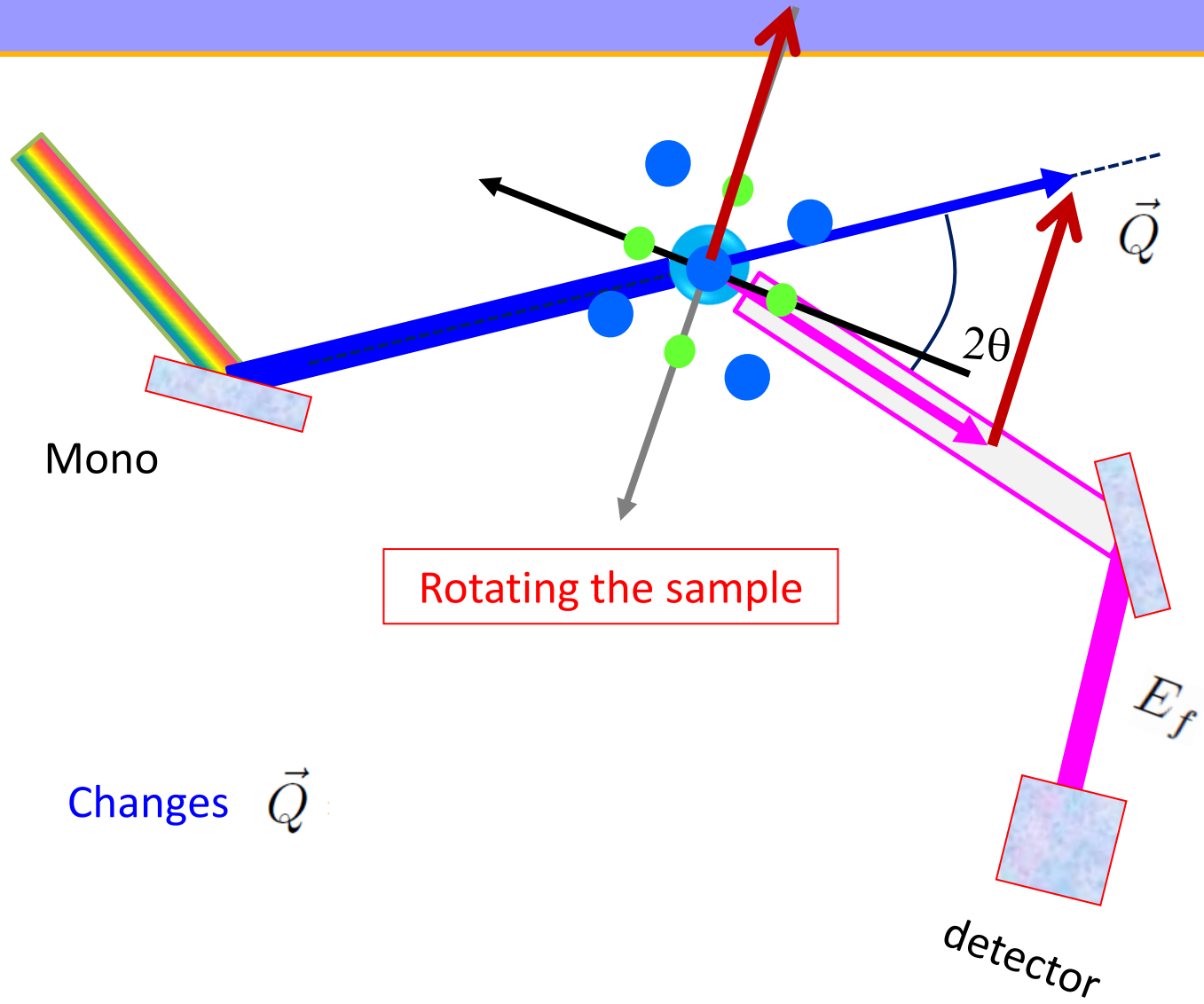
$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$



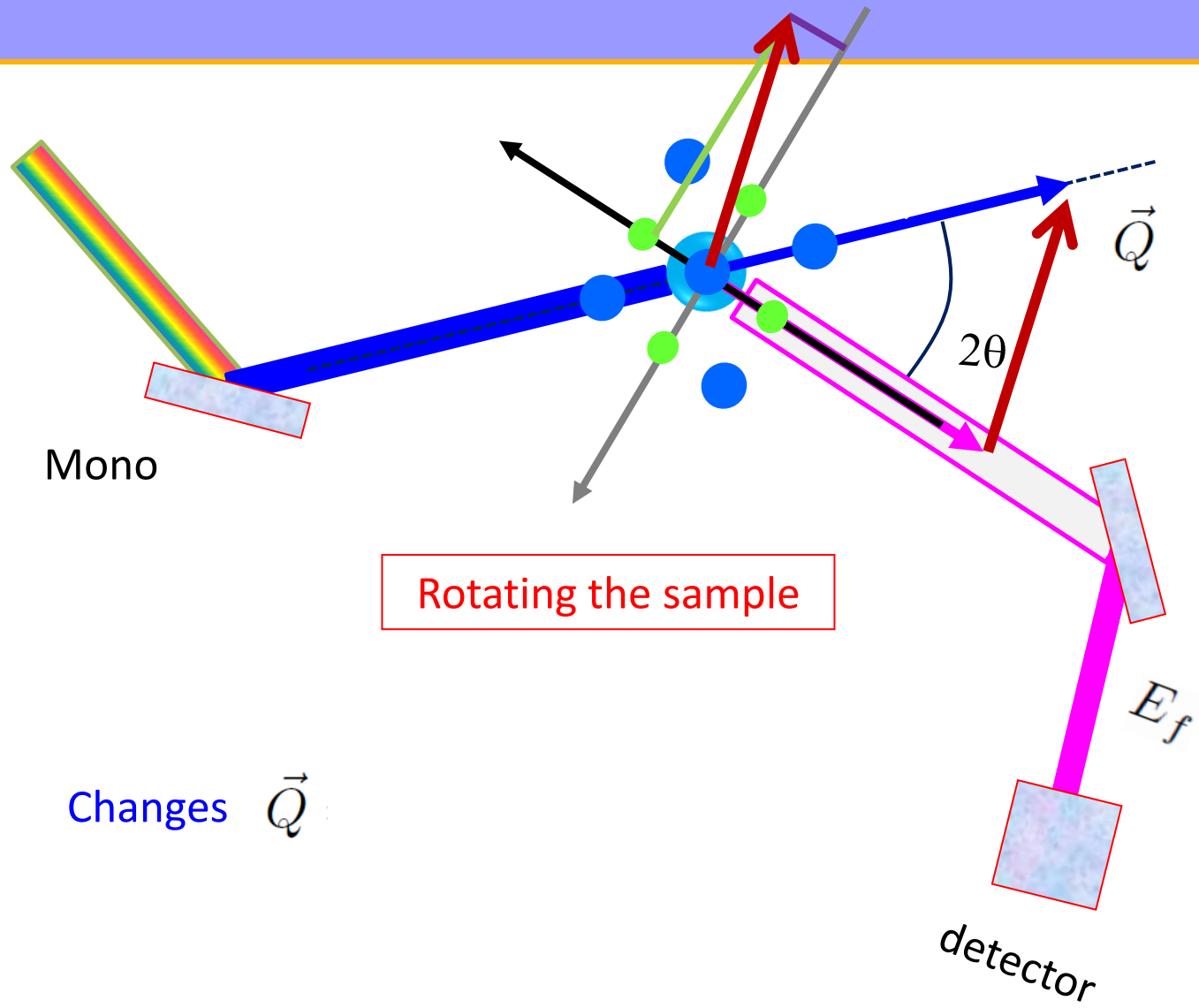
Changes $\vec{Q}$



Changes $\vec{Q}$

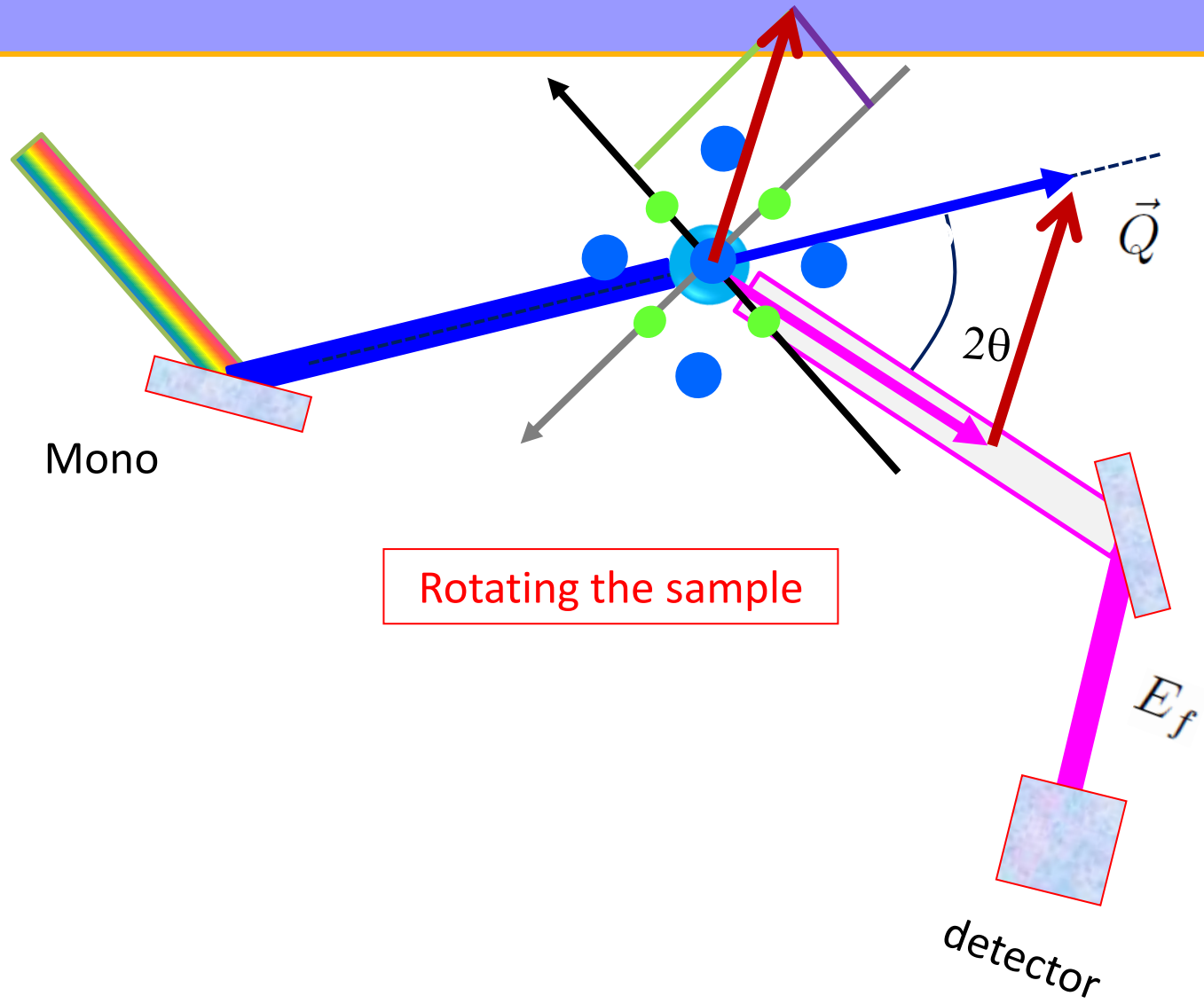


Changes $\vec{Q}$



Changes $\vec{Q}$

TAS

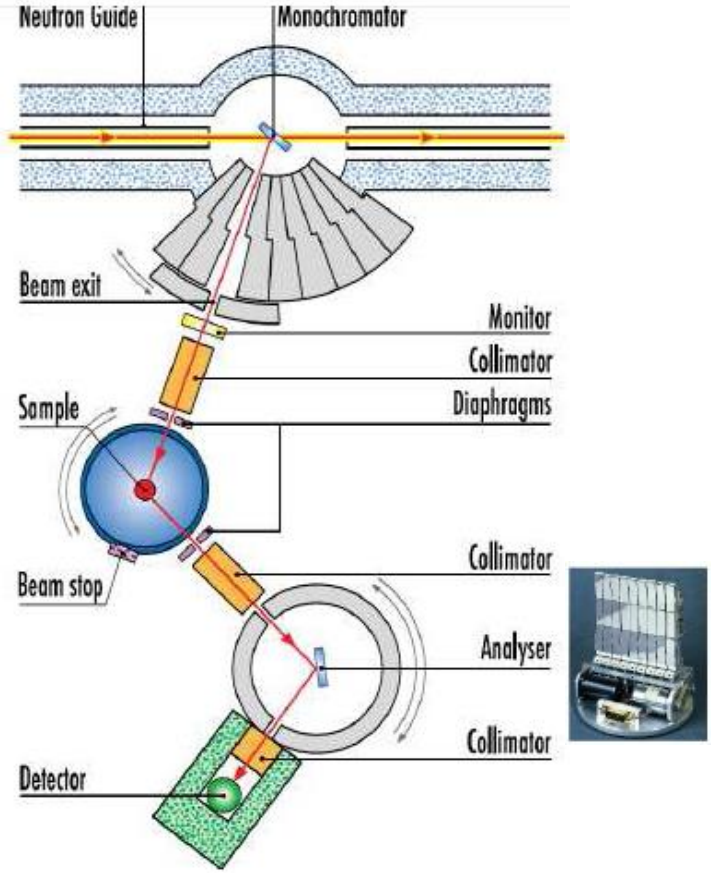


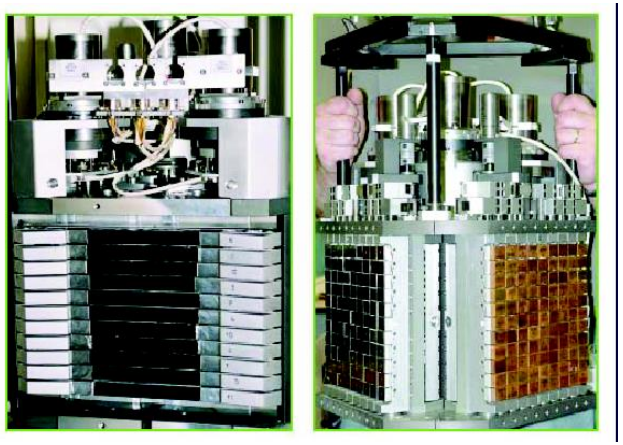
Rotating the sample

Time consumming ….

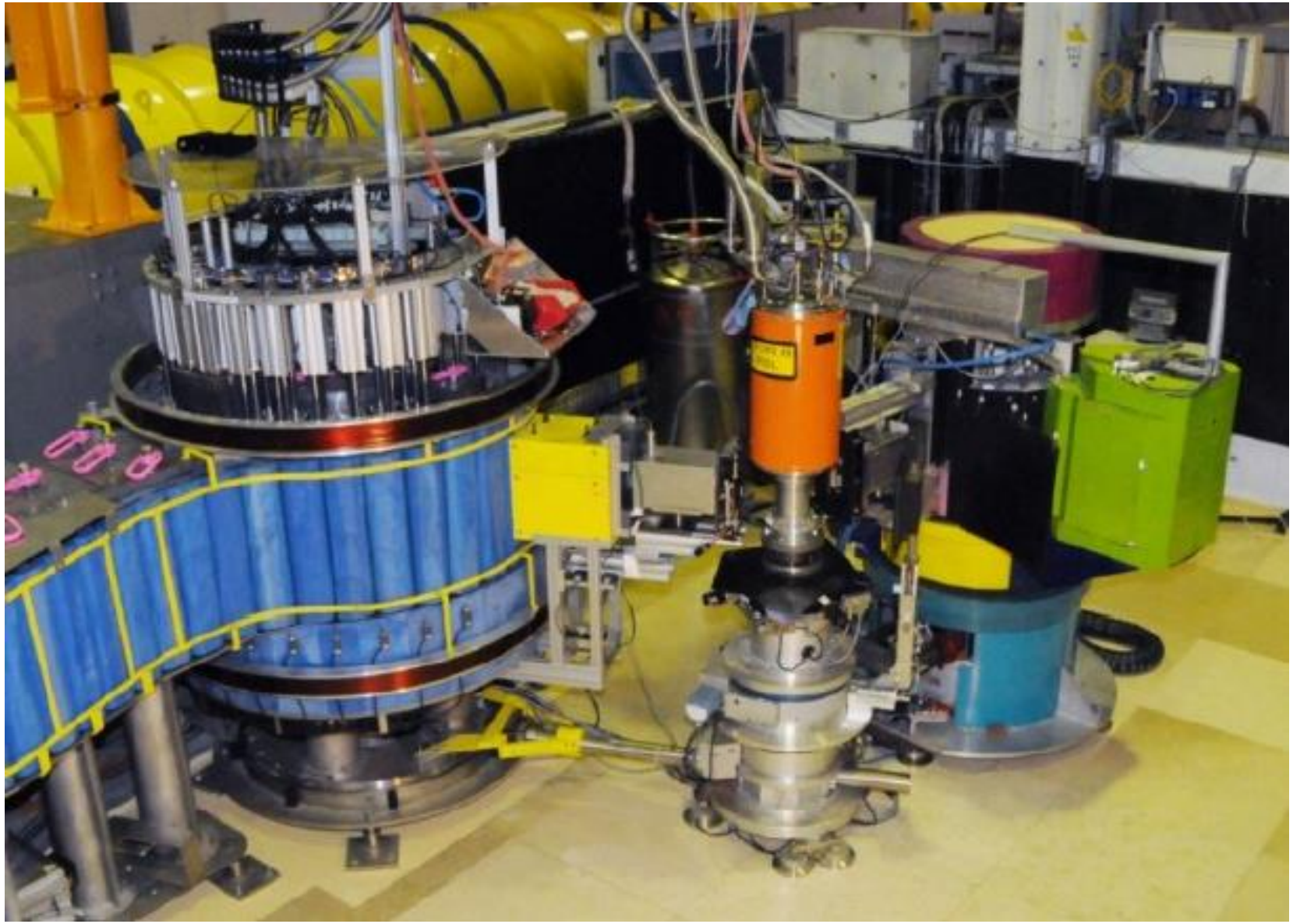
TAS

Triple axes spectrometer
(IN8, IN20, IN12, IN22 @ ILL)





TAS



6. What about the neutron spin ?
Is it possible to manipulate it?

Polarized neutrons

$$
\begin{aligned}
I_x^{++} &\propto |N|^2 \\
I_x^{--} &\propto |N|^2 \\
I_x^{+-} &\propto |M_\perp|^2 - M_{ch} \\
I_x^{-+} &\propto |M_\perp|^2 + M_{ch} \\
I_y^{++} &\propto |N|^2 + |M_\perp^y|^2 + R_y \\
I_y^{--} &\propto |N|^2 + |M_\perp^y|^2 - R_y \\
I_y^{+-} &\propto |M_\perp^z|^2 \\
I_y^{-+} &\propto |M_\perp^z|^2 \\
I_z^{++} &\propto |N|^2 + |M_\perp^z|^2 + R_z \\
I_z^{--} &\propto |N|^2 + |M_\perp^z|^2 - R_z \\
I_z^{+-} &\propto |M_\perp^y|^2 \\
I_z^{-+} &\propto |M_\perp^y|^2
\end{aligned}
$$

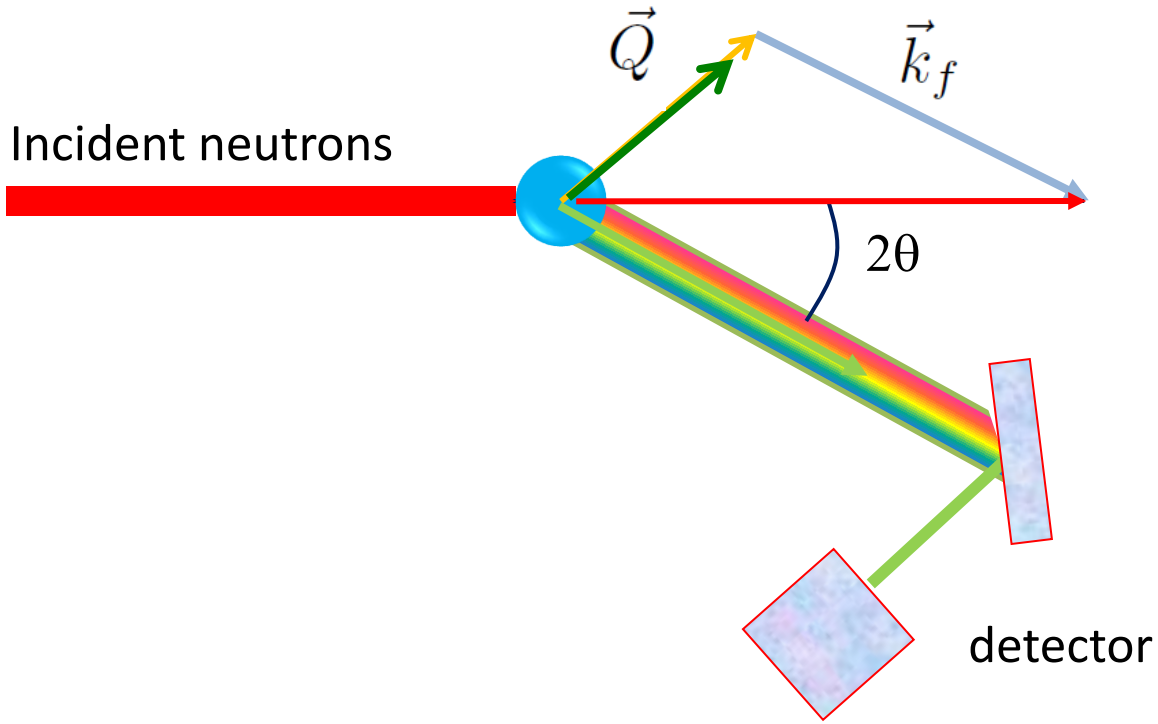
Depending on the spin direction wrt Q, new correlation functions appear

$M = M^z + M^y$

and

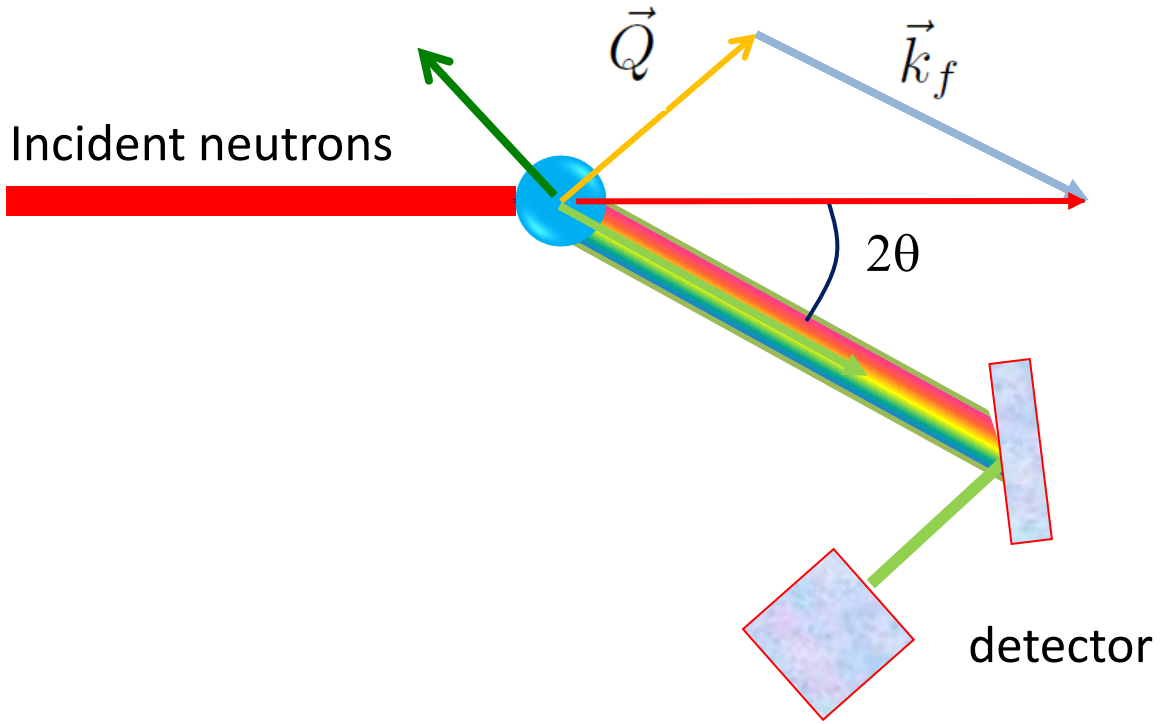
$M^y \quad M^z \quad M_{ch}$

Polarized neutrons



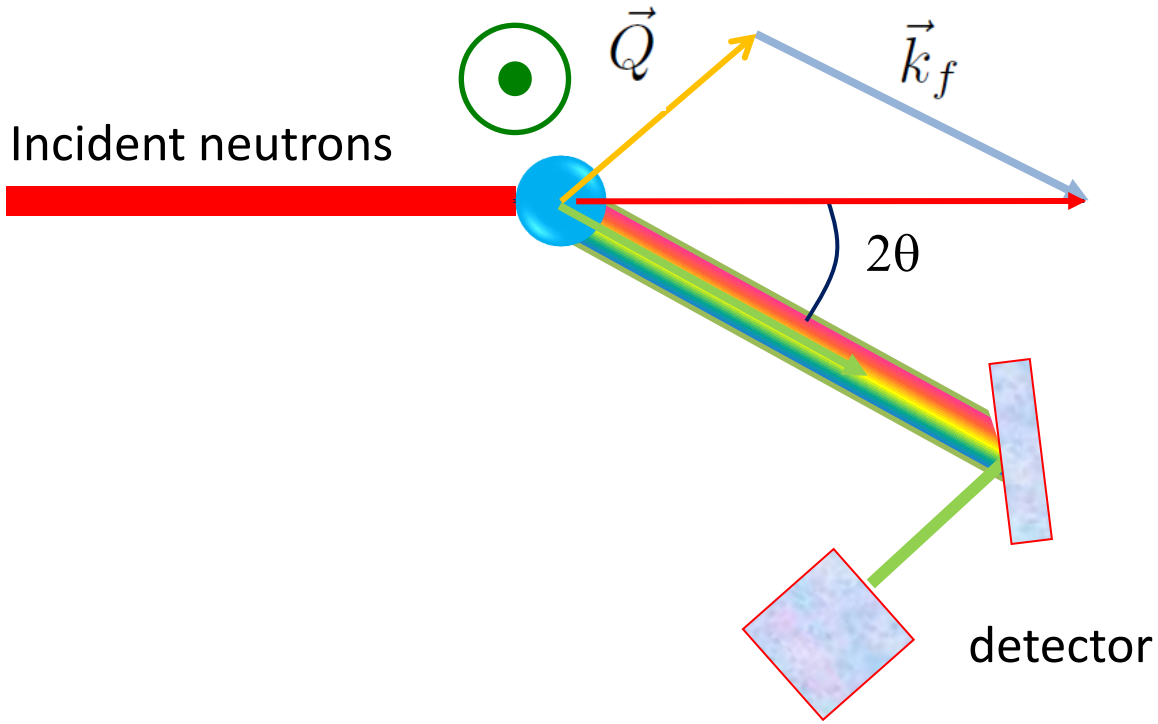
Neutron spin // Q (« x »)

