Neutron Spin Echo Spectroscopy

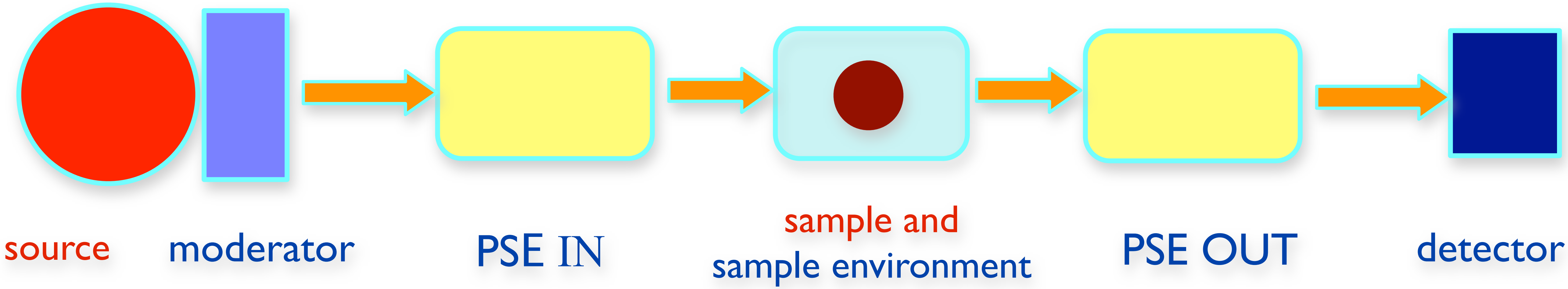
Catherine Pappas

TU Delft

uncluding slides and animations from

R. Gähler, R. Cywinski, W. Bouwman

from the source to the detector



Neutron flux

$$\varphi = \Phi \, \eta \, dE \, d\Omega \, / \, 4\pi$$

- Φ: source flux distribution
- η: intensity losses
- $dE \, d\Omega$: field of neutron instrumentation

definition of the beam : Q, E and polarisation

Neutron Spin Echo

why ?

very high resolution

how ?

using the transverse components of beam polarization

Larmor precession

Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : Larmor precession

III: NSE : semi-classical description

IV: movies

V: quantum mechanical approach

VI: examples

VII: NSE and structure

Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : classical description

III: NSE : quantum mechanical description

IV: movies

V: NSE and coherence

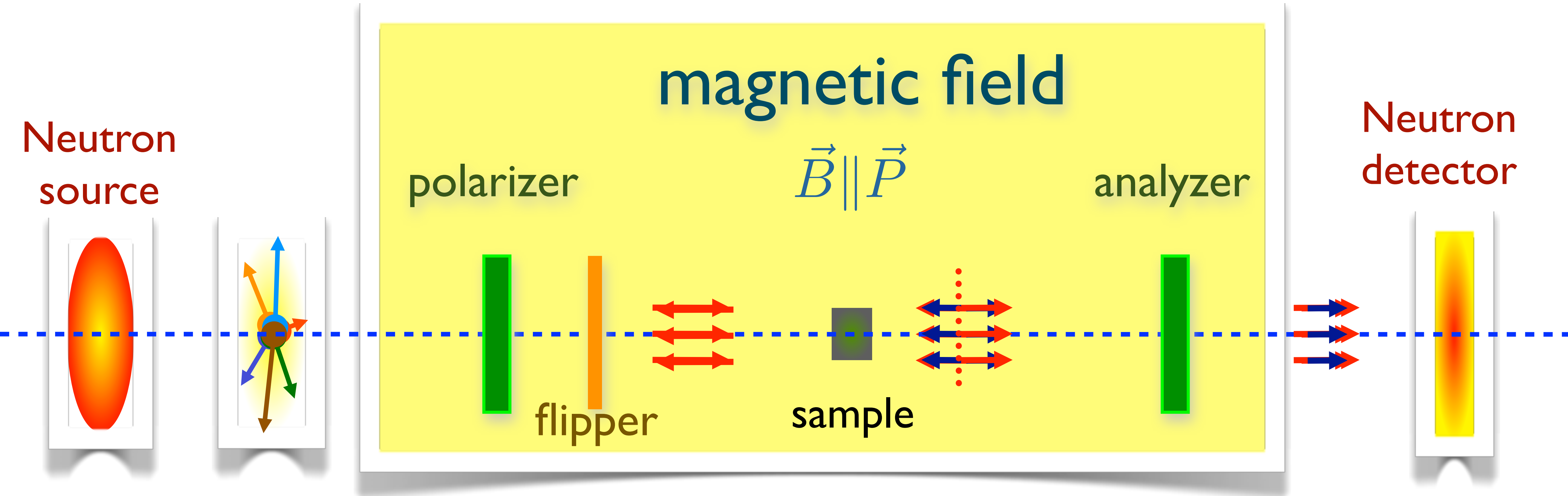
VI: exemples

VII: NSE and structure

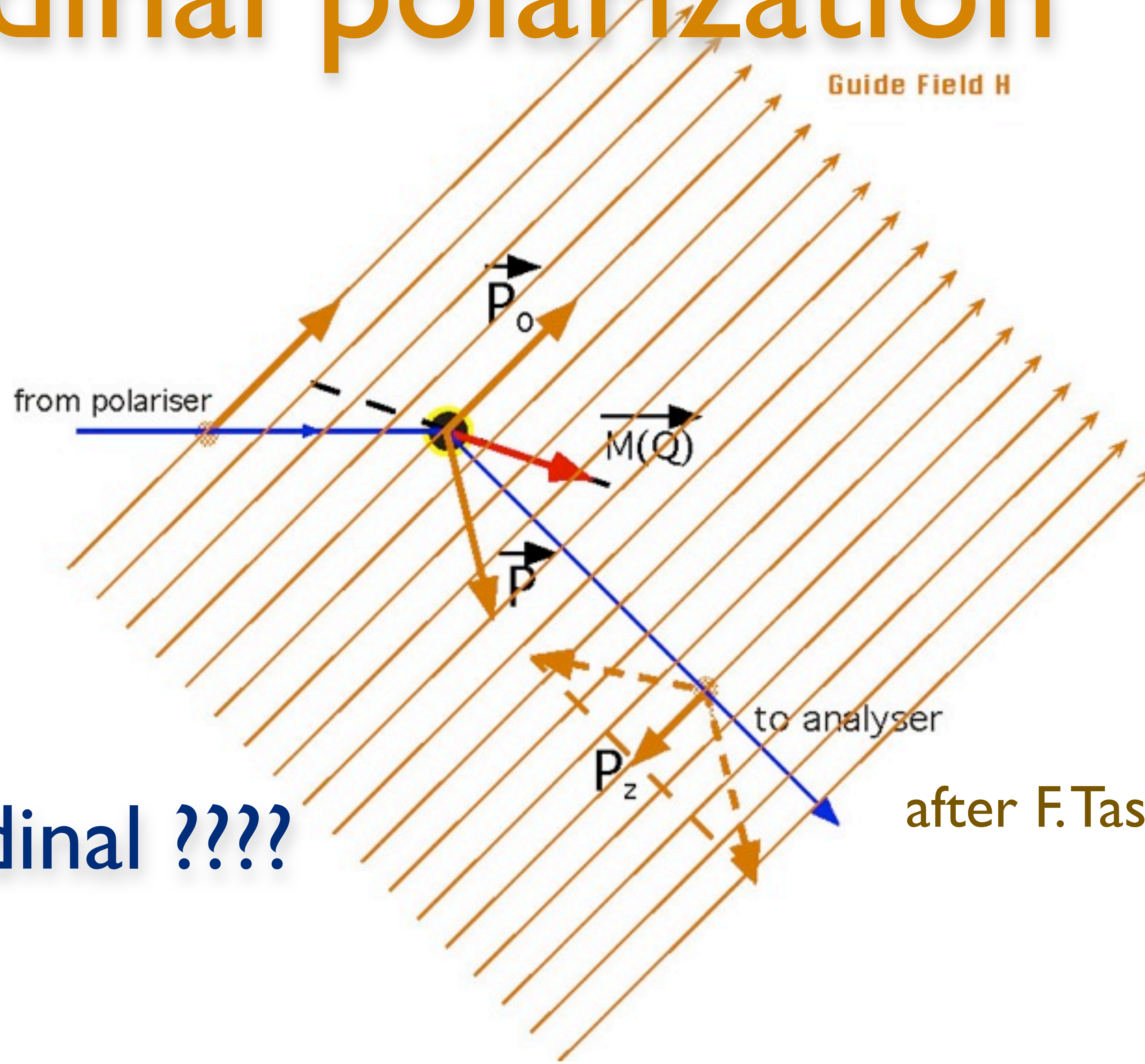
Polarized Neutrons

- polarizer
- analyzer

magnetic field (guide - precession)



Longitudinal polarization analysis



after F. Tasset

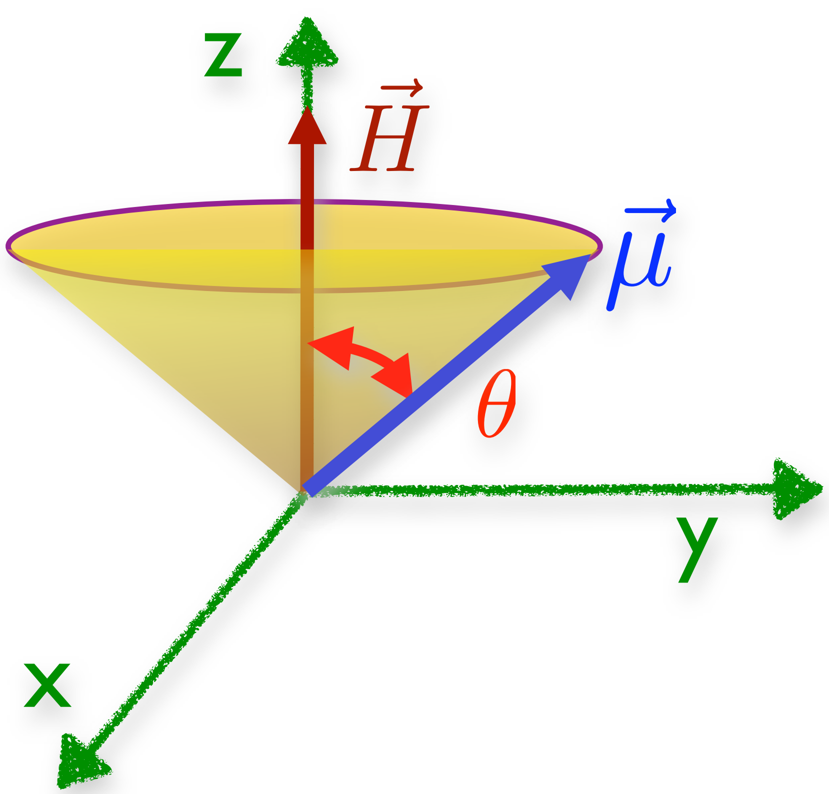
Why longitudinal ????

because we apply a magnetic field and measure the projection of the polarization vector along this field

Larmor Precession

Motion of the polarization of a neutron beam in a magnetic field

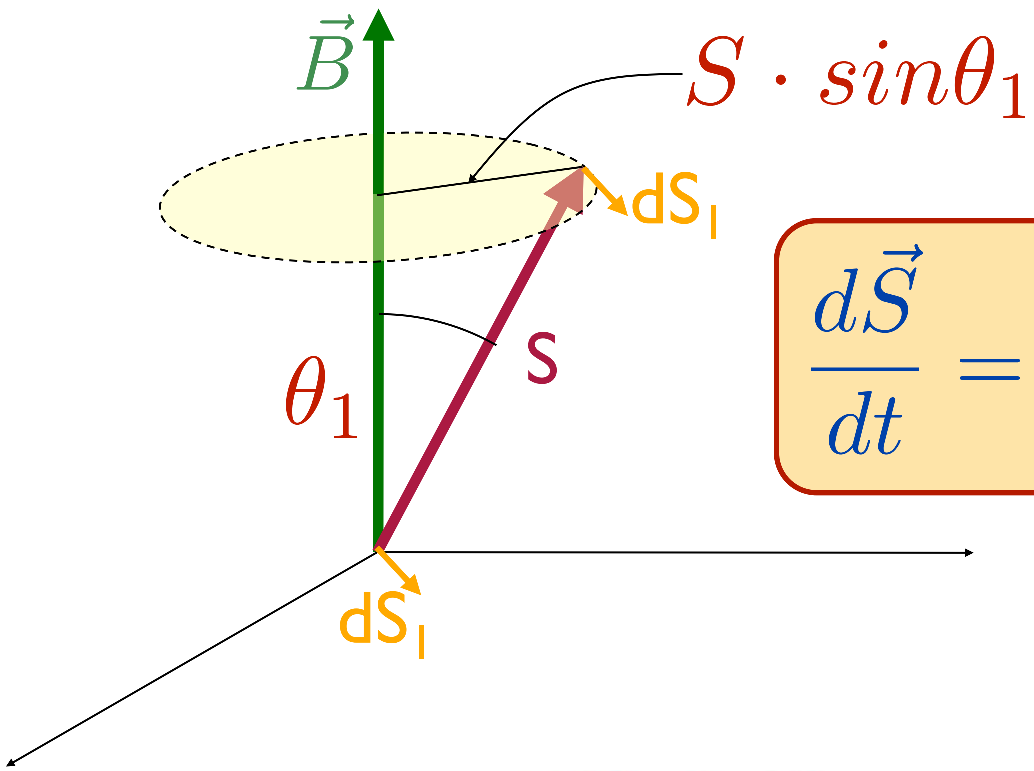
$$\frac{d\vec{\mu}}{dt} = \gamma \cdot (\vec{\mu} \times \vec{B}) = \vec{\mu} \times \vec{\omega}_L$$



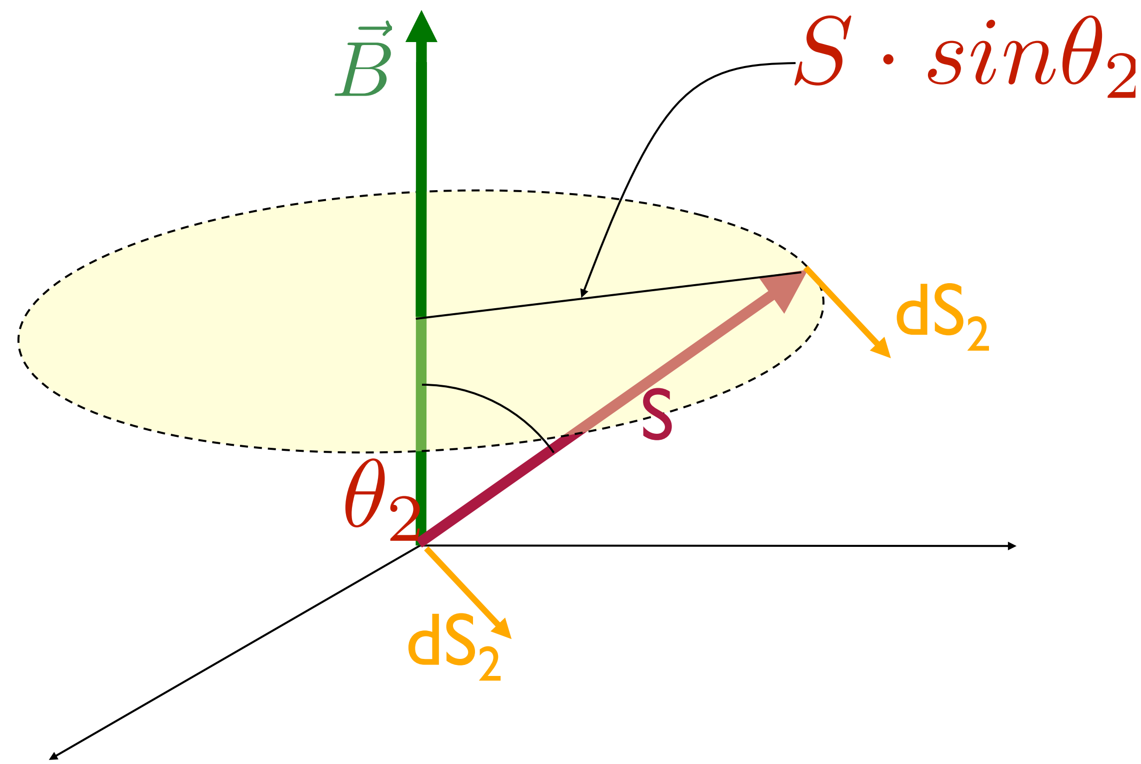
"gyromagnetic ratio" of neutrons

$$\gamma = 2.9\ kHz/G$$

Larmor Precession



$$\frac{d\vec{S}}{dt} = \gamma \cdot (\vec{S} \times \vec{B})$$



$d\vec{S} \perp \vec{B} \quad \Rightarrow$ precession around B

$d\vec{S} \perp \vec{S} \quad \Rightarrow$ precession frequency is constant;

in both cases $dS \propto S\,sin\theta$

during dt, the angular change of $S\,sin\theta$ around B is constant:

