Principles of inelastic neutron scattering

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Plan of module N.1

1. Introductory notes
2. Overview of Neutron Properties
3. General description of a scattering experiment
4. Cross section: definitions
5. Cross section calculation (Q.M.)
6. Integration over final energies (diffraction)
7. Coherent and incoherent (atomic) scattering

The discovery of neutron
(Chadwick, 1932)

1930 - Bothe and Becker bombard Be with α-particles obtaining a very penetrating and non-ionizing radiation, that was assumed to be composed by very energetic γ-rays.

Soon after, Curie and Joliot observe that this radiation, hitting a target of paraffin, give rise to energetic protons (5.3 MeV). Where this radiation composed by γ-particles, their energy should have been of some 52 MeV, quite unlikely.

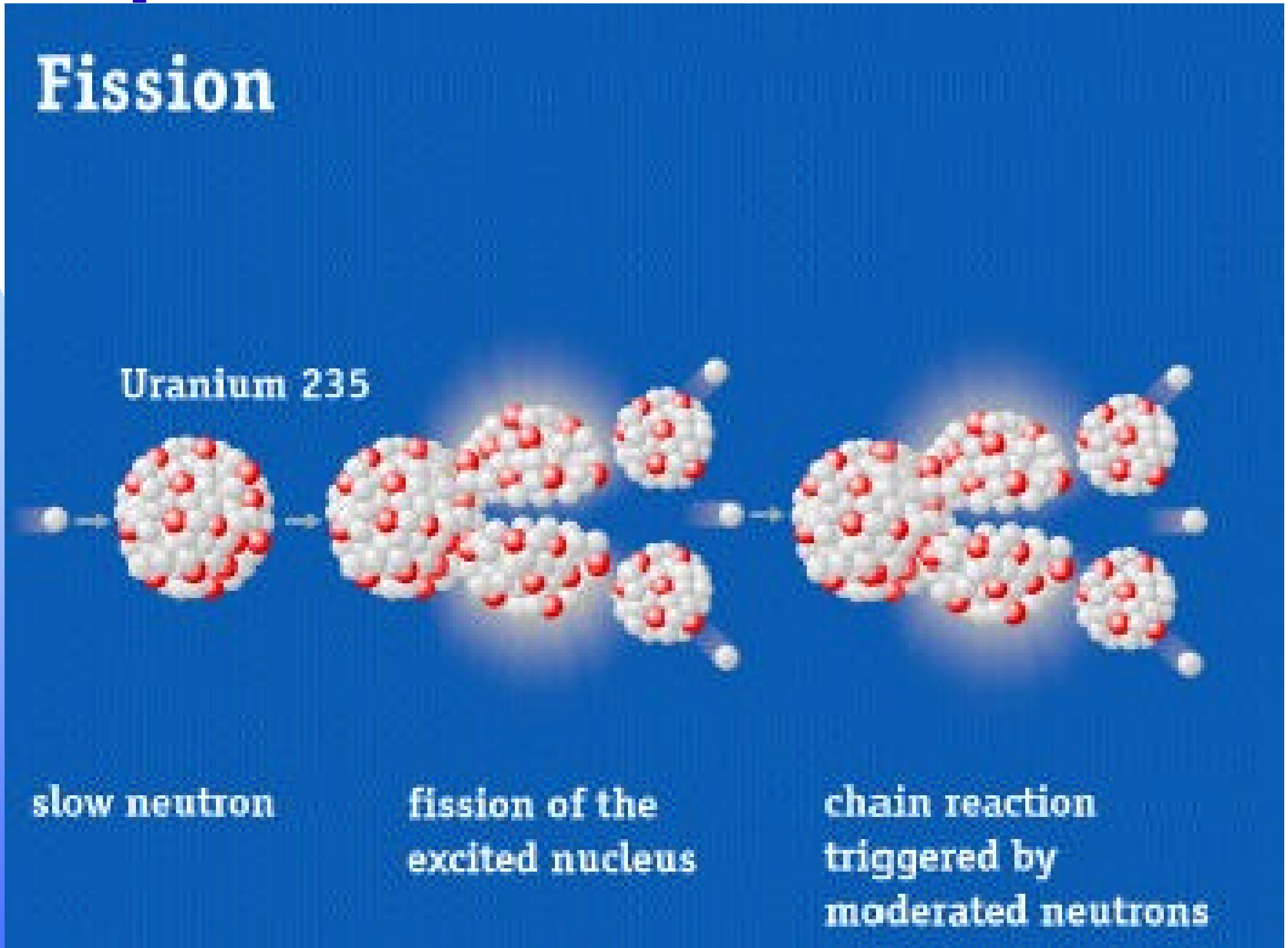
1932 - Chadwick identifies this radiation as neutral particles with a mass similar to that of proton.

The neutron is officially born!

neutron properties

- Free neutrons are unstable, with half-life τ = 10.6 min. (β-decay)
- Bound neutrons are (generally) stable
- Mass: m = 1.6749286 a.m.u.
- Electric d.m. < 10^{-25} (e cm)
- Spin: s = 1/2
- Magnetic d.m.: $\mu = g_s\, s\, \mu_N$
  - For a neutral point particle $g_s = 0$
  - Instead, $\mu = -1.9130418\, \mu_N$
- $\Rightarrow$ neutron is NOT a point particle