Polarized neutrons



Neutron spin perpendicular to Q within the scattering plane (« y »)

Polarized neutrons



Neutron spin perpendicular to Q and to the scattering plane (« z »)

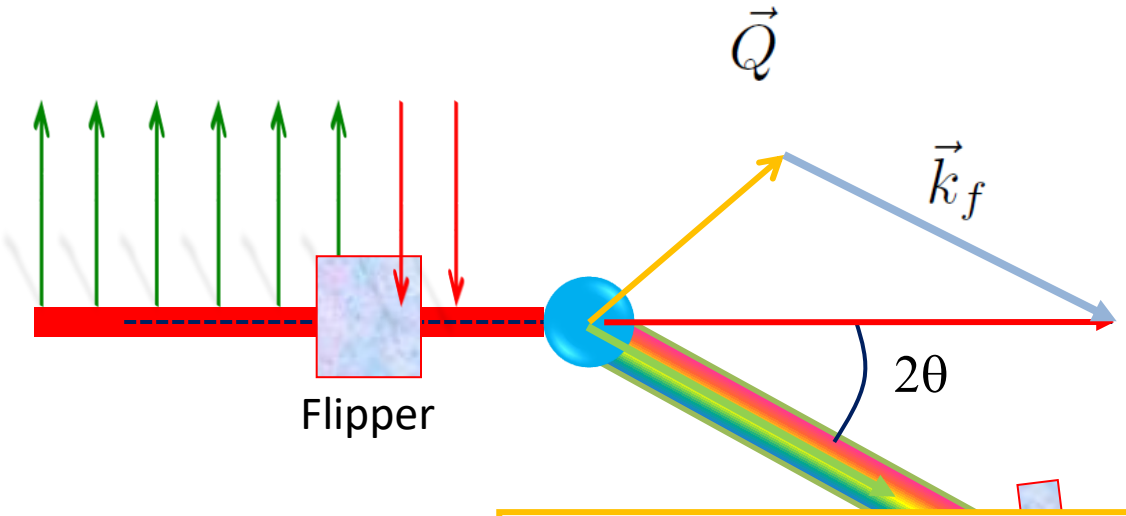
Incoming neutron spin

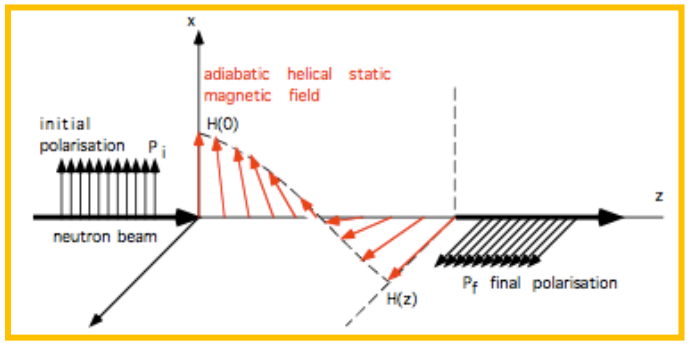
Bender

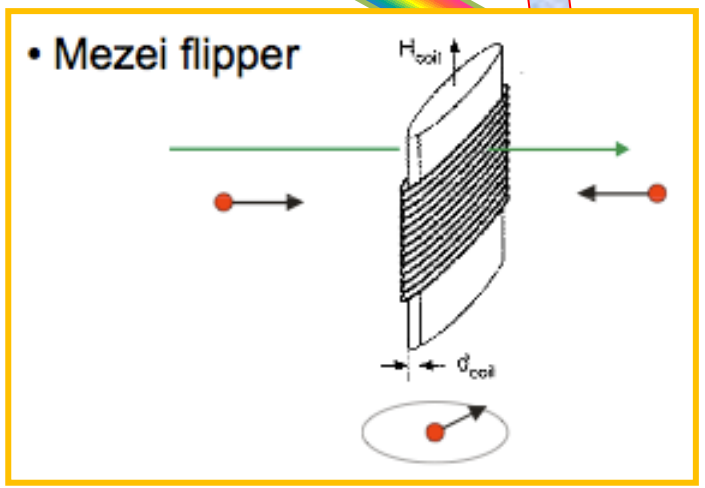
Mono
Heussler

Flipper

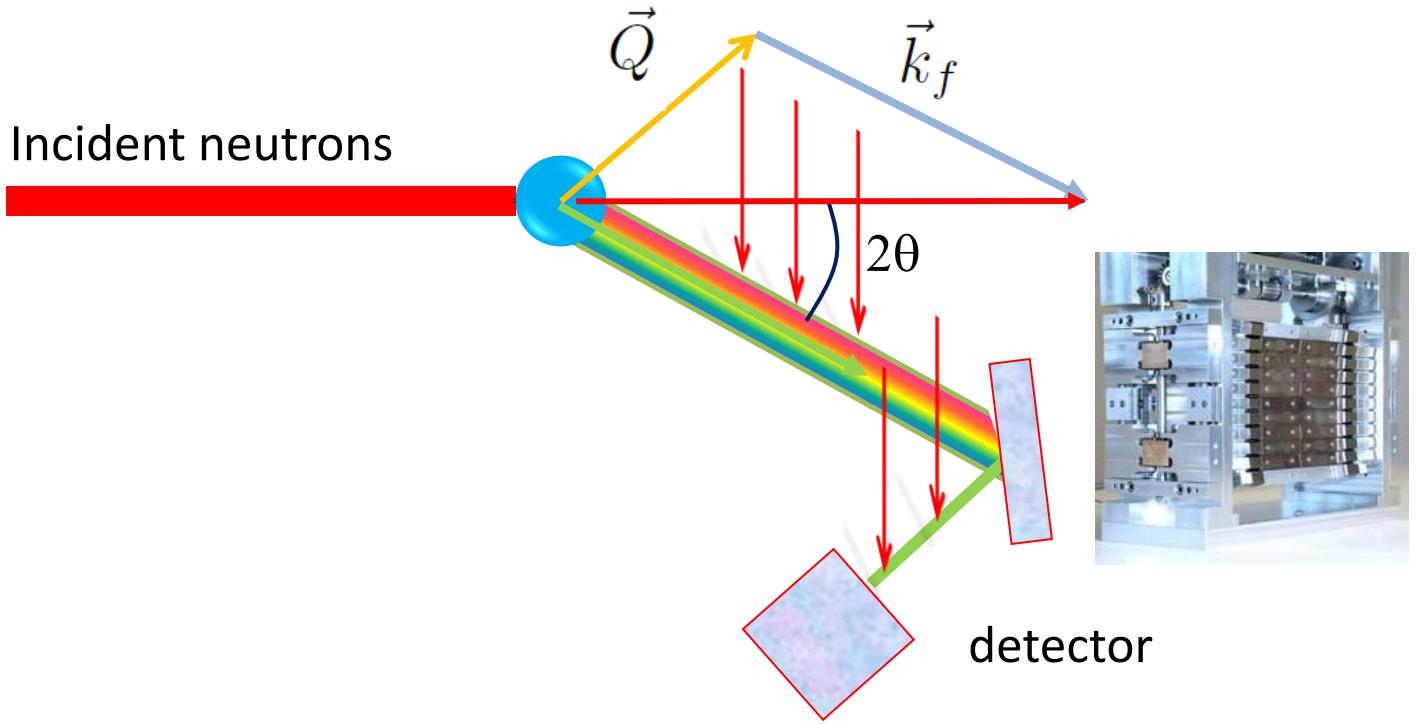
Incoming neutron spin





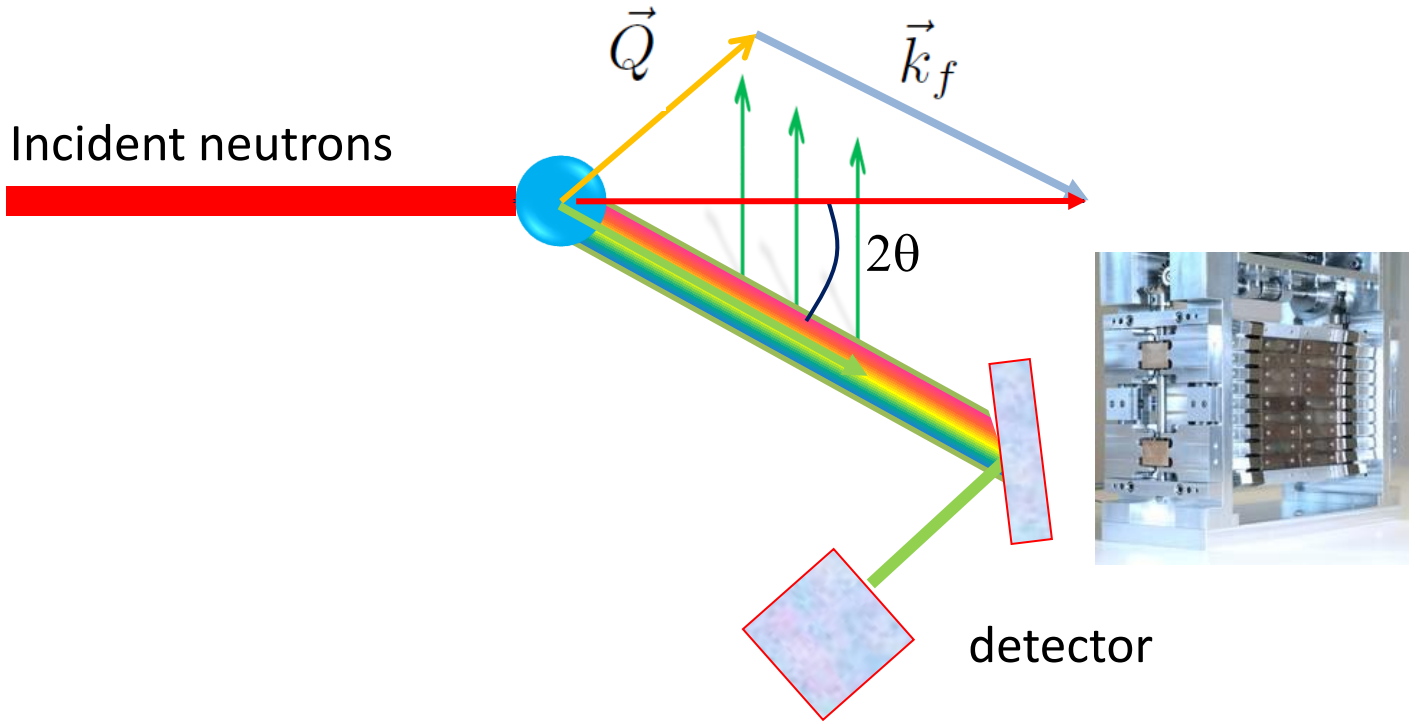


Scattered neutron spin



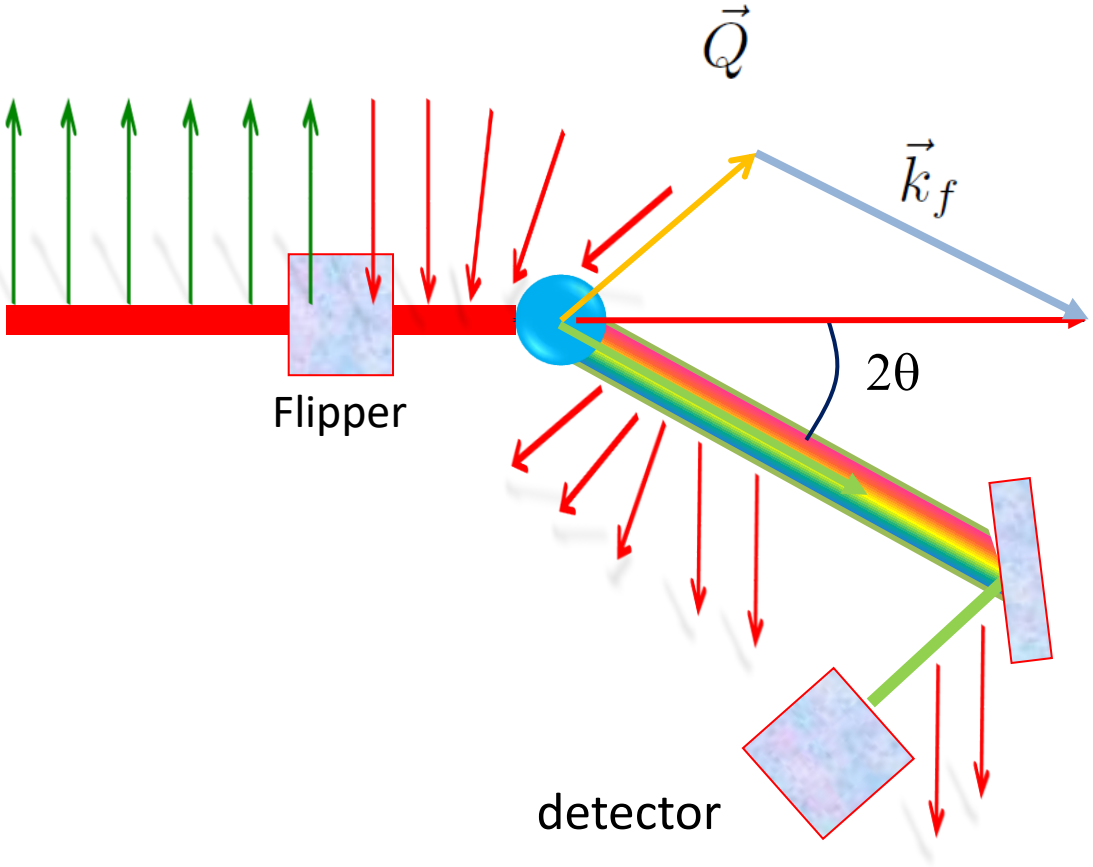
The analyzer selects the final polarization.
Projects onto a given direction (fixed by set up of the instrument)

Scattered neutron spin



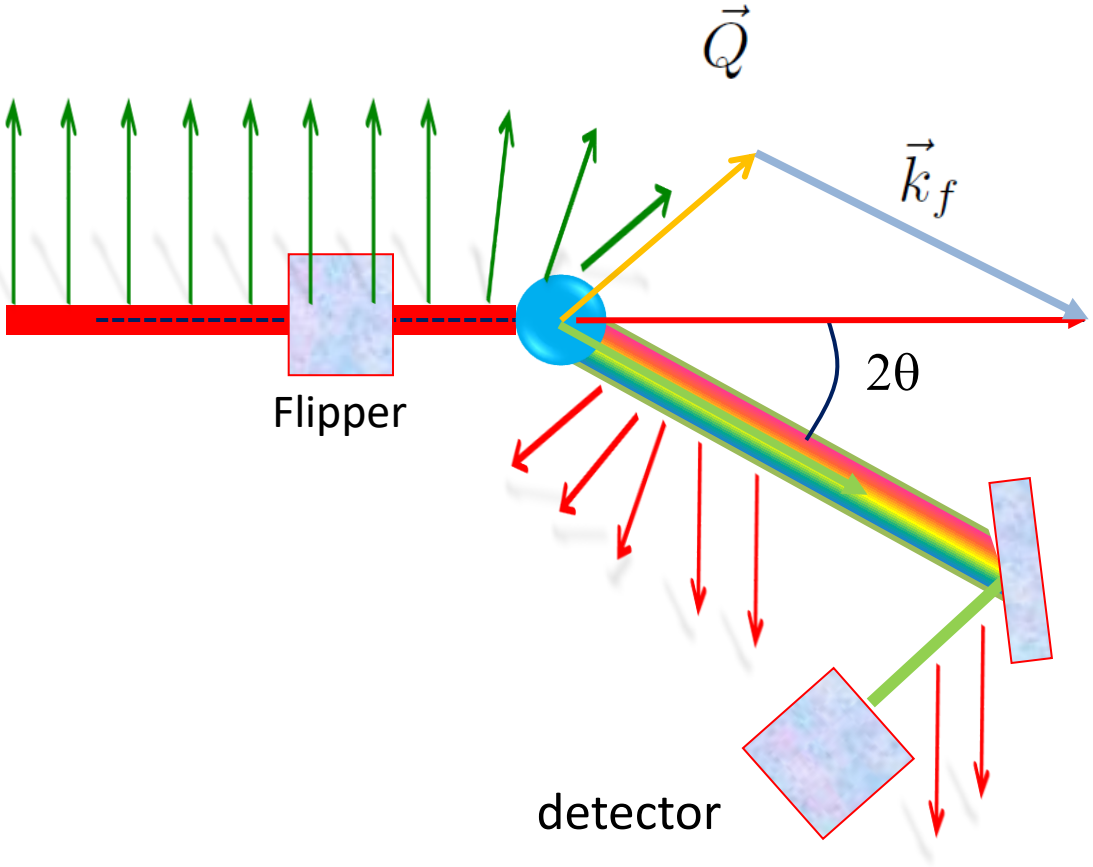
The analyzer selects the final polarization.
Projects onto a given direction (fixed by set up of the instrument)

Polarized neutrons



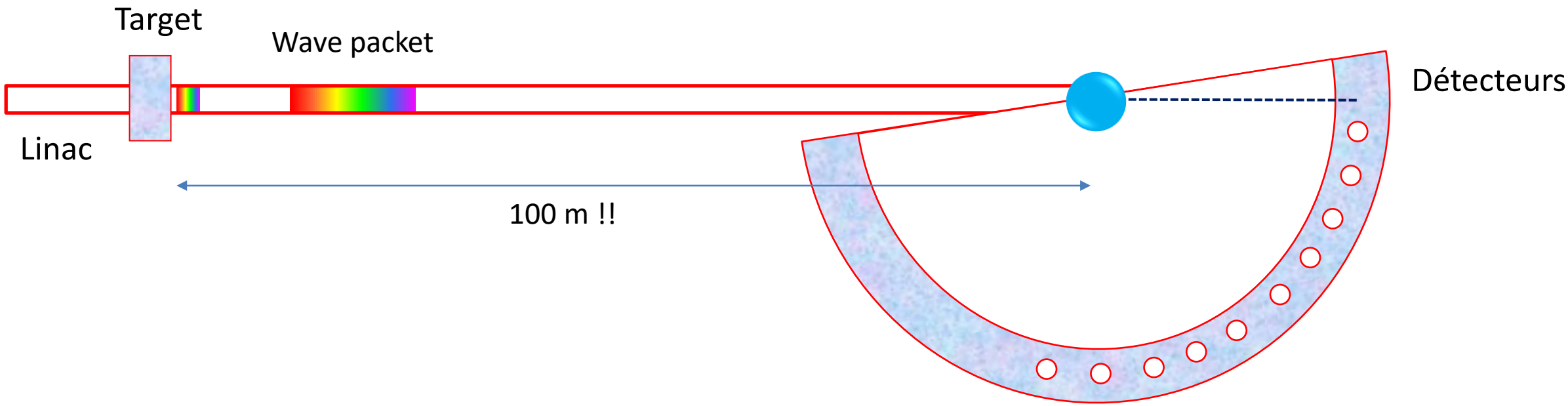
Process I^{--}_{x}

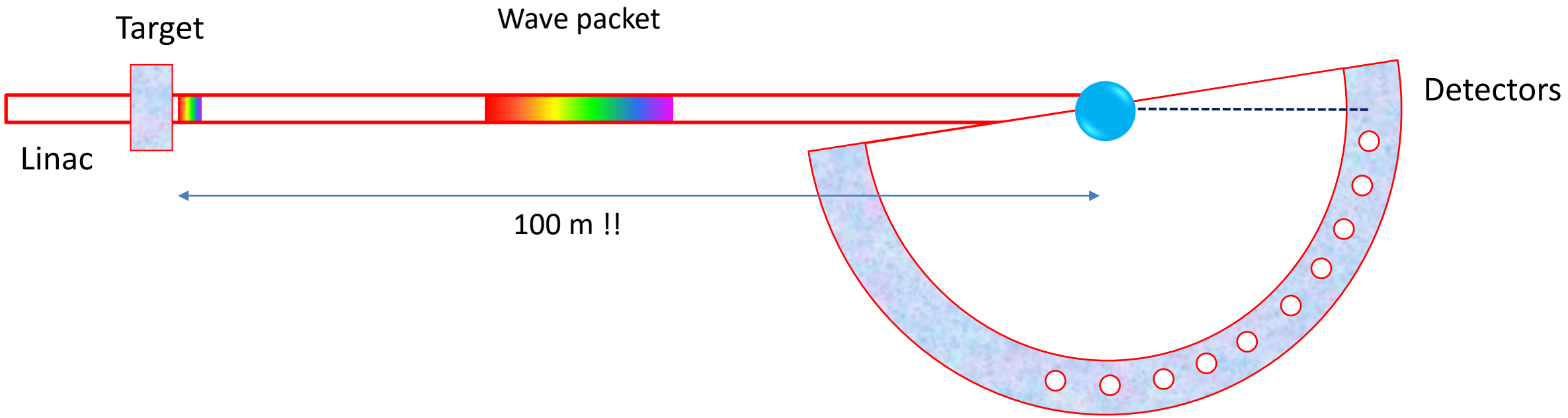
Polarized neutrons

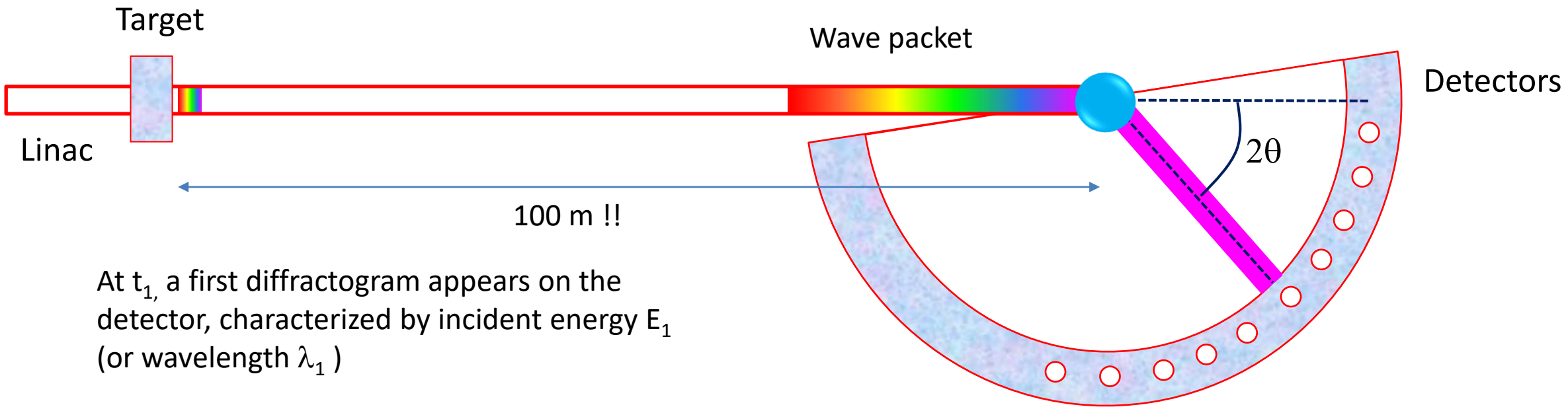


Process I^{+-}_{x}

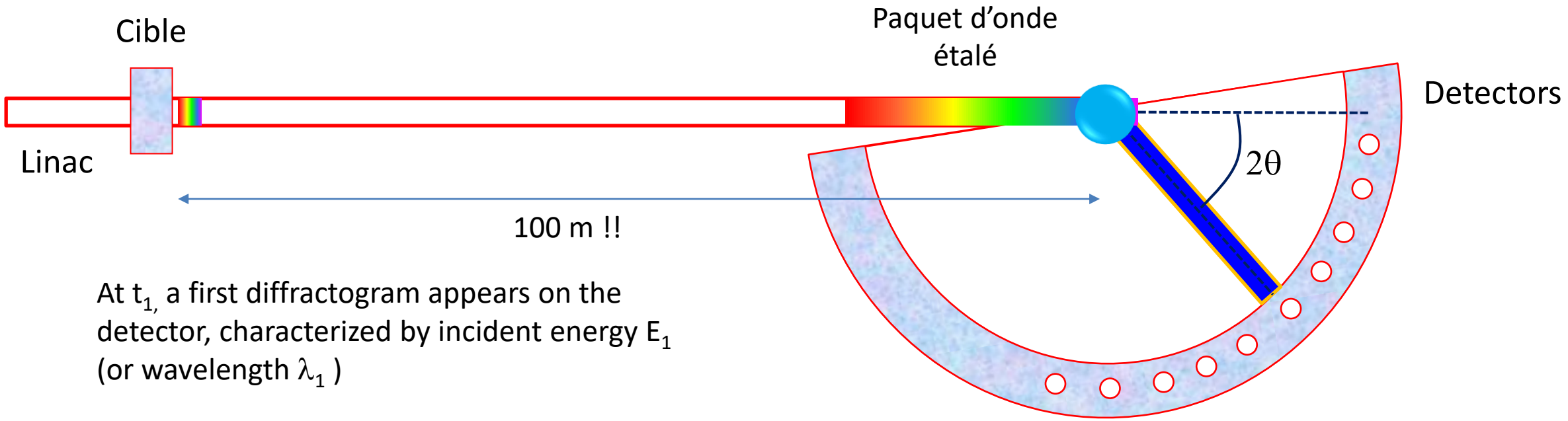
7. ESS and polychromatic pulses


Target
Wave packet
Détecteurs
Linac
100 m !!