$\Rightarrow$ the precession 'Larmor' frequency ω_L does not depend on θ

Why Precession

relation spin - magnetic moment

nucleons

$$\mu_N = \frac{e\hbar}{2m_p}$$

electrons

$$\mu_B = \frac{e\hbar}{2m_e}$$

e is the elementary charge, $\hbar$ is the reduced Planck's constant,

m_p is the proton rest mass	m_e is the electron rest mass

The values of nuclear magneton

SI 5.050×10^{-27} J·T^{-1}

CGS 5.050×10^{-24} erg•G^{-1}

The values of Bohr magneton

SI 9.274×10^{-24} J•T^{-1}

CGS 9.274×10^{-21} erg•G^{-1}

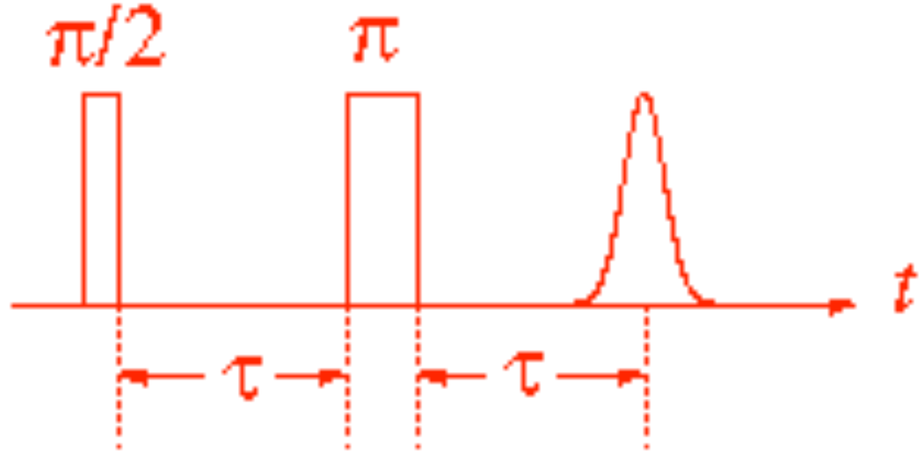
ratio ~ 1800

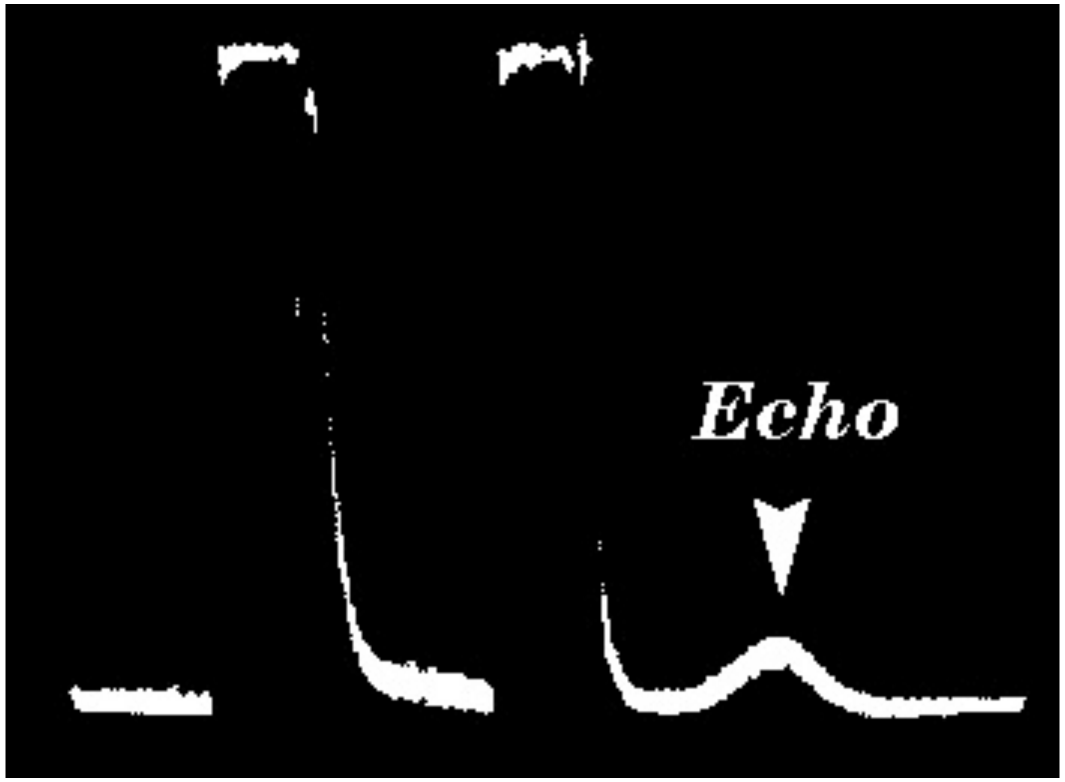
Larmor Precession

NMR spin echo

Erwin Hahn 1950

$$\frac{d\vec{\mu}}{dt} = -\gamma\,\vec{\mu} \times \vec{H} = \vec{\mu} \times \vec{\omega}_L$$

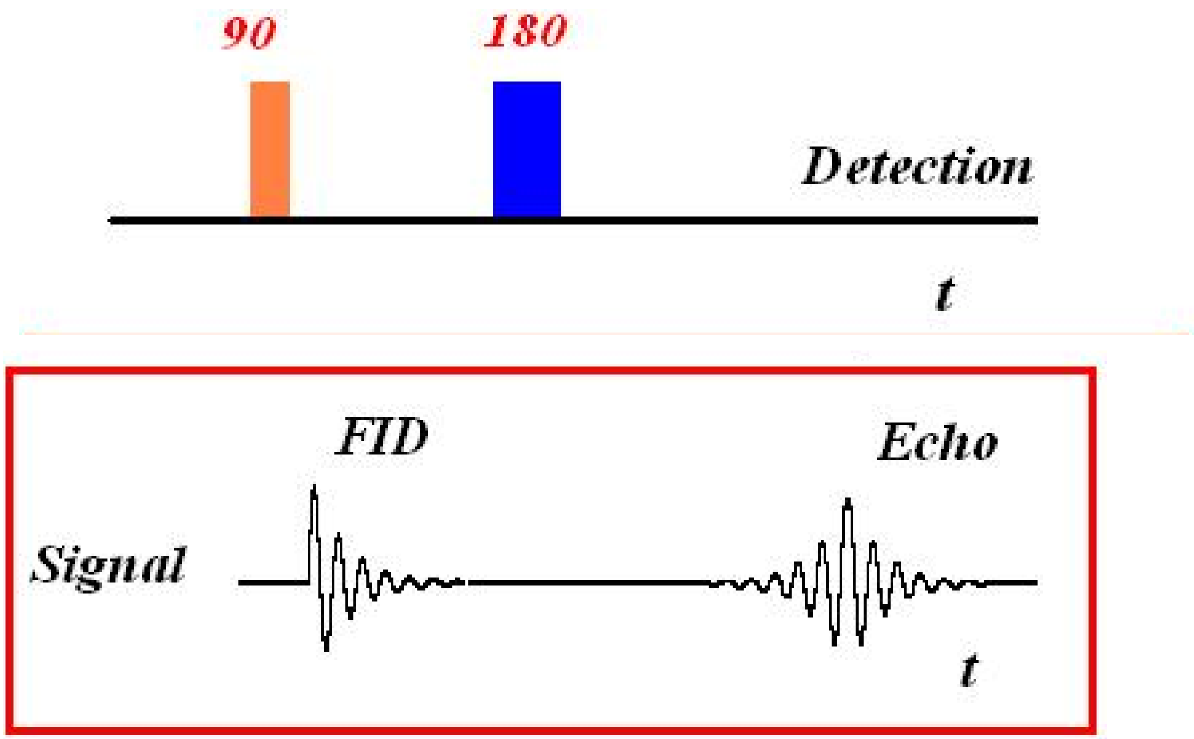




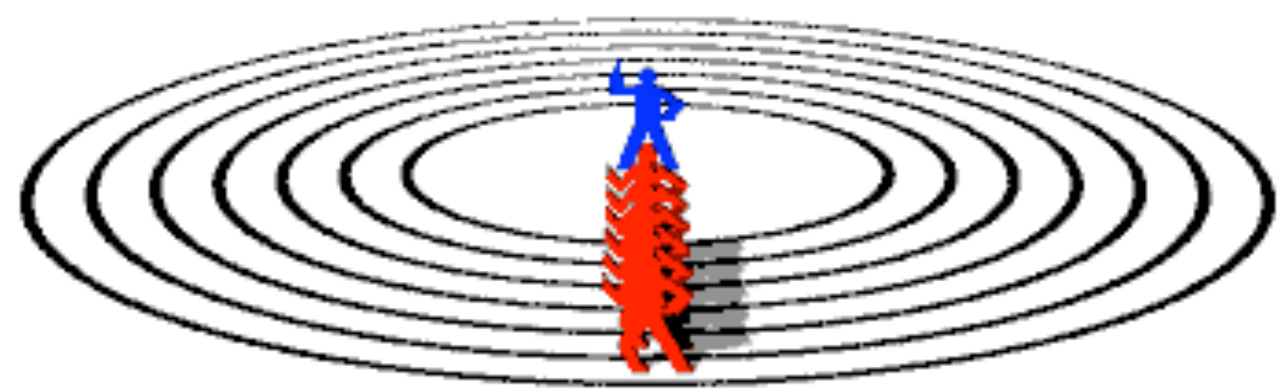
Larmor Precession

NMR spin echo

Erwin Hahn 1950



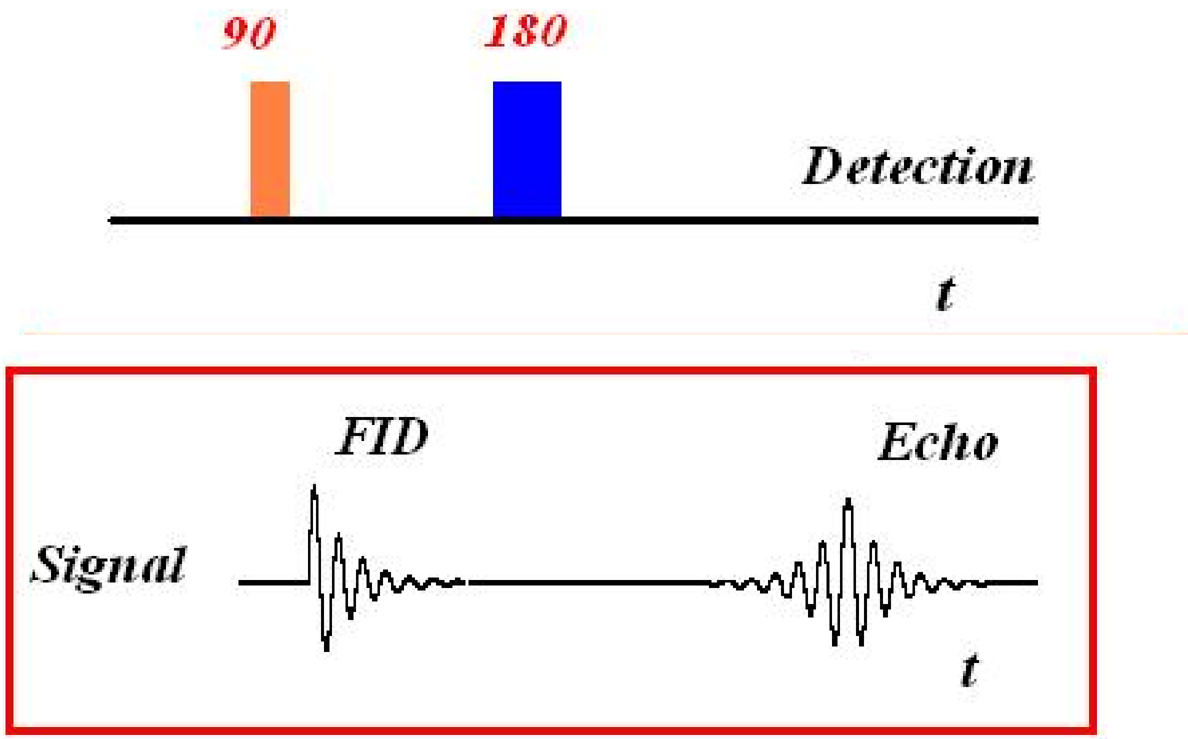
$$\frac{d\vec{\mu}}{dt} = -\gamma\, \vec{\mu} \times \vec{H} = \vec{\mu} \times \vec{\omega}_L$$