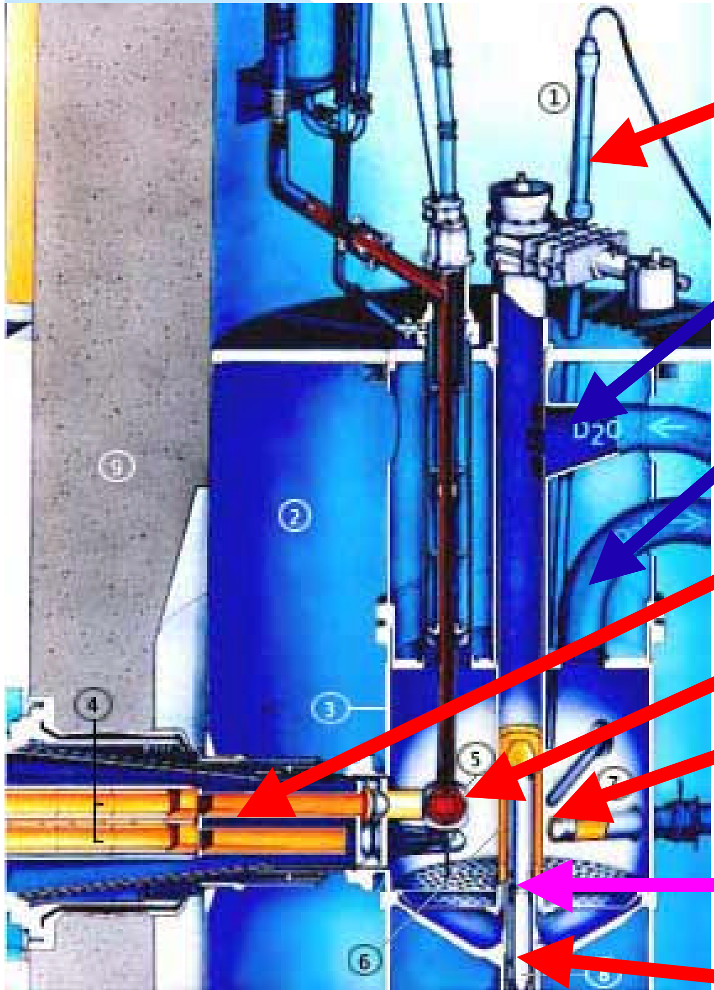
Neutron production: nuclear fission



2-3 neutrons / fission

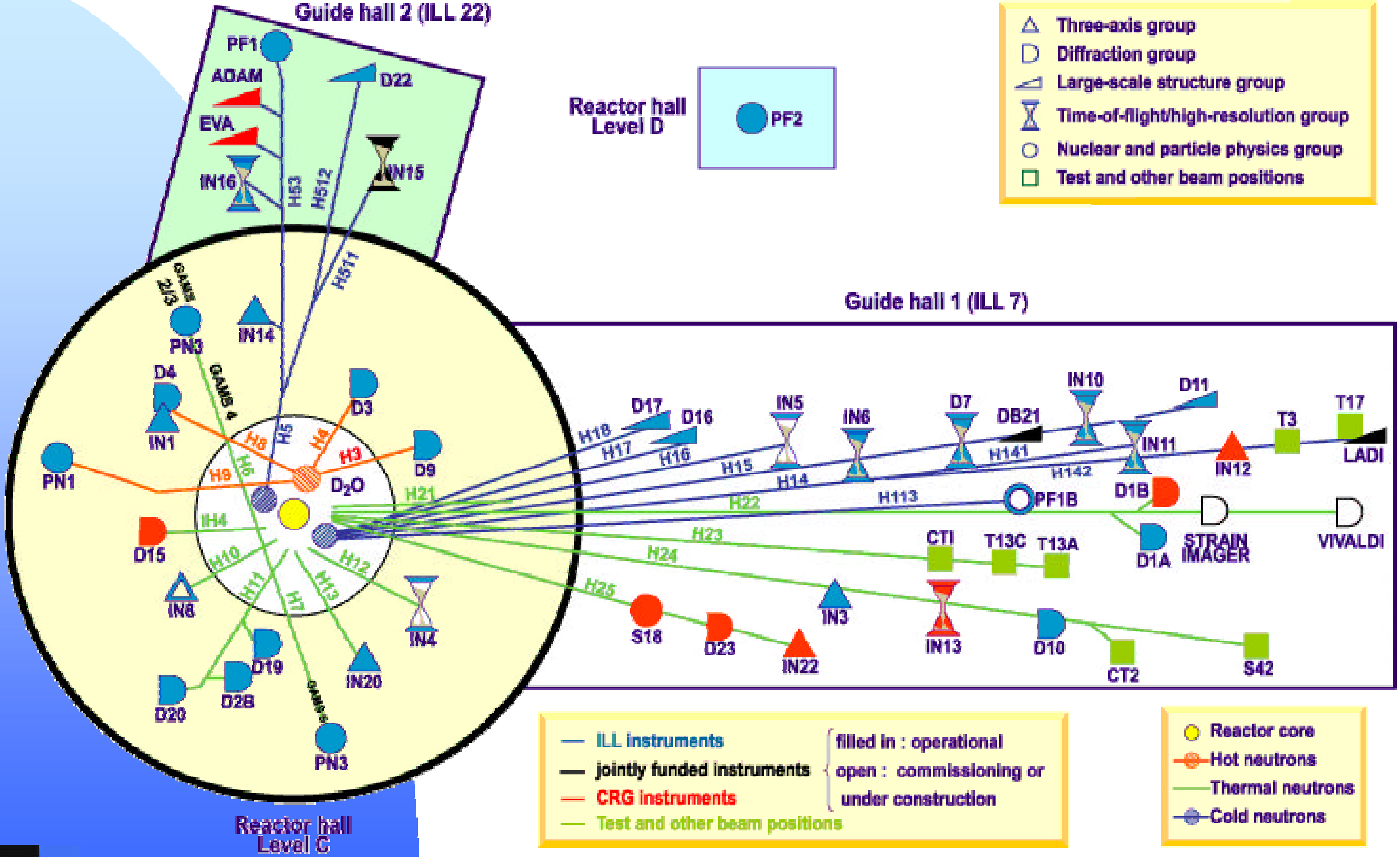
Example: ILL reactor (58 MW)

4.3×10^{18} neutrons / s (fission)