Target
Wave packet
Detectors
Linac
100 m !!

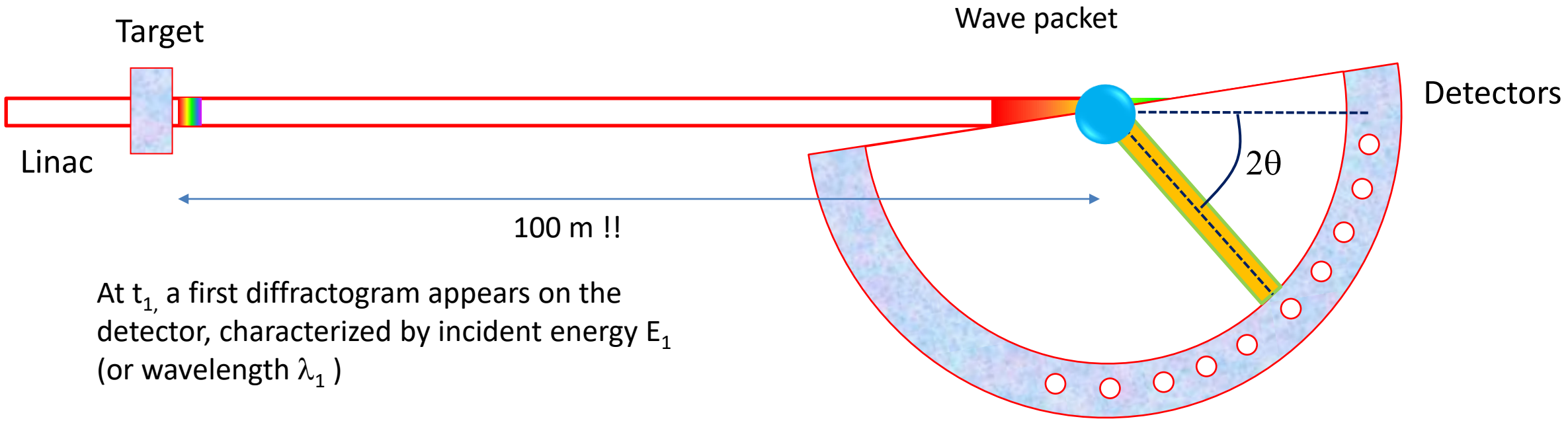


At $t_{1,}$ a first diffractogram appears on the detector, characterized by incident energy E_1 (or wavelength λ_1)



At t_1, a first diffractogram appears on the detector, characterized by incident energy E_1 (or wavelength λ_1)

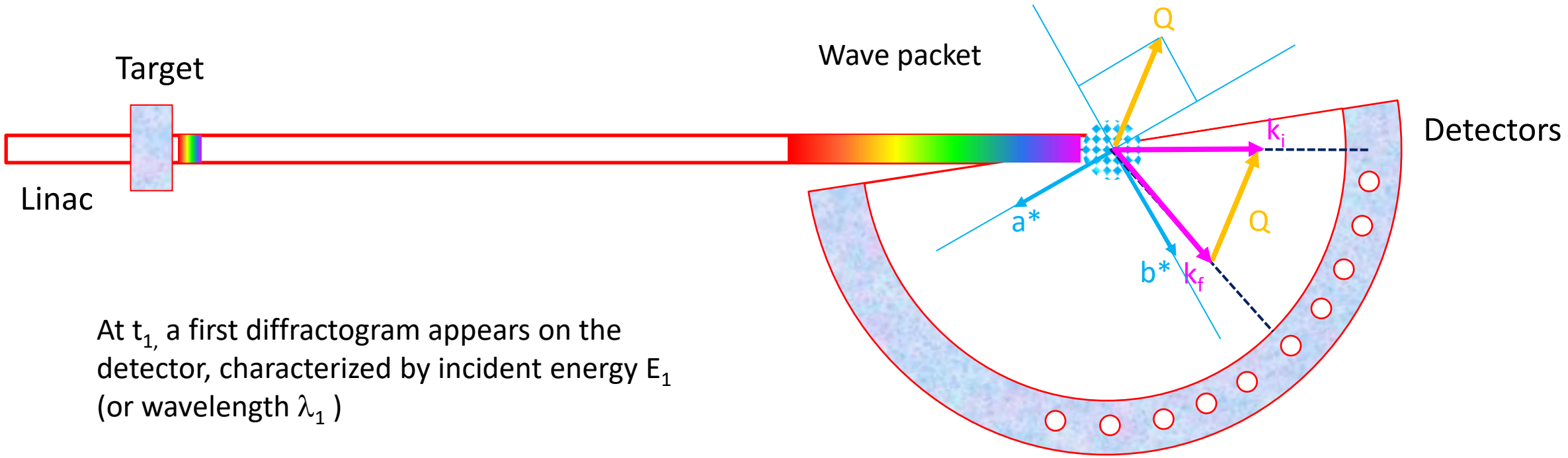
A $t_2 = t_1 + \delta t$, a new one forms, characterized by incident energy E_2 (wavelength λ_2)



At t_1, a first diffractogram appears on the detector, characterized by incident energy E_1 (or wavelength λ_1)

A $t_2 = t_1 + \delta t$, a new one forms, characterized by incident energy E_2 (wavelength λ_2)

… and so on for E_i all in the wave packet.



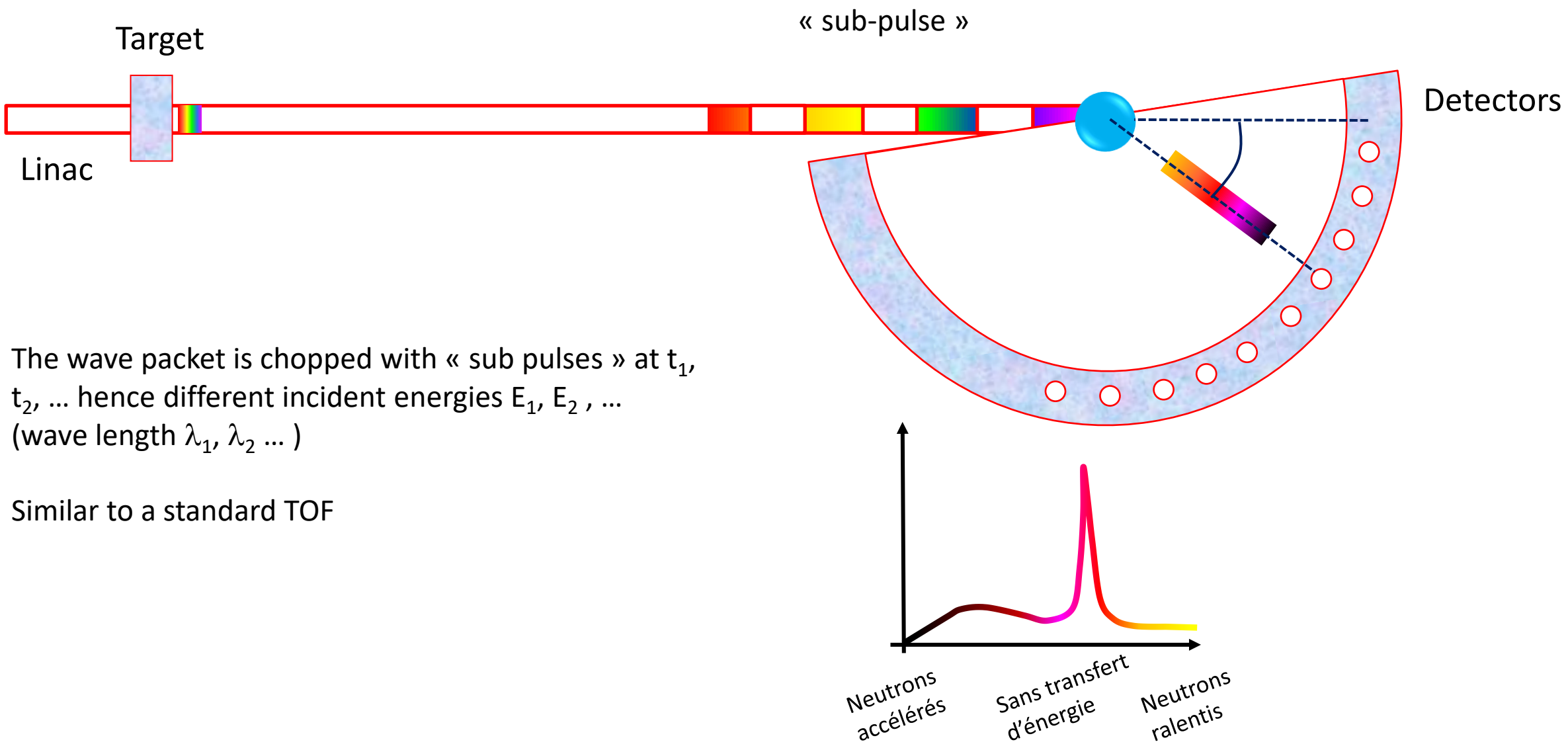
At t_1, a first diffractogram appears on the detector, characterized by incident energy E_1 (or wavelength λ_1)

A $t_2 = t_1 + \delta t$, a new one forms, characterized by incident energy E_2 (wavelength λ_2)

… and so on for E_i all in the wave packet.

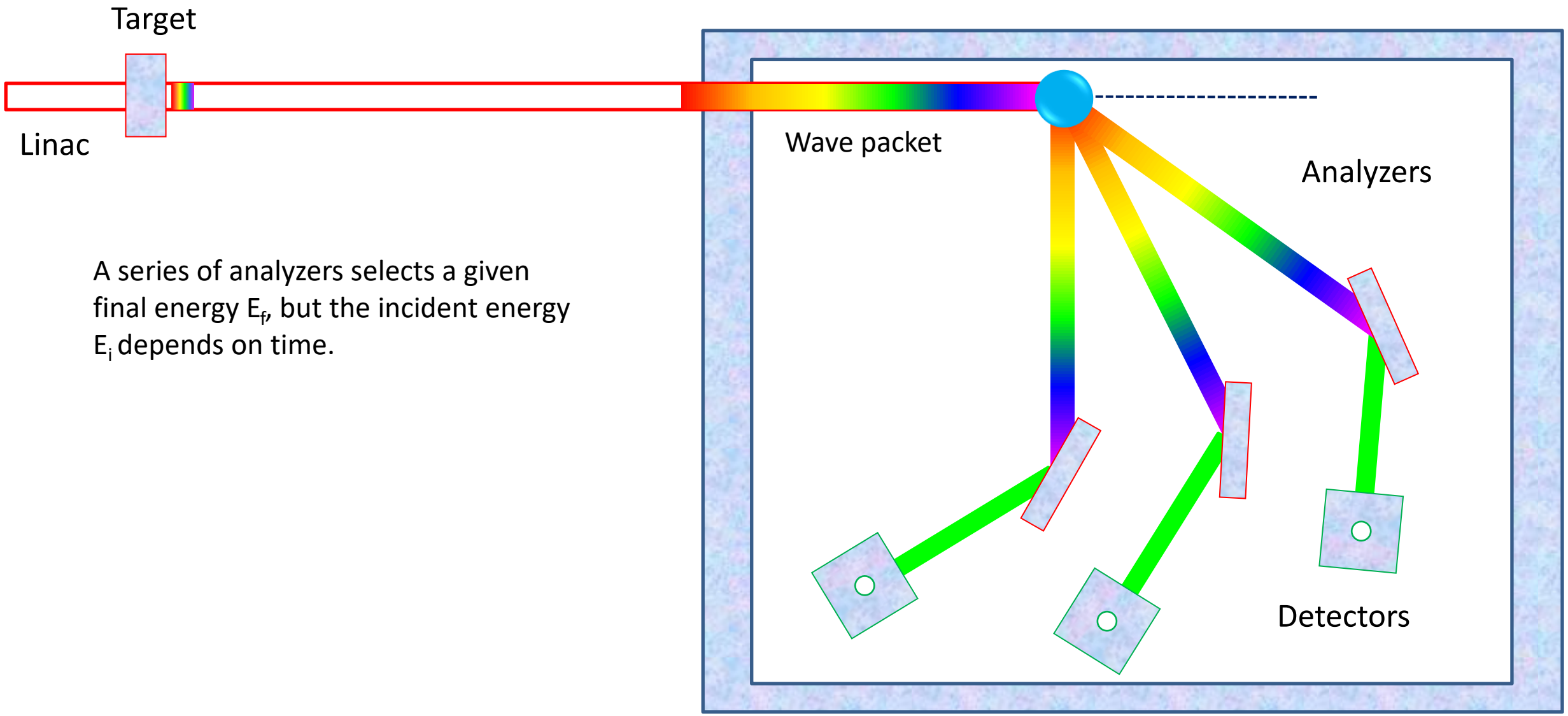
During the pulse, for a given 2θ, Q (and its coordinates) are changing continuously.

ISSUE = DATA REDUCTION

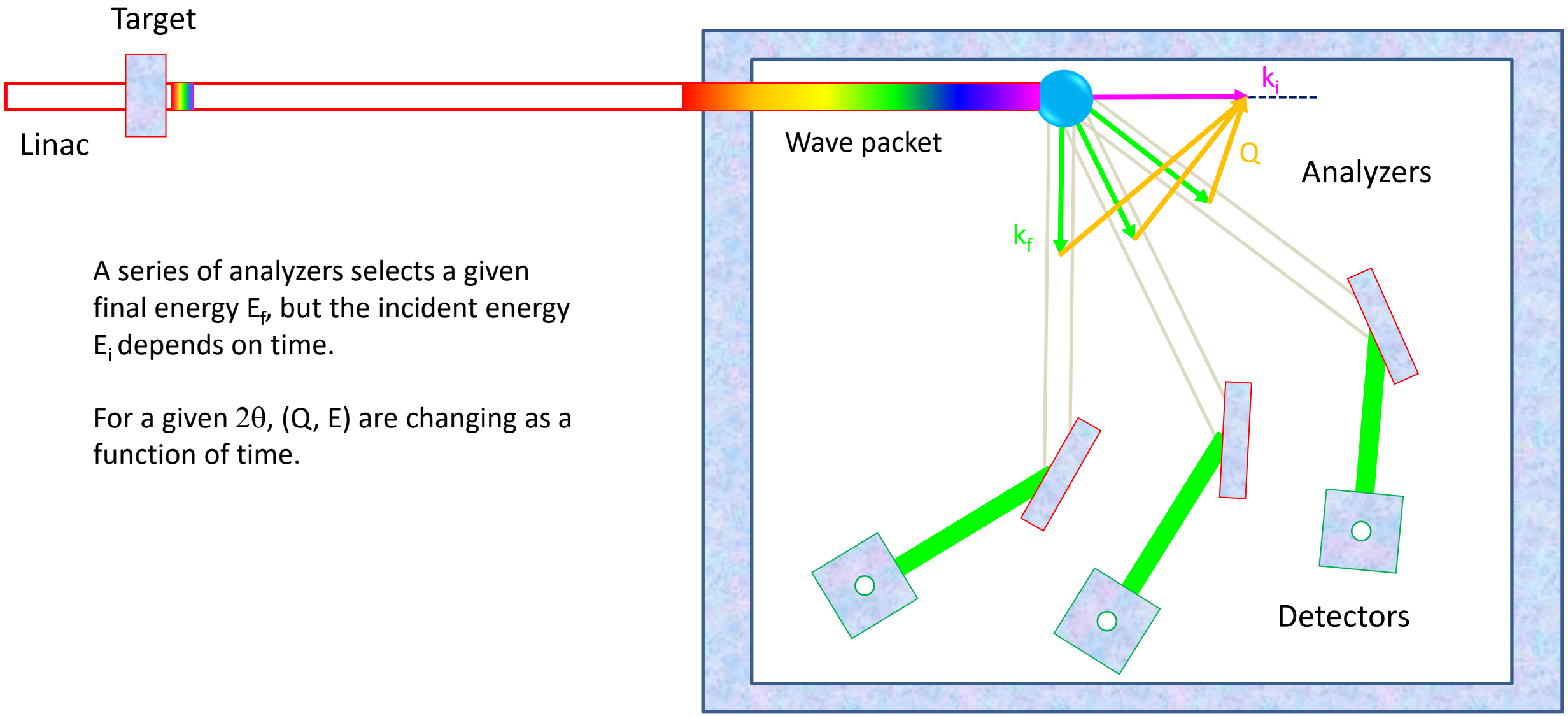


The wave packet is chopped with « sub pulses » at t_1, t_2, … hence different incident energies E_1, E_2 , …
(wave length λ_1, λ_2 …)

Similar to a standard TOF

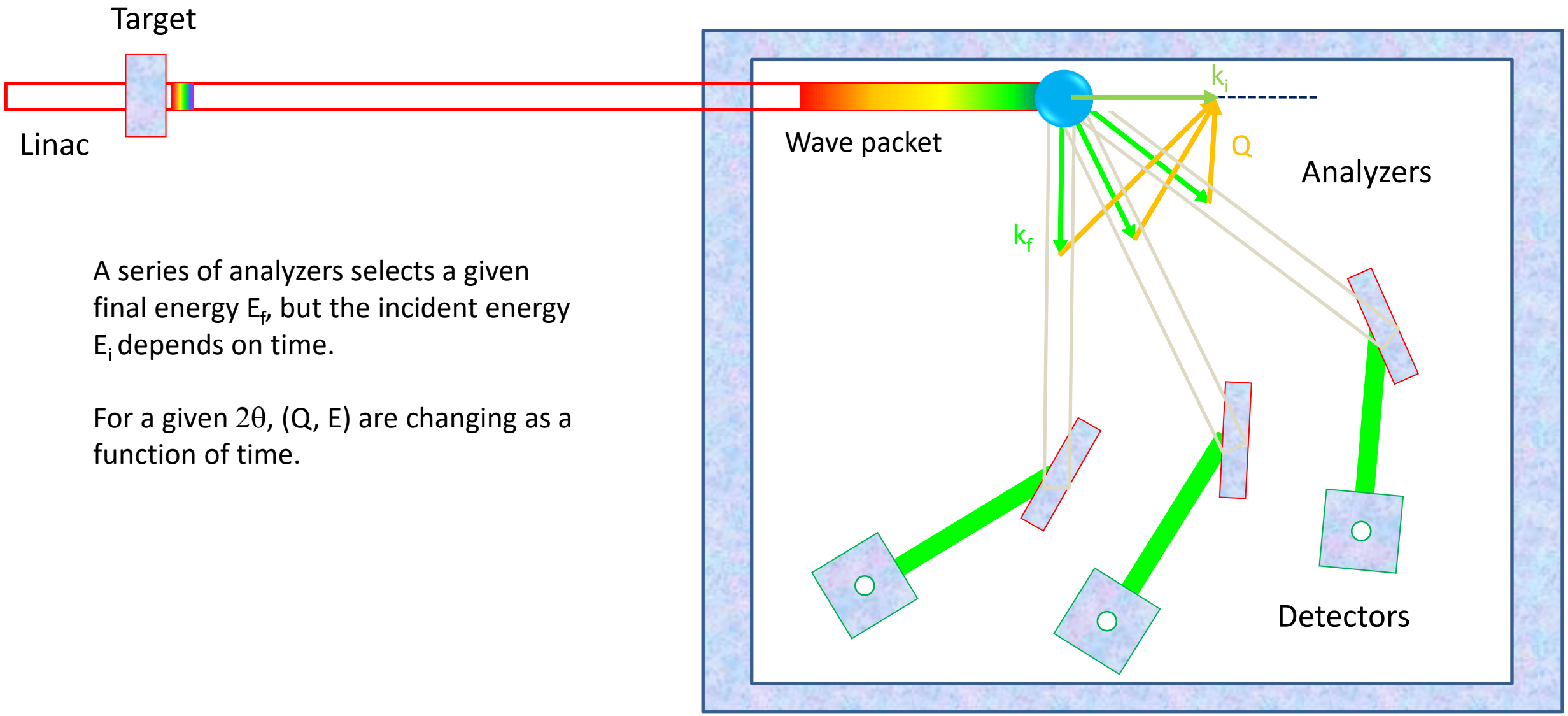


A series of analyzers selects a given final energy E_f, but the incident energy E_i depends on time.



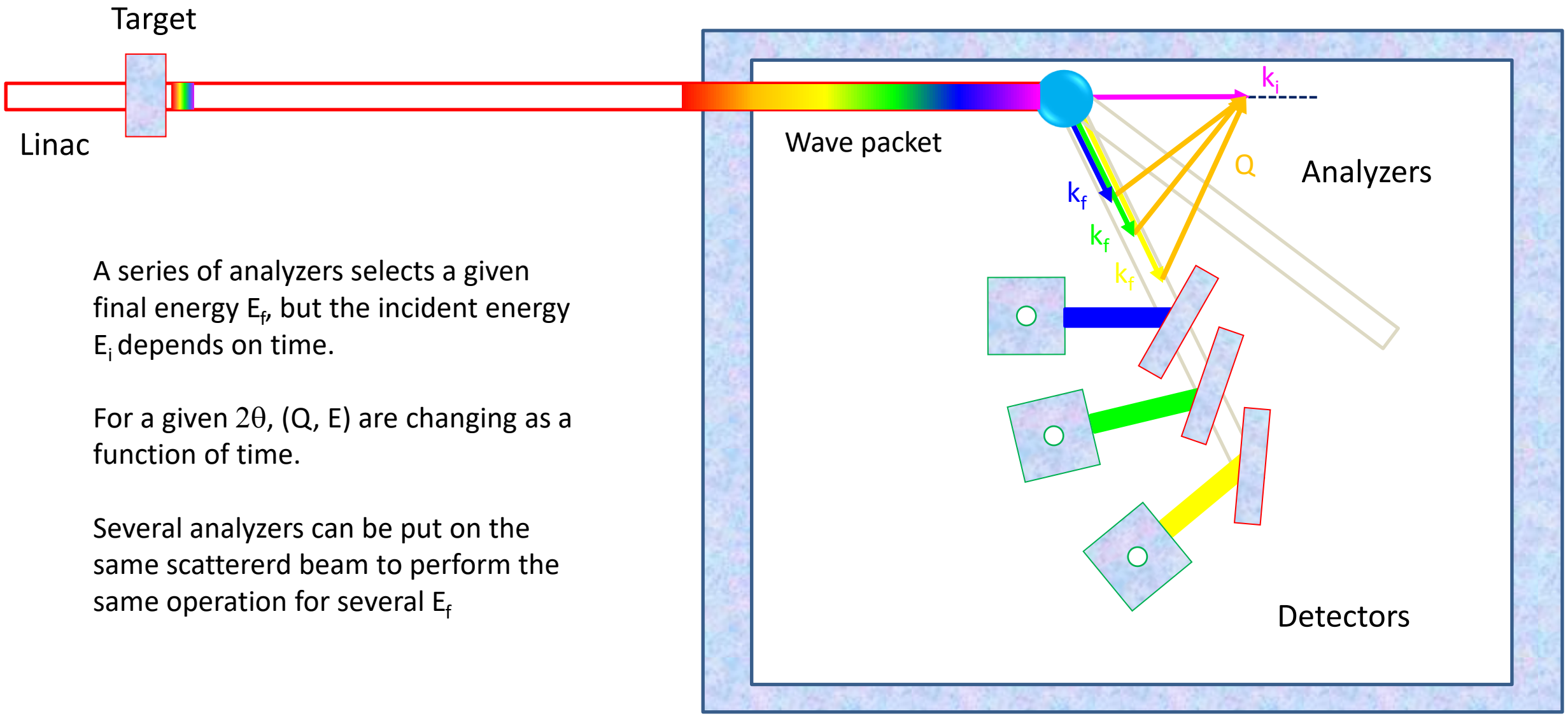
A series of analyzers selects a given final energy E_f, but the incident energy E_i depends on time.