Larmor Precession

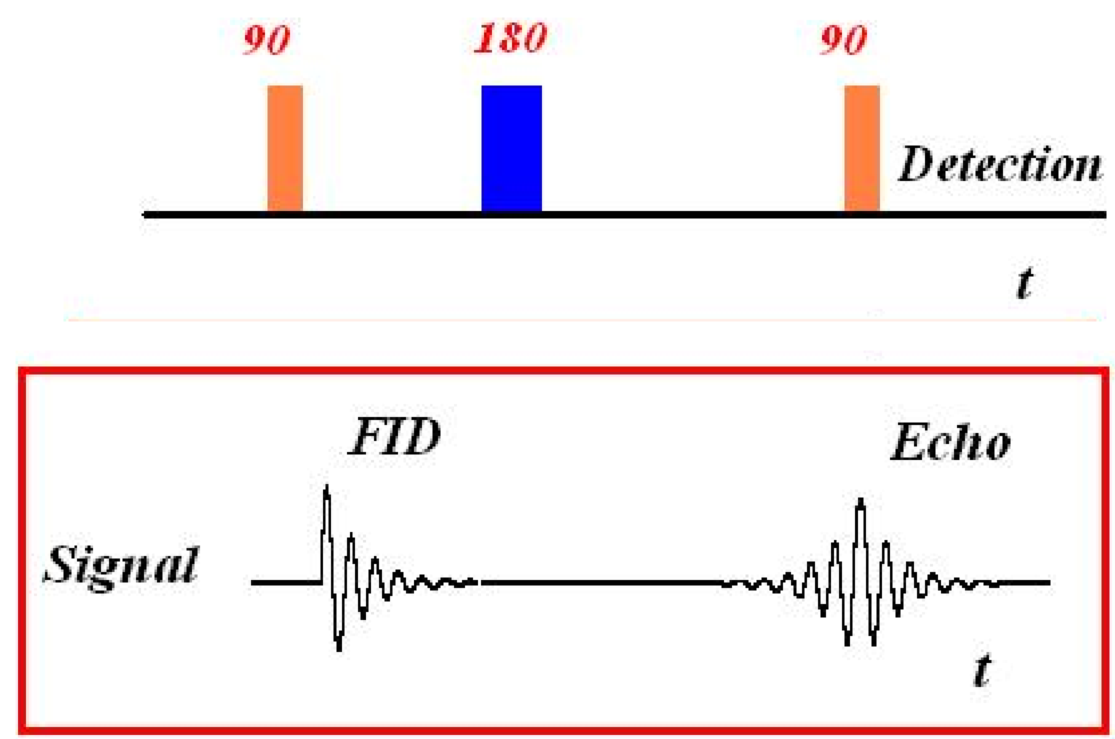
NMR spin echo

Erwin Hahn 1950

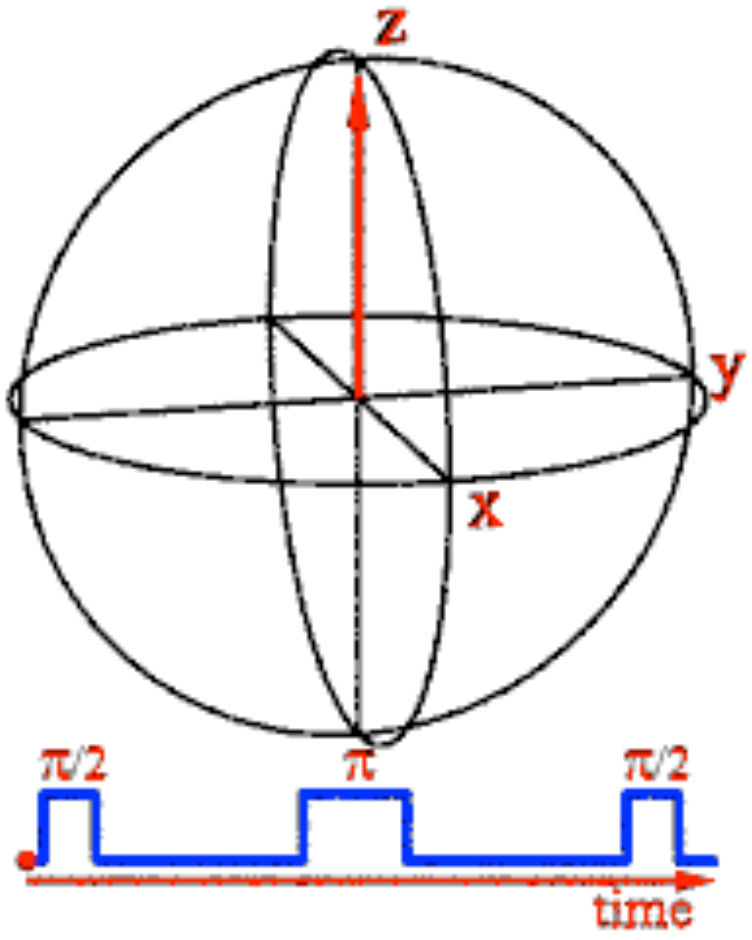


Neutron spin echo

Ferenc Mezei 1972

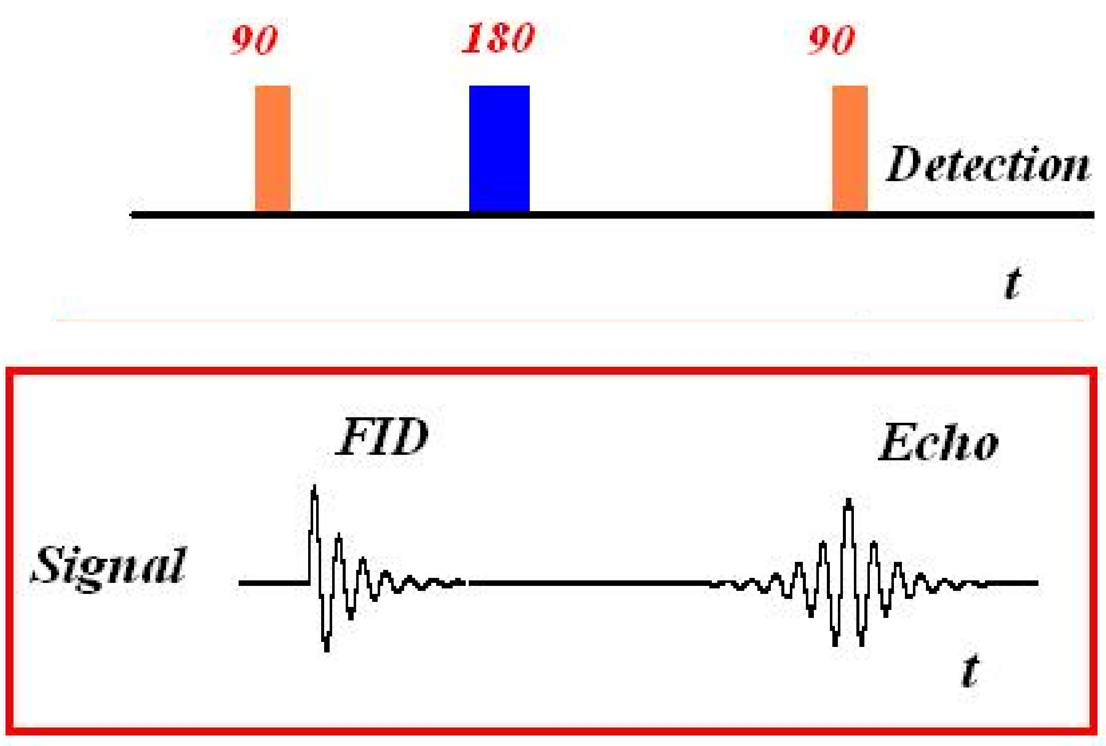


Larmor Precession



Neutron spin echo

Ferenc Mezei 1972



Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : Larmor precession

III: NSE : semi-classical description

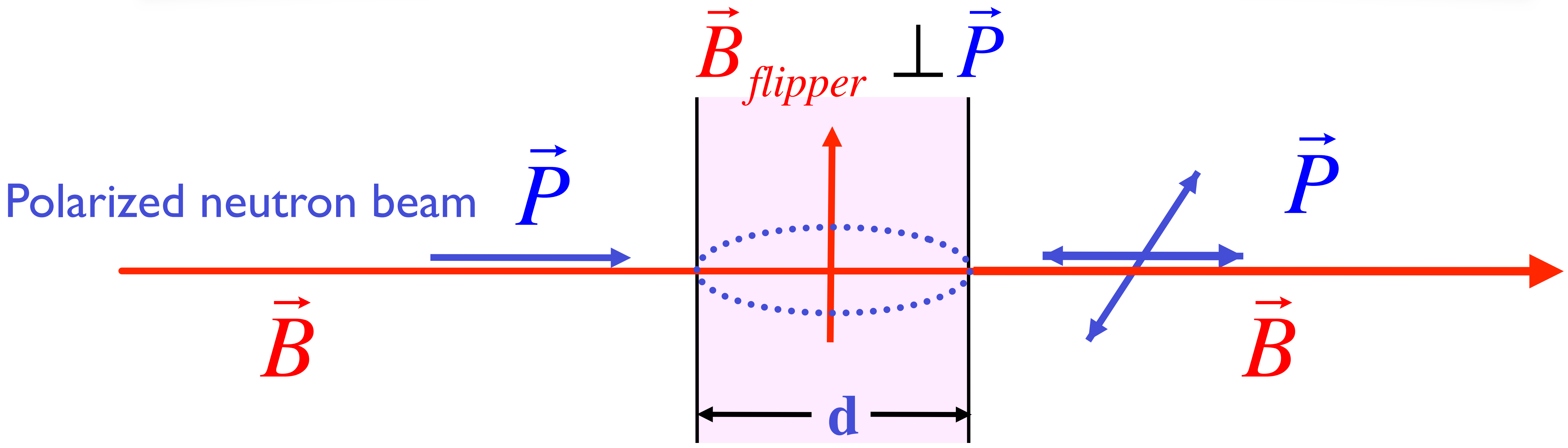
IV: movies

V: quantum mechanical approach

VI: examples

VII: NSE and structure

Larmor precession and flippers



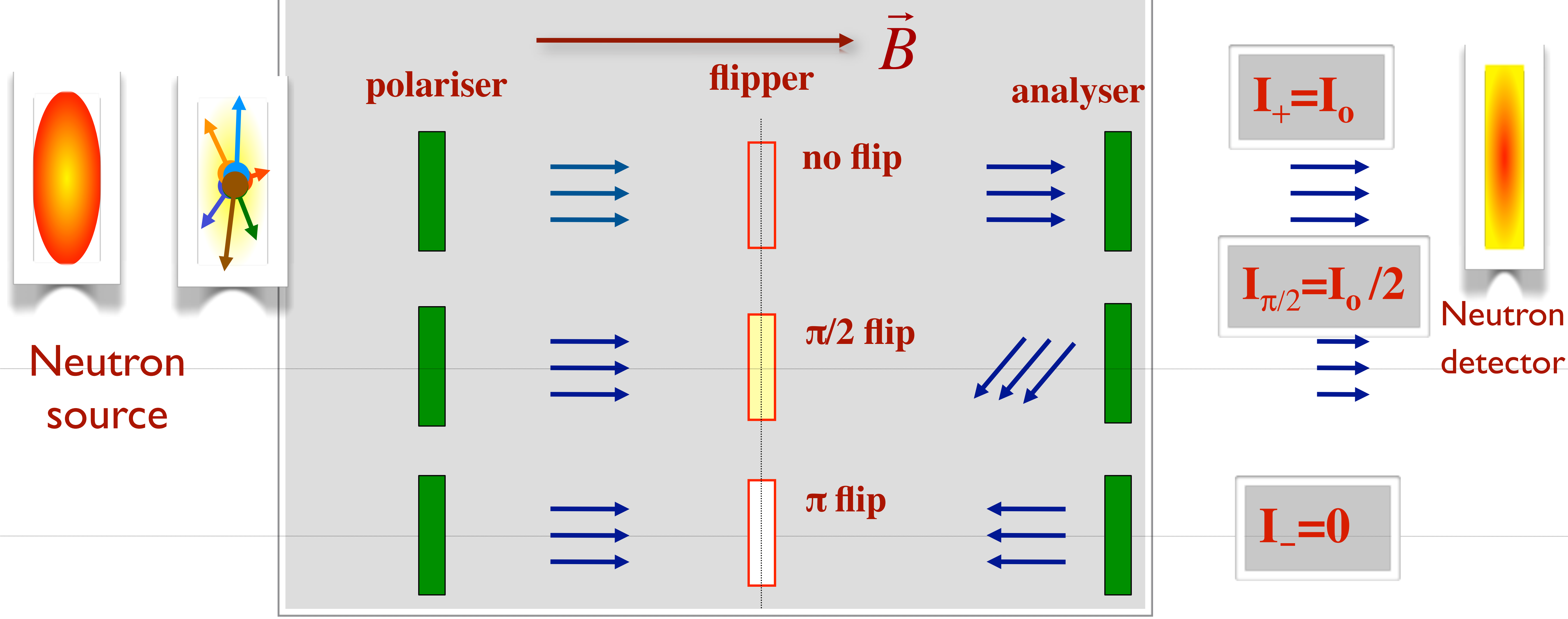
Precession angle

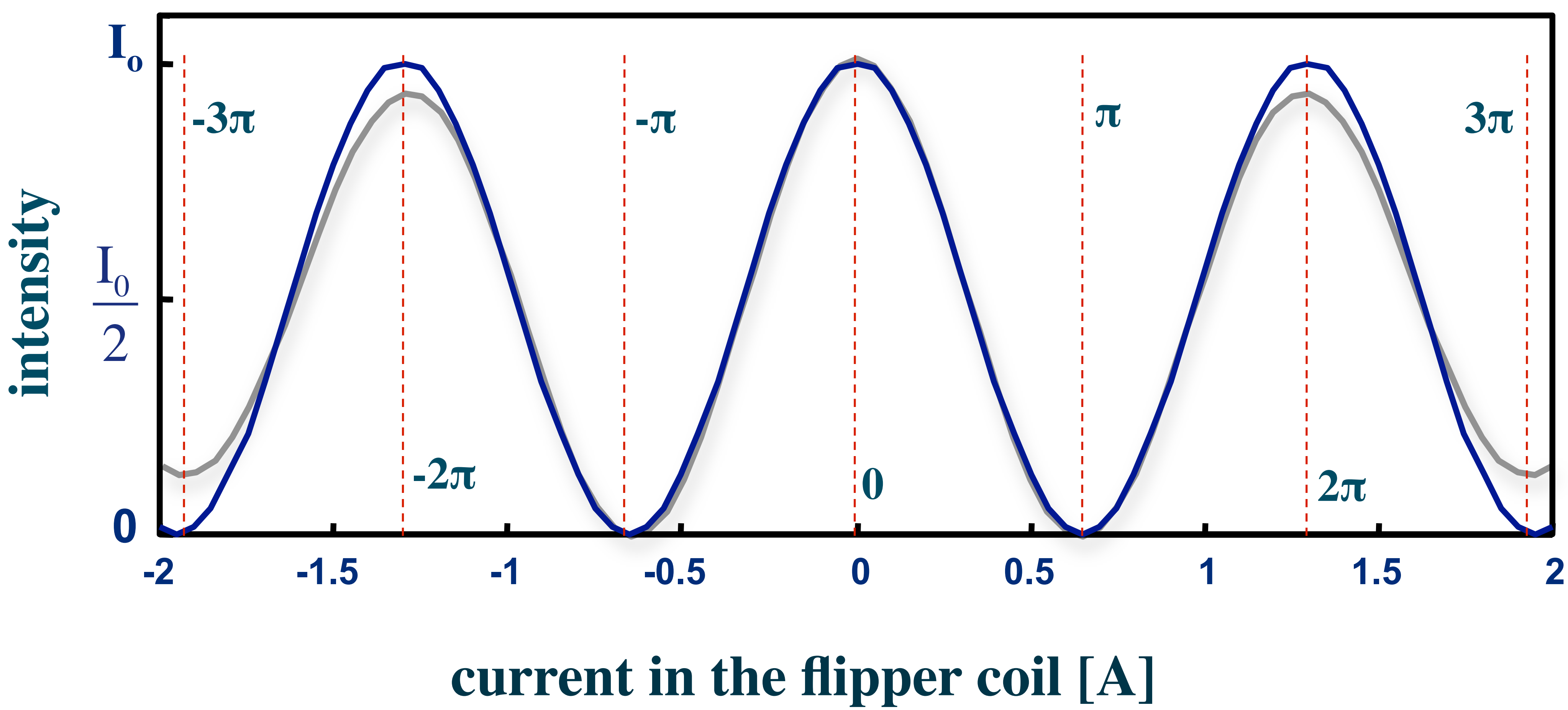
$\varphi = \omega_L t = \gamma B t = \gamma B d / v$

$\varphi = 2916.4 \text{ Hz/G} * 2\pi * B\,[G] * d[cm] * \lambda\,[Å] / 395600$

For $\varphi = 2\pi$

$B d = 135.7 \text{ G.cm}/ \lambda\,[Å] = 1.357\ 10^{-3} \text{ T.m}/ \lambda\,[nm]$



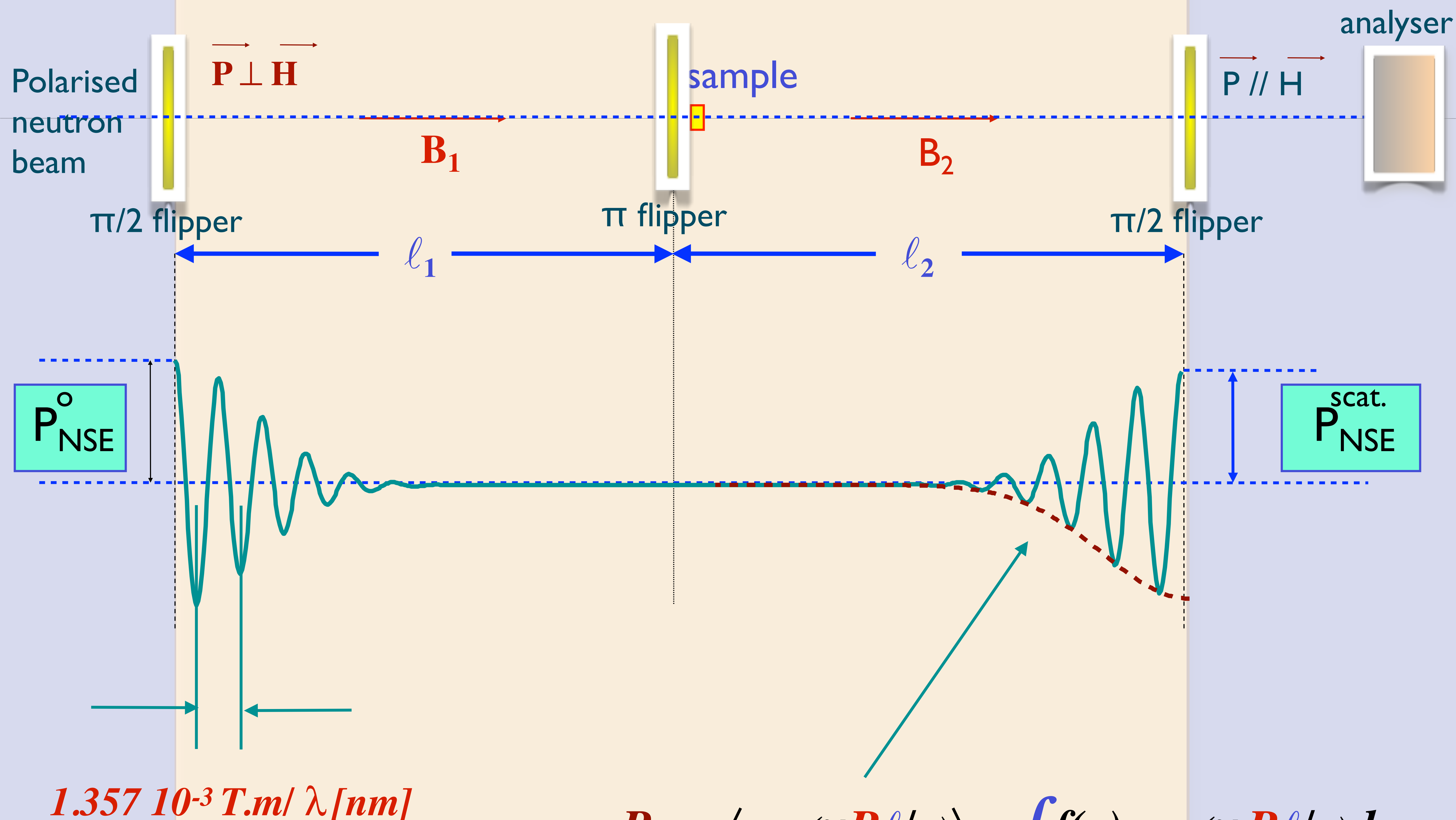


Beam Polarization

$$|\vec{P}| = \frac{I_+ - I_-}{I_+ + I_-}$$

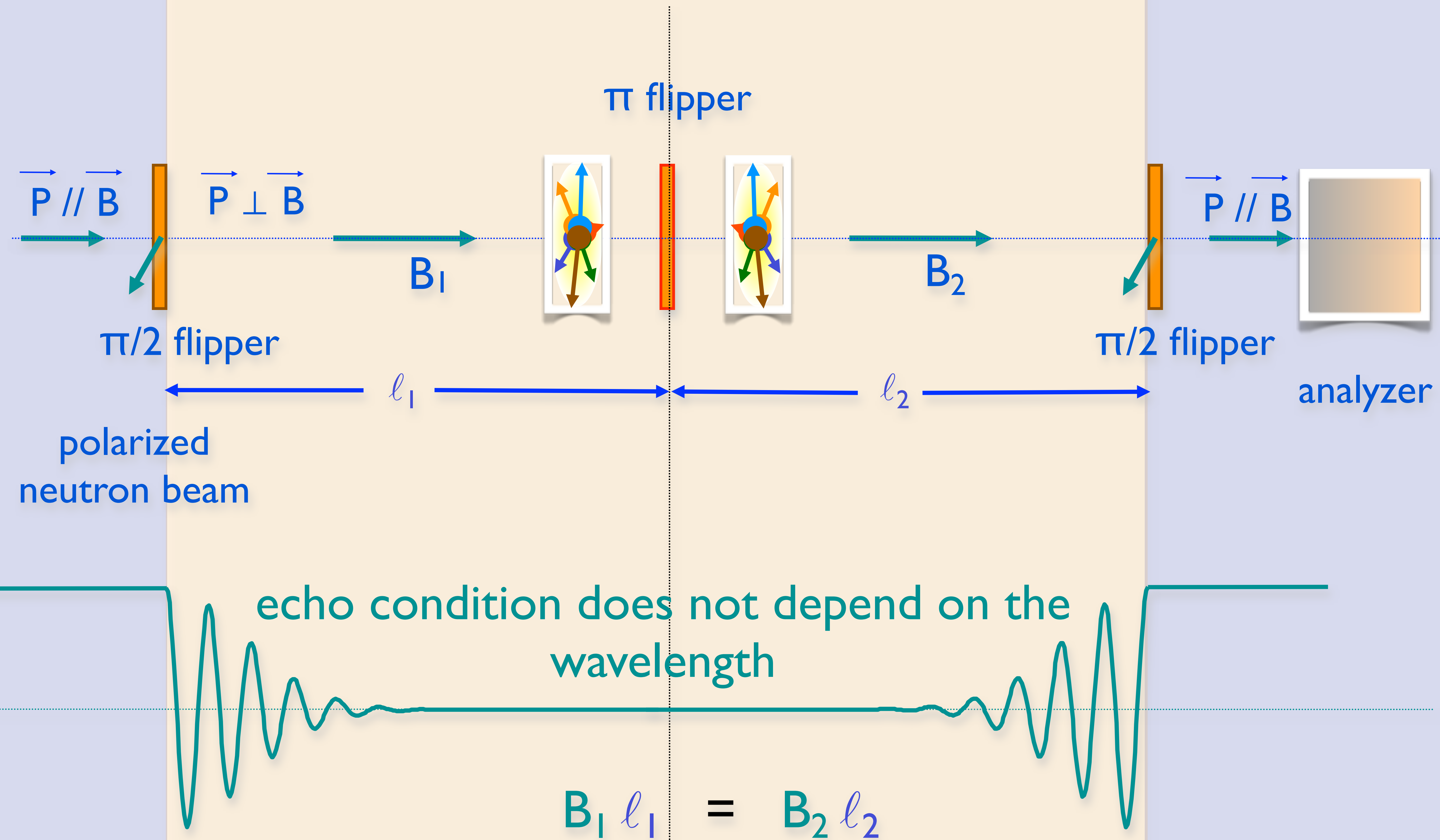
$$\Delta\phi \propto \Delta\lambda$$

neutron spin echo



$$P_{//\vec{B}} = \langle \cos(\gamma B \ell / v) \rangle = \int f(v) \cos(\gamma B \ell / v) dv$$