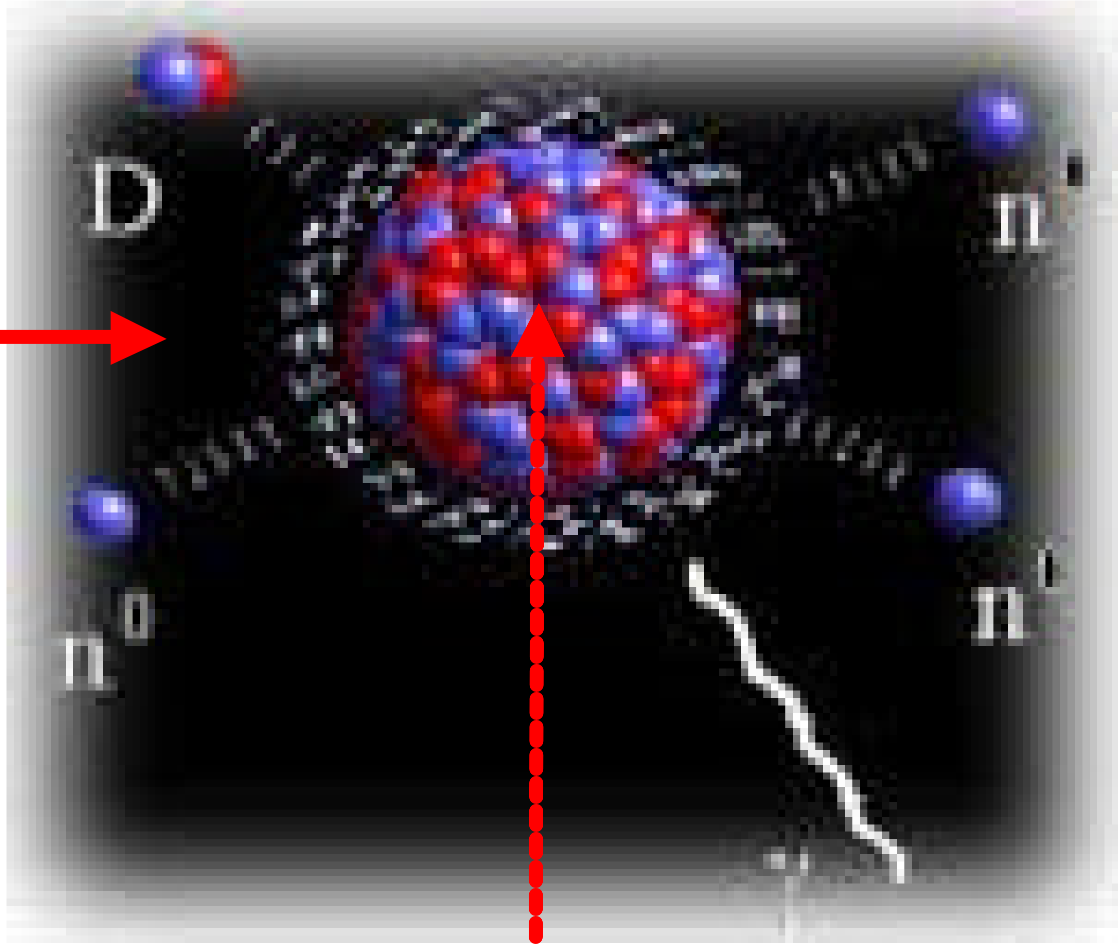
- 1: security rod
- 2: heavy water inlet
- 3: heavy water outlet
- 4: neutron double guide
- 5-7: cold sources
- 6: reactor core (uranium 235)
- 8: Boron control rod

ILL: instrument map



Neutron production: spallation
(to spall = to splinter, break away)