For a given 2θ, (Q, E) are changing as a function of time.



A series of analyzers selects a given final energy E_f, but the incident energy E_i depends on time.

For a given 2θ, (Q, E) are changing as a function of time.



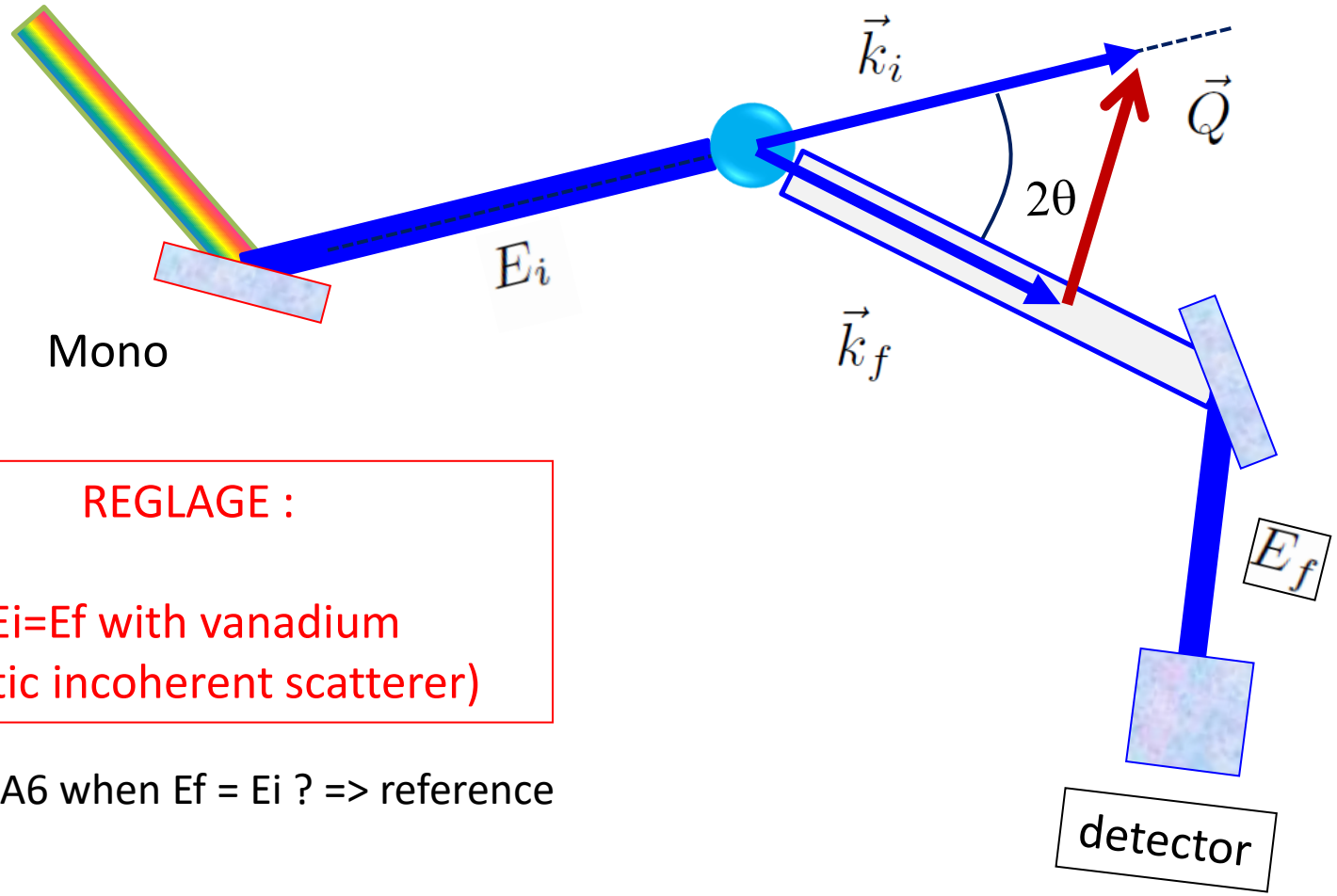
A series of analyzers selects a given final energy E_f, but the incident energy E_i depends on time.

For a given 2θ, (Q, E) are changing as a function of time.

Several analyzers can be put on the same scattererd beam to perform the same operation for several E_f

IN12

Reglage



REGLAGE :

Ei=Ef with vanadium
(elastic incoherent scatterer)

Ex : A5, A6 when Ef = Ei ? => reference

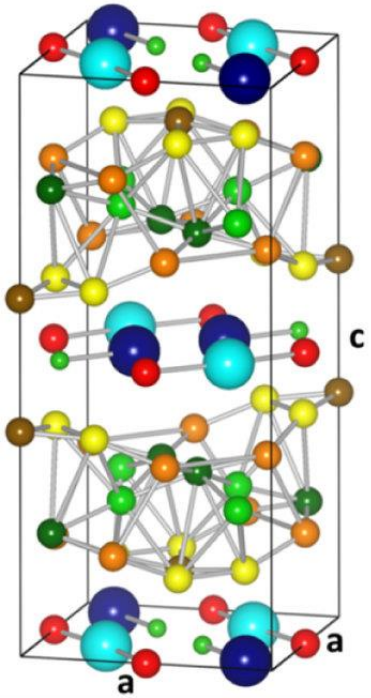
Sample II for tutorial : $Nd_2Fe_{14}B$

a = b = 8.8 Å
c = 12.2 Å

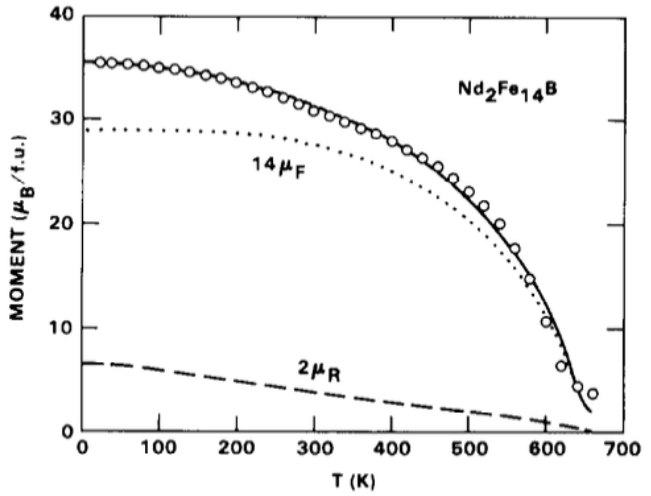
Space group : $P4_2/mnm$ Z=4

Magnetic ordering below $T_{Curie} \simeq 585$ K

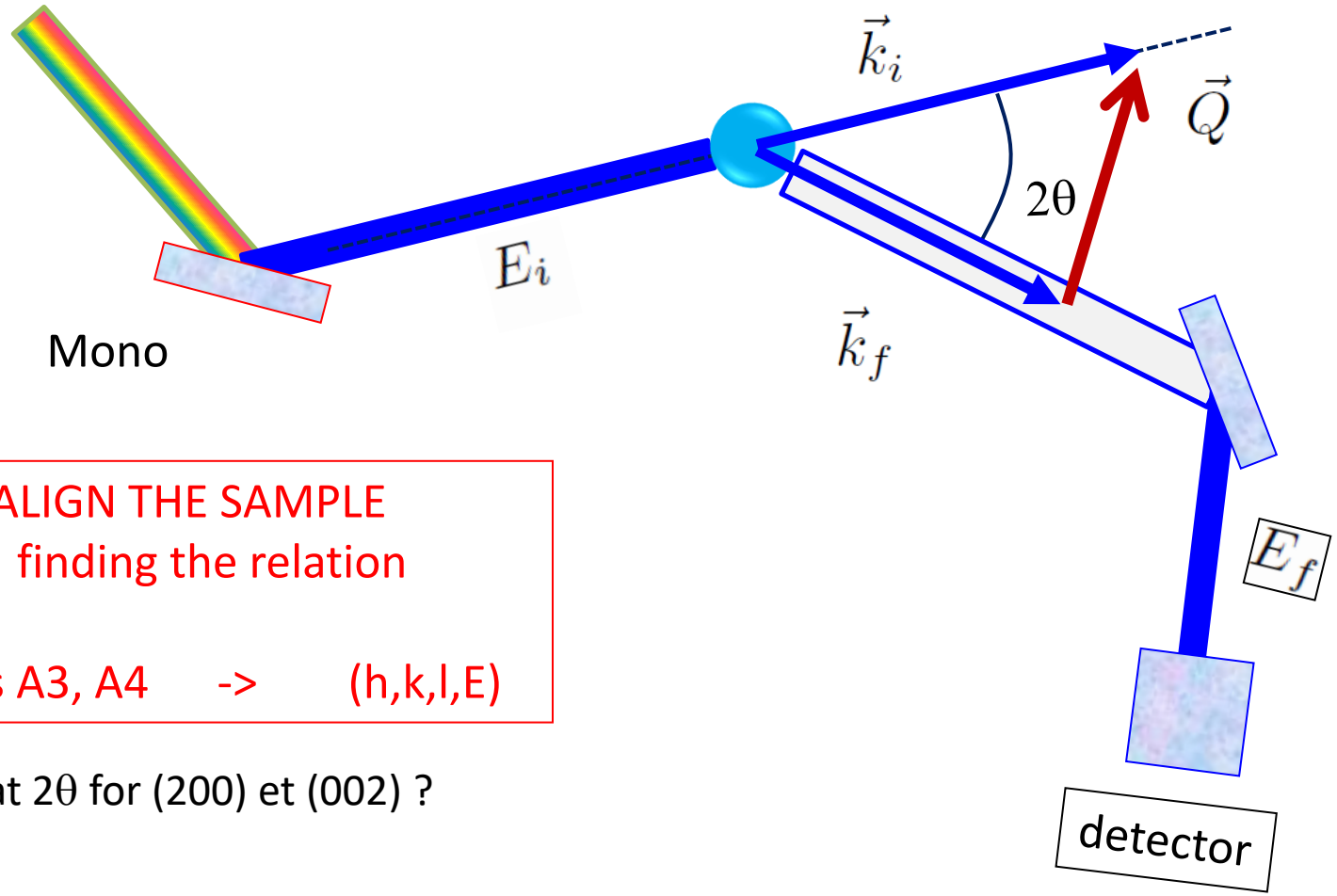
Ferromagnetic m//c down to 135 K



Atom	x	y	z
Nd(4f)	0.268	0.268	0.0
Nd(4g)	0.140	-0.140	0.0
Fe(16k$_1$)	0.223	0.567	0.127
Fe(16k$_2$)	0.037	0.360	0.176
Fe(8j$_1$)	0.098	0.098	0.204
Fe(8j$_2$)	0.317	0.317	0.246
Fe(4e)	0.5	0.5	0.114
Fe(4c)	0.0	0.5	0.0
B(4g)	0.371	-0.371	0.0



Tutorial

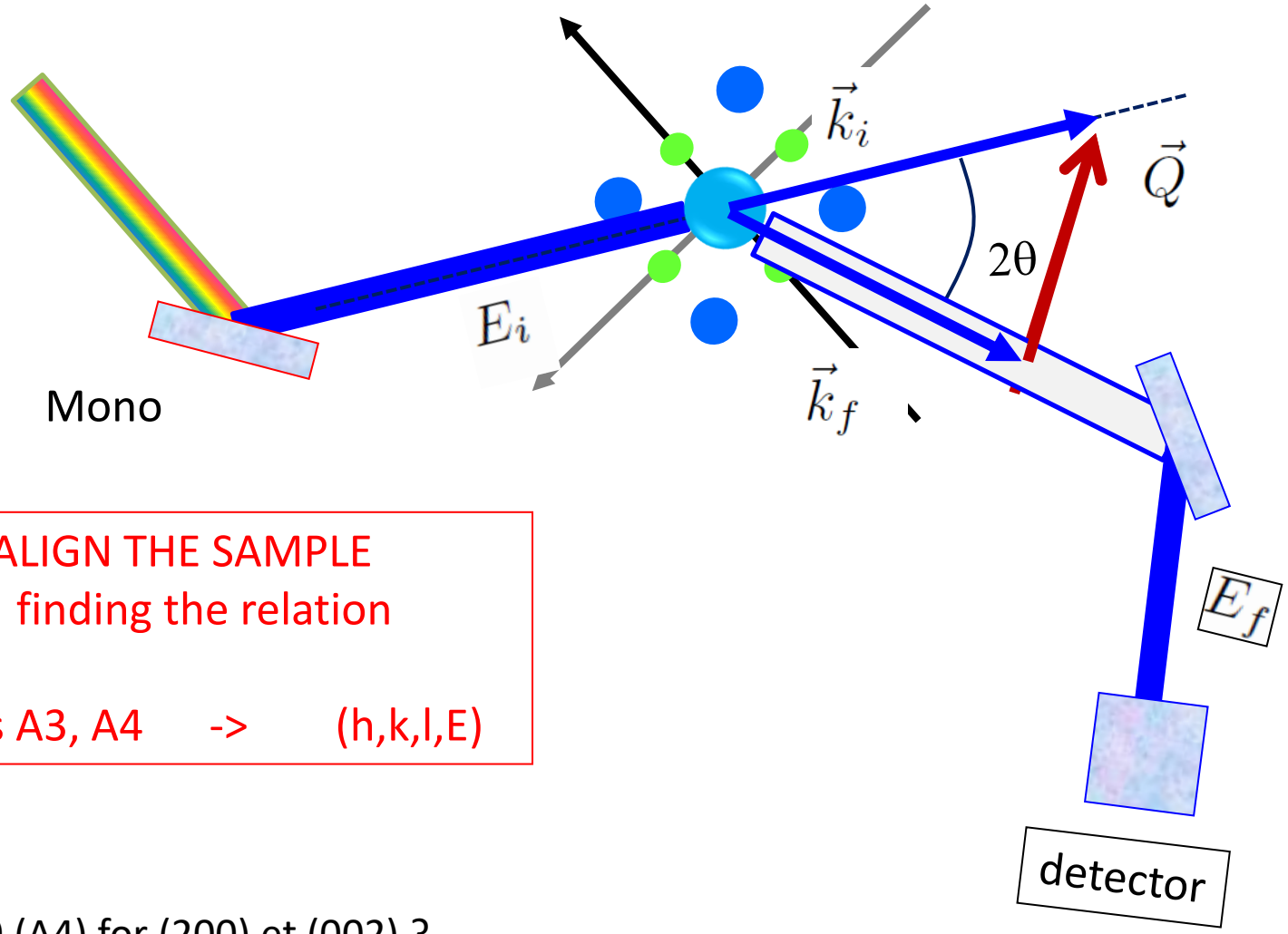


ALIGN THE SAMPLE
= finding the relation

angles A3, A4 -> (h,k,l,E)

Ex : what 2θ for (200) et (002) ?

Tutorial



ALIGN THE SAMPLE
= finding the relation

angles A3, A4 -> (h,k,l,E)

Ex :

what 2θ (A4) for (200) et (002) ?
What sample rotation (A3) ?

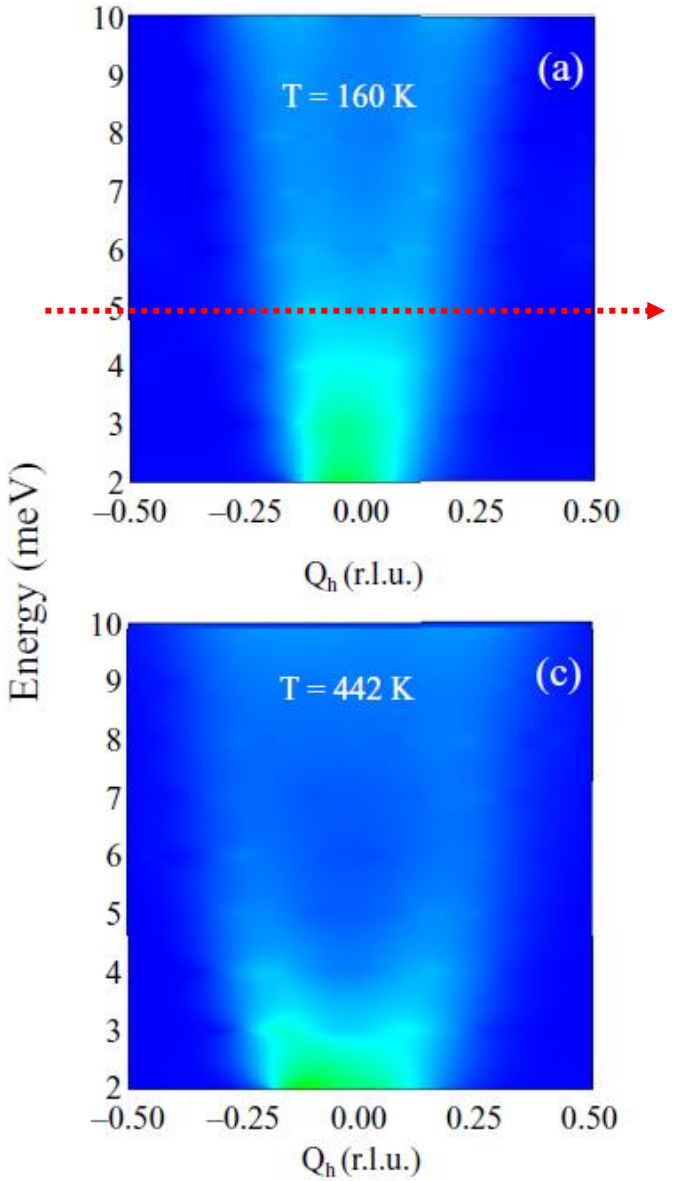
PHYSICAL REVIEW B **102**, 014443 (2020)

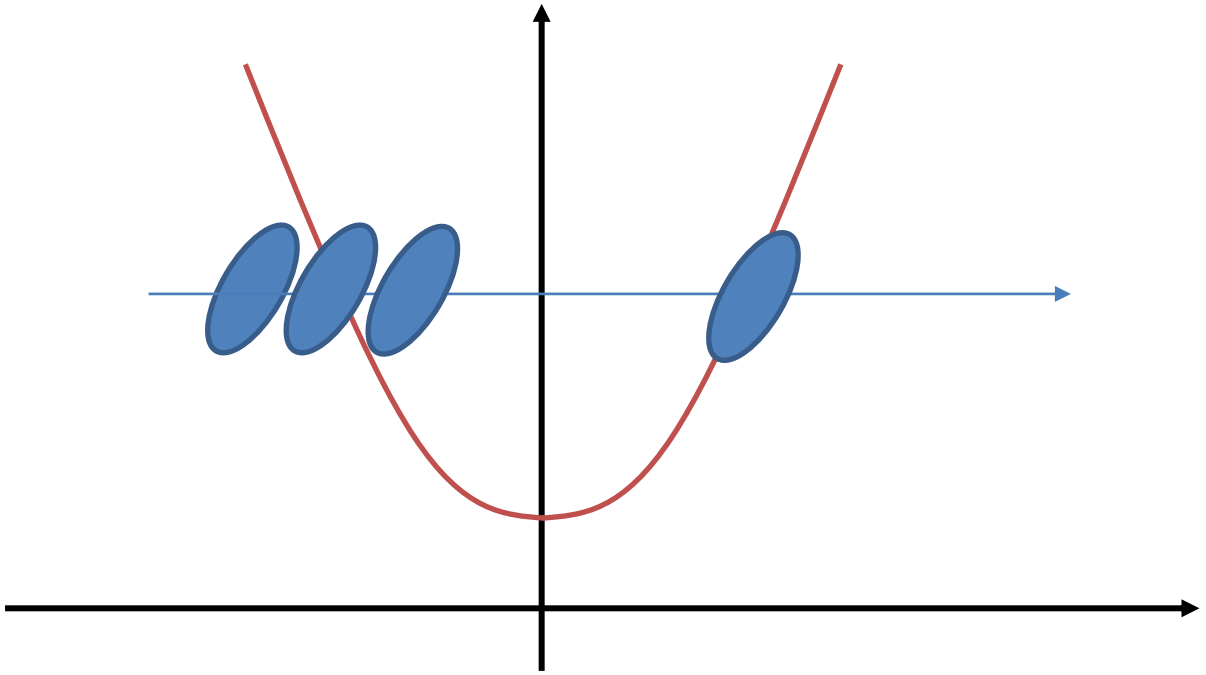
Anisotropy and temperature dependence of the spin-wave stiffness in $Nd_2Fe_{14}B$: An inelastic neutron scattering investigation

H. Naser,[1] C. Rado,[1] G. Lapertot,[2] and S. Raymond[3,*]
[1]*CEA, LITEN, Université Grenoble Alpes, 38000 Grenoble, France*
[2]*Université Grenoble Alpes, CEA, IRIG, PHELIQS, IMAPEC, 38000 Grenoble, France*
[3]*Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38000 Grenoble, France*

Determine
the spin wave dispersion relation
propagating along (q_h0 0)
and stemming from the zone
center (002).

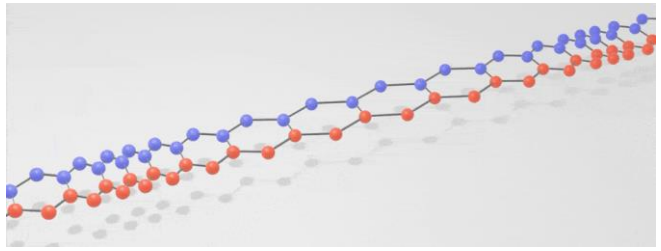
D q_h^2 law ?