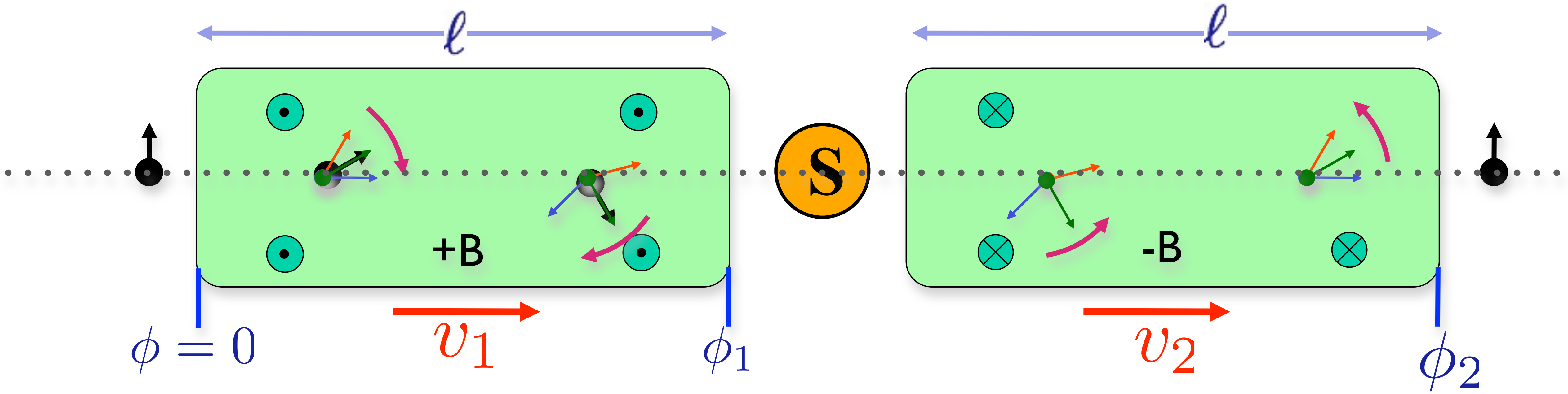
neutron spin echo



echo condition does not depend on the wavelength

$$B_1 \ell_1 = B_2 \ell_2$$

basic equations

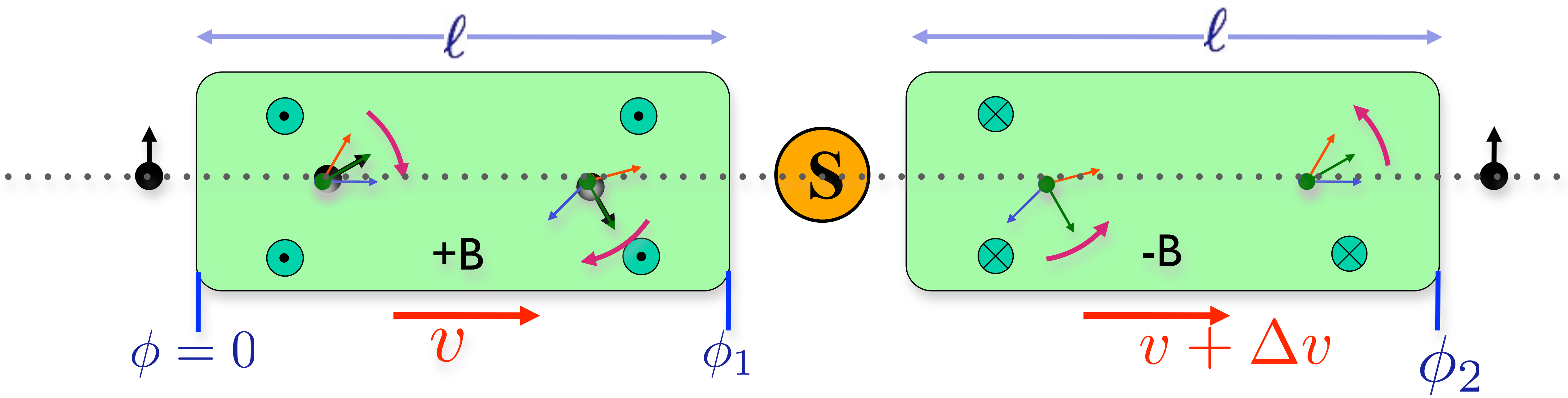


$$\phi_1 = \omega_L \cdot \ell / v_1 \qquad \phi_2 = \omega_L \cdot \ell (1/v_1 - 1/v_2)$$

for $v_1 = v$ and $v_2 = v + \Delta v \;\Rightarrow$

$$\phi_2 = \omega_L \, \ell \, [1/v - 1/(v + \Delta v)] \approx \omega_L \, \ell \, \Delta v / v^2 = \omega_L \, t \, \Delta v / v$$

basic equations



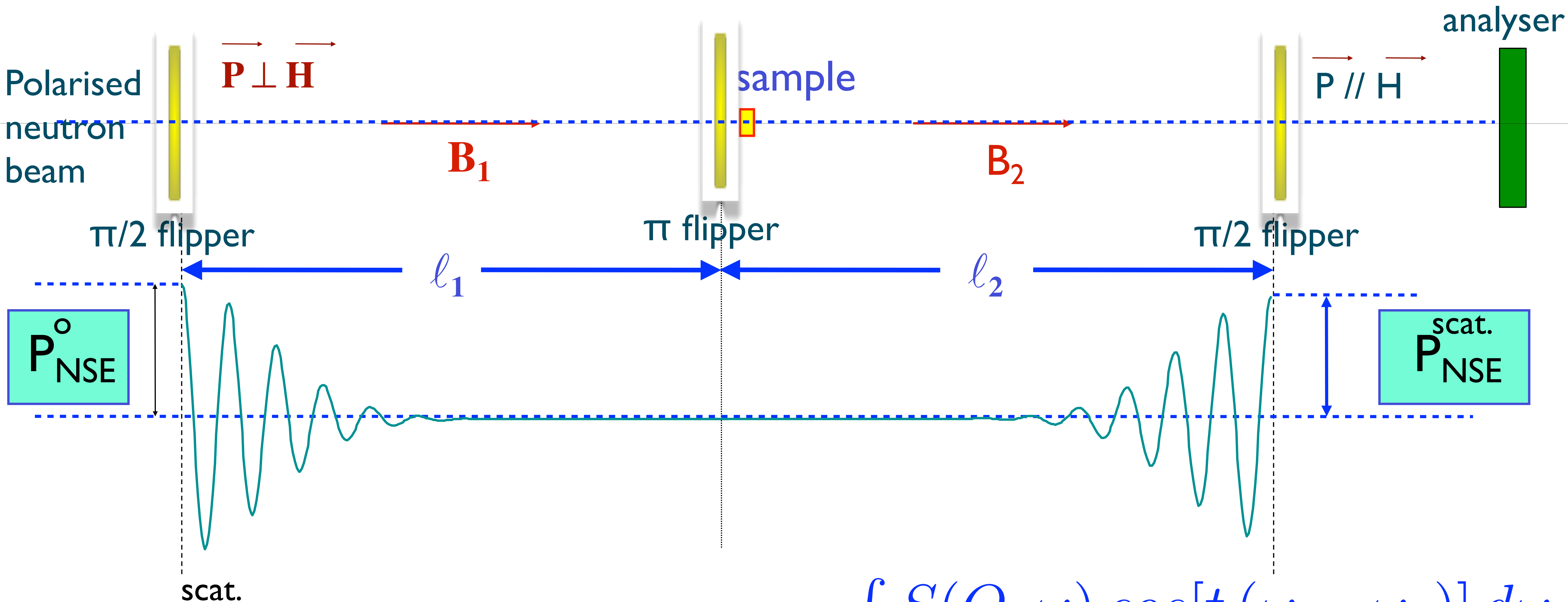
scattering theory : $\Delta v \rightarrow \omega$

$$\hbar\omega = m/2 \cdot (v_1^2 - v_2^2) = m/2 \cdot (v_1 + v_2)(v_1 - v_2) \approx m \cdot v \cdot \Delta v$$

$$\phi_2 = \omega_L \,\ell\, [1/v - 1/(v + \Delta v)] \approx \omega_L \,\ell\, \Delta v / v^2 = \omega_L \, t \, \Delta v / v$$

$$\Rightarrow \phi_2 = t_{NSE}\, \omega$$

and $t_{NSE} = \omega_L \cdot \ell \cdot \hbar / (m v^3) = \omega_L \cdot t / (2\omega_o)$



$$P_{NSE} = P_s \langle cos(\phi - \langle \phi \rangle) \rangle = P_s \frac{\int S(Q,\omega)\, cos[t\,(\omega - \omega_o)]\, d\omega}{\int S(Q,\omega)\, d\omega}$$

for quasi-elastic scattering $\omega_o = 0$

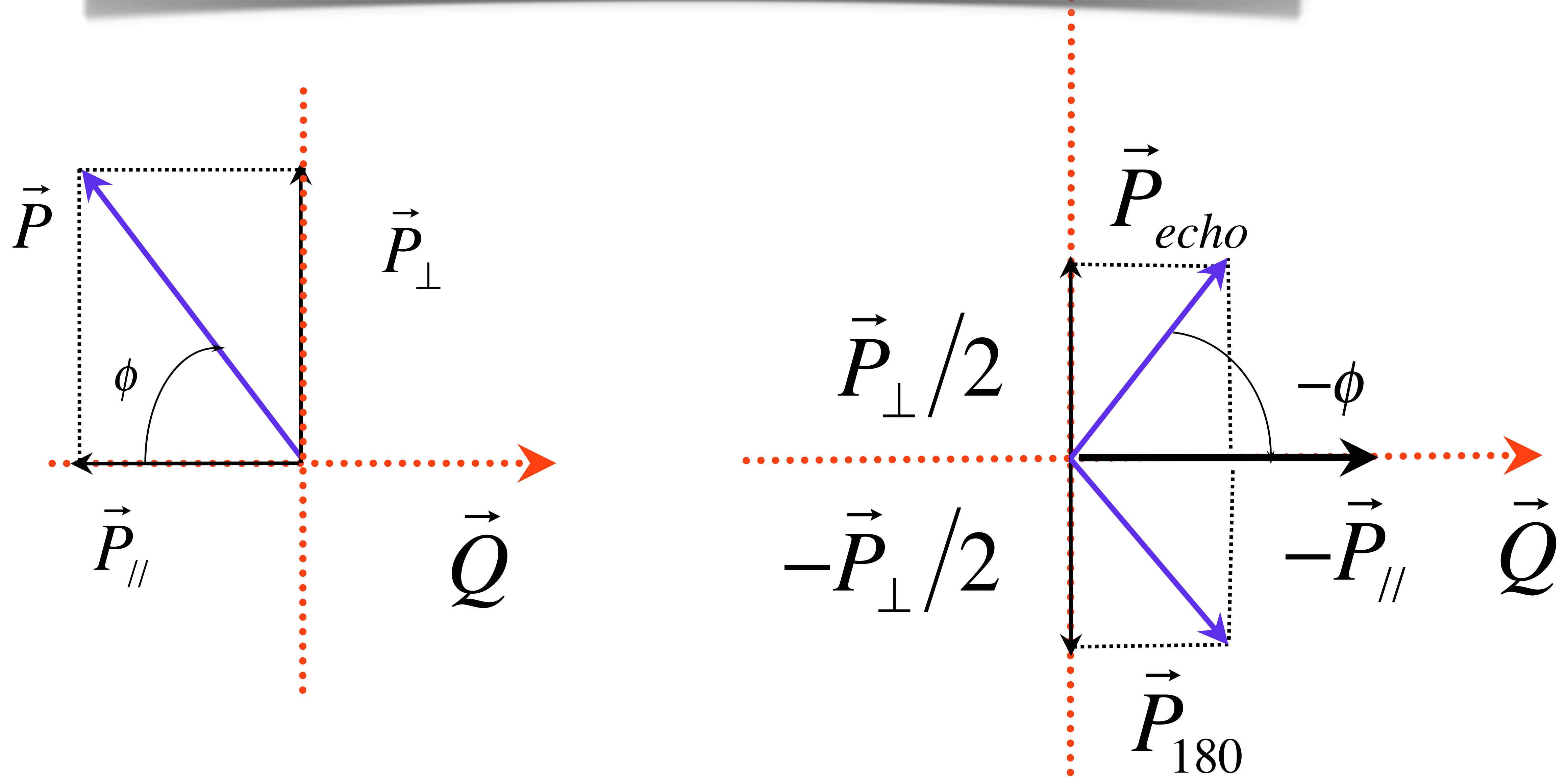
$$P^{scat}_{NSE}/P_s = \Re\,[S(Q,t)]/S(Q) = I(Q,t)$$

most generaly $\phi - \langle \phi \rangle = f(\vec{q},\omega) \propto S(\vec{(Q)},t)$

locally

paramagnetic scattering :

$$P' = -\hat{Q}\,(\hat{Q}\cdot\vec{P})$$

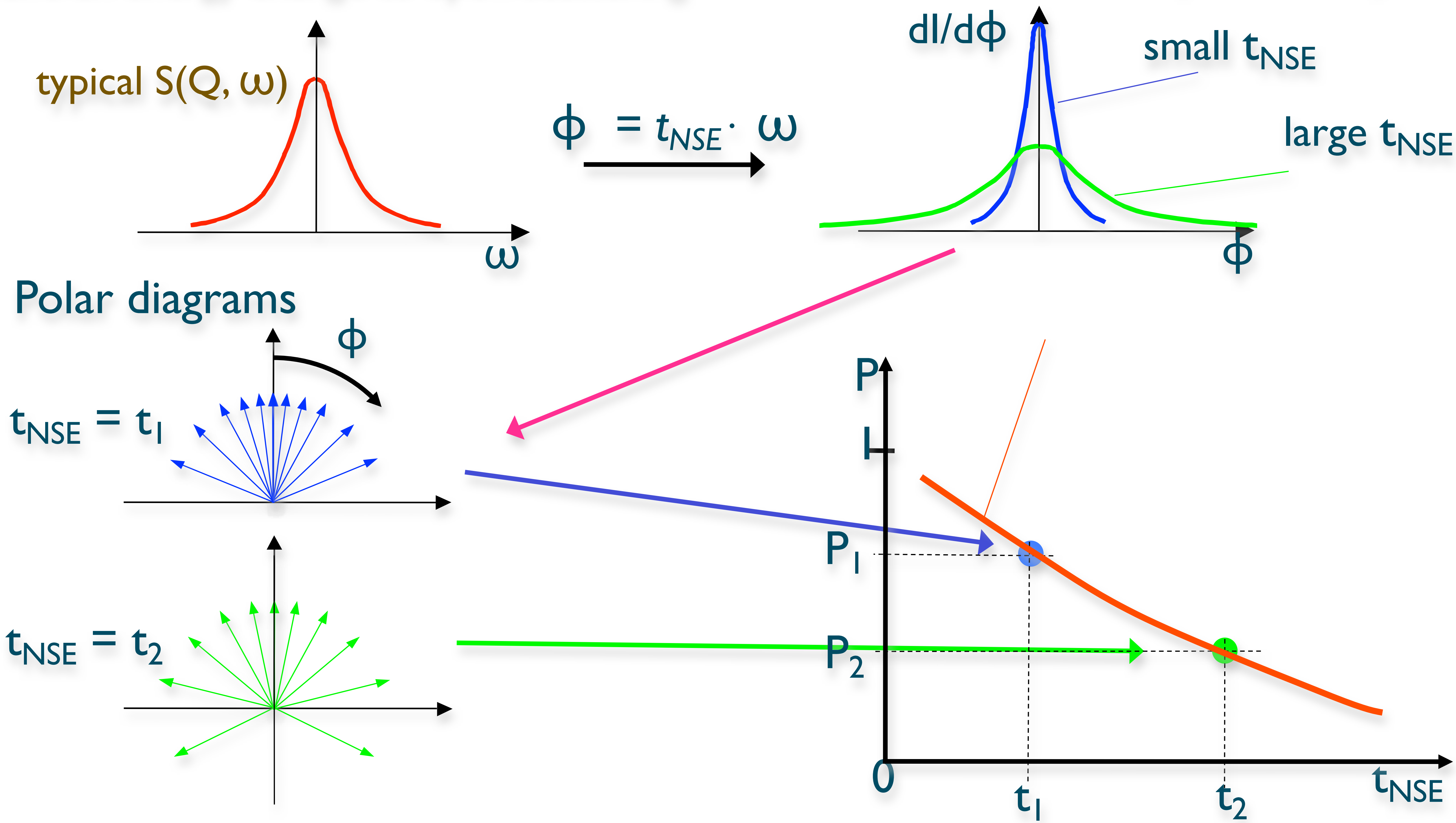


the π flipper is the sample

measuring principle

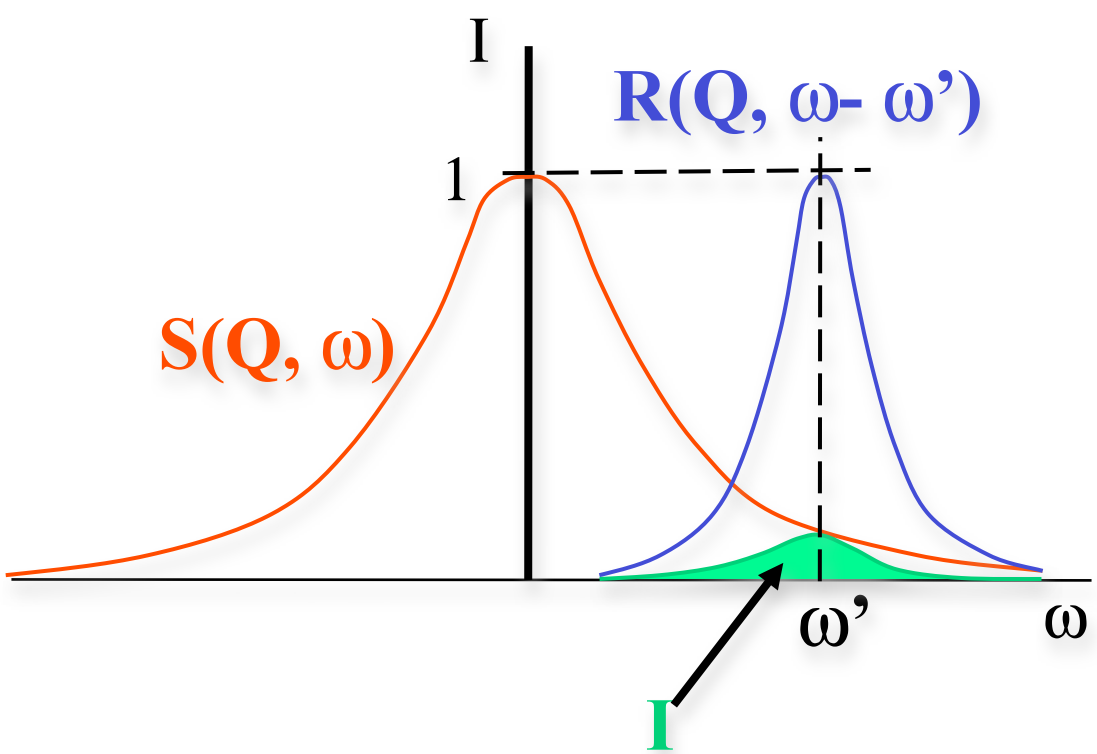
$S(Q, \omega)$: probability for a momentum change Q and an energy change ω upon scattering

distribution of spins at analyzer



Fourier transform and resolution

Let S(Q, ω) be the scattering function and let R(Q, ω) be the resolution function.