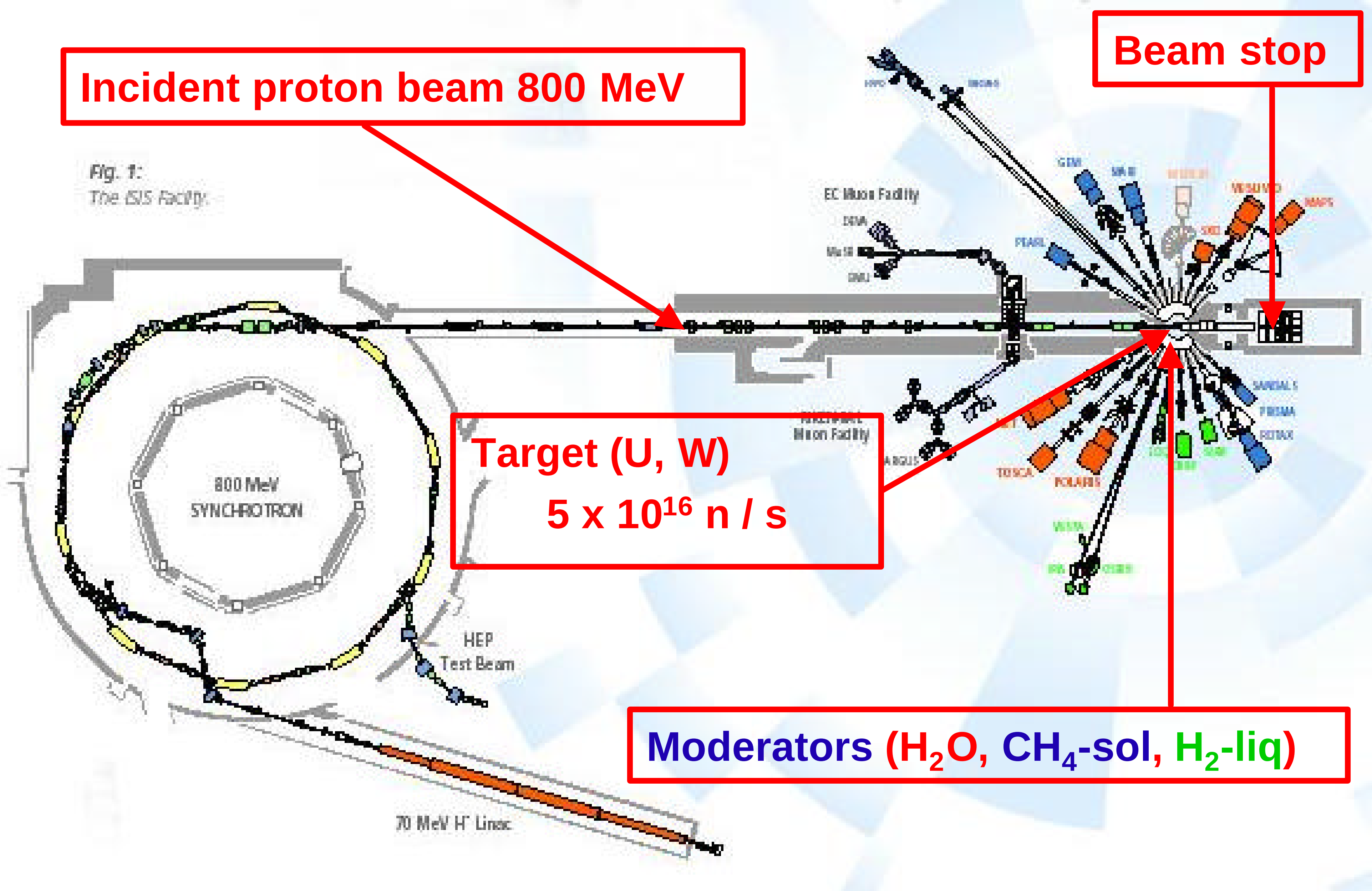
800 MeV protons



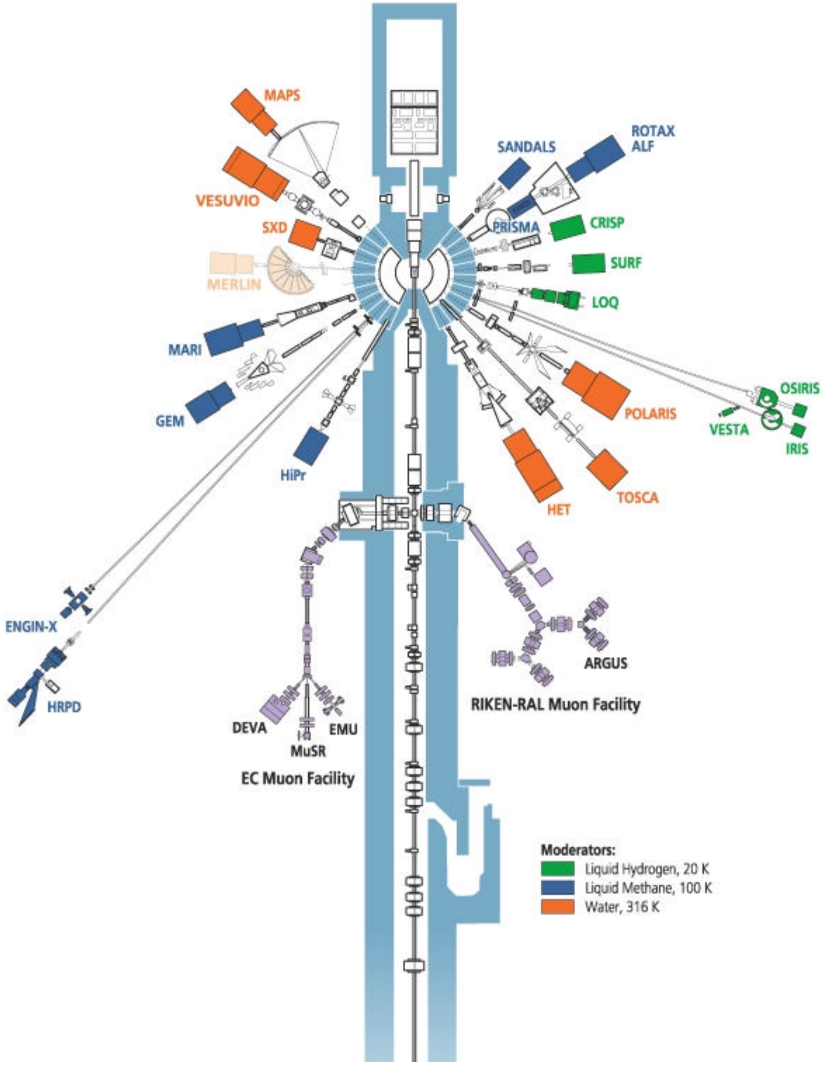
Tungsten target

- High nuclear excitation
- Nuclear relaxation
  - Radiative decay
  - Light nuclides evaporation
- 15-30 neutrons / event

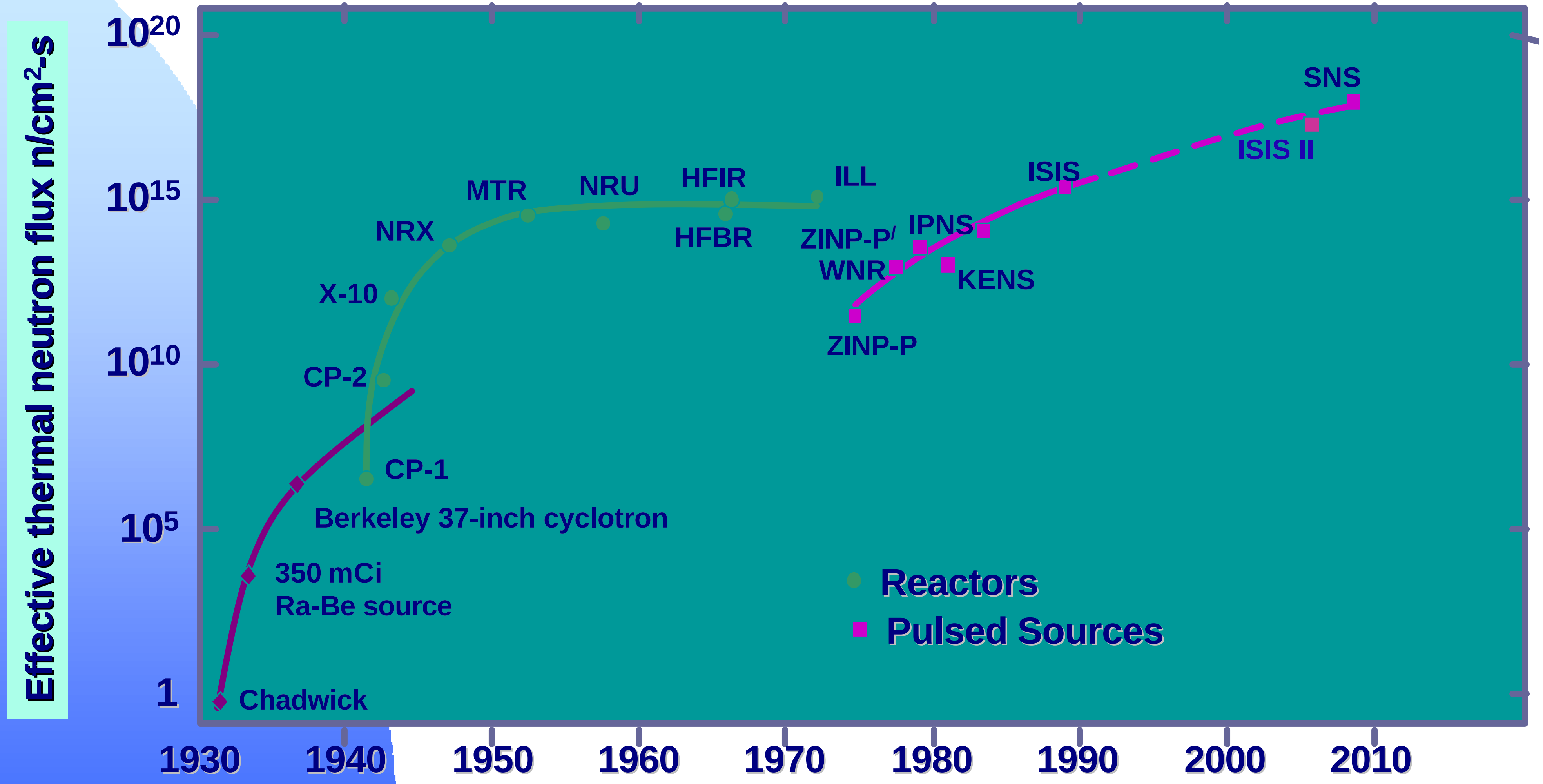
Schematics of pulsed source ISIS



Neutron pulsed source ISIS (160 kW)
(Oxford, UK)