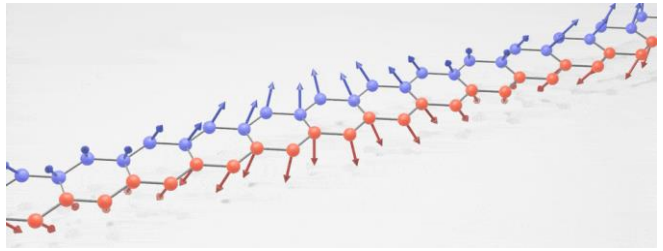
Elastic and Inelastic

Lattice dynamics



Atomic force constants

Spin dynamics



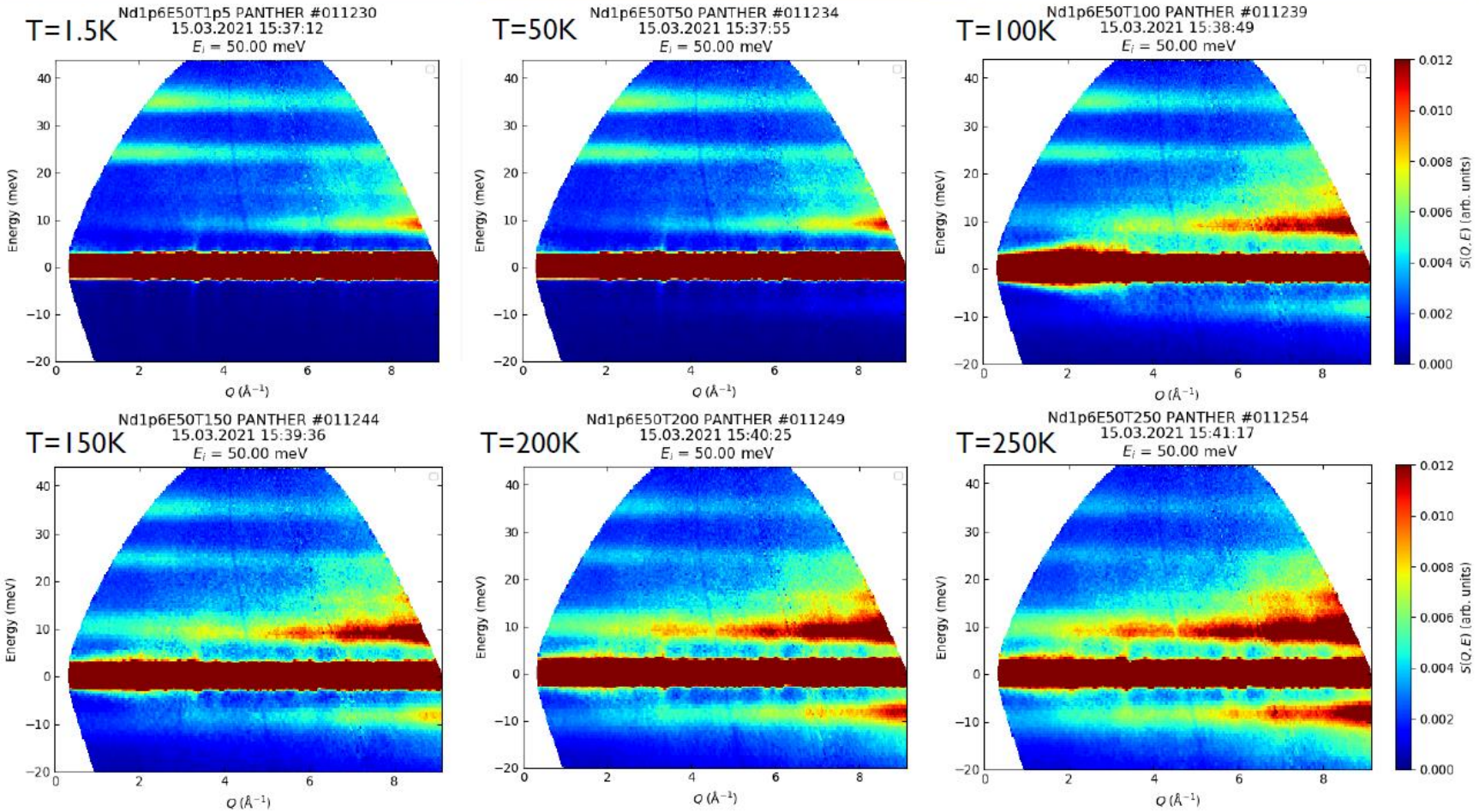
Magnetic exchange

THANK YOU FOR YOUR ATTENTION

8. More …

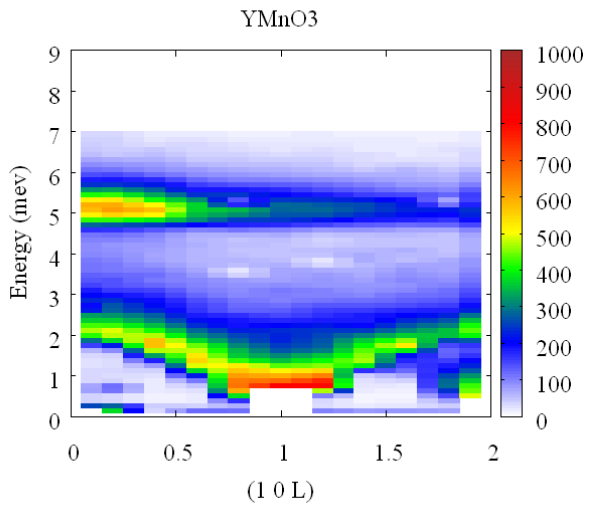
Crystal field

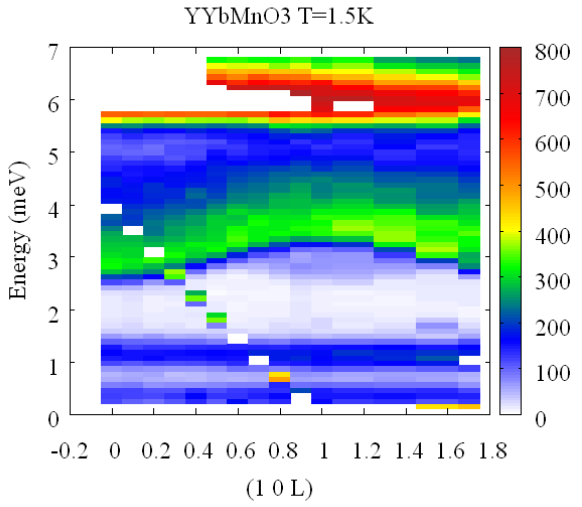
$ND_{1.6}LA_{0.4}ZR_2O_7$



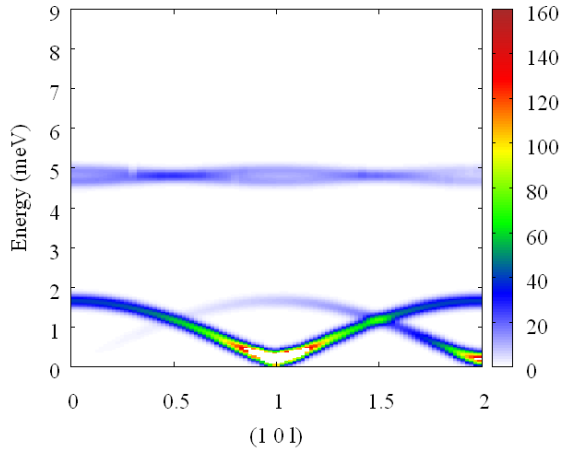
Triangular lattice

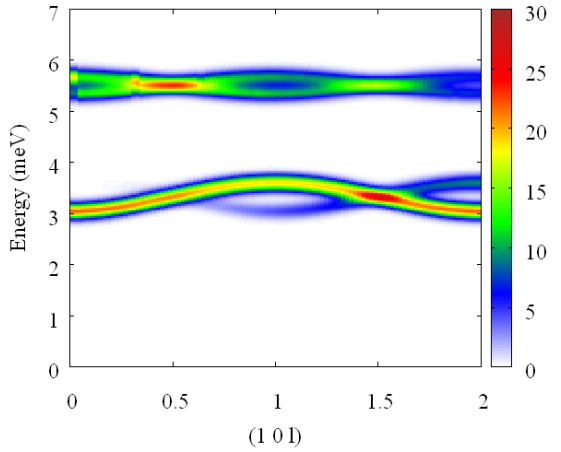
$YMnO_3$





$YbMnO_3$





Pyrochlore ferromagnet $Yb_2Ti_2O_7$

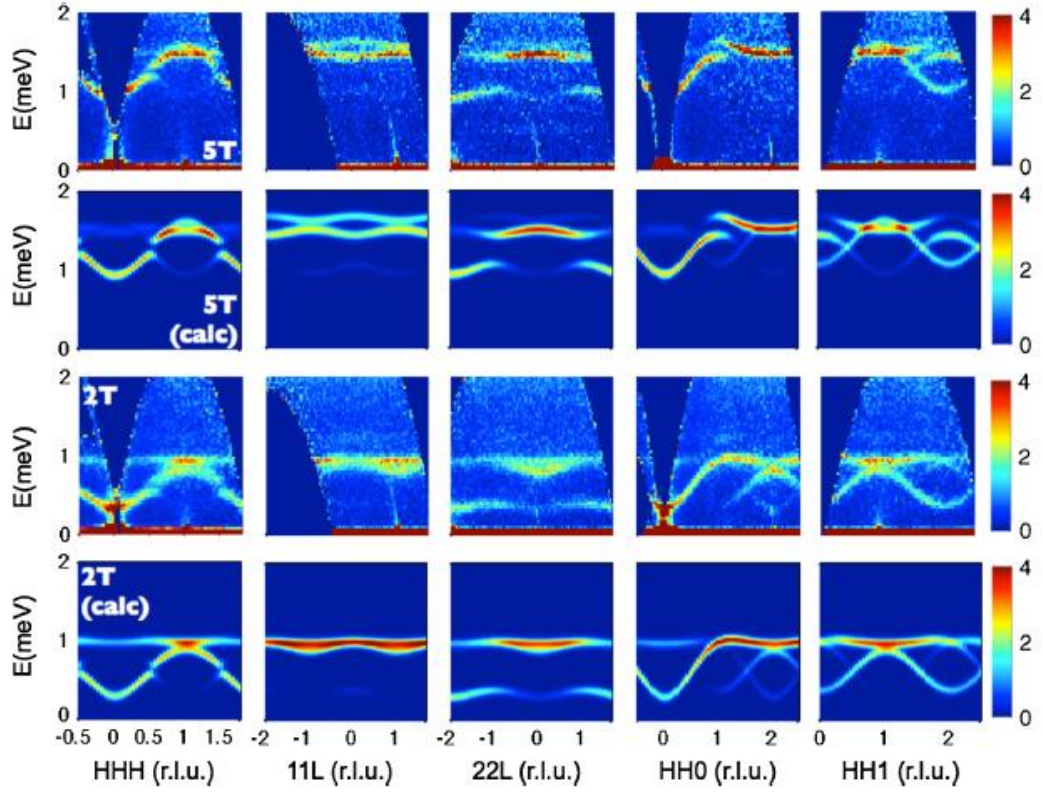


FIG. 1. The measured $S(\mathbf{Q}, \omega)$ at $T = 30$ mK, sliced along various directions in the HHL plane, for both $H = 5$ T (first row) and $H = 2$ T (third row). The second and fourth rows show the calculated spectrum for these two field strengths, based on an anisotropic exchange model with five free parameters (see text) that were extracted by fitting to the 5 T data set. For a realistic comparison to the data, the calculated $S(\mathbf{Q}, \omega)$ is convoluted with a Gaussian of full-width 0.09 meV. Both the 2 T and 5 T data sets, composed of spin wave dispersions along five different directions, are described extremely well by the same parameters. (Note that r.l.u. stands for reciprocal lattice units.)

Pyrochlore antiferromagnet $Er_2Ti_2O_7$

Order by Quantum Disorder in $Er_2Ti_2O_7$

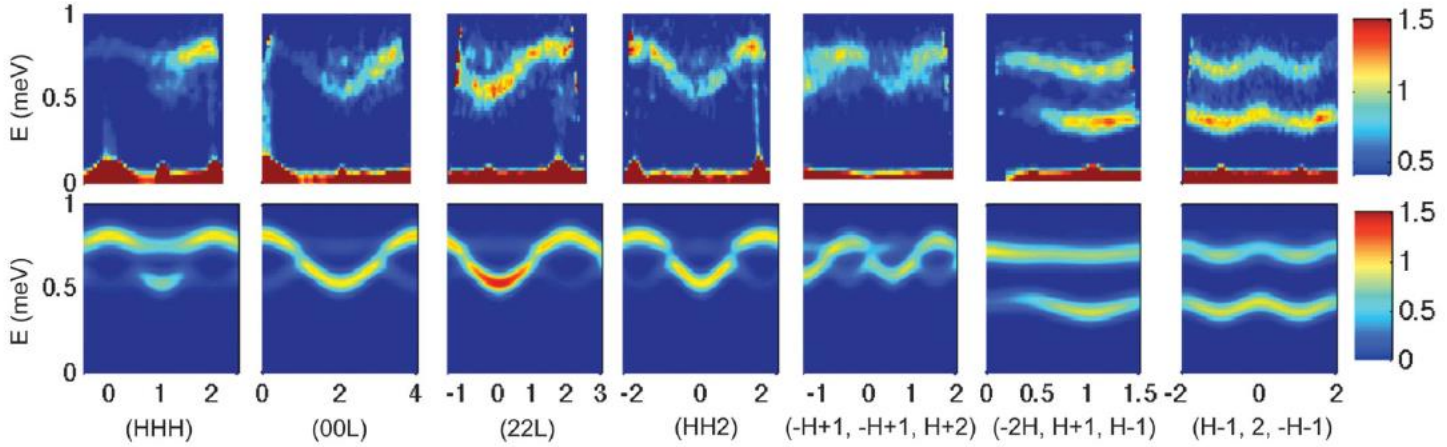
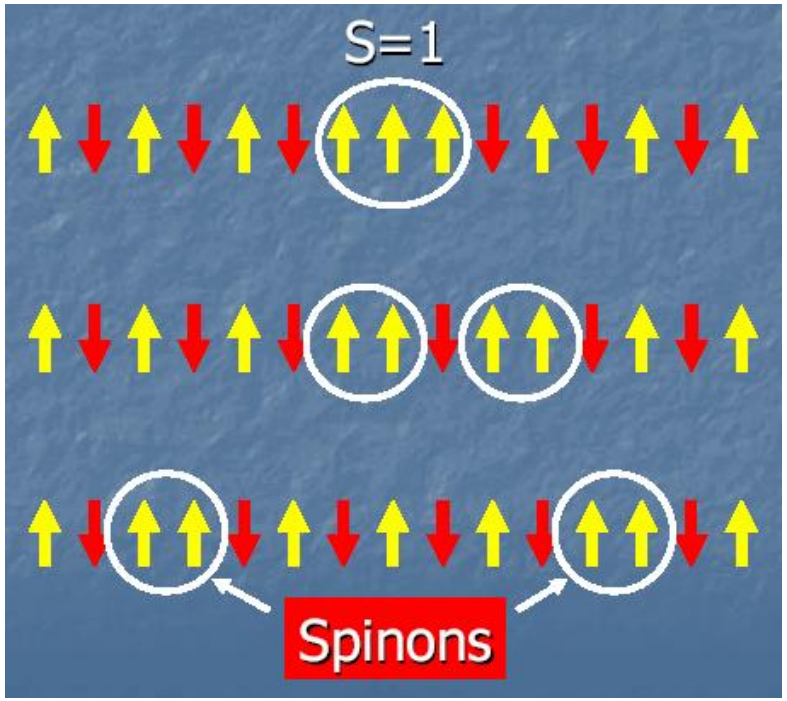


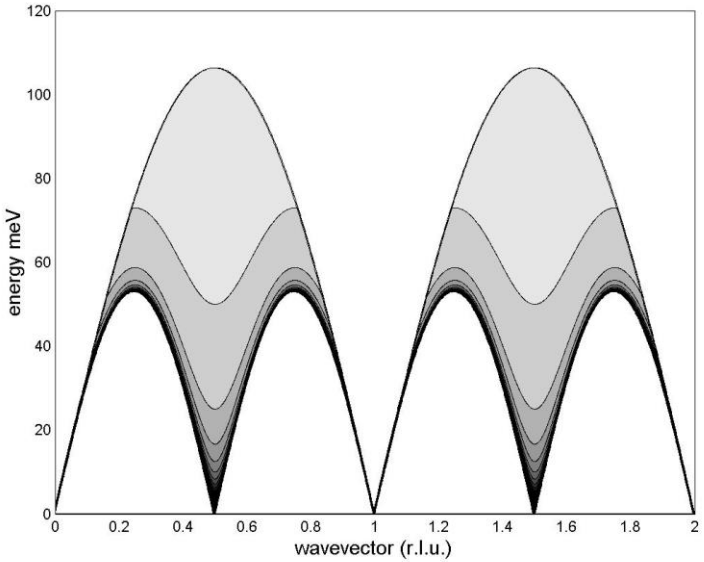
FIG. 1 (color). The measured $S(\mathbf{Q}, \omega)$ at $T = 30$ mK, $H = 3$ T sliced along several directions. The first five columns show $S(\mathbf{Q}, \omega)$ in the *HHL* plane, with the field applied along $[1\bar{1}0]$, while the last two columns show $S(\mathbf{Q}, \omega)$ for the field along [111]. Top row: measured $S(\mathbf{Q}, \omega)$. Bottom row: calculated $S(\mathbf{Q}, \omega)$, based on an anisotropic exchange model with six free parameters (see text) that were extracted by fitting to the measured dispersions.

Quantum magnets

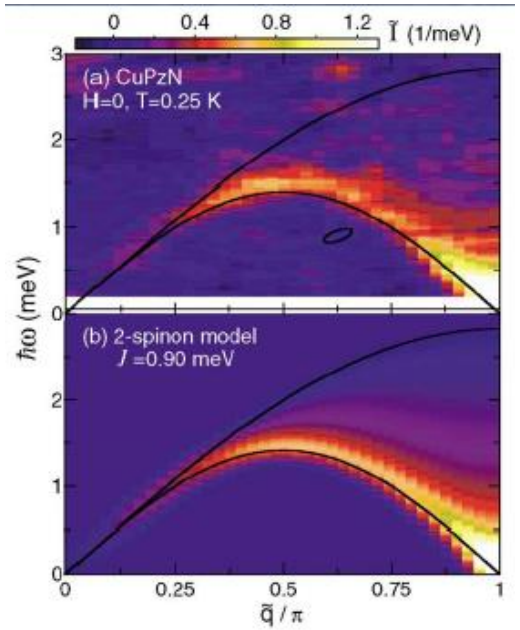
Spin waves fractionalize into spinons (also called deconfined excitations)



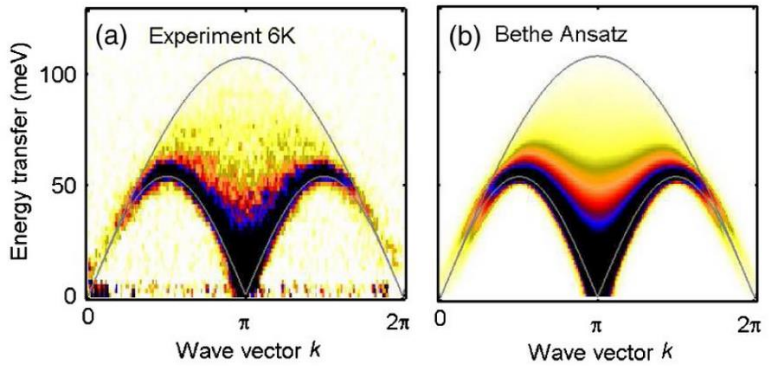
Cartoon by F. Mila



Quantum magnets



CuPzN, Stone et al, PRL 2003



$KCuF_3$, Lake et al, Nature Materials 2005

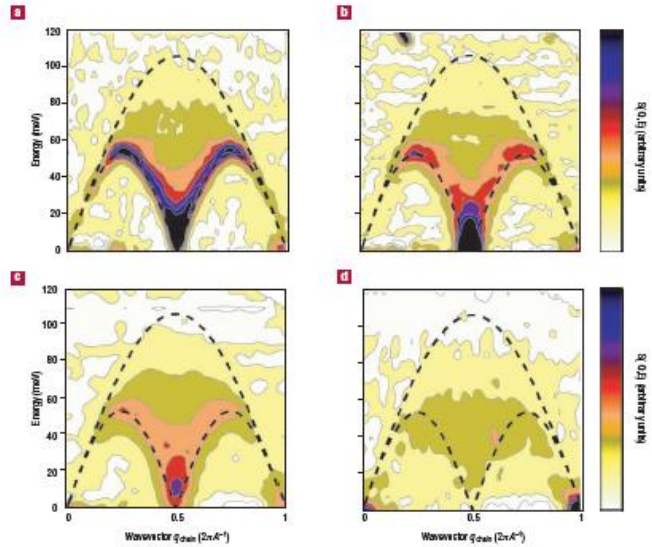
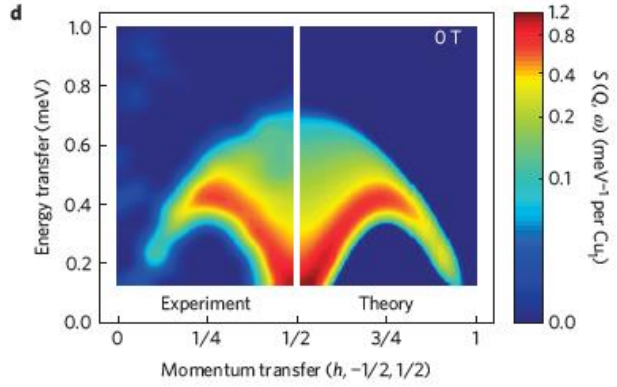


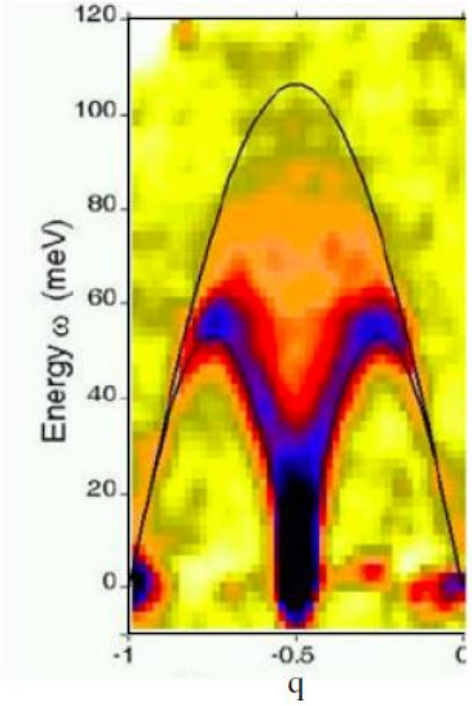
Figure 1 Inelastic neutron scattering data for $KCuF_3$. The data is plotted as a function of E and q parallel to the chains for the temperatures a, $T = 6$ K, b, $T = 50$ K, c, $T = 150$ K and d, $T = 300$ K. The colours indicate the size of the neutron scattering cross-section $S(q,E)$ and the superimposed black dashed lines indicate the region where the multi-spinon continuum is predicted at $T = 0$ K by the Muller Ansatz equation (1). The data was collected using the MAPS time-of-flight spectrometer at ISIS, Rutherford Appleton Laboratory, UK.

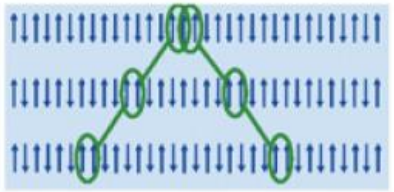


$CuSO_4$ $5D_2O$ Mourigal et al, Nature Physics 2013

Quantum magnets

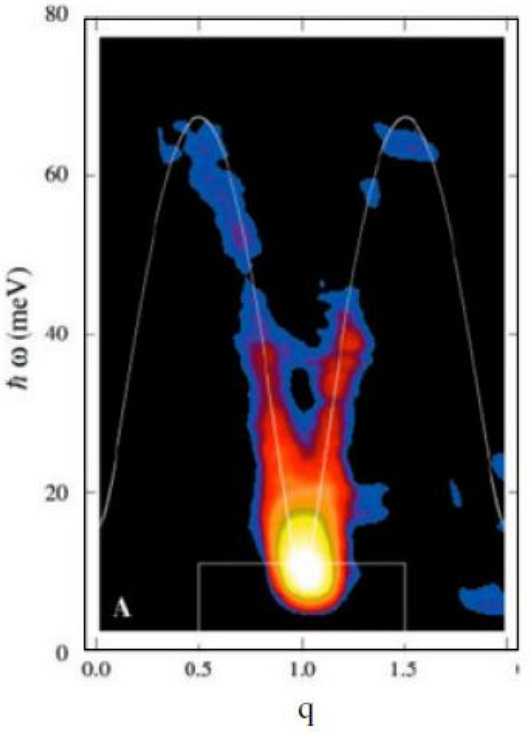
S= ½ $KCuF_3$

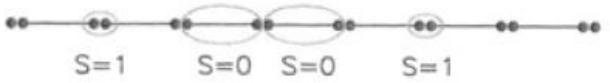




Spin correlations decay as power law
Spin ½ particles : continuum
gapless

S= 1 Y_2BaNiO_5





Spin correlations decay exponentially
Spin 1 excitation : well defined mode
(Haldane) Gapped spectrum

The susceptibility (hence the correlations) are sensitive to nesting properties of the Fermi surface

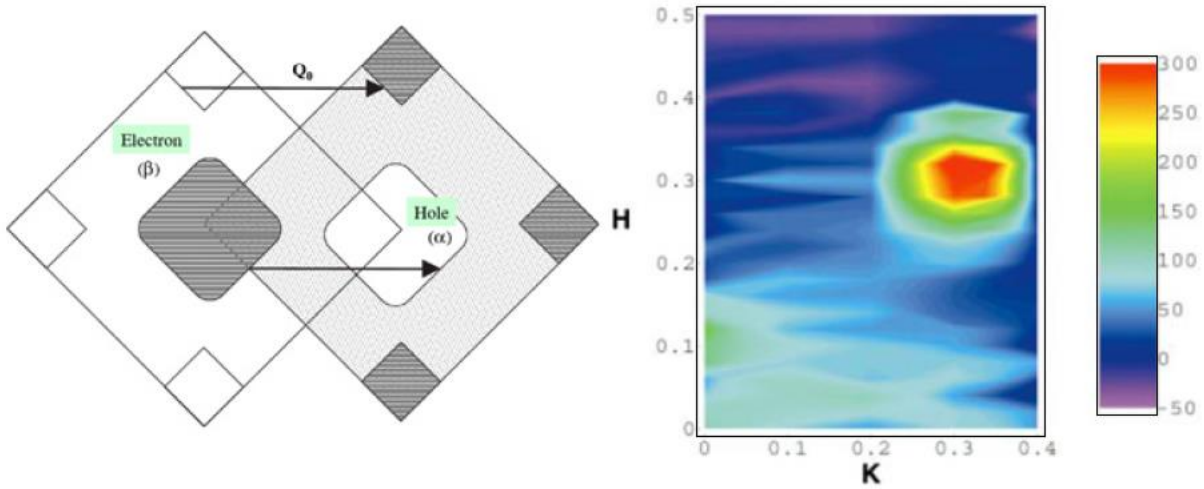
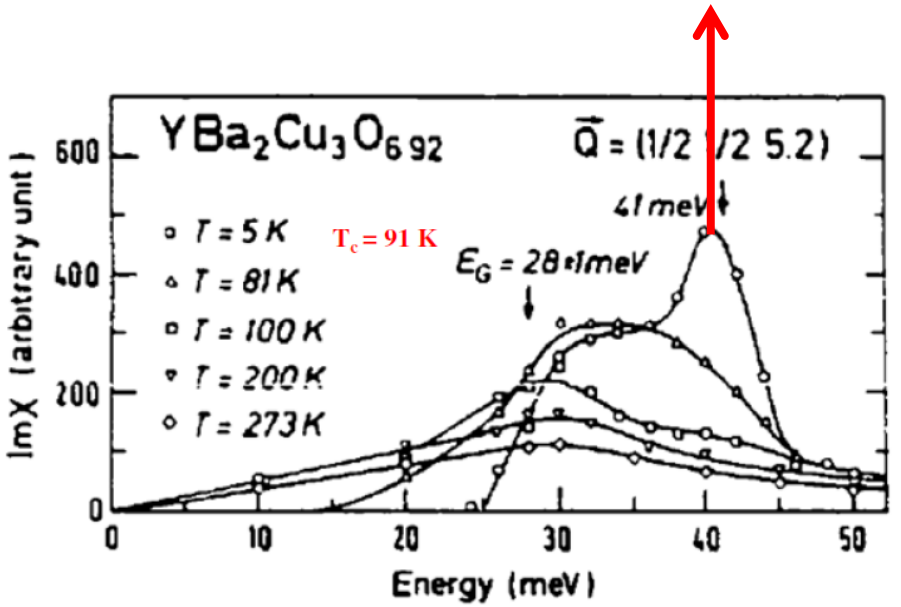


Figure 10. Left: sketch of the nesting feature between α and β bands of Sr_2RuO_4. Right: (H, K) map of the magnetic excitations in Sr_2RuO_4 at 10 K for an energy transfer of 4.1 meV [21].