If a spectrometer is set to ω', then the norm. countrate is:

$$I(Q,\omega') = \int S(Q,\omega)\, R(Q,\omega-\omega')\, d\omega$$

$$= S \otimes R\text{; convolution;}$$

The function R(Q, ω- ω') should be the same over the range, where S(Q, ω) is significant;

If, like in spin echo, the Fourier Transform of I is the signal, then the convolution of S and R can be written as

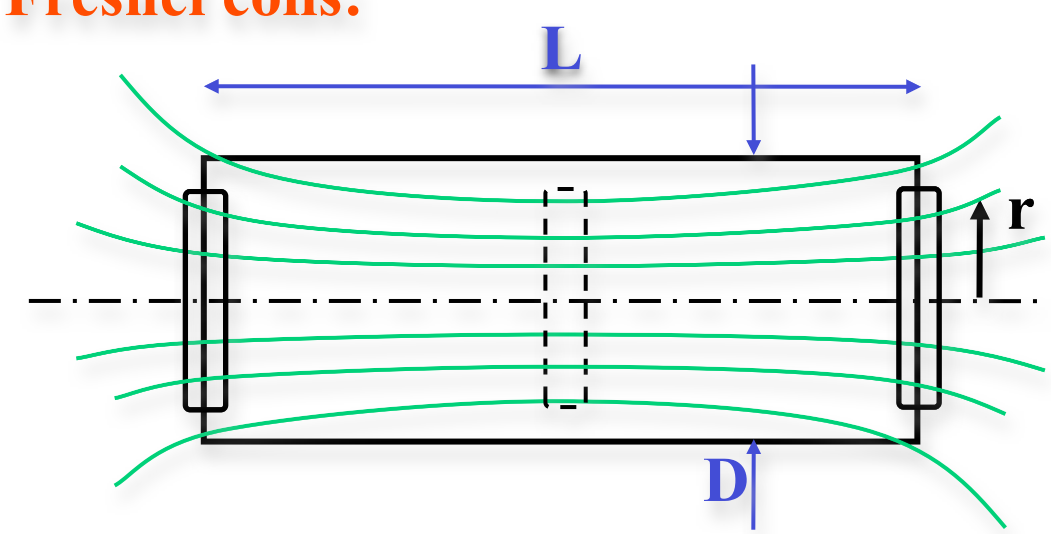
$$FT(I) = FT\{S \otimes R\} = FT\{S\} \cdot FT\{R\}$$

For NSE: $FT(I) = FT\left\{\frac{\gamma^2}{\gamma^2+\omega^2} \otimes \frac{\gamma_o^2}{\gamma_o^2+\omega^2}\right\} = e^{-\gamma t} e^{-\gamma_o t} = e^{-(\gamma+\gamma_o)t}$

Subtleties of NSE

- fields are mostly longitudinal;
- adiabatic transitions at ends;
- ‘π/2 coils’ to start or end precession;
- ‘π coils’ to reverse effective field direction; (Hahn’s echoes; NMR-imaging);
- ‘Fresnel coils’ to compensate field inhomogeneities
- Adiabaticity parameter; at sample; at coils;
- How to measure polarization?
- Spin flip due to spin-incoherent (2/3)
  or paramagnetic scattering (depends on $O(\vec{P}, \vec{Q})$)
- Spin echo for ferromagnetic samples;

Fresnel coils:



Standard cylindrical coil:

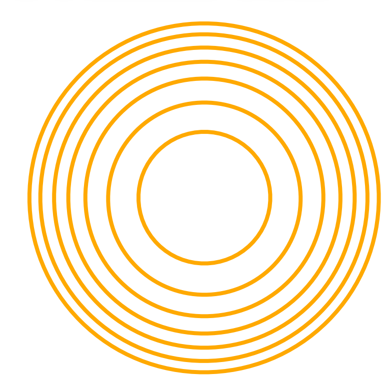
$\int Bdl \approx B_0 L + B_0 r^2/2D;$

Correction by current loops:

$\int B_F\, df \sim I ;$

Current around loop

Fresnel coil



density of loops increases with r^2;

Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : Larmor precession

III: NSE : semi-classical description

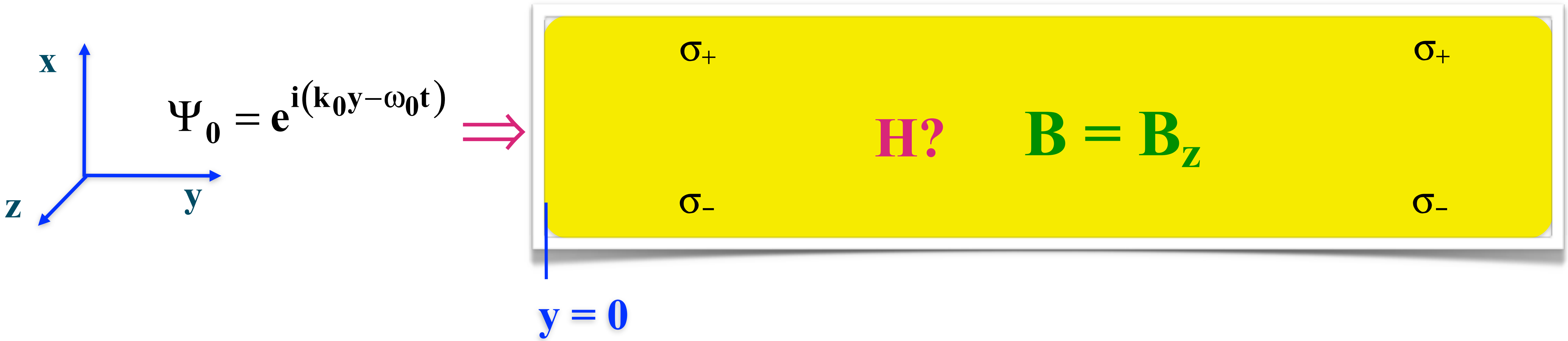
IV: movies

V: quantum mechanical approach

VI: examples

VII: NSE and structure

Plane wave entering a static B-field



$$\Psi_0 = e^{i(k_0 y - \omega_0 t)} \Rightarrow$$

the 2 states Ψ_+ and Ψ_- have different kinetic energies $E_0 \pm \mu \cdot B$

Static case [dB/dt = 0]: no change in total energy ($\omega = \omega_0$) but change in k

$$\frac{\hbar^2 k_\pm^2}{2m} = \frac{\hbar^2 k_0^2}{2m} \pm \mu B; \quad \Rightarrow \quad \frac{\hbar^2}{2m}\left(k_\pm^2 - k_0^2\right) = \pm \mu B;$$

$$\mu \cdot B \,,\, E_{kin} \quad \Rightarrow \quad \left(k_\pm^2 - k_0^2\right) \approx \left(k_\pm - k_0\right) 2k_0 = \Delta k_\pm \cdot 2k_0; \qquad \Delta k_\pm = \frac{2m}{\hbar^2}\frac{\mu B}{2k_0} = \frac{\mu B}{\hbar \times v}$$

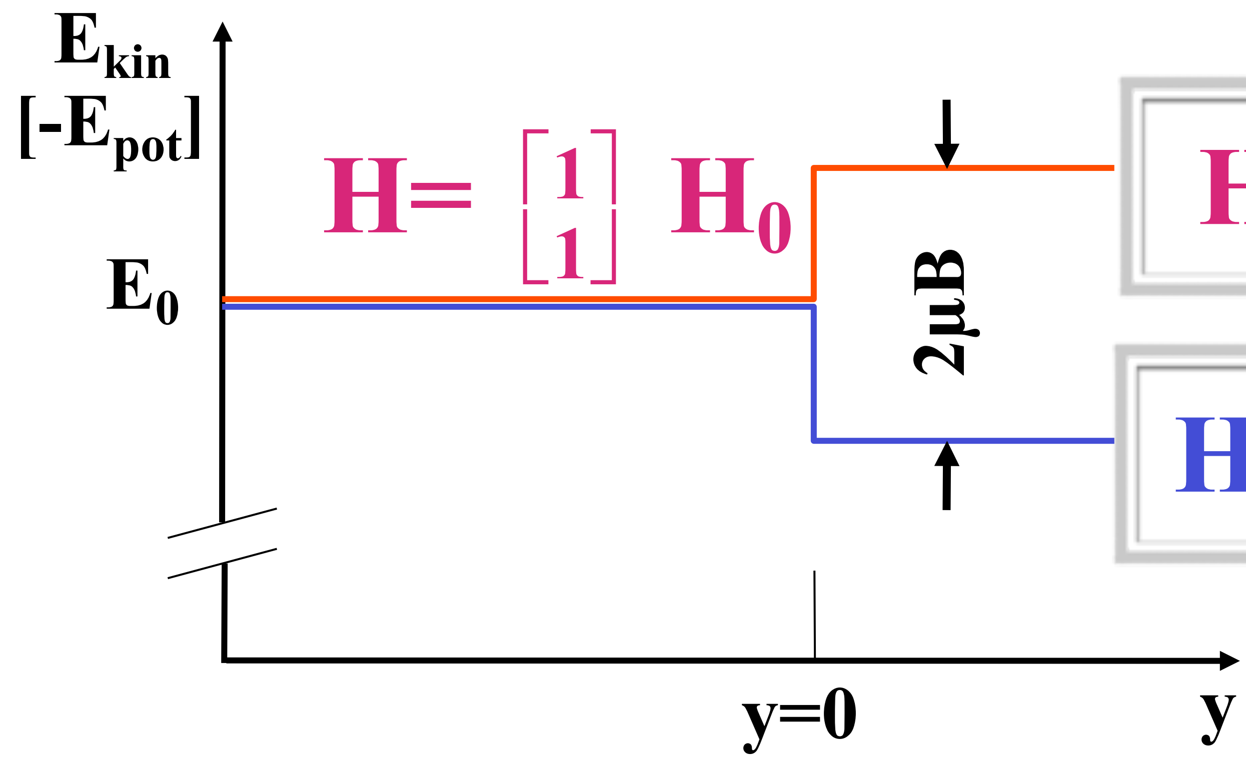
v is the classical neutron velocity

$$\Psi = \begin{vmatrix} \Psi_+ \\ \Psi_- \end{vmatrix} = \begin{vmatrix} e^{i(y\mathrm{k}_+ - \omega_o t)} \\ e^{i(y\mathrm{k}_- - \omega_o t)} \end{vmatrix} = e^{i(y\mathrm{k}_o - \omega_o t)} \begin{vmatrix} e^{+iy\Delta\mathrm{k}} \\ e^{-iy\Delta\mathrm{k}} \end{vmatrix}$$

Both states have equal amplitudes, as the initial polarization is perpendicular to the axis of quantization (z-axis);

These amplitudes $\frac{1}{\sqrt{2}}$ are set to 1 here.

Energy diagram:

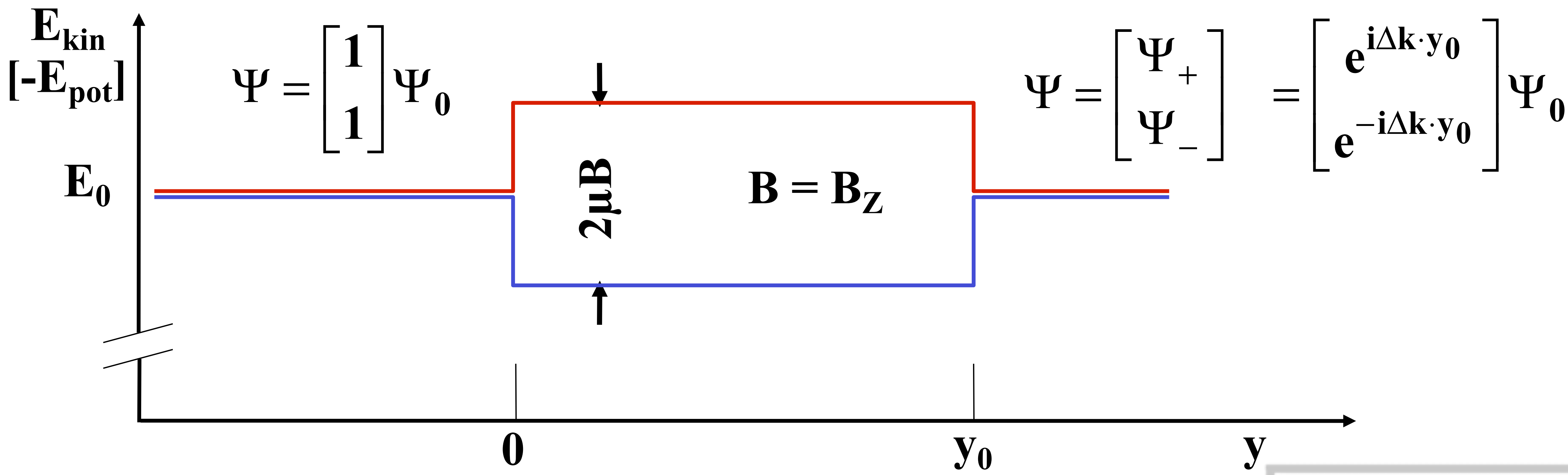


$$\mathbf{H_+ = H_0 \cdot e^{i\,\Delta k\,y}}$$

$$\mathbf{H_- = H_0 \cdot e^{-i\,\Delta k\,y}}$$

$$\mathbf{\Delta k = \mu \cdot B/\hbar v}$$

in a magnetic field



$$\Delta k = \mu \cdot B/\hbar v$$
$$t_0 = y_0/v$$

Setting the polarizer to x-direction:

$$I_x = \frac{1}{\sqrt{2}}(\Psi_+ + \Psi_-) \quad \times CC \quad = \frac{1}{2}\left(e^{i\Delta k \cdot y_0} + e^{-i\Delta k \cdot y_0}\right)\left(e^{-i\Delta k \cdot y_0} + e^{i\Delta k \cdot y_0}\right)$$

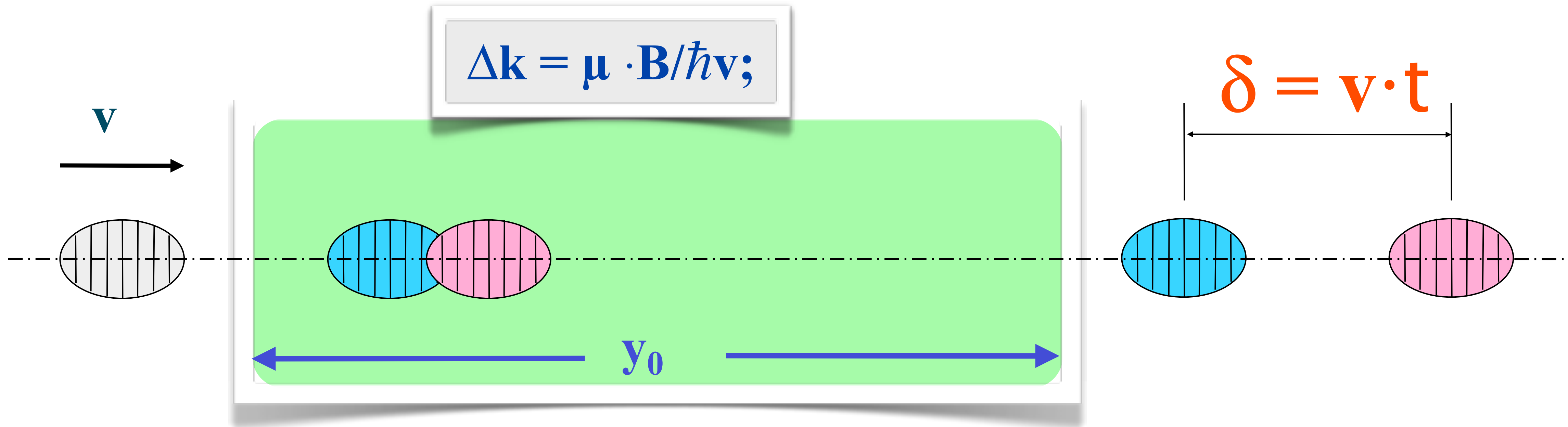
$$I_x = \frac{1}{2}\left(1 + 1 + e^{2i\Delta k \cdot y_0} + e^{-2i\Delta k \cdot y_0}\right) = 1 + \cos(2\Delta k \cdot y_0) = 1 + \cos\left(\frac{2\mu B}{\hbar v} \cdot y_0\right)$$

$I_x = 1 + \cos(\omega_L t_0)$; $\left[I_y = 1 + \sin(\omega_L t_0)\right]$; $\omega_L = 2\mu B/\hbar$; Larmor precession!

wavepackets instead of plane waves

wavepacket (bandwidth $\Delta\lambda$) of length Δy and lateral width $\Delta x = \Delta z$;

$\Delta y \approx \lambda^2/\Delta\lambda$; $\Delta x \approx \lambda/(2\pi\theta)$; θ = beam divergence; typ. values: $\Delta x, \Delta y \approx 100$ Å

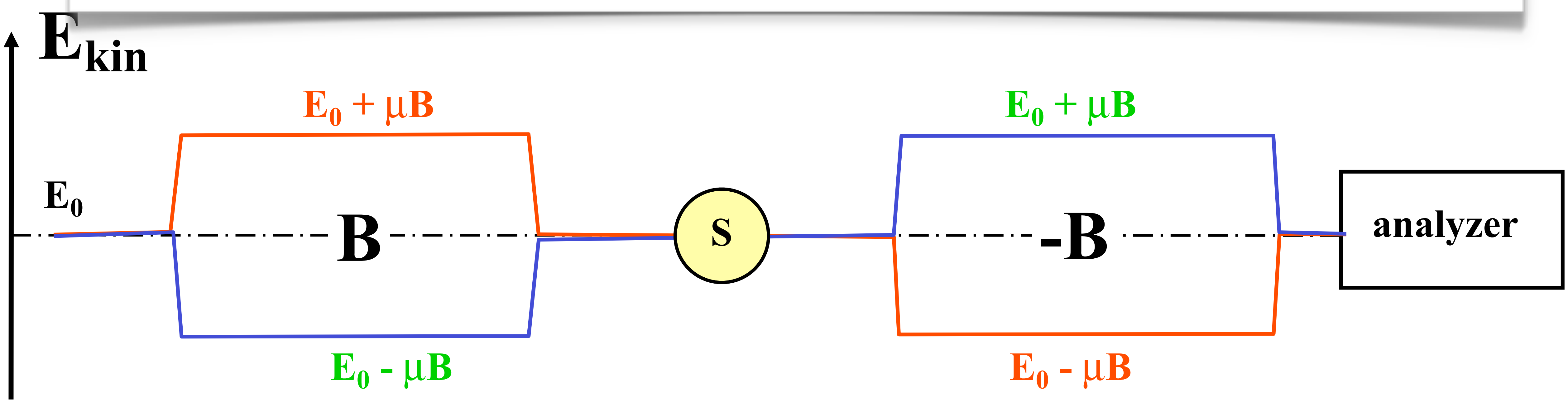


Time splitting dt = t of the two wave packets, separated by the propagation through the field of length $\mathbf{y}_0$:

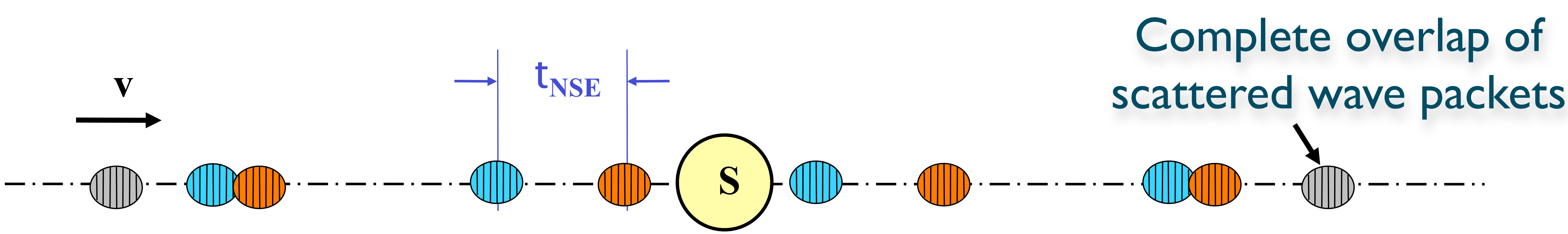
$$\frac{dE}{E} = \frac{2t}{t_o} \Rightarrow t = \frac{y_o}{2V} \cdot \frac{2\mu B}{\frac{1}{2} m V^2} = \frac{2\mu B \cdot y_o}{m V^3} = \frac{\omega_L \cdot t}{2\omega_o}$$

For fields of typ. 1 kG and length of m, t is in the ns range for cold neutrons;
In Neutron Spin echo spectroscopy, t is the ‘spin echo time’;

semi-classical description: measuring principle



- The first field splits the wavepacket into two
- the second one overlaps them again;
- The analyser superposes both packets;



Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : Larmor precession

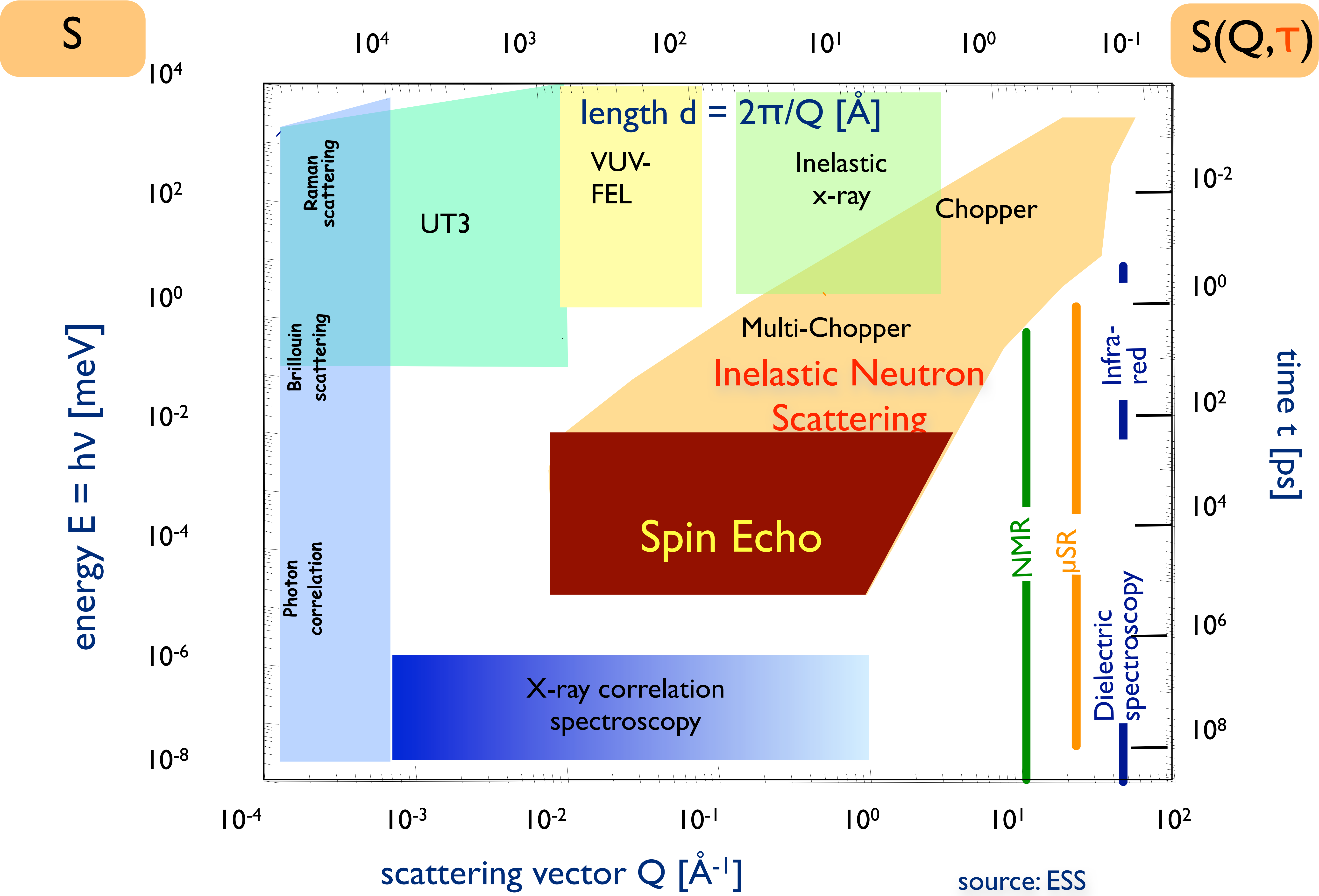
III: NSE : semi-classical description

IV: movies

V: quantum mechanical approach

VI: examples

VII: NSE and structure


S
S(Q,τ)
10⁴
10³
10²
10¹
10⁰
10⁻¹
length d = 2π/Q [Å]
Raman scattering
UT3
VUV-FEL
Inelastic x-ray
Chopper
Brillouin scattering
Multi-Chopper
Inelastic Neutron Scattering
Spin Echo
Photon correlation
X-ray correlation spectroscopy
NMR
μSR
Infra-red
Dielectric spectroscopy
energy E = hν [meV]
10⁴
10²
10⁰
10⁻²
10⁻⁴
10⁻⁶
10⁻⁸
time τ [ps]
10⁻²
10⁰
10²
10⁴
10⁶
10⁸
10⁻⁴
10⁻³
10⁻²
10⁻¹
10⁰
10¹
10²
scattering vector Q [Å⁻¹]
source: ESS

Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : Larmor precession

III: NSE : semi-classical description

IV: movies

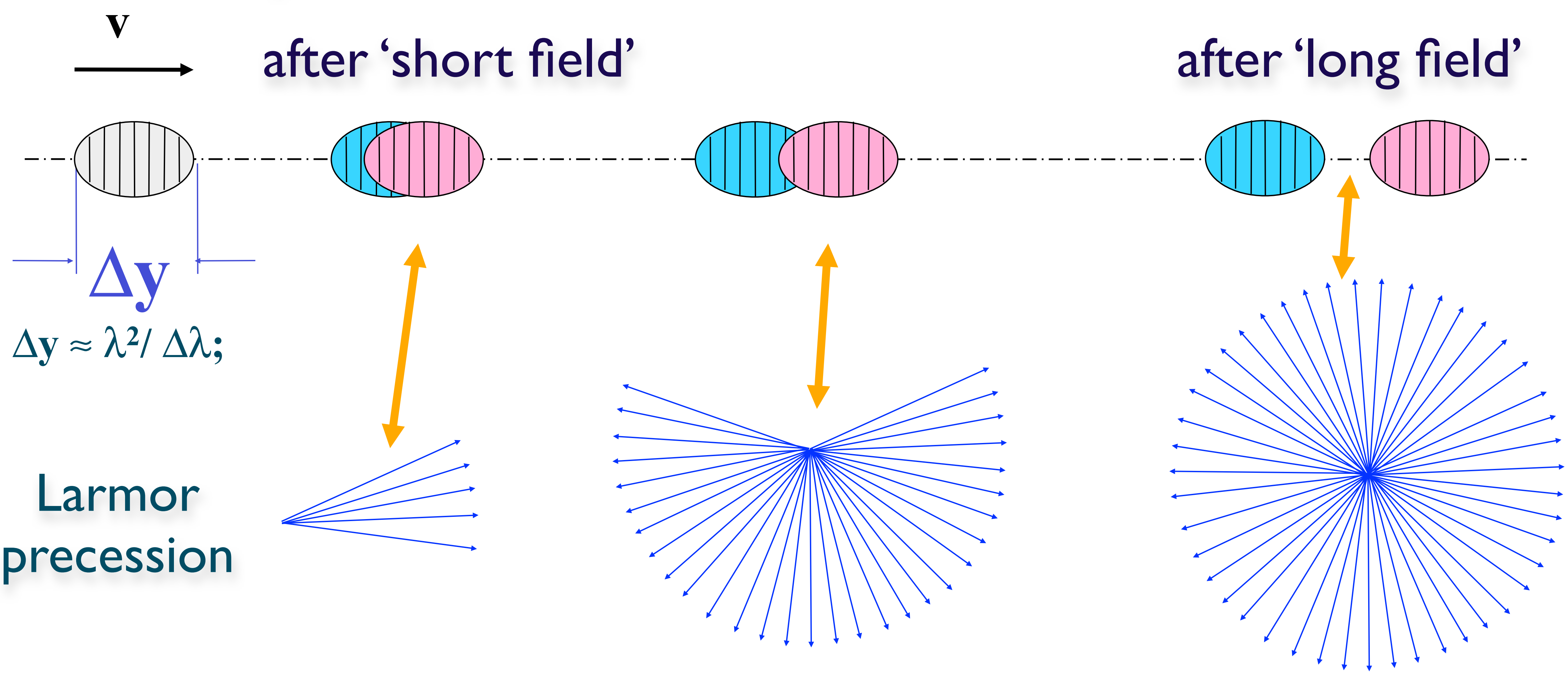
V: quantum mechanical approach

VI: examples

VII: NSE and structure

what is the real life - what is fantasy ?

semi-classical picture:



Directions of the individual spins of the polychromatic beam after passage through B fields of different lengths

Complete separation of the two packets implies that no coherent superposition of both states exists any more what is the real life - what is fantasy ?

what is a spin ?

what is the coherent superposition of states ?

quantum mechanics

=

plane waves

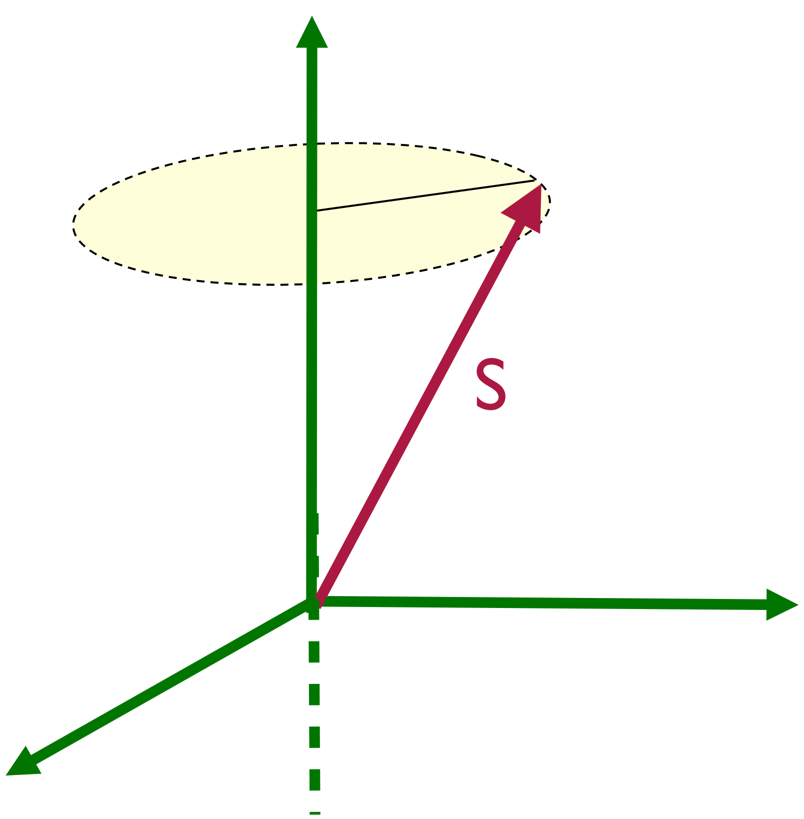
is a coherent superposition of the two states their “sum” ?

$$|+\rangle + |-\rangle$$ vs. the spin in the plane

the spin is not a vector (classical view)

what is classical what is quantum mechanical coherent superposition of states

the spin is not a vector (classical)

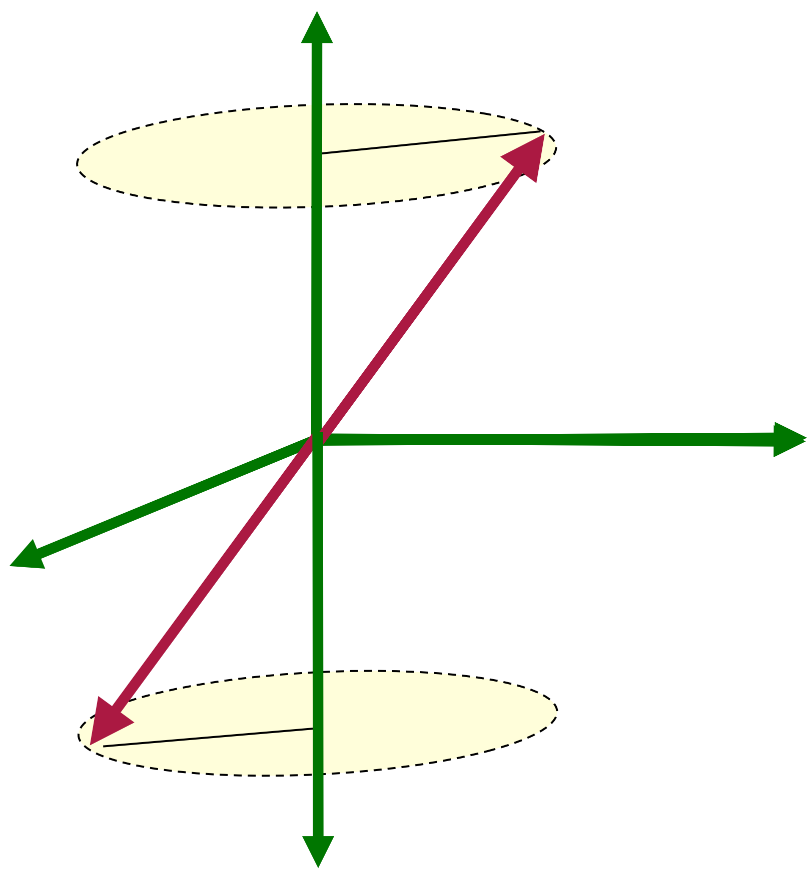


$s = 1/2$

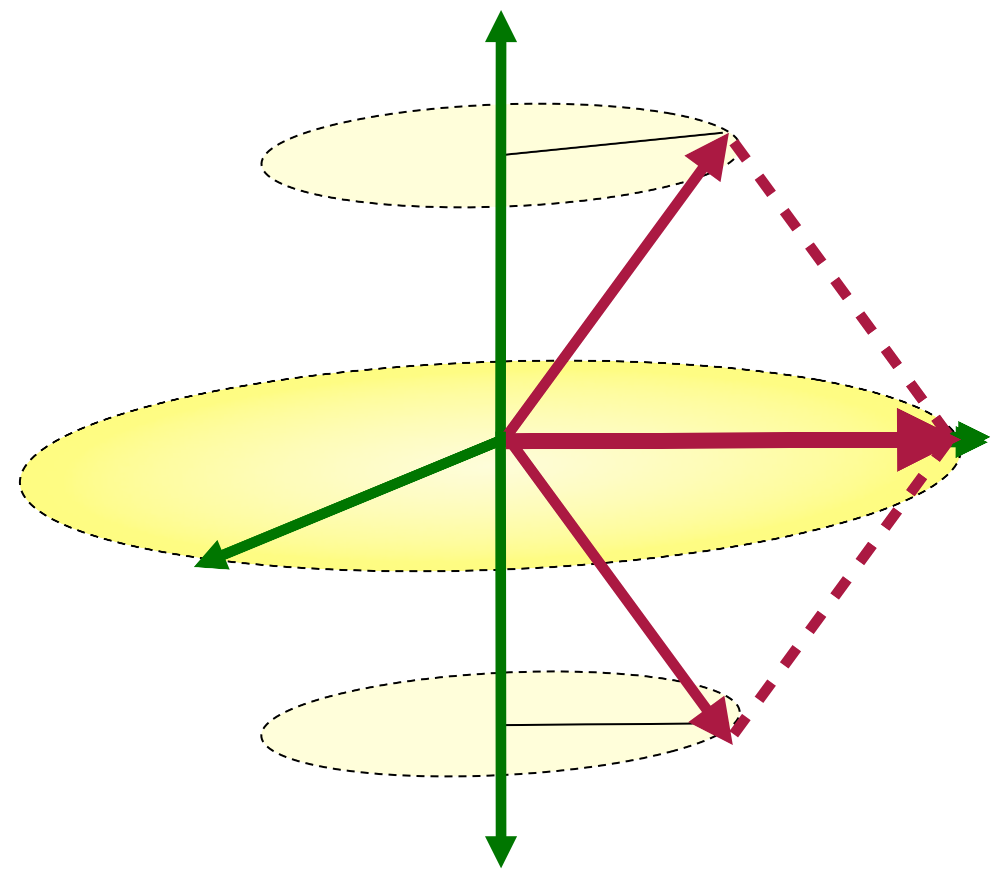
$$s_z = \begin{cases} +1/2 \\ -1/2 \end{cases}$$

coherent superposition of states

spin 1 case gives a hint: two $s_z=0$ states



singlet

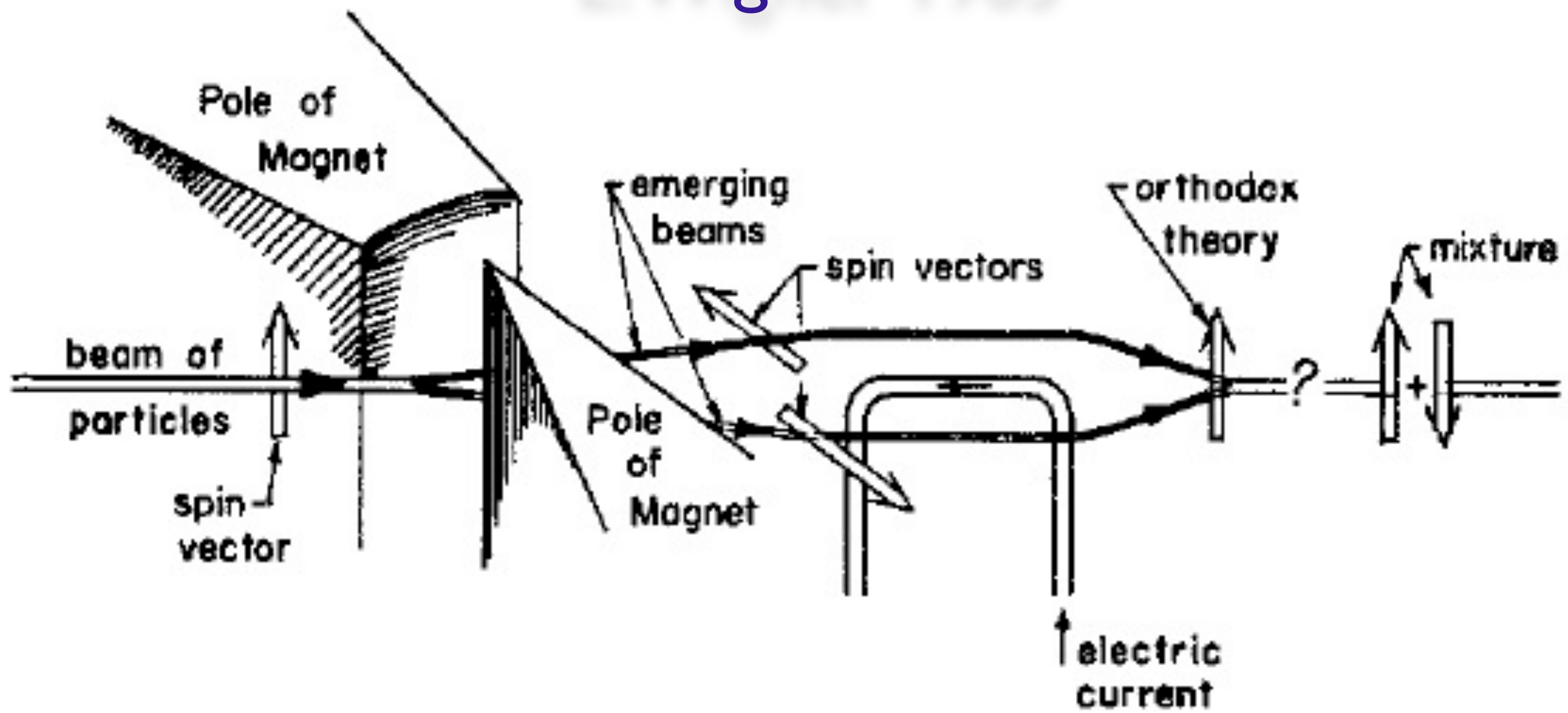


$s_z=0$ of the S=1 state

coherent superposition of states

Basics of QM :
2 slit experiment
wave - particle duality
The classical - "Copenhangen" - description of QM