Intensity of neutron sources:
hystorical sketch (and beyond)



(Updated from *Neutron Scattering*, K. Skold and D. L. Price, eds., Academic Press, 1986)

Properties of neutrons

De Broglie: $$\lambda = \frac{h}{p} = \frac{h}{m\,\mathrm{v}}$$

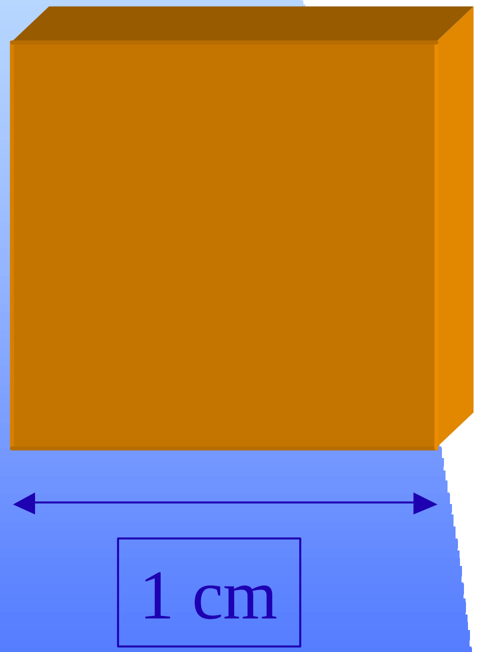
Momentum: $$\mathbf{p} = \hbar \mathbf{k}$$

Energy: $$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m}$$

Why neutrons?

Copper block: 1x1x1 cm^3

density = 8.96 atomic weight: 63.54



- **Microscopic Structure:**
  - **N = 8.492 x 10^{22} atoms**
  - **density = 84.92 atoms/nm^3**
  - **<ℓ> = 2.27 Å = 0.227 nm**
- **Dynamics:**
  - **Kin. Energy = 3/2 k_BT (not true)**
  - **<E>= 38 meV**
  - **<v> = 343 m/s**
  - **<t> = 0.6 ps**

Thermal neutron properties

Moderator: T = 300 K

- **E = 25.8 meV**

  ~ elementary excitations energy

- **λ = 1.78 A**

  ~ interatomic distances in condensed matter

- **neutral particles**

  High penetration power in dense condensed matter

X-rays too may possess the right wavelength ...

<E> = 10 keV

l = 1.24 A

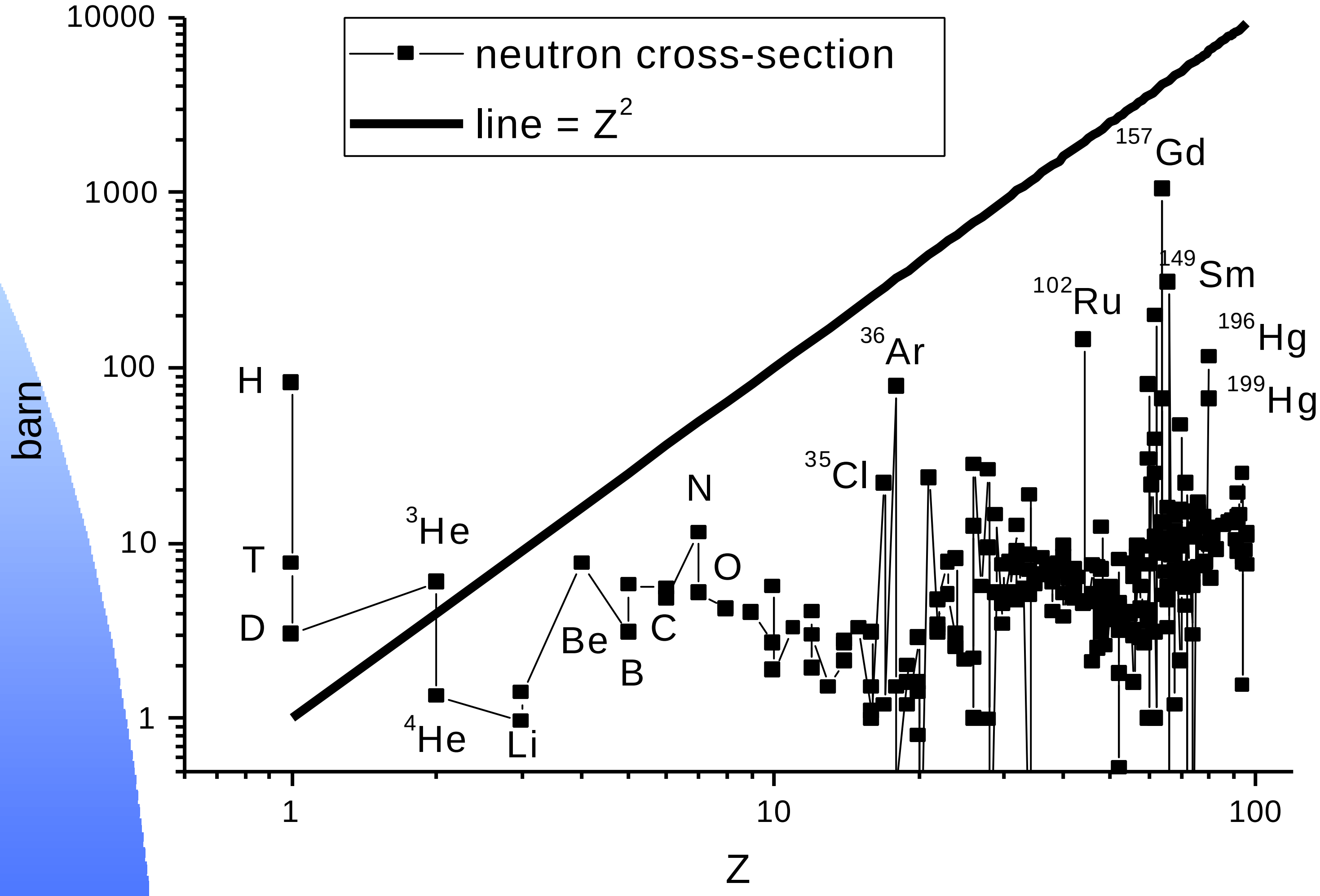
thus ...