Interactions may create a bound state (spin exciton)
Resonance peak in High Tc superconductors and heavy fermions ?

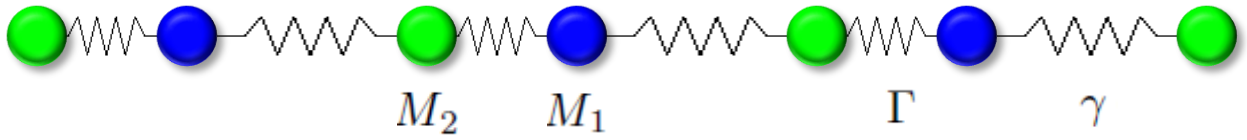
$$\chi_0(\mathbf{q},\omega) = -2\mu_B^2 \sum_{\mathbf{k}} \frac{f_{\mathbf{k}+\mathbf{q},\sigma'} - f_{\mathbf{k},\sigma}}{\epsilon_{\mathbf{k}+\mathbf{q},\sigma'} - \epsilon_{\mathbf{k},\sigma} - \hbar\omega + i\epsilon}$$

$$\chi_0(\mathbf{q},\omega) = -2\mu_B^2 \sum_{\mathbf{k}} \left(1 - \frac{\Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{k}+\mathbf{q}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}}\right) \frac{f_{\mathbf{k}+\mathbf{q},\sigma'} + f_{\mathbf{k},\sigma} - 1}{E_{\mathbf{k}+\mathbf{q},\sigma'} - E_{\mathbf{k},\sigma} - \hbar\omega + i\epsilon}\,.$$



Example 2 : Phonons

Di-atomic chain



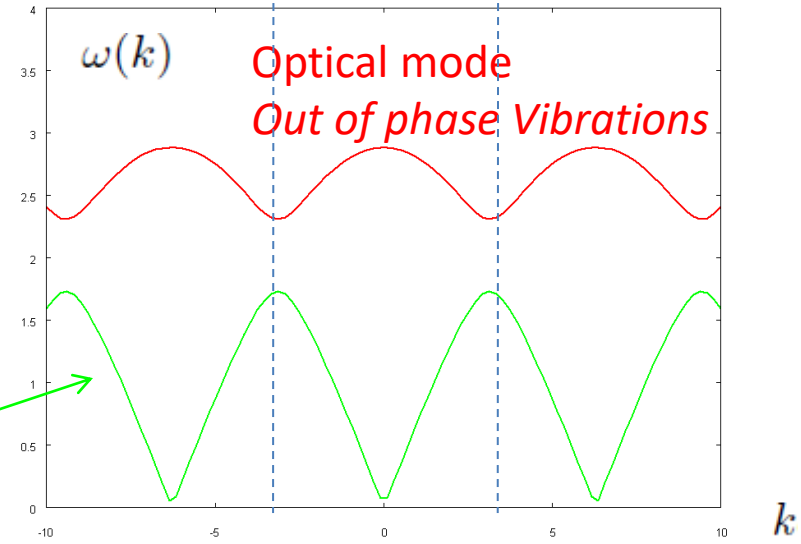
$$M_1 \frac{d^2}{dt^2} u_{m,1} = \Gamma\ (u_{m,2} - u_{m,1}) + \gamma\,(u_{m-1,2} - u_{m,1})$$

$$M_2 \frac{d^2}{dt^2} u_{m,2} = \Gamma\ (u_{m,1} - u_{m,2}) + \gamma\,(u_{m+1,1} - u_{m,2})$$

Force constants between atoms

Fourier transform: for each k, eigenvalue problem

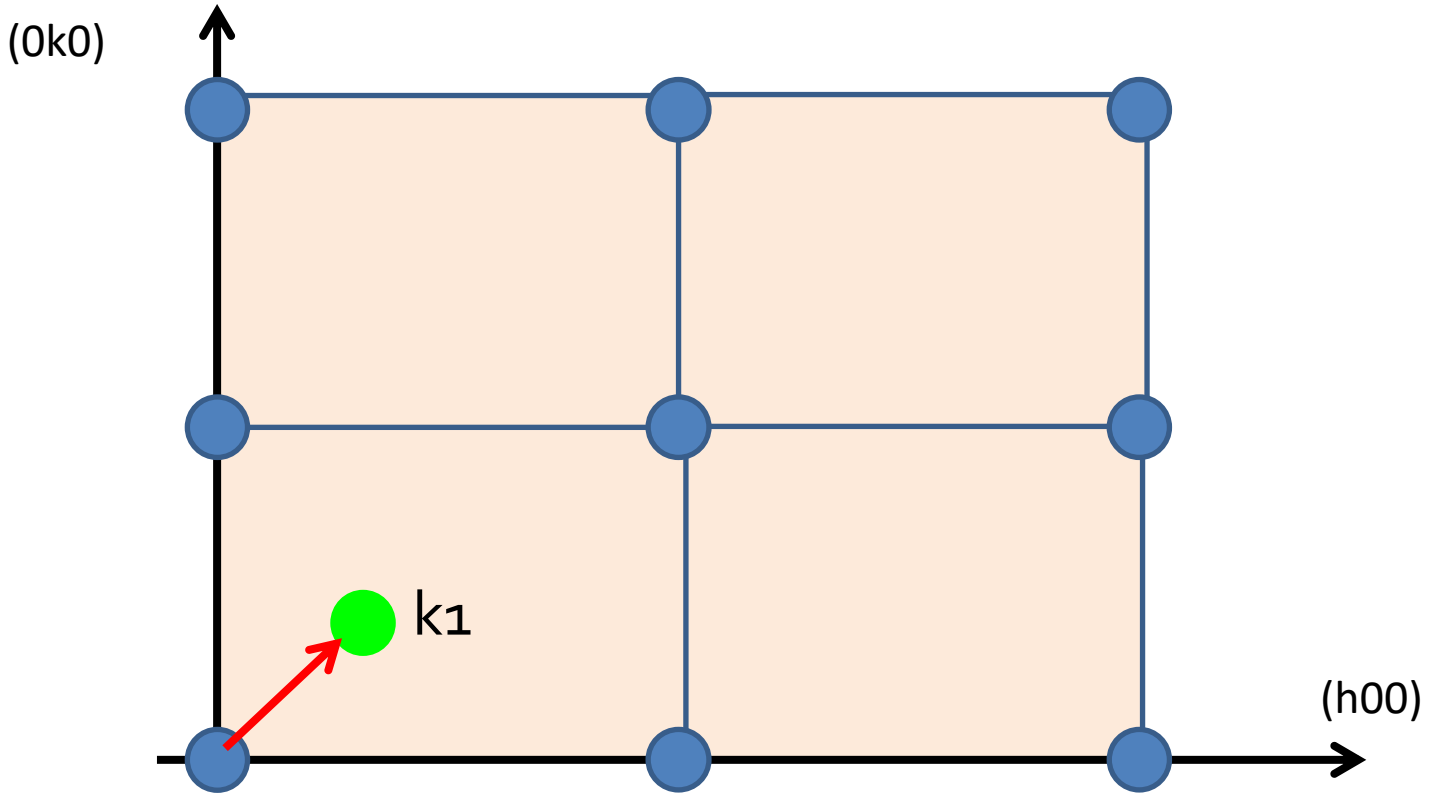
$$\begin{pmatrix} \omega^2 - \frac{\Gamma+\gamma}{M_1} & \frac{\Gamma+\gamma e^{-ika}}{\sqrt{M_1 M_2}} \\ \frac{\Gamma+\gamma e^{ika}}{\sqrt{M_1 M_2}} & \omega^2 - \frac{\Gamma+\gamma}{M_2} \end{pmatrix} \begin{pmatrix} \sqrt{M_1}u_1 \\ \sqrt{M_2}u_2 \end{pmatrix} = 0$$



Example 2 : Phonons

In real material :

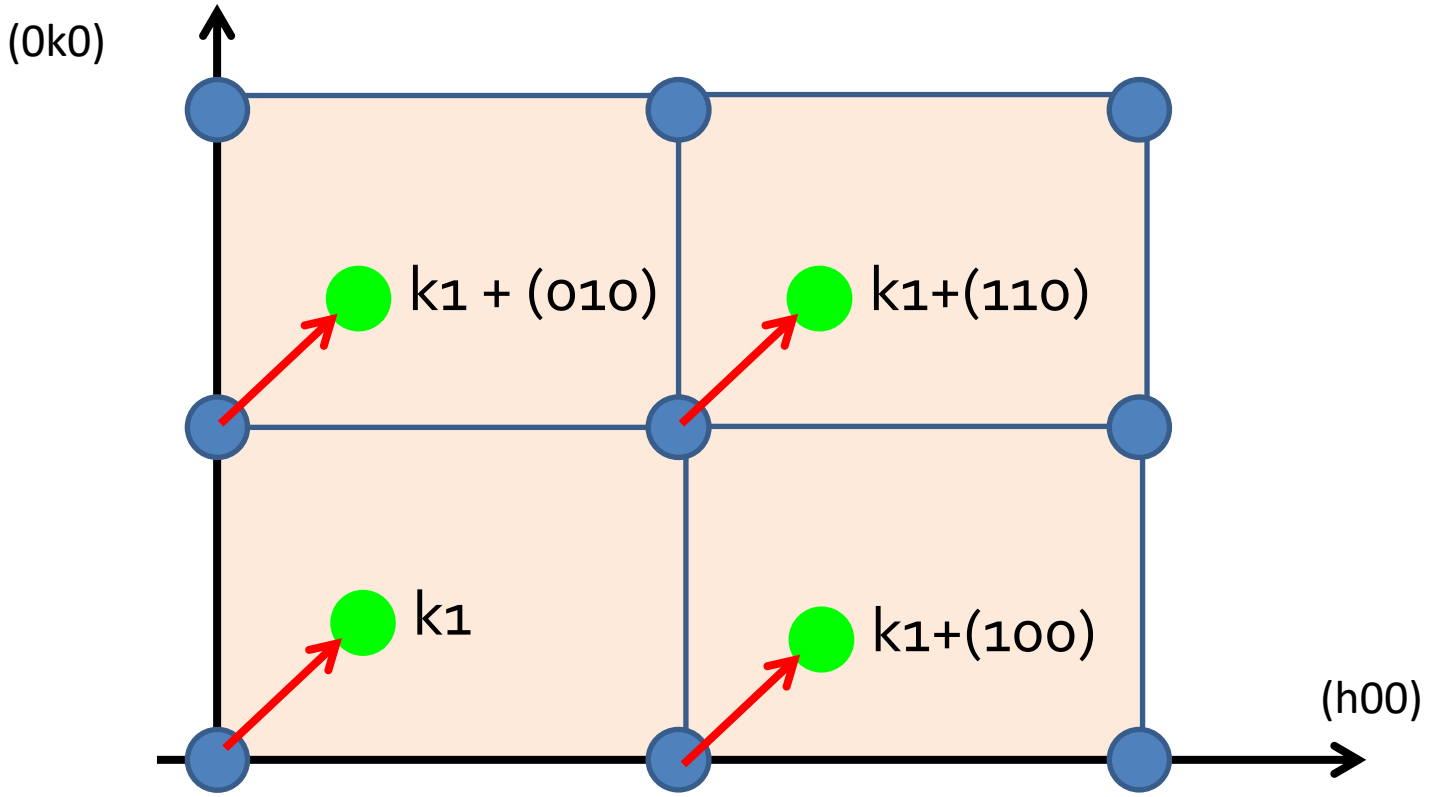
- 3N branches (3 acoustic)
- periodic dispersion (Brillouin zone, lattice invariance)



Example 2 : Phonons

In real material :

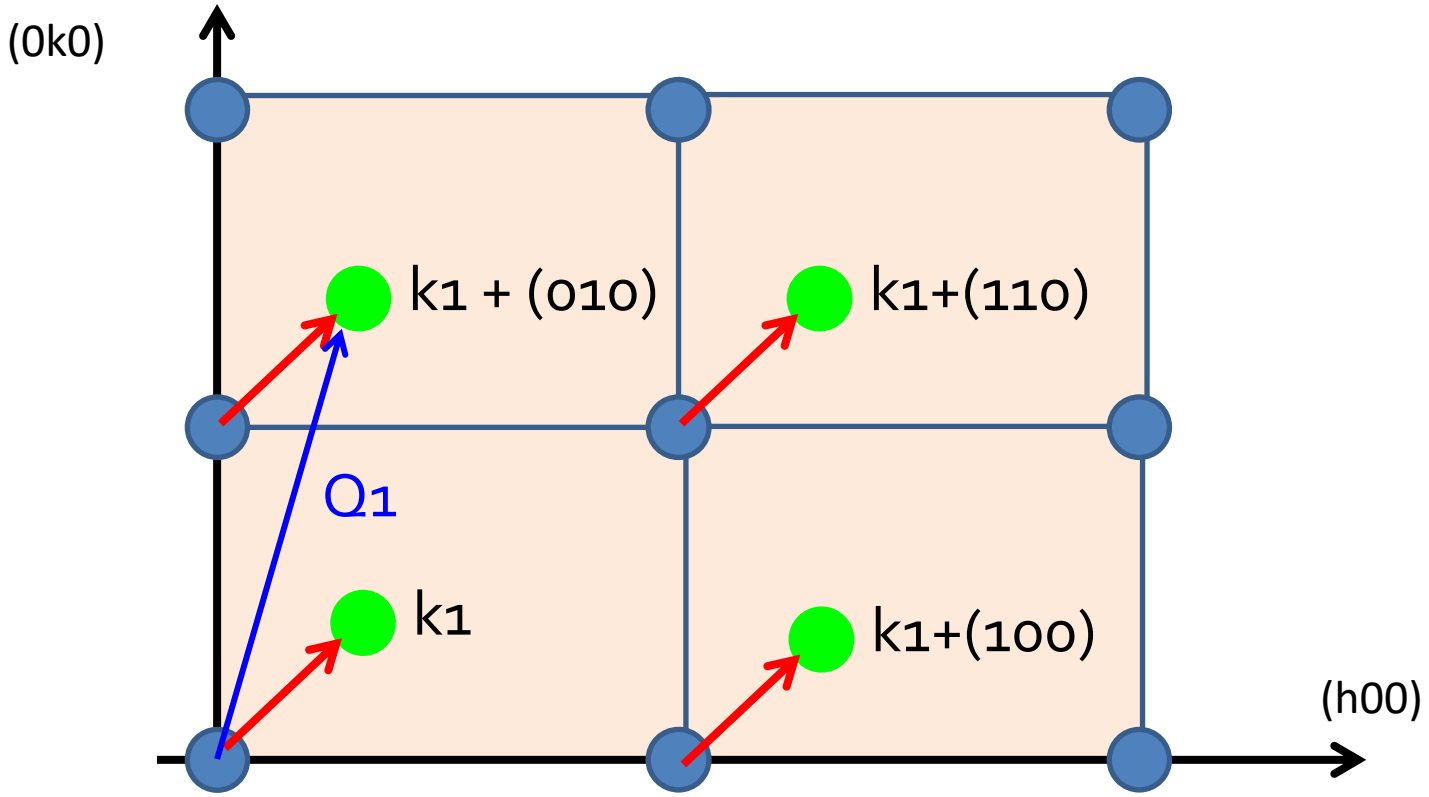
- 3N branches (3 acoustic)
- periodic dispersion (Brillouin zone, lattice invariance)



Example 2 : Phonons

In real material :

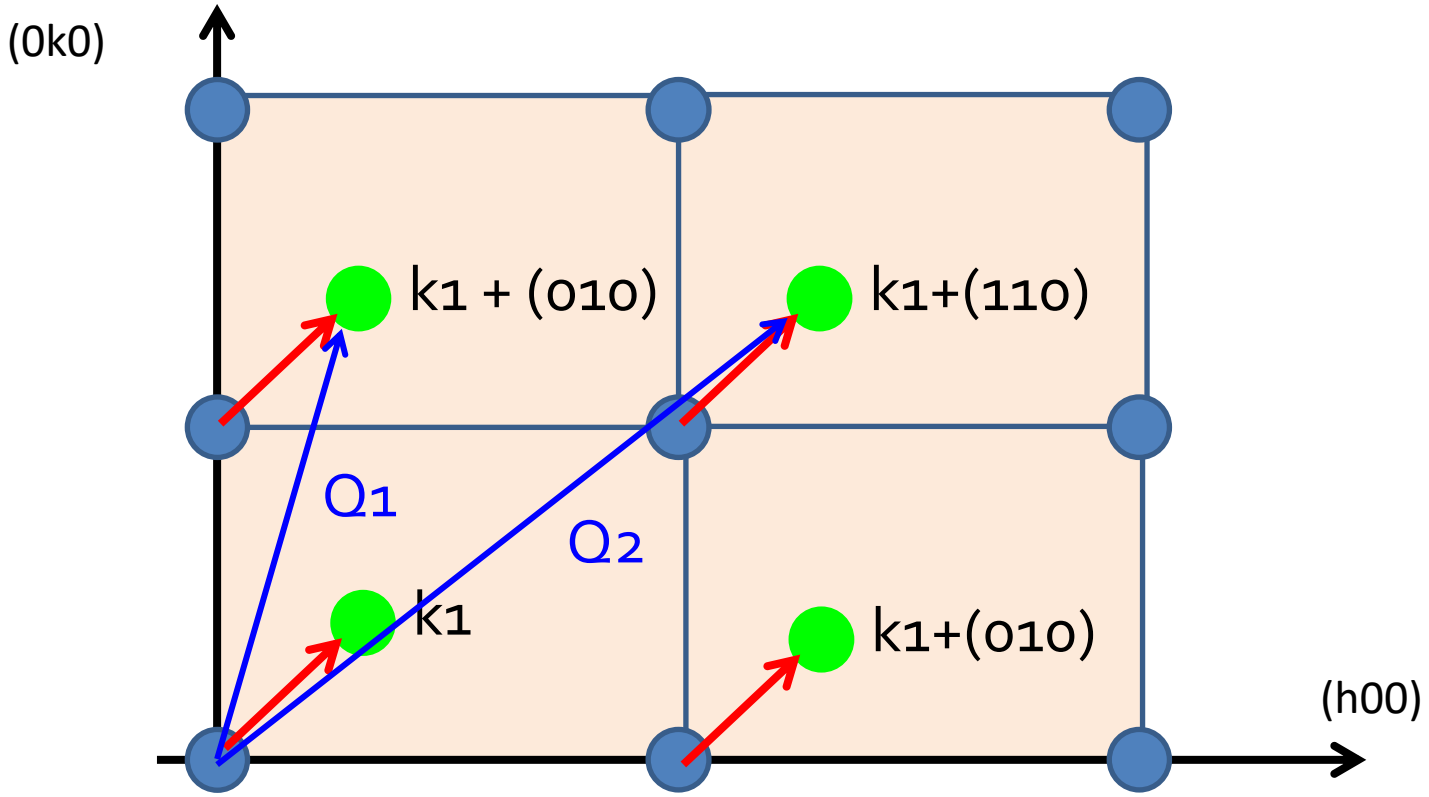
- 3N branches (3 acoustic)
- periodic dispersion (Brillouin zone, lattice invariance)



Example 2 : Phonons

In real material :

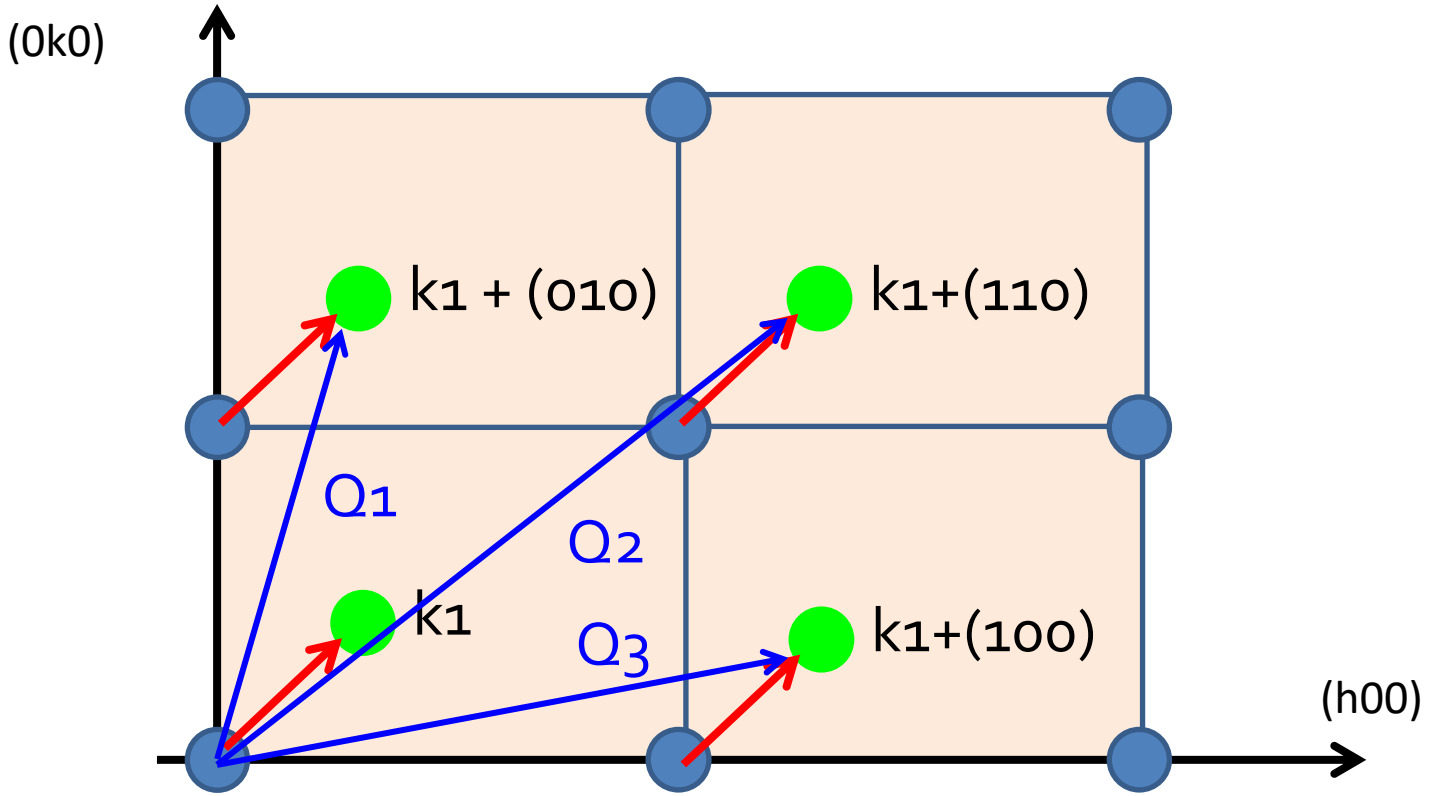
- 3N branches (3 acoustic)
- periodic dispersion (Brillouin zone, lattice invariance)



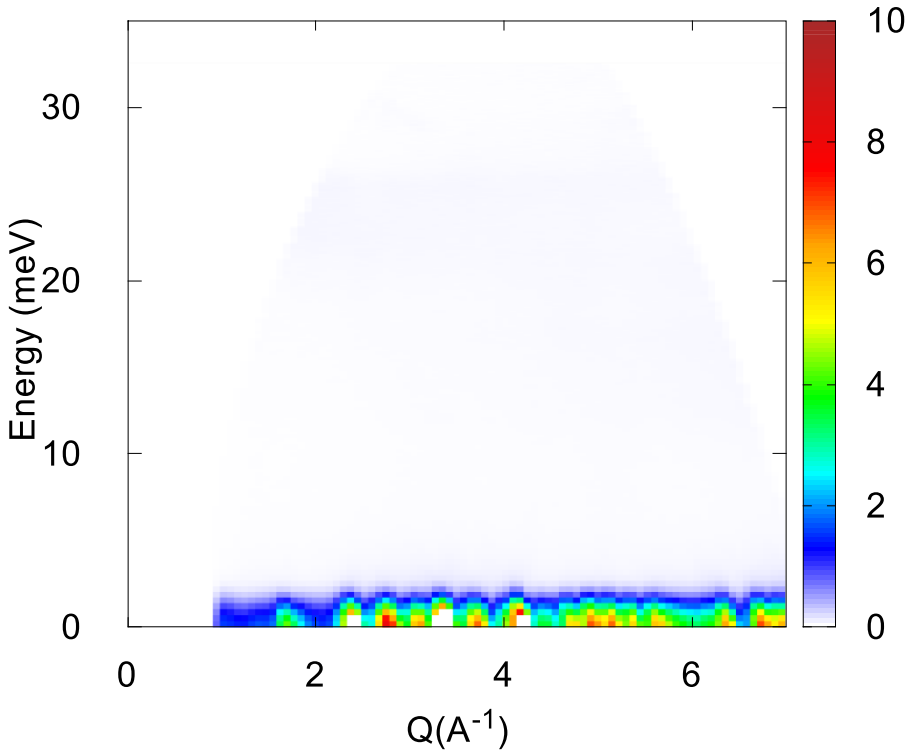
Example 2 : Phonons

In real material :

- 3N branches (3 acoustic)
- periodic dispersion (Brillouin zone, lattice invariance)