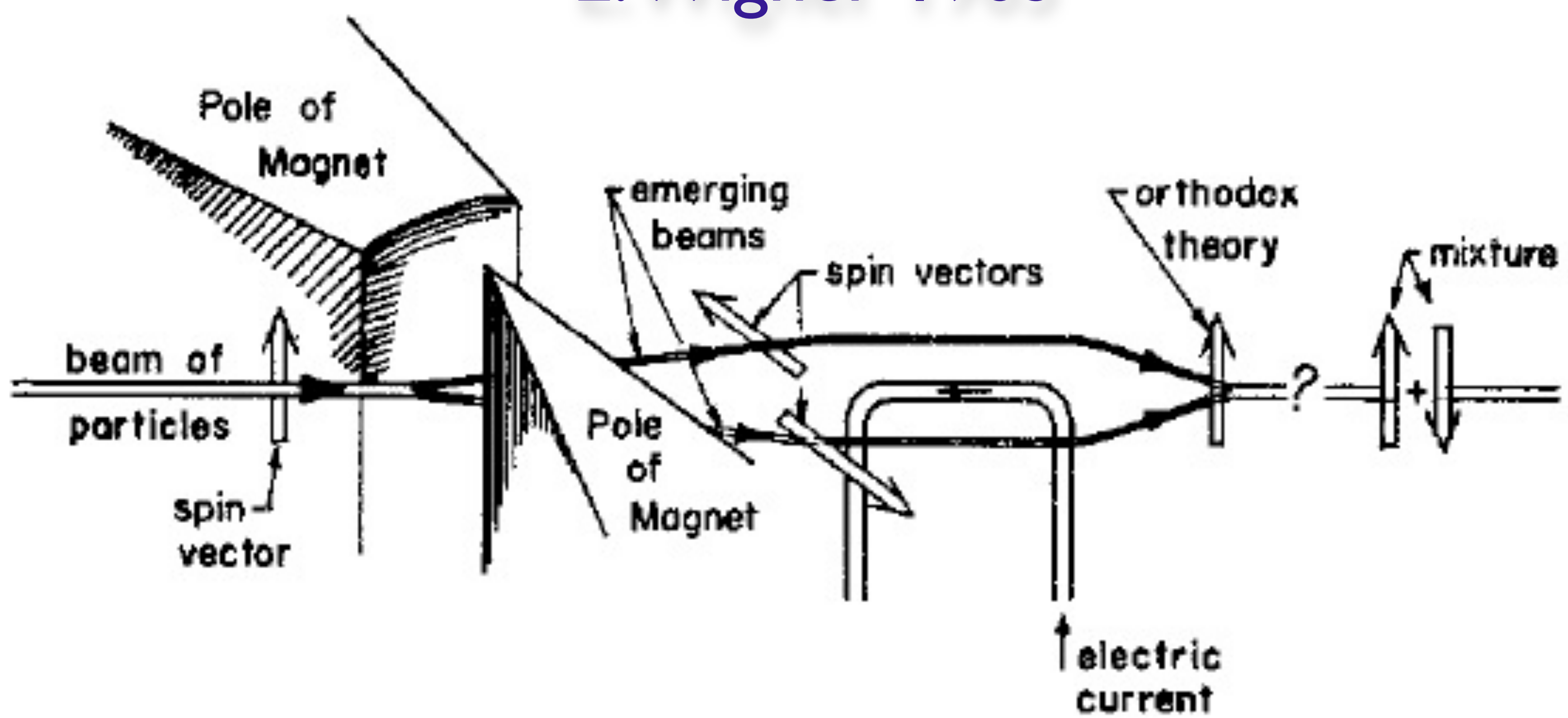
The Problem of Measurement
E. Wigner 1963



coherent superposition of states

Basics of QM :
2 slit experiment
wave - particle duality
The classical - "Copenhangen" - description of QM

The Problem of Measurement
E. Wigner 1963



Neutron Spin Echo

I: polarized neutrons - Larmor precession

II: NSE : Larmor precession

III: NSE : semi-classical description

IV: movies

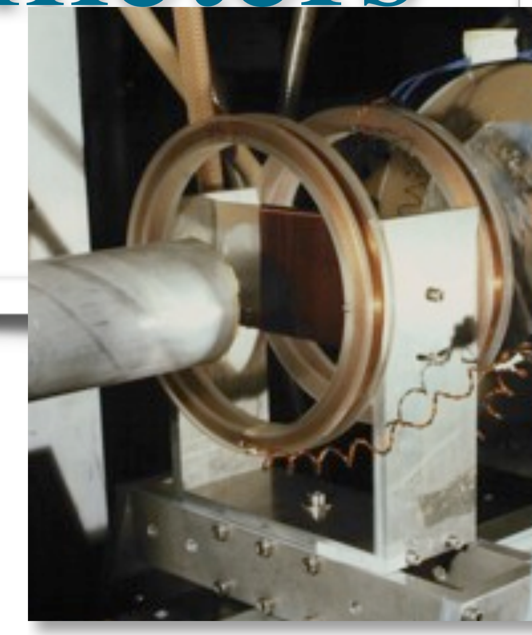
V: quantum mechanical approach

VI: examples

VII: NSE and structure

Neutron spin echo spectrometers-

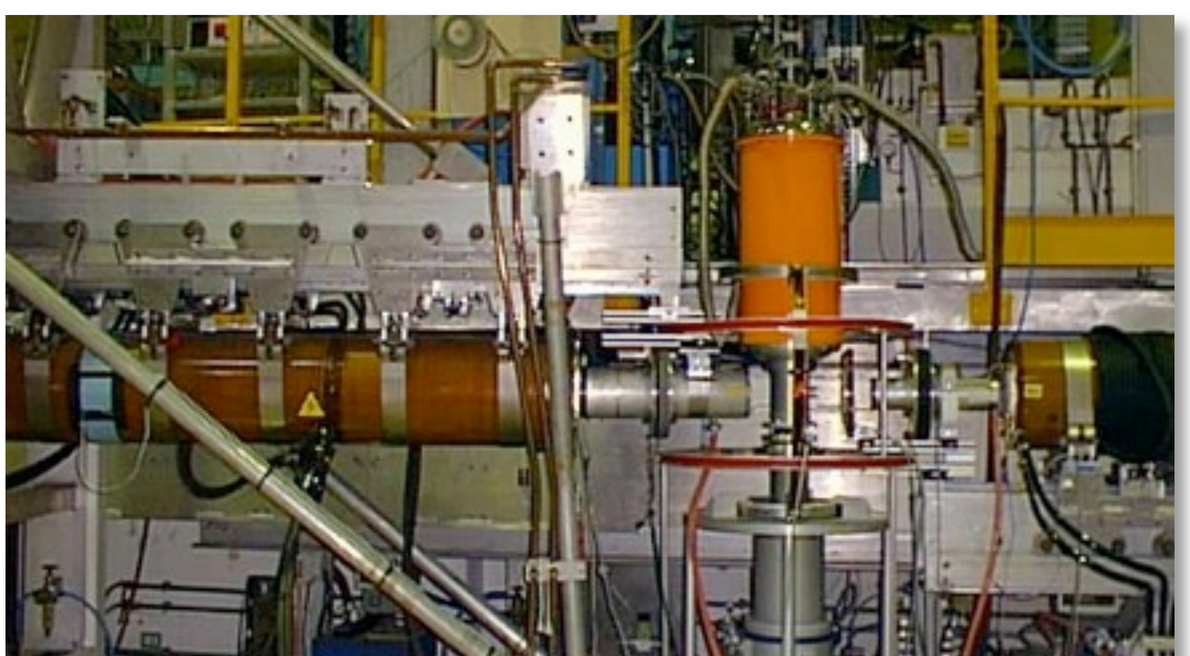
above: Mezei's first spin echo precession coils



right: π /2 flipper coils

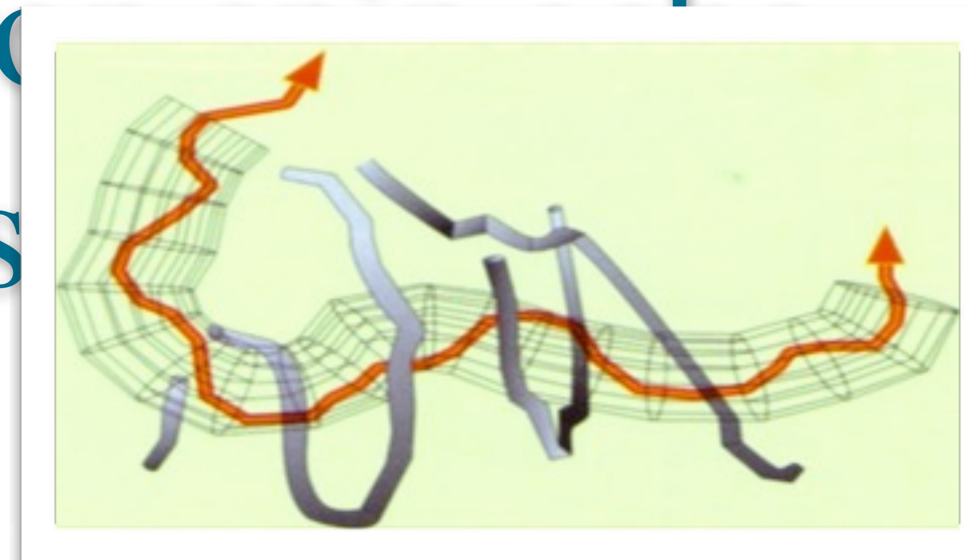
HZ Berlin

below: IN11



Examples of neutr studies

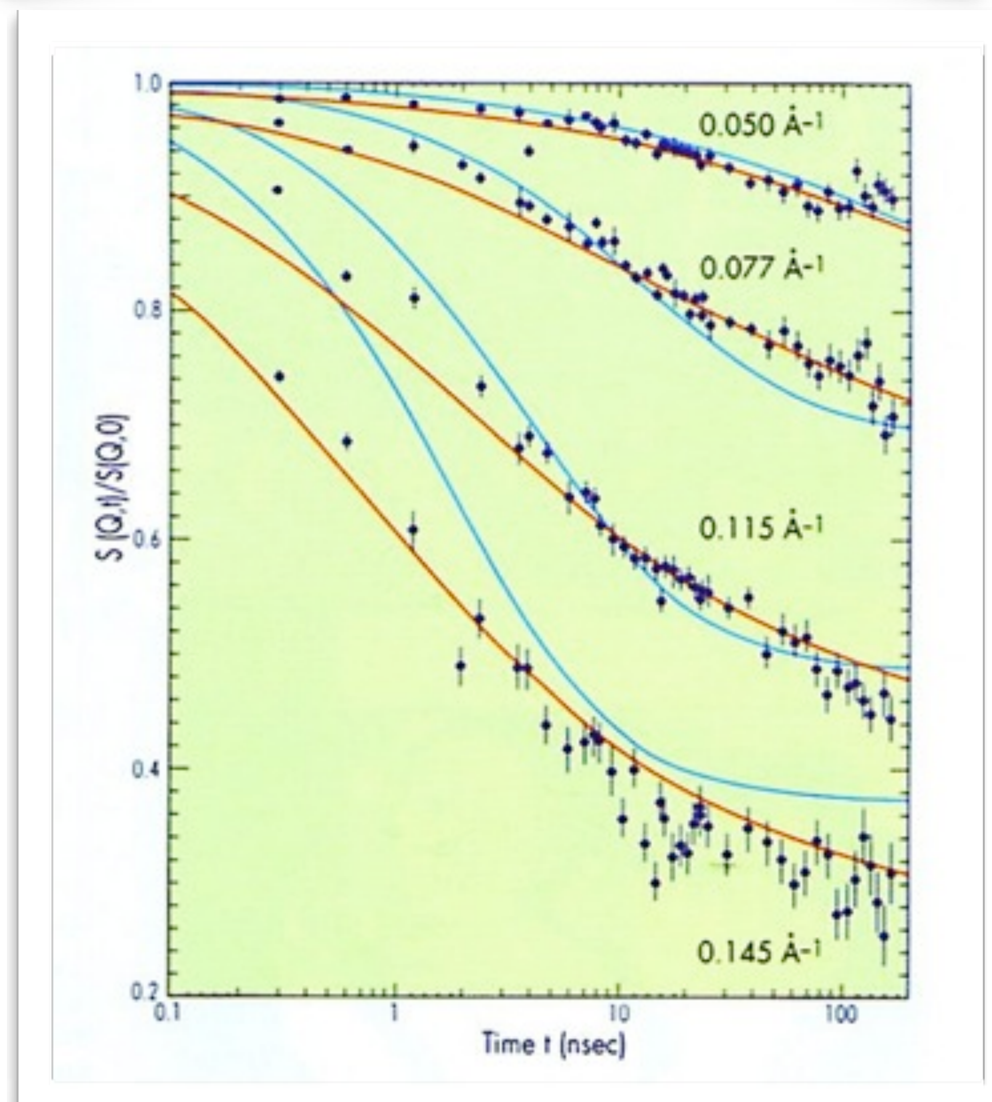
Reptation in polyethelene



The dynamics of dense polymeric systems are dominated by entanglement effects which reduce the degrees of freedom of each chain

de Gennes formulated the reptation hypothesis in which a chain is confined within a “tube” constraining lateral diffusion – although several other models have also been proposed

The measurements on IN15 are in agreement with the reptation model. Fits to the model can be made with one free parameter, the tube diameter, which is estimated to be 45Å

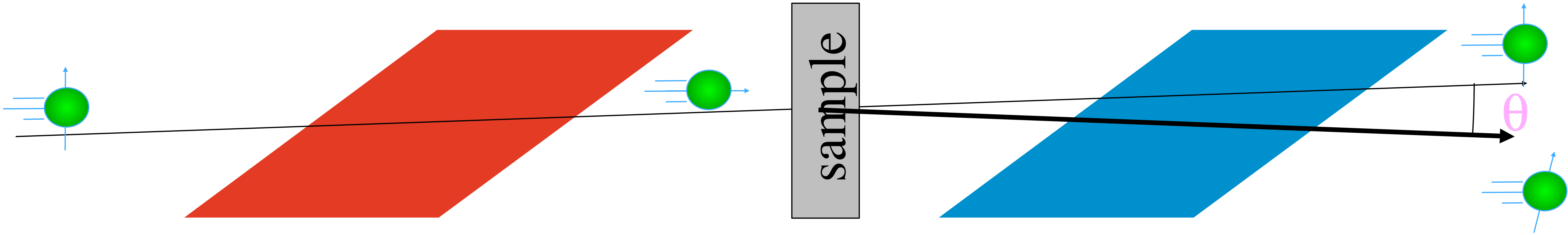


Schleger et al, Phys Rev Lett 81, 124 (1998)

Neutron Spin Echo

- I: polarized neutrons - Larmor precession
- II: NSE : Larmor precession
- III: NSE : semi-classical description
- IV: movies
- V: quantum mechanical approach
- VI: examples
- VII: NSE and structure

Larmor precession codes scattering angle



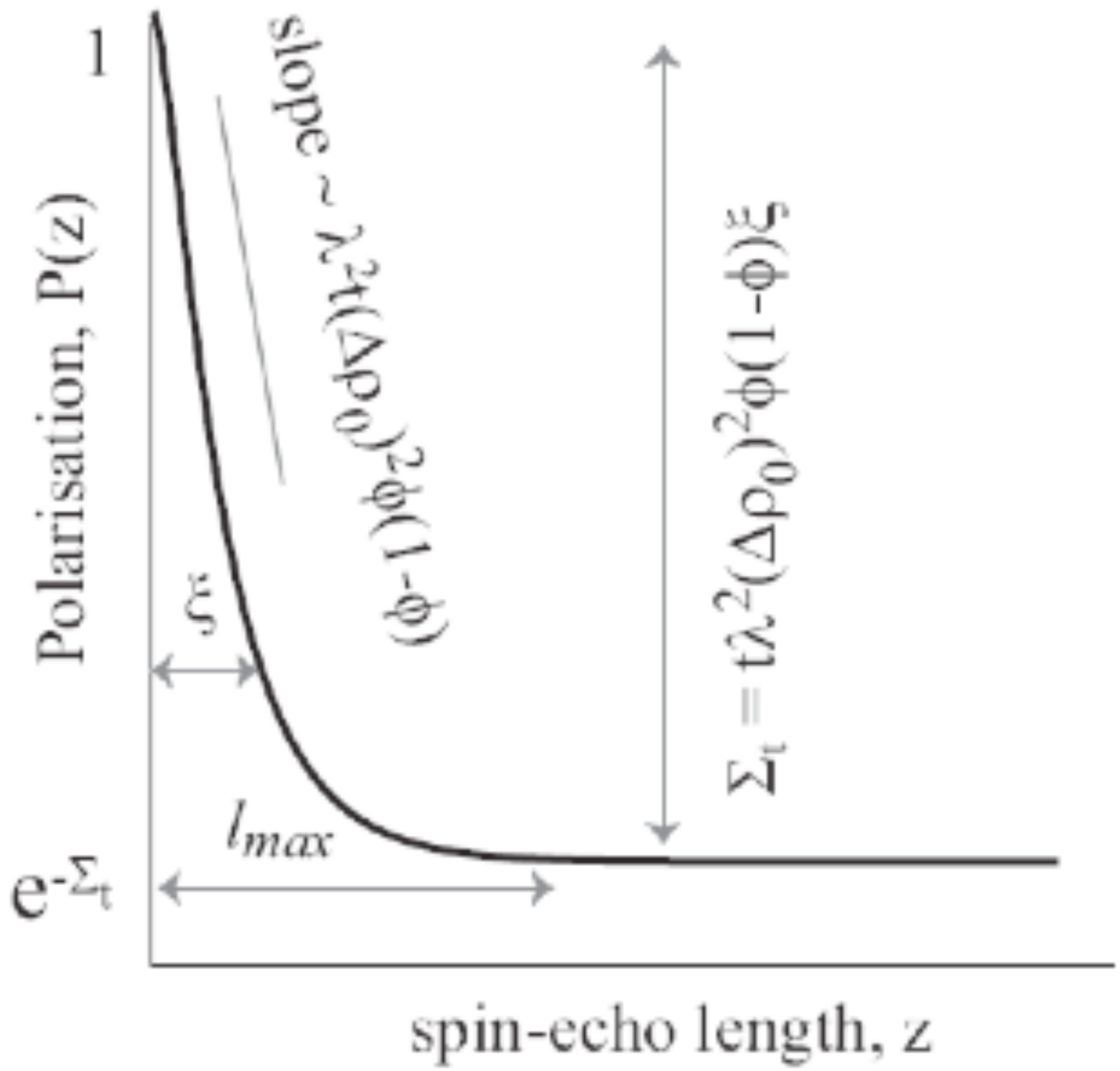
Unscattered beam gives spin echo at $\varphi = 0$
Independent of height and angle

Scattered wave vector transfer Q_z
results in precession ϕ $\qquad \phi \cong zQ_z$
Proportional to the **spin echo length** z

Measure polarisation: $P(z) = \cos(zQ_z)$
Fourier transform scattering cross-section:
real space density correlation function $G(z)$

Keller *et al.* Neutron News **6**, (1995) 16
Rekveldt, NIMB **114**, 366 (1996).