- Good for probing the microscopic structure of dense matter

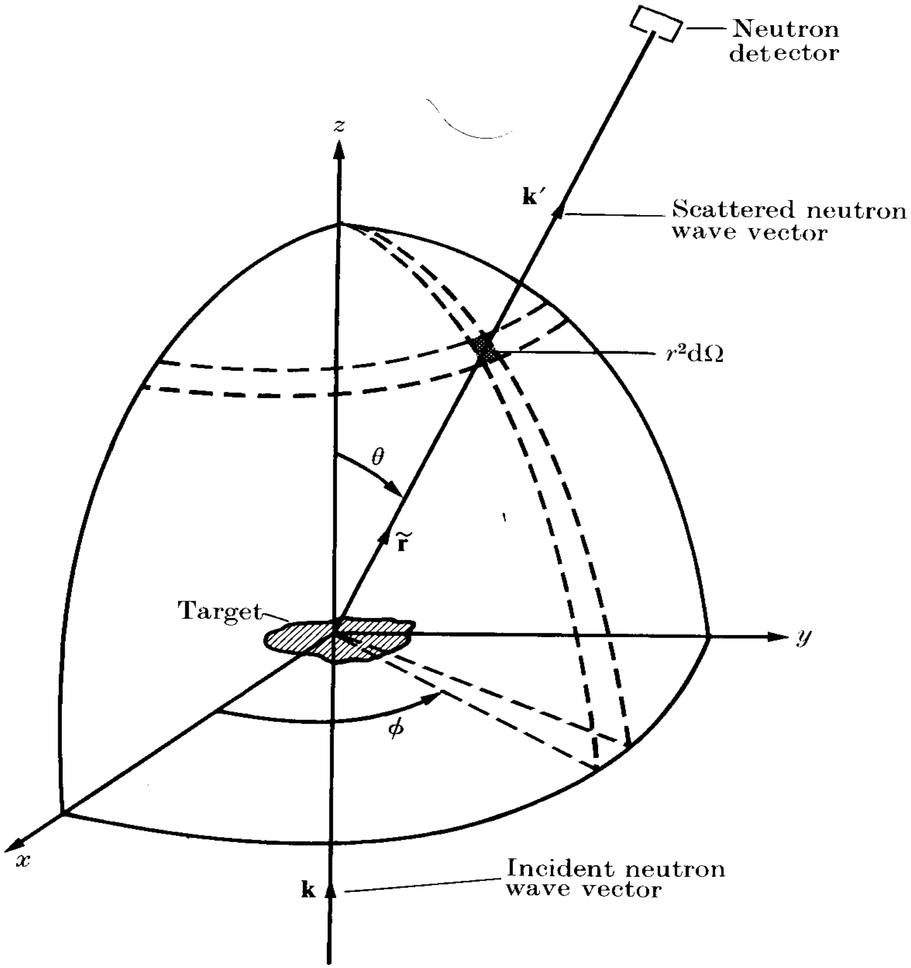
however ...

- Energy too large to probe effectively the microscopic dynamics !

neutron and x-ray cross sections

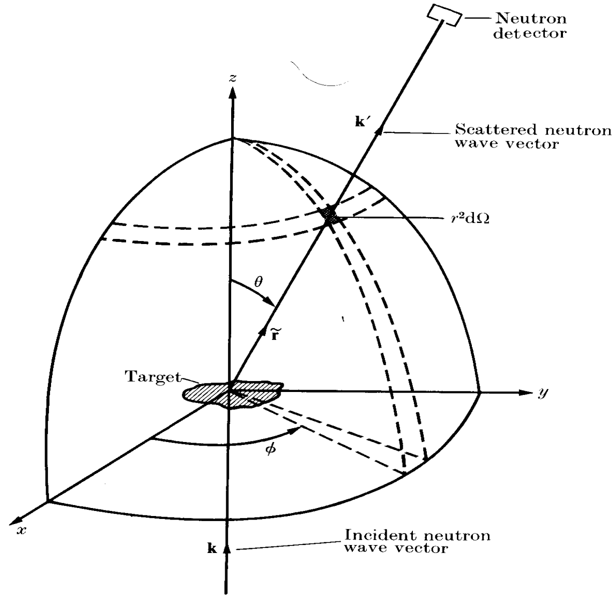


A neutron scattering experiment



- Incident neutron $\left\{ e_0 , \hbar\vec{k}_0 \right\}$
- Scattered neutron $\left\{ e_1 , \hbar\vec{k}_1 \right\}$
- Energy transfer $E = e_0 - e_1$
- Momentum transfer $\boldsymbol{k} = \boldsymbol{k}_0 - \boldsymbol{k}_1$

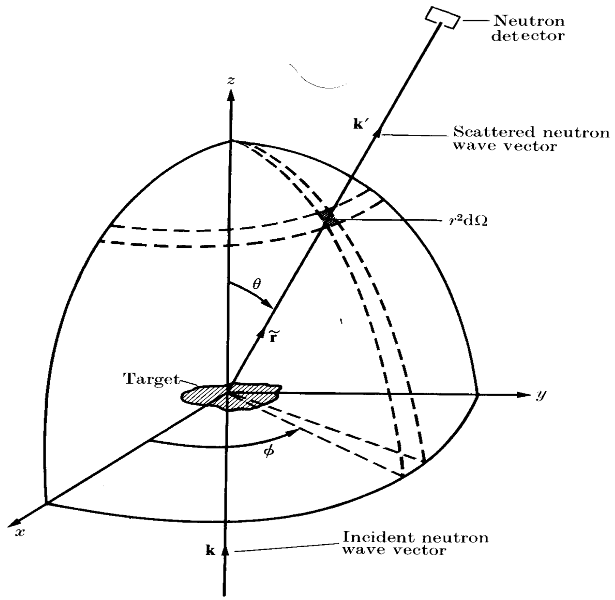
Scattering cross section: definition



$$d I = N \; j\,(e_0) de_0 \, \frac{d^2 s}{d\Omega\, de} \, d\Omega\, de_1$$

- dI =neutrons collected (neutrons /sec)
- N =number of elements in scattering volume
- $\varphi(\varepsilon_0)$ =Inc. neutron flux (neutrons/meV/sec/cm^2)
- $d\varepsilon_0$ =Incident neutrons energy window (meV)
- $d\varepsilon_1$ = Scattered neutrons energy window (meV)
- $d\Omega$ =Collection solid angle