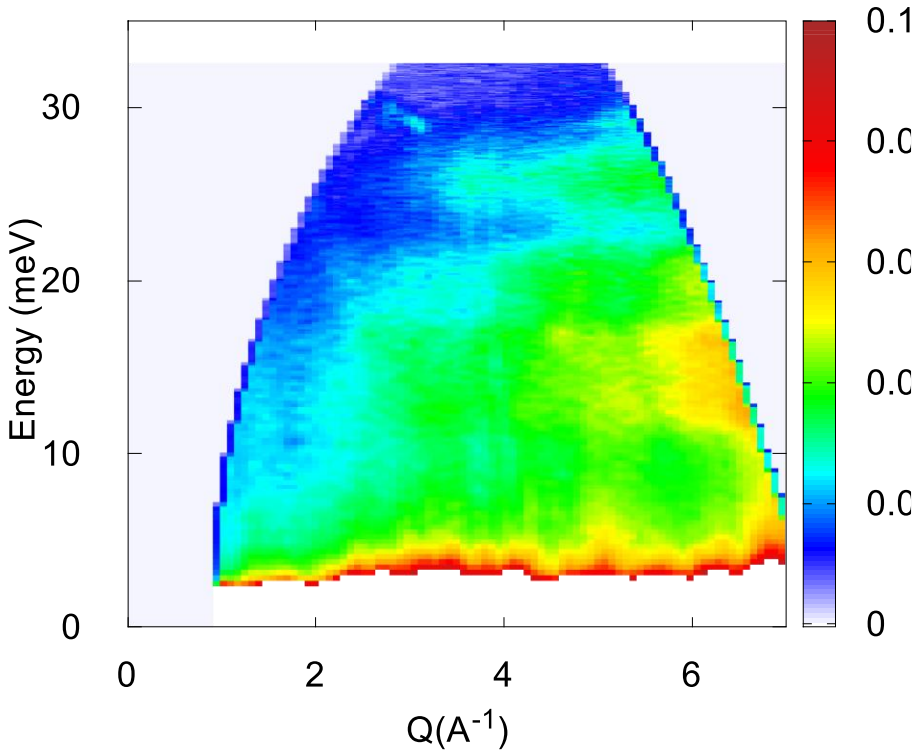


$YNiO_3$



- $YNiO_3$ powder sample
  T = 200 K
- Not much to see,
  except the elastic line

$YNiO_3$



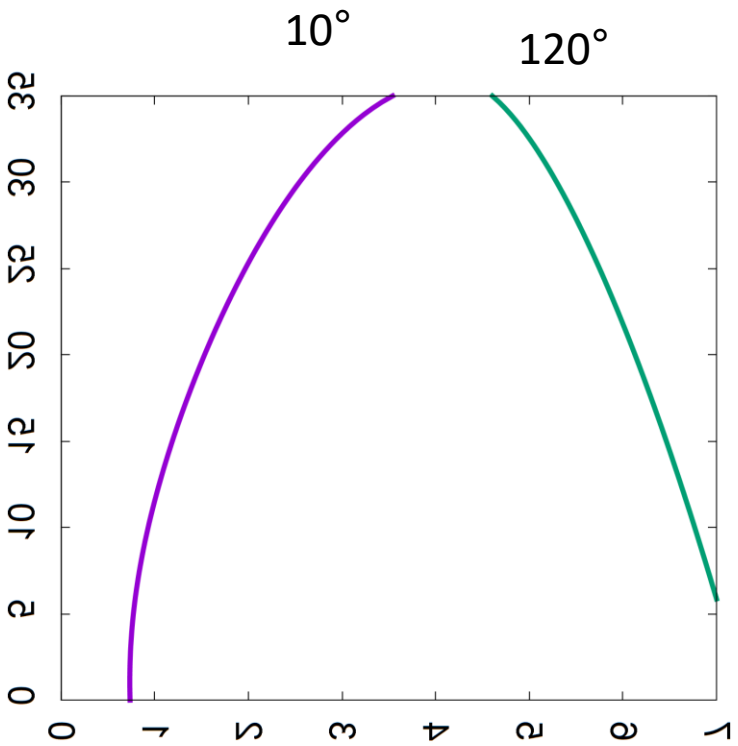
- $YNiO_3$ powder sample
  T = 200 K
- Not much to see,
  except the elastic line

  Change color-scale !!
- Enveloppes

$$E = \hbar\omega = E_i - E_f$$

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

$YNiO_3$



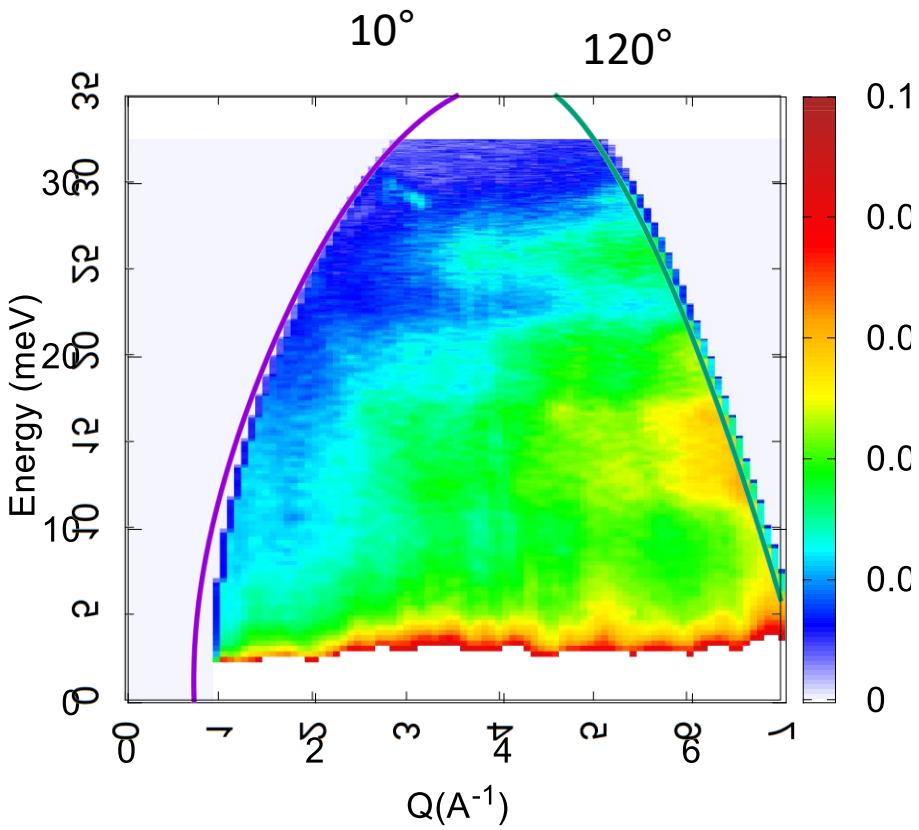
- Enveloppes $\vec{Q} = \vec{k}_i - \vec{k}_f$

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$

$$\frac{\hbar^2 Q^2}{2m} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$$

$$\frac{\hbar^2 Q^2}{2m} = 2E_i - E - 2\sqrt{E_i(E_i - E)}\cos 2\theta$$

$YNiO_3$



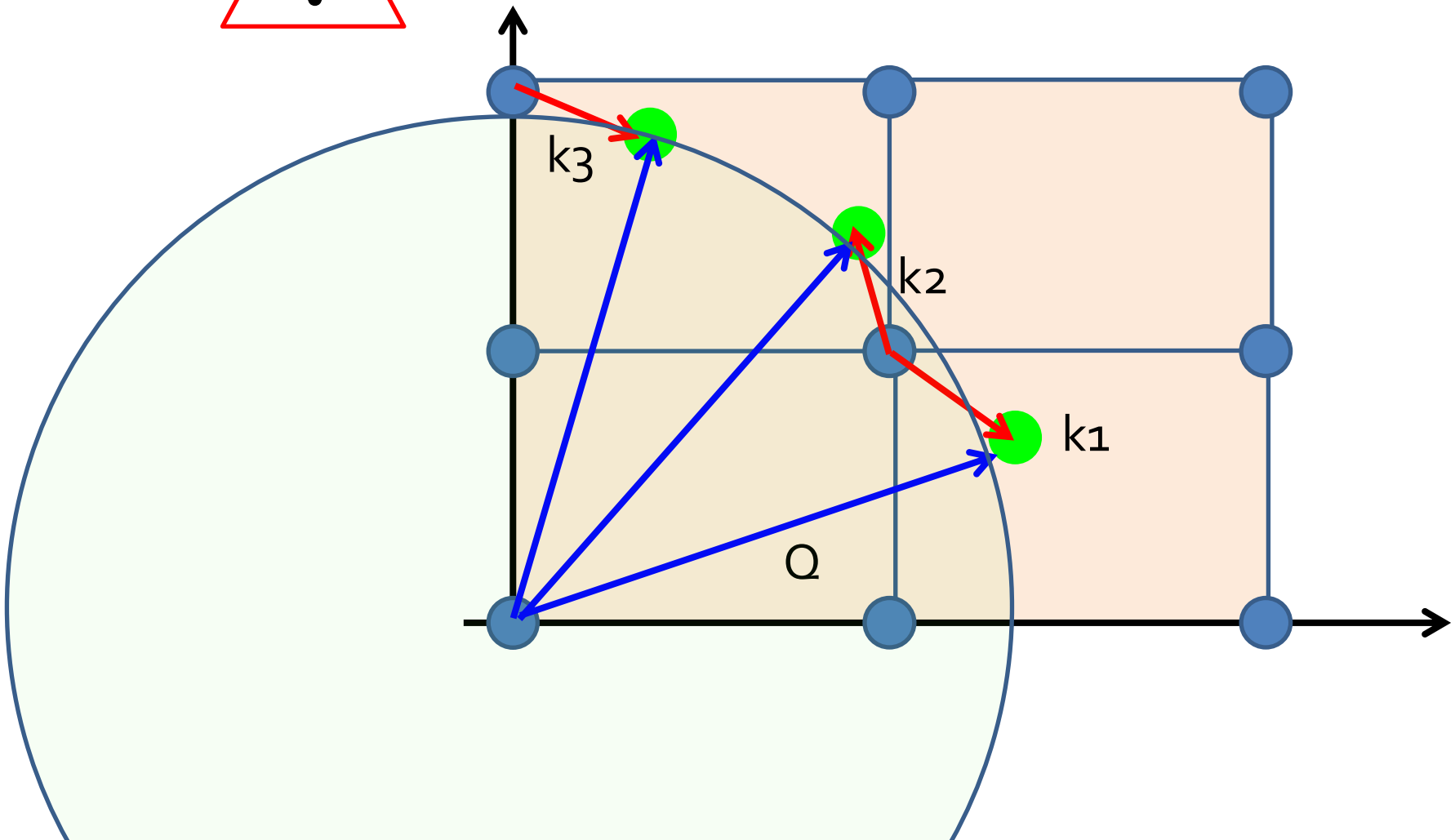
- Enveloppes $\vec{Q} = \vec{k}_i - \vec{k}_f$

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$

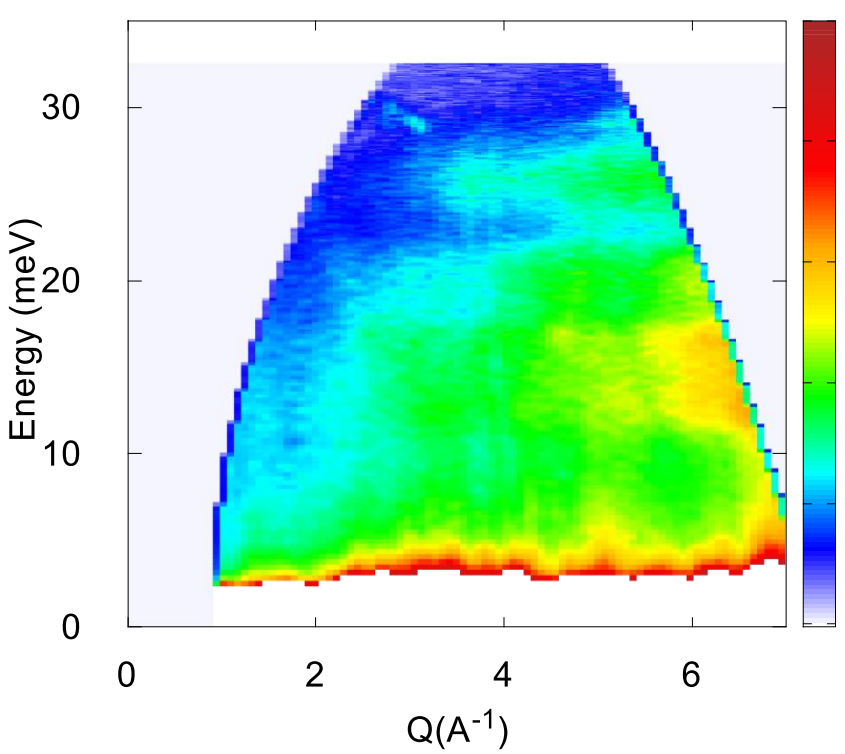
$$\frac{\hbar^2 Q^2}{2m} = E_i + E_f - 2\sqrt{E_i E_f}\cos 2\theta$$

$$\frac{\hbar^2 Q^2}{2m} = 2E_i - E - 2\sqrt{E_i(E_i - E)}\cos 2\theta$$

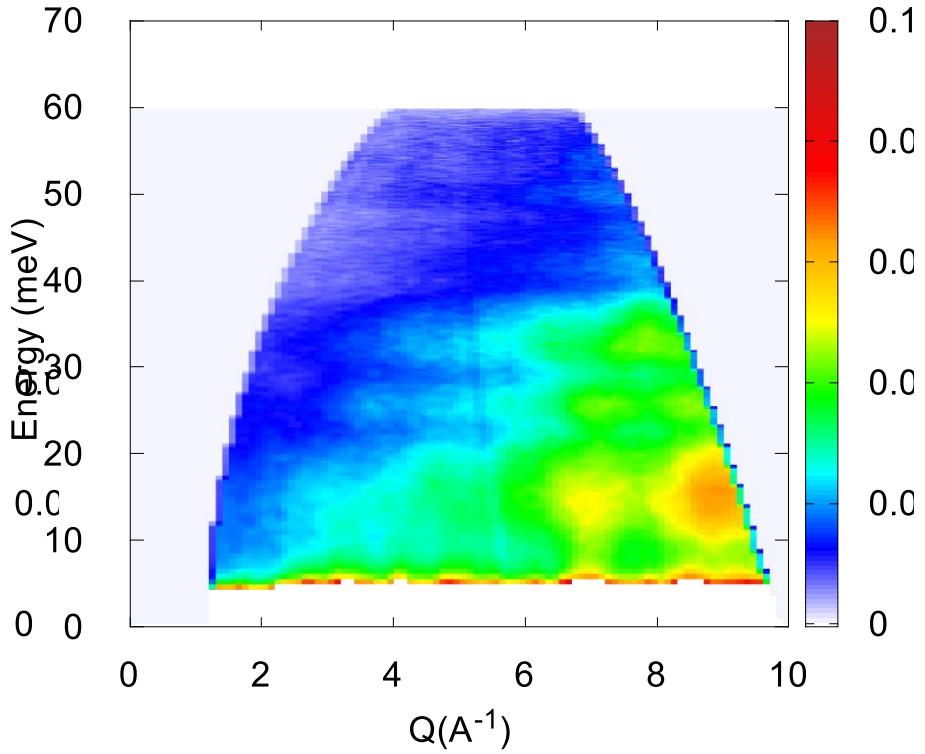
Because of the powder average, different phonon states with different k's but same modulus of Q are summed together, leading to a ***partial density of states***



- Changing Ei to modify energy range and energy resolution



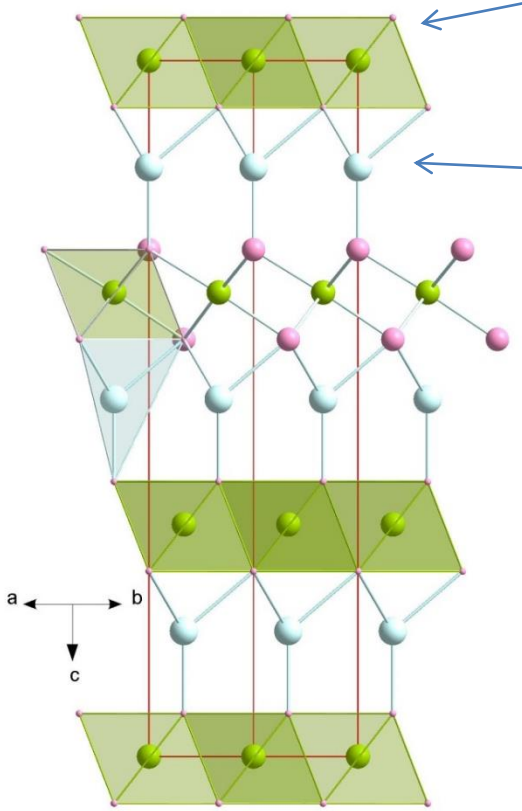
λ = 1.5 Å



λ = 1.1 Å

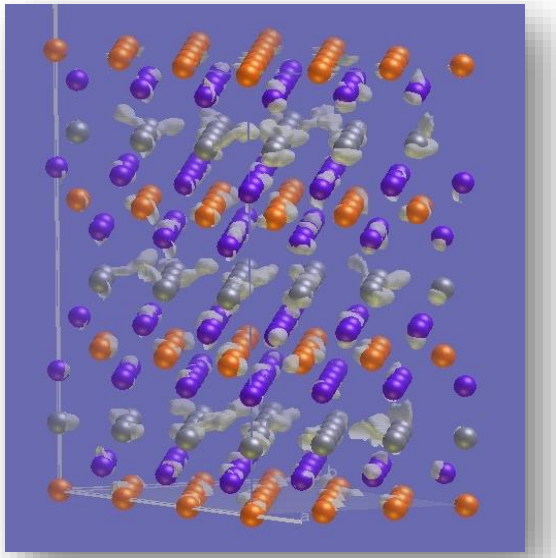
Example 3 : $AgCrSe_2$

Why this example ? because the lattice dynamics is remarkable



CrS_6 or $CrSe_6$ compact layers, perfect triangular lattice

Ag^+ layers

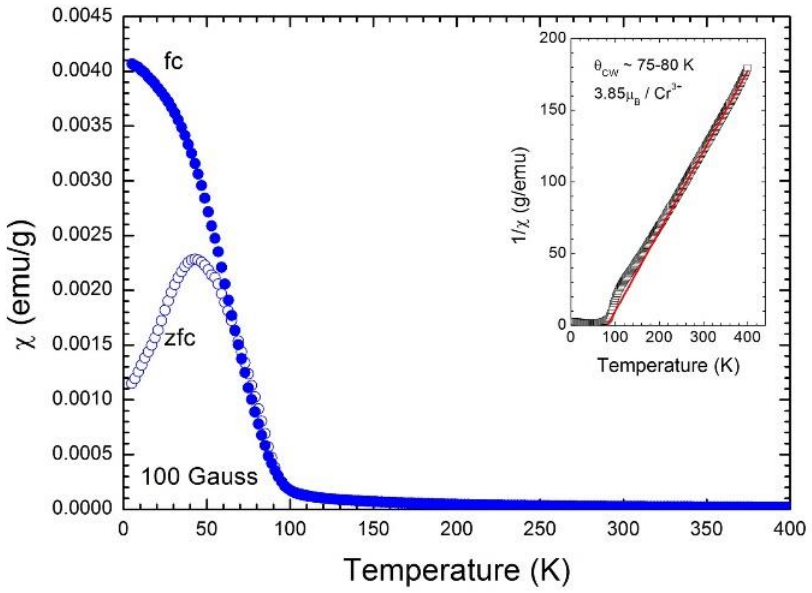


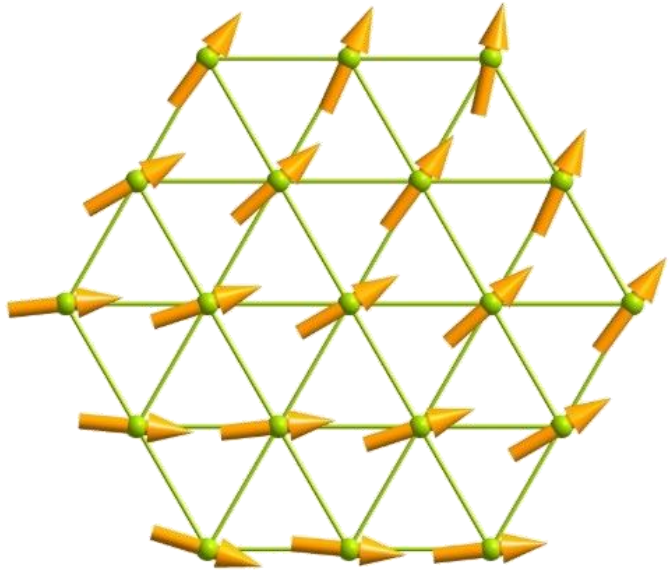
Ag atoms (grey) have tunnel-like trajectories bridging two sites, even as low as 150 K.

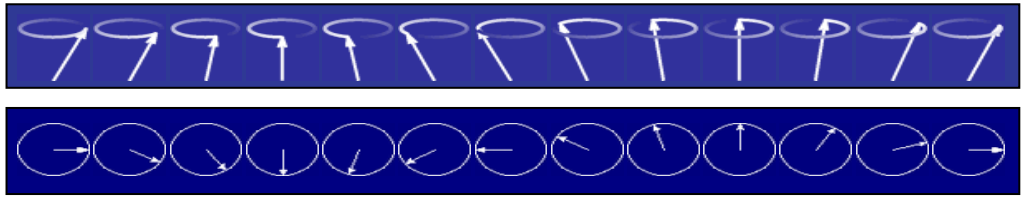
Example 3 : $AgCrSe_2$

And also because AgCrSe2 is magnetic and thus hosts magnetic excitations

T_N = 51 K

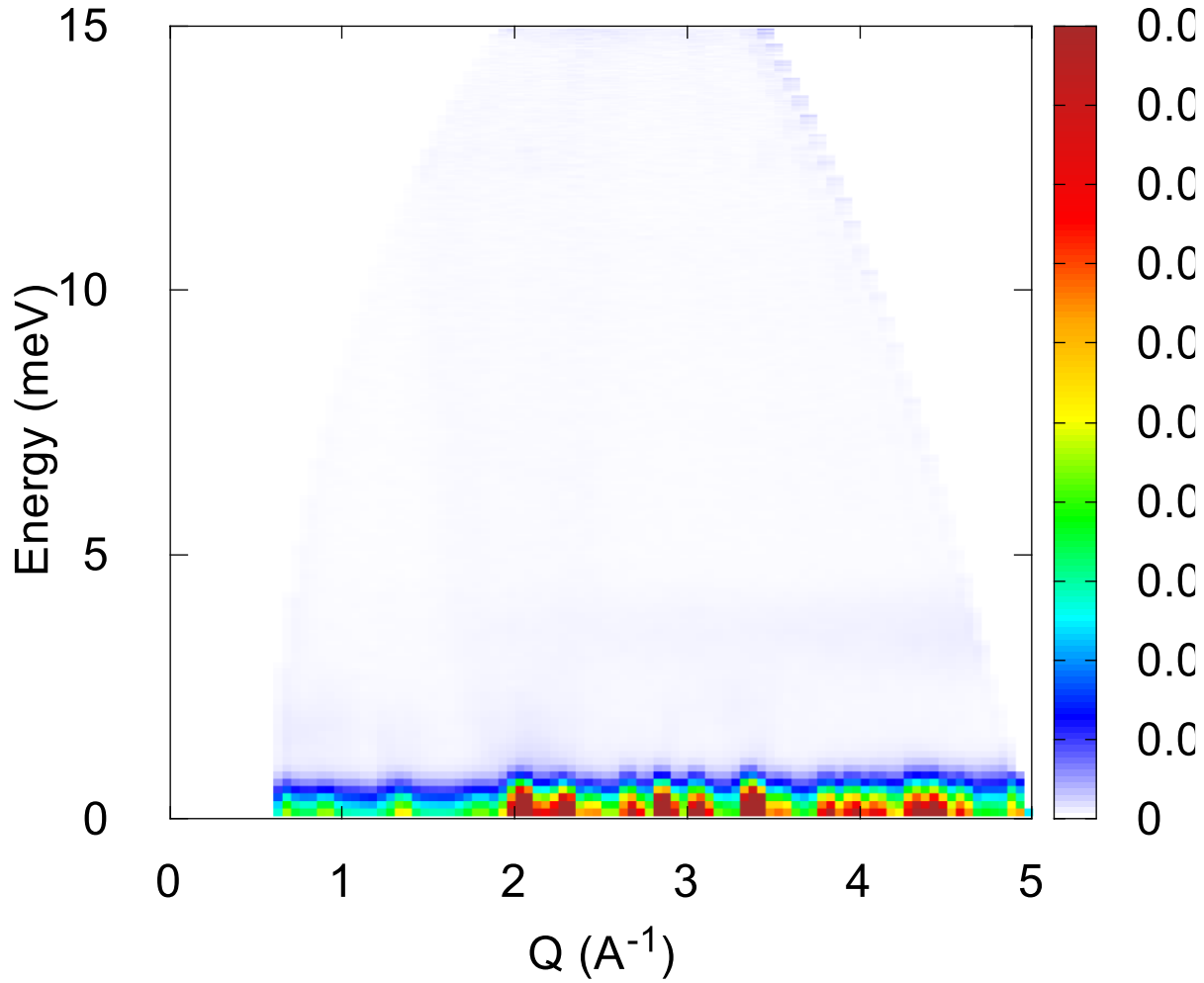






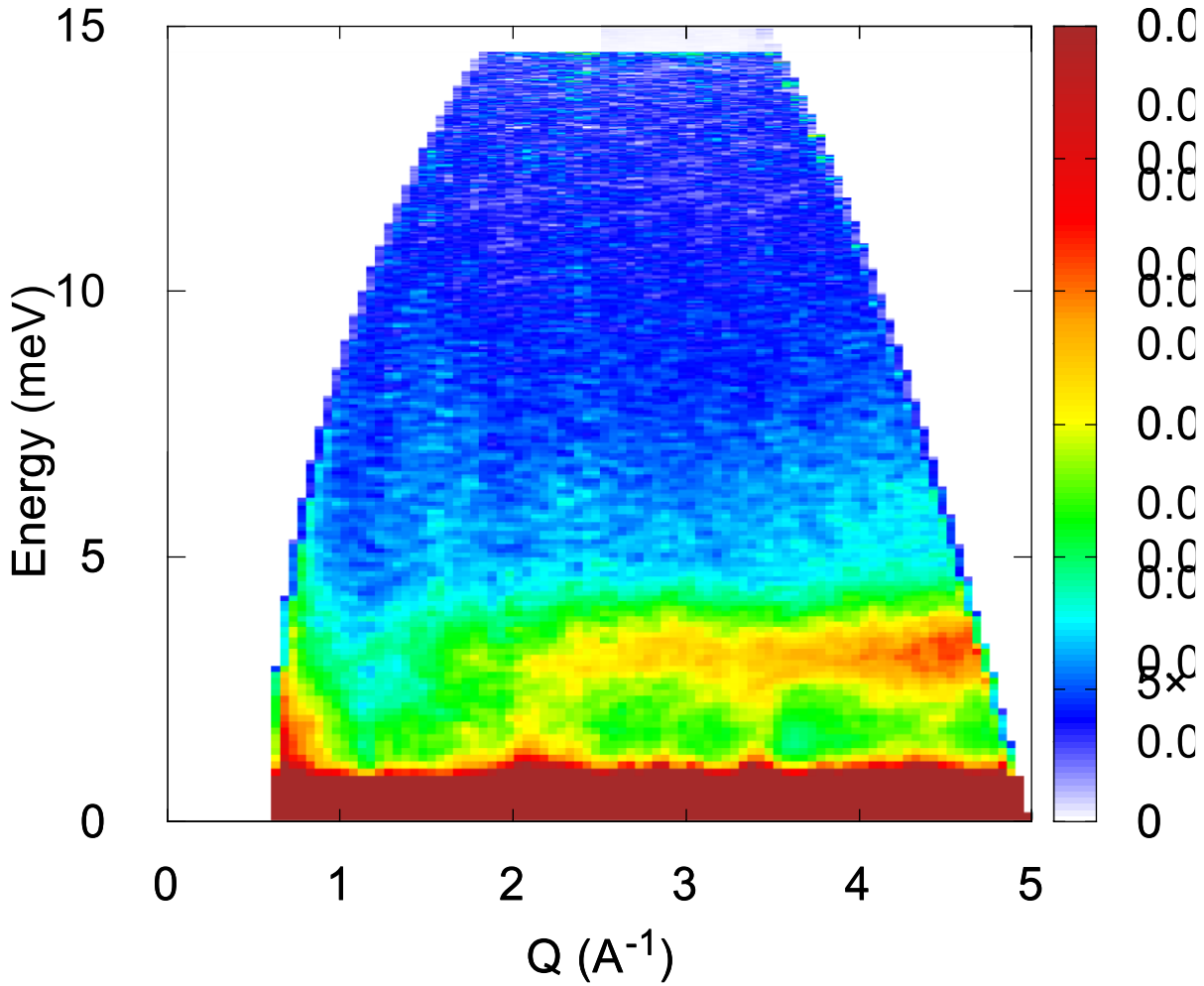
Example 3 : $AgCrSe_2$

Again, not much to see, except the elastic line : change color-scale !!