Direct information in measurement



Ordering

Compactness

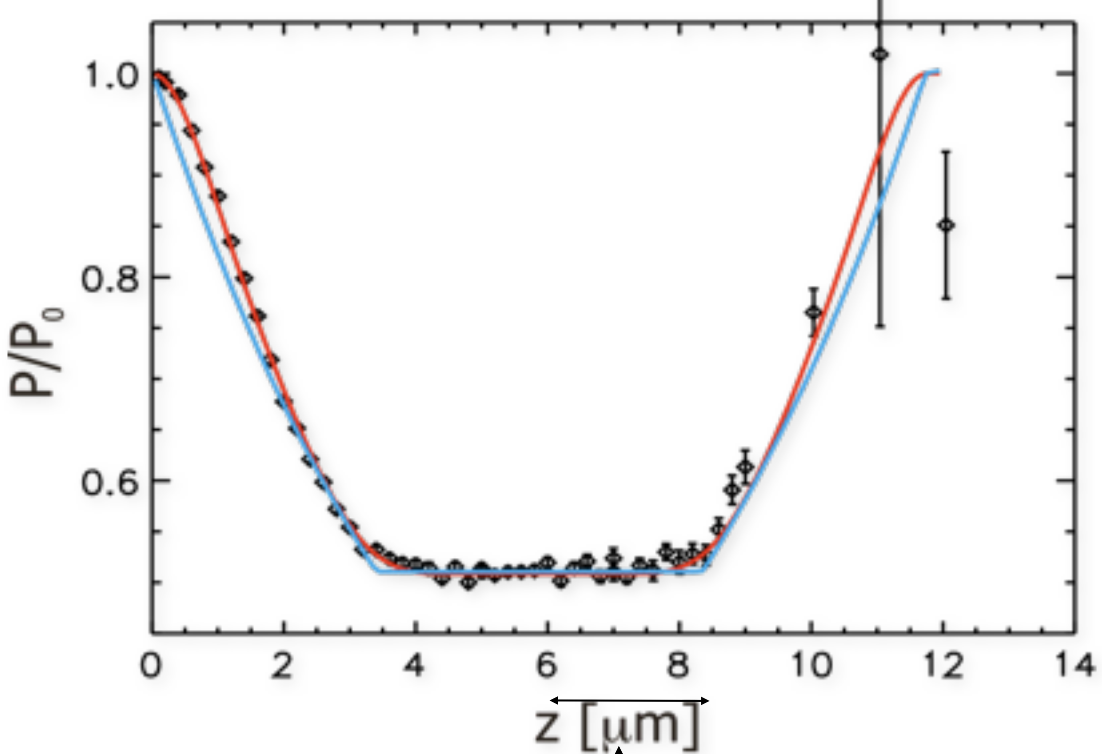
Correlation lengths

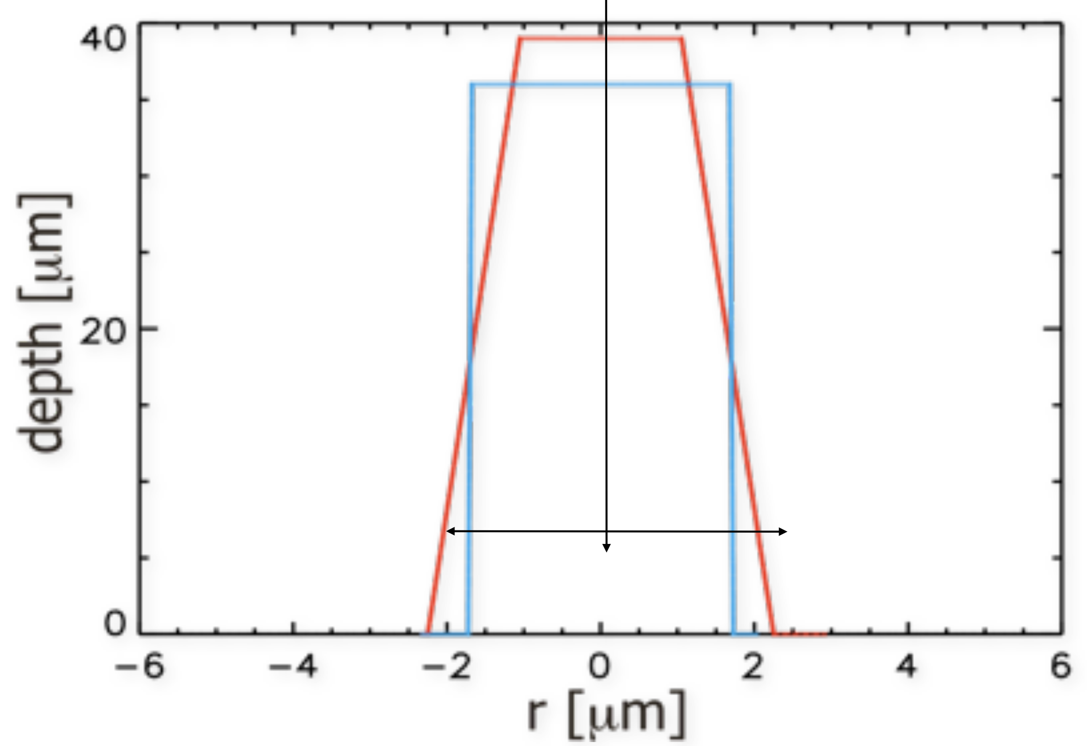
Fractal dimensions

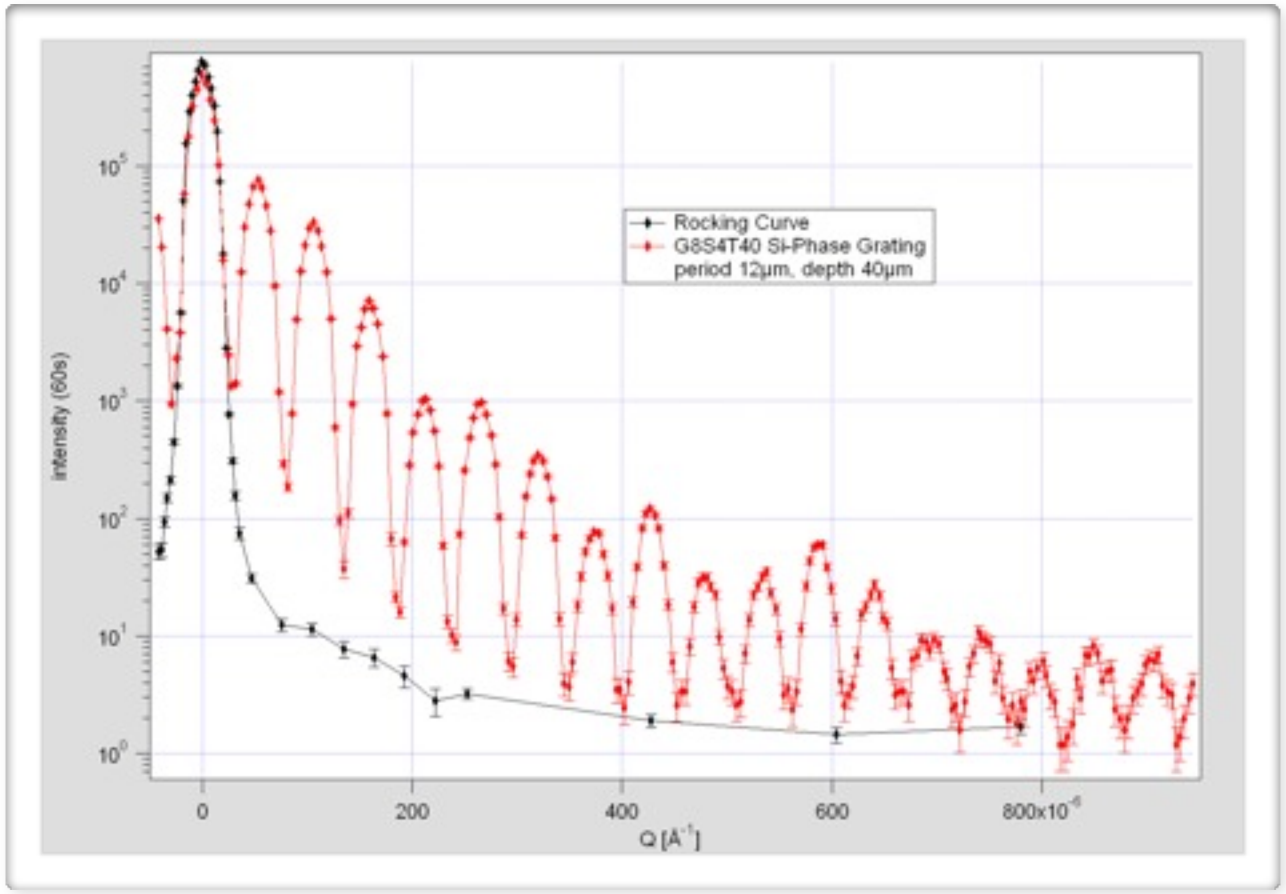
Specific surfaces

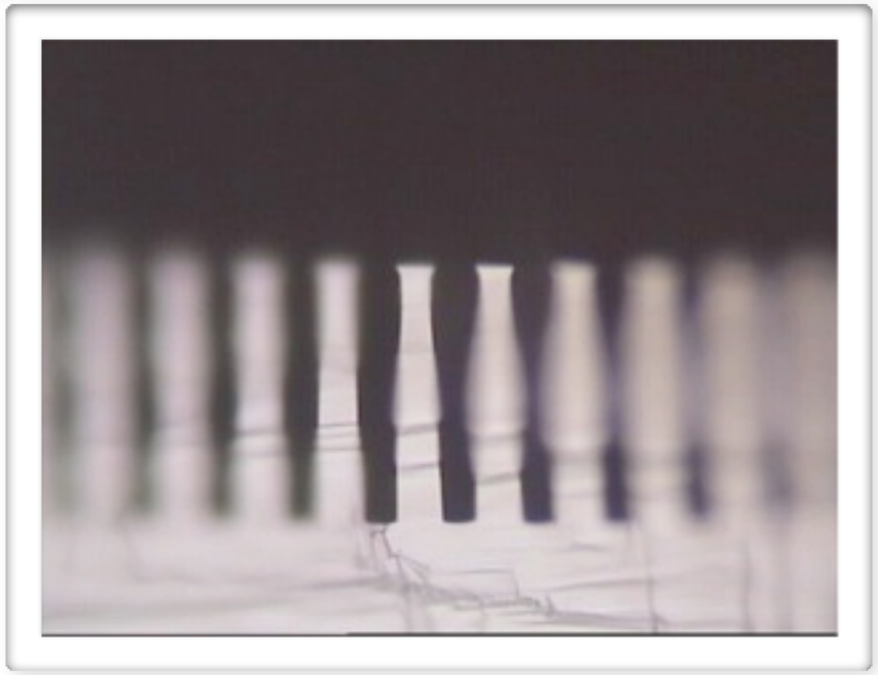
Etc…

SESANS measures directly shape ridges





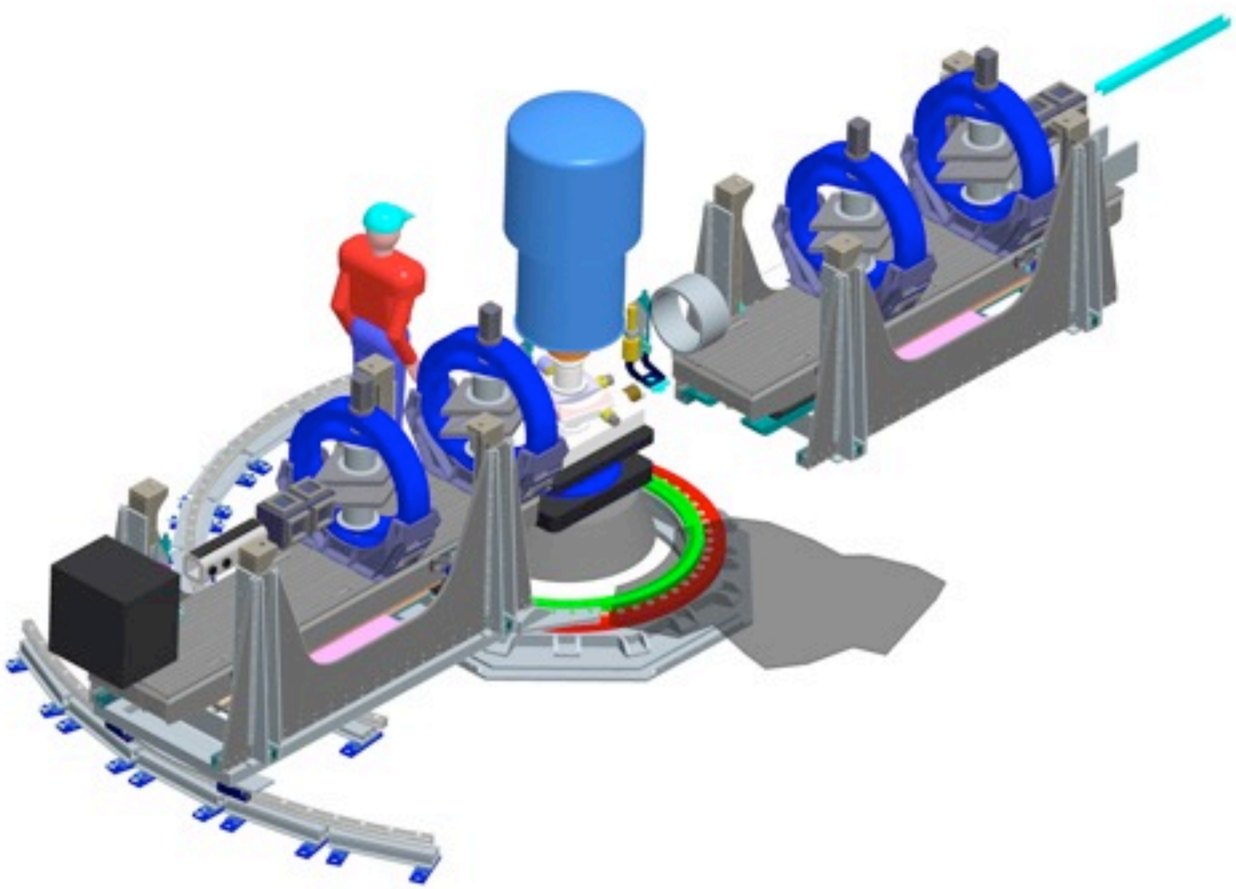




Realisation SESANS

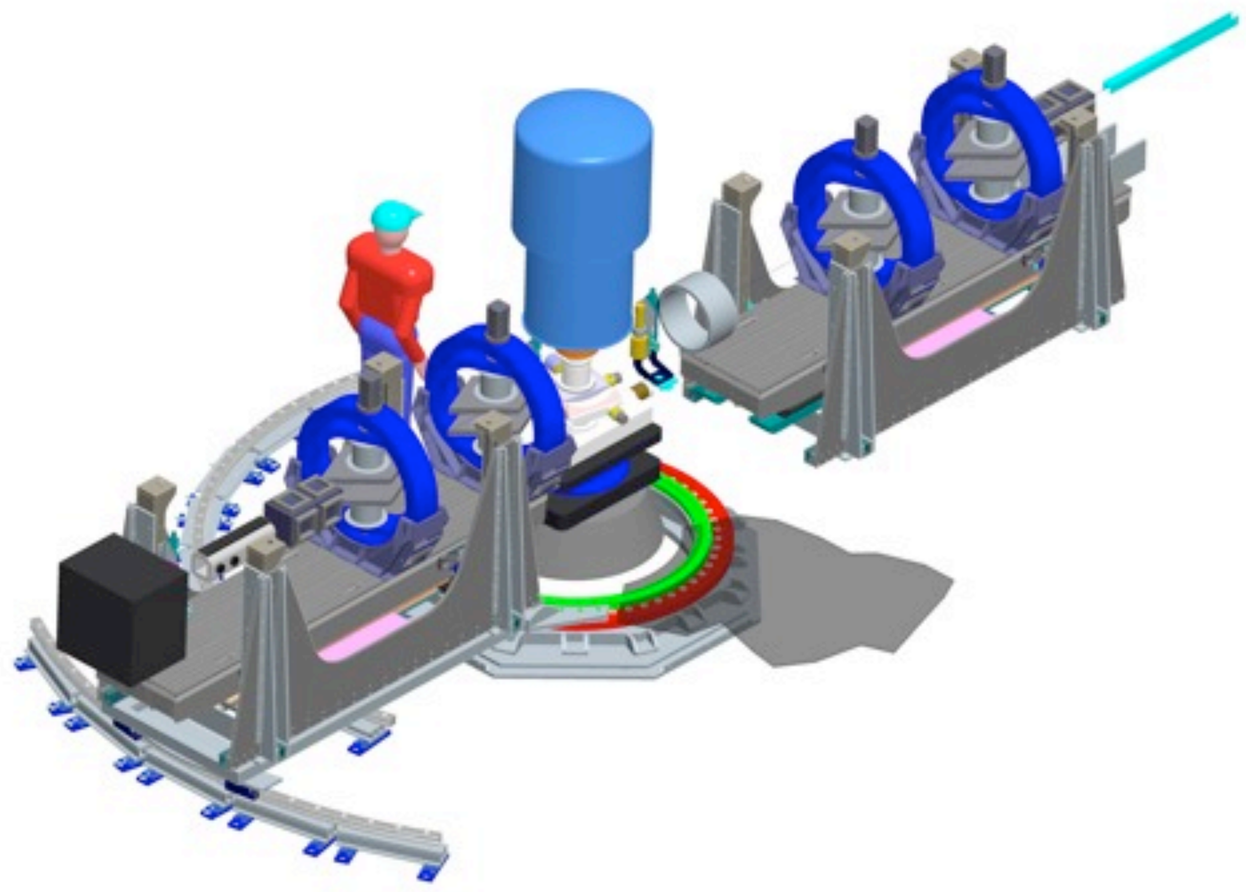
Spin-echo reflectometer OffSPEC

- Off-specular to measure in-plane scattering
- Specular reflectivity of bent surfaces high-resolution
- Separation specular and off-specular



ISIS 2nd target station
Off specular reflectometer
Spin-echo components for
High resolution without
collimation

Thank you !



TS2 ISIS

TU Delft