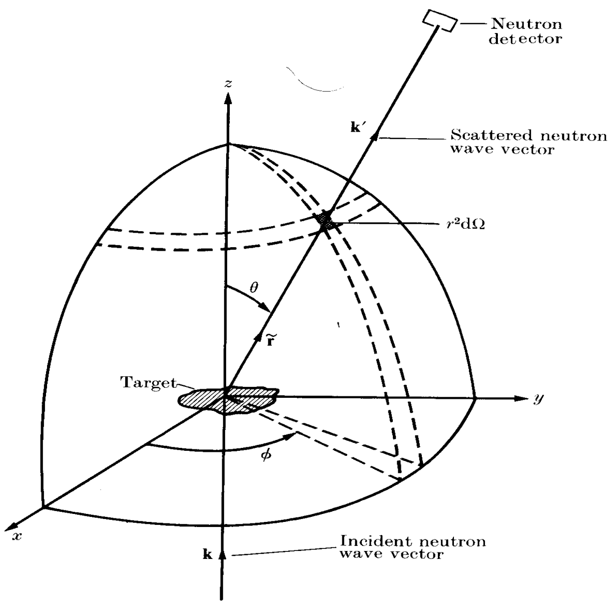
Conservation rules: energy



- Energy conservation: $$E = e_0 - e_1$$

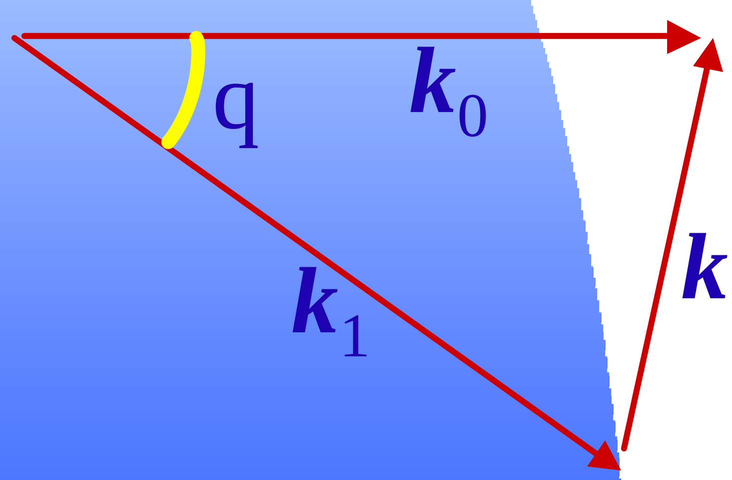
- E = energy lost by the neutron
- E = energy gained by the system
  - Collective excitations
  - Molecular excitations
  - Nuclear recoil

Conservation rules: momentum

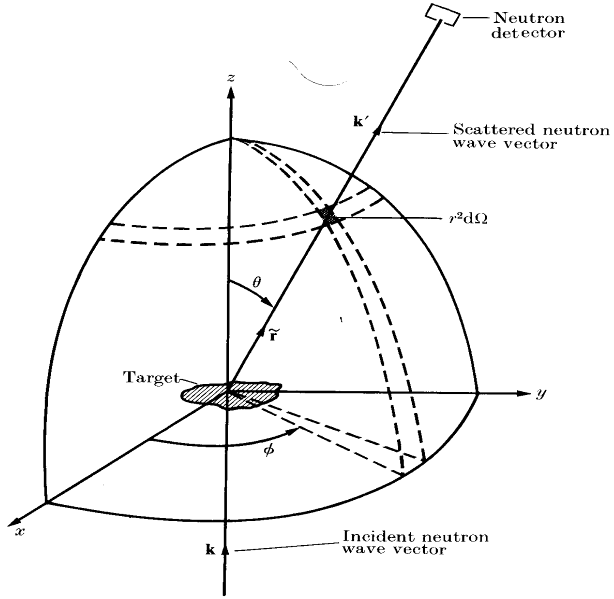


- Momentum conservation: $$\hbar \mathbf{k} = \hbar \mathbf{k}_0 - \hbar \mathbf{k}_1$$

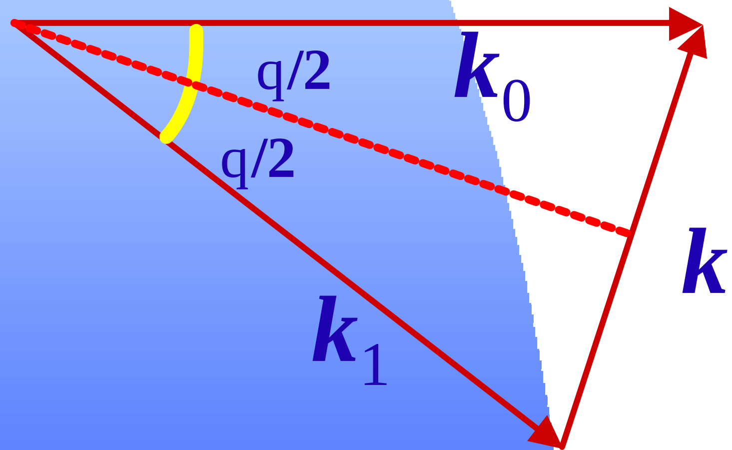
- k_0 =incident neutron wavenumber
- k_1 =scattered neutron wavenumber
- $\hbar k$ =momentum transferred to the system
  - Collective excitations
  - ~~Molecular excitations~~
  - Nuclear recoil