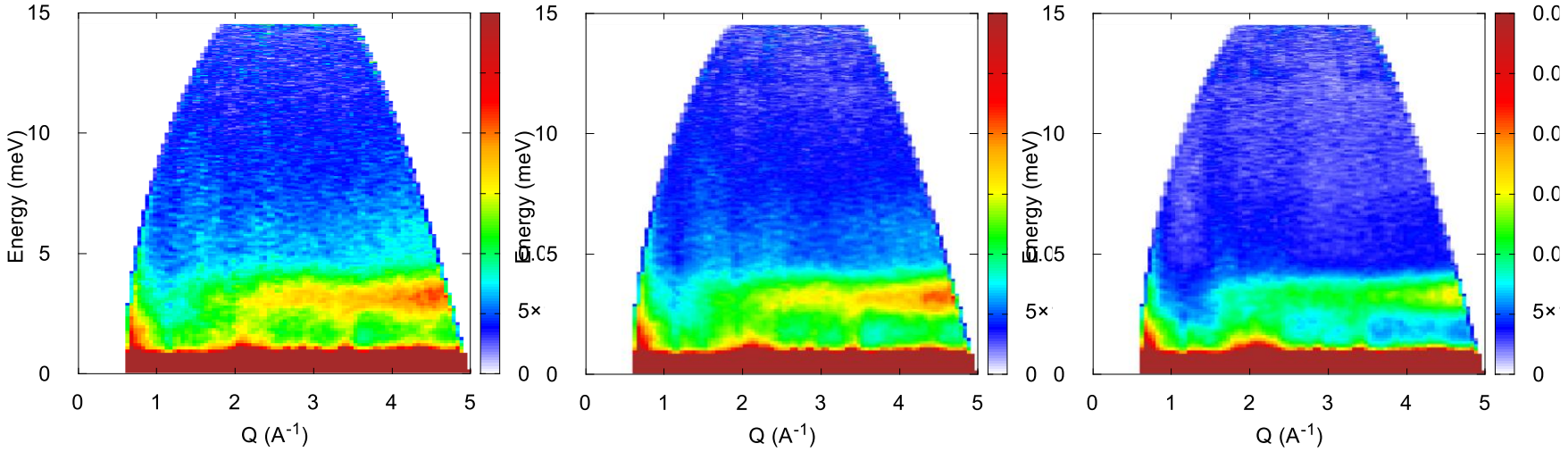


Example 3 : $AgCrSe_2$

Again, not much to see, except the elastic line : change color-scale !!



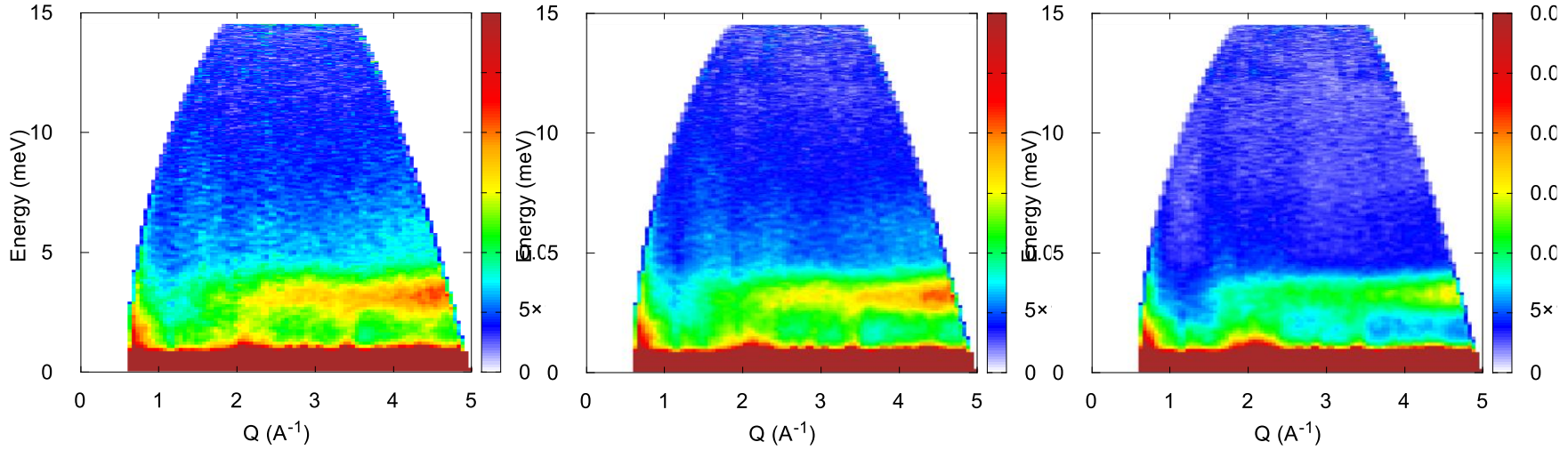
Example 3 : $AgCrSe_2$



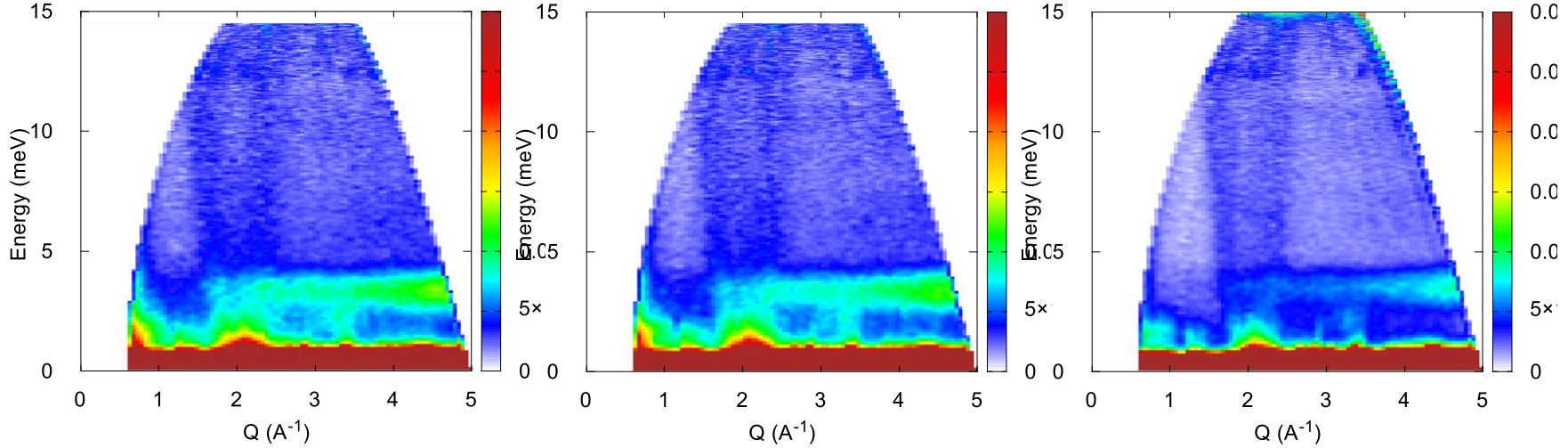
Intrinsic temperature dependence (phonons are bosons) $1 + \frac{1}{\exp E/k_B T - 1}$

Anomalous low energy band at about 3 meV due to Ag jumps

Example 3 : $AgCrSe_2$

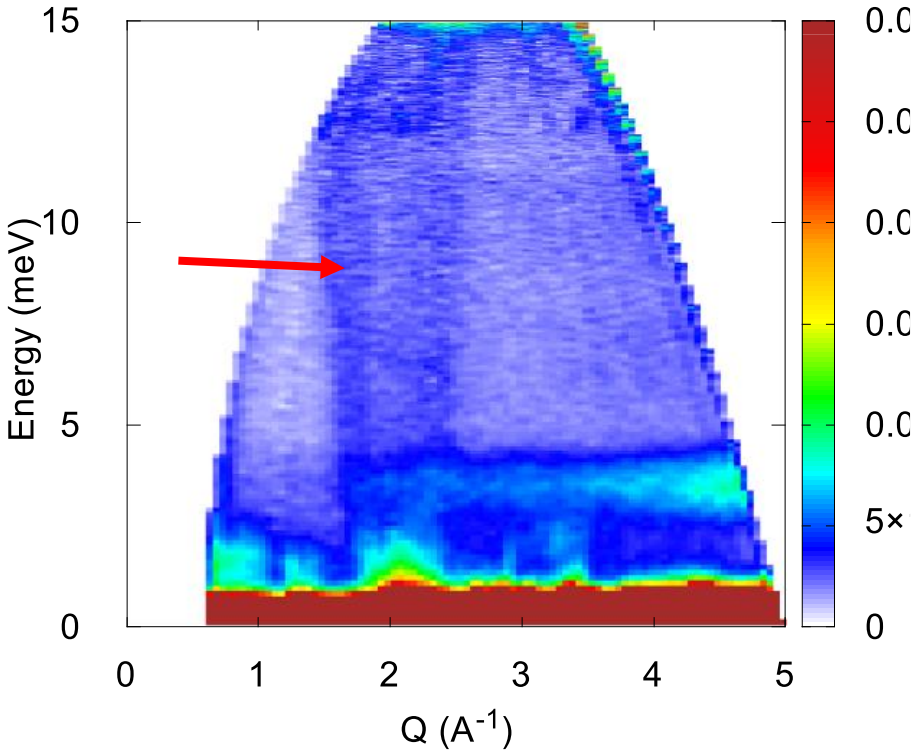


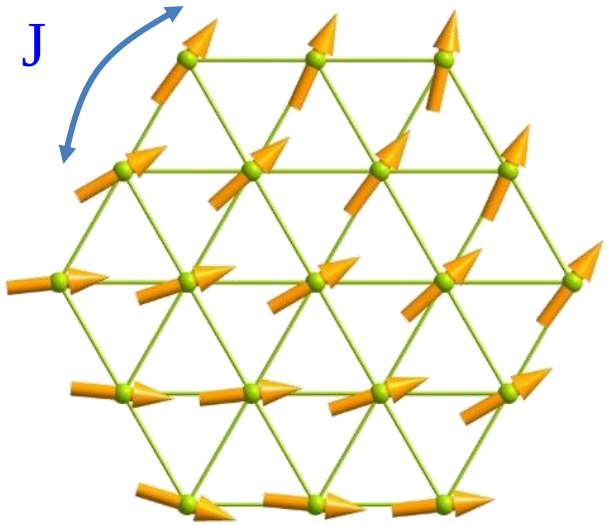
Additional signal due to Cr spins below T_N



Example 3 : $AgCrSe_2$

As for phonons, this is the partial density of states of magnetic excitations

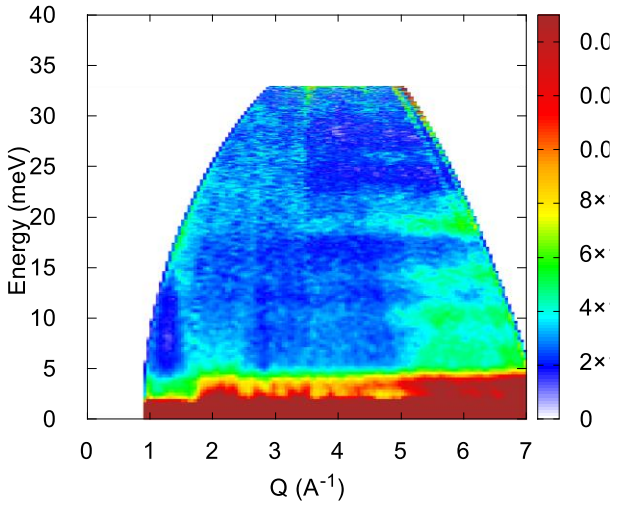




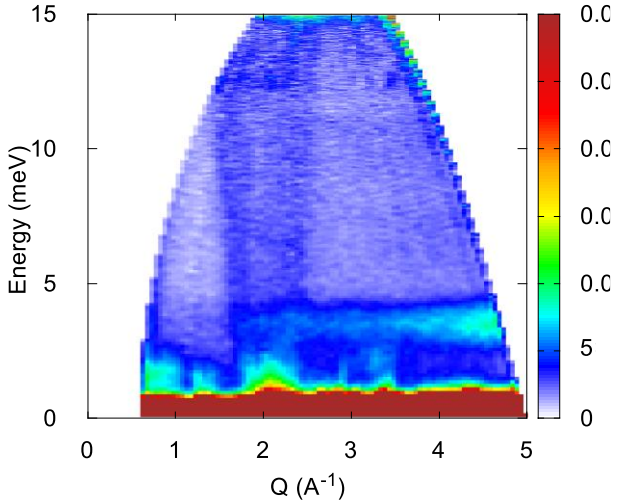
$$\mathcal{H} = \sum_{\langle ij \rangle} J(\mathbf{r}_i - \mathbf{r}_j)\mathbf{S}_i \cdot \mathbf{S}_j,$$

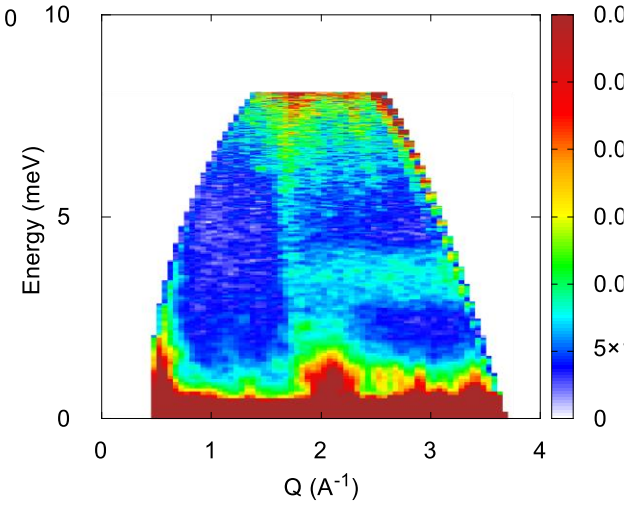
Determine exchange interactions between spins

Example 3 : $AgCrSe_2$

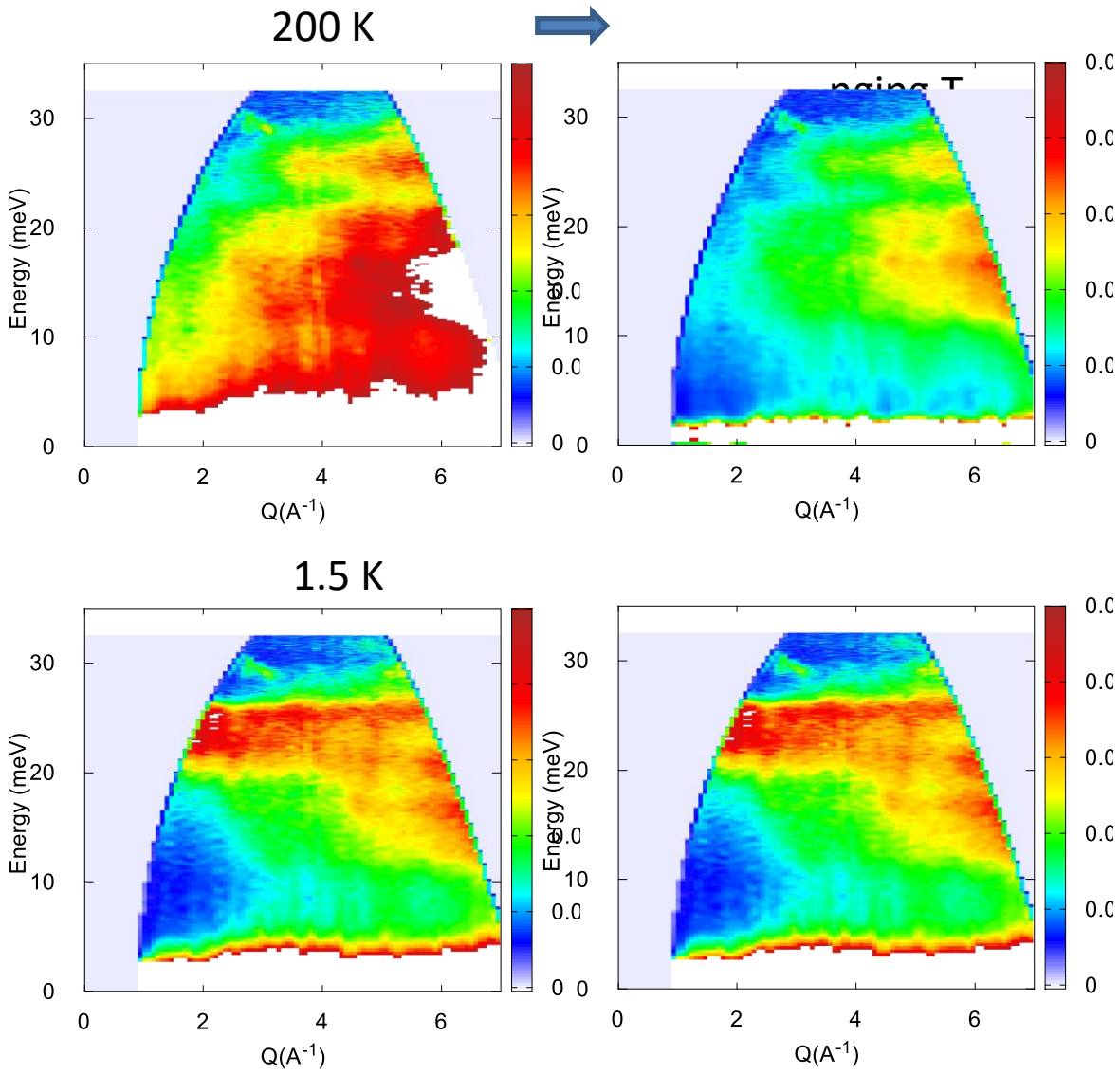


Change Ei to modify energy range and energy resolution





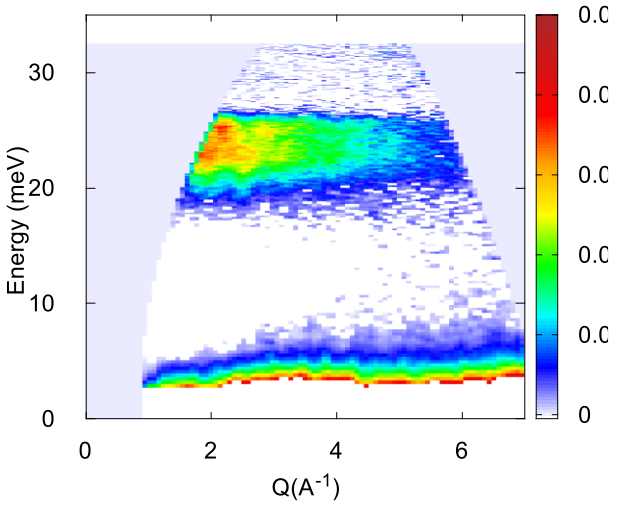
Back to $YNiO_3$



Correct for the Bose factor

$$1 + \frac{1}{\exp E/k_B T - 1}$$

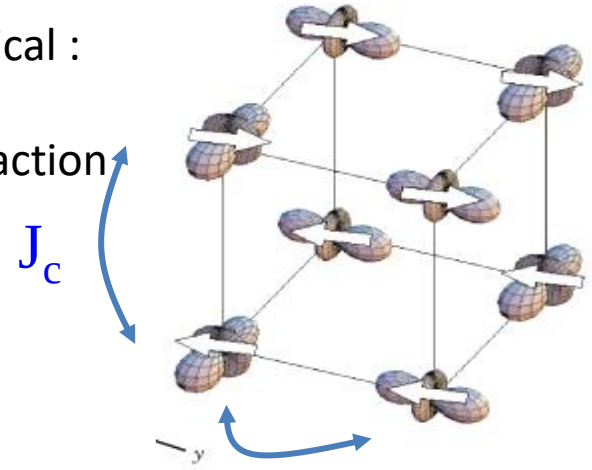
Take the difference

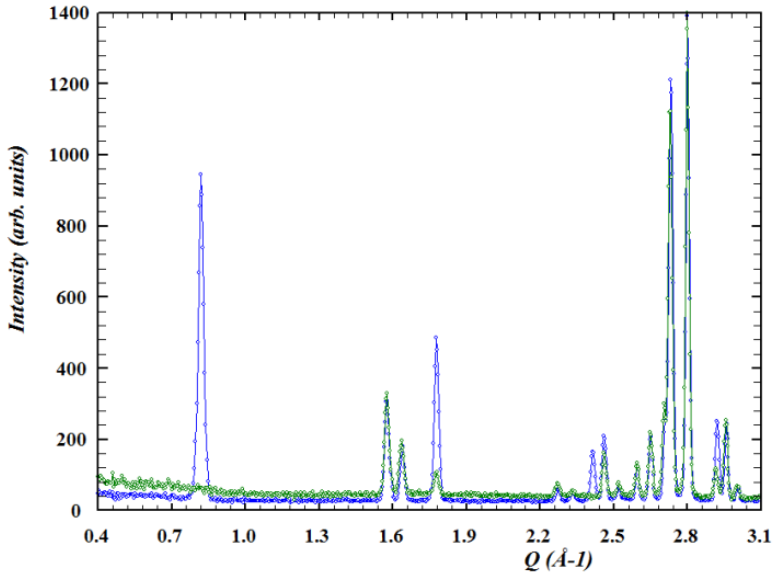


to reveal Ni spin excitations

Example 4 : $LaMnO_3$

Tomorrows' practical : see the magnetic transition by diffraction





But what about the values of Jc and Jab ?

$$\mathcal{H} = \sum_{\langle ij \rangle} J(\mathbf{r}_i - \mathbf{r}_j)\mathbf{S}_i \cdot \mathbf{S}_j,$$