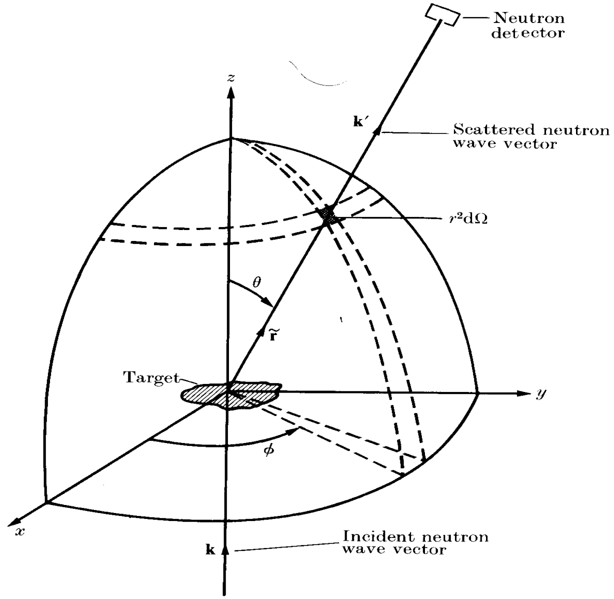
Elastic Scattering



$$e_0 = e_1 \qquad \hbar k_0 = \hbar k_1$$

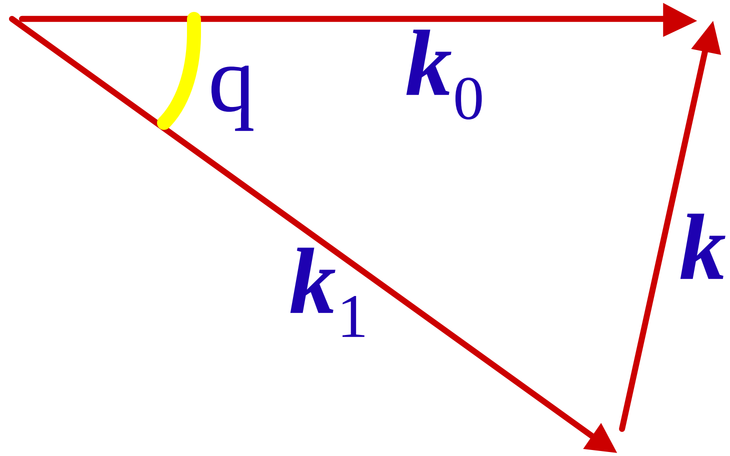


$$k = 2k_0 \sin(q / 2)$$



Inelastic Scattering

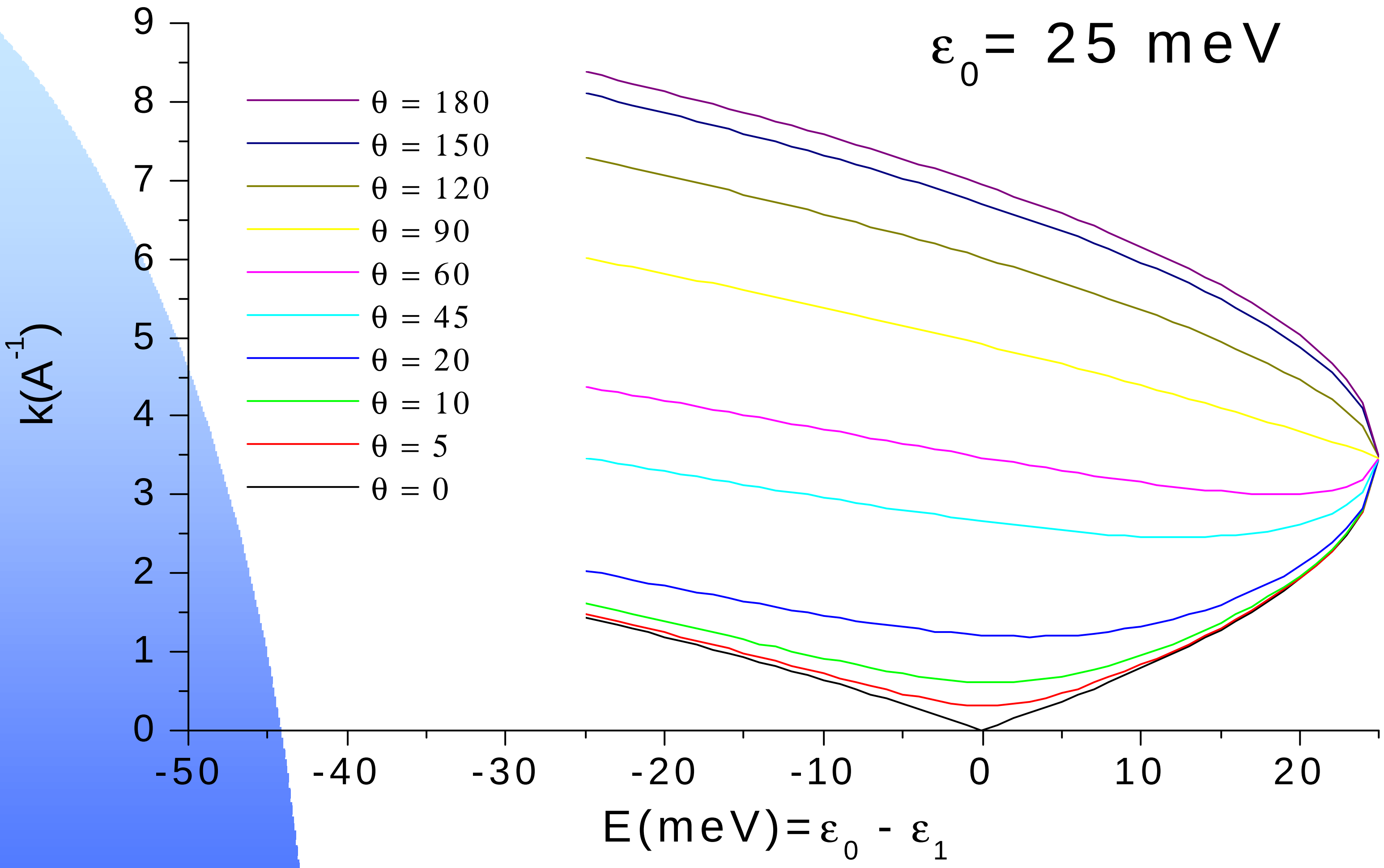
$$e_0 \neq e_1 \qquad \hbar k_0 \neq \hbar k_1$$



$$\mathbf{k}^2 = (\mathbf{k}_0 - \mathbf{k}_1)^2 = k_0^2 + k_1^2 - 2k_0 k_1 \cos(q)$$

From which a kinematically allowed region can be drawn:

Kinematically allowed region



q = scattering angle in degrees

Calculation of scattering cross section

Initial State: $|0\rangle = |\mathbf{k}_0, \mathbf{s}_0; \Lambda_0, s_0\rangle$

- Neutron
  - $\mathbf{k}_0$, ε_0 = momentum and energy
  - $\mathbf{s}_0$ = spin state
- Target
  - E_0= target energy
  - σ_0= target spin state
  - Λ_0=ALL degrees of freedom
    - ✓Collective motions
    - ✓ Molecular excitations

Final State: $|1\rangle = |\mathbf{k}_1, \mathbf{s}_1; \Lambda_1, s_1\rangle$

- Neutron
  - $\mathbf{k}_1$, ε_1 = momentum and energy
  - $\mathbf{s}_1$ = spin state
- Target
  - E_1= target energy
  - σ_1= target spin state
  - Λ_1=ALL degrees of freedom
    - ✓Collective motions
    - ✓ Molecular excitations

1st order perturbation theory
(1st Born approximation)

$$w_{0\to 1} = \frac{2p}{\hbar}\left|\langle 1|\hat{V}|0\rangle\right|^2 r(1)$$

- Fermi “golden rule”,
  where:

- V = interaction Hamiltonian
- ρ(1) = density of final states (1)

Neutrons as plane waves:

Neutron states:
Normalized plane waves

$$|\mathbf{k}_0\rangle = \frac{1}{L^{3/2}} e^{-i\mathbf{k}_0\cdot\mathbf{r}} \qquad |\mathbf{k}_1\rangle = \frac{1}{L^{3/2}} e^{-i\mathbf{k}_1\cdot\mathbf{r}}$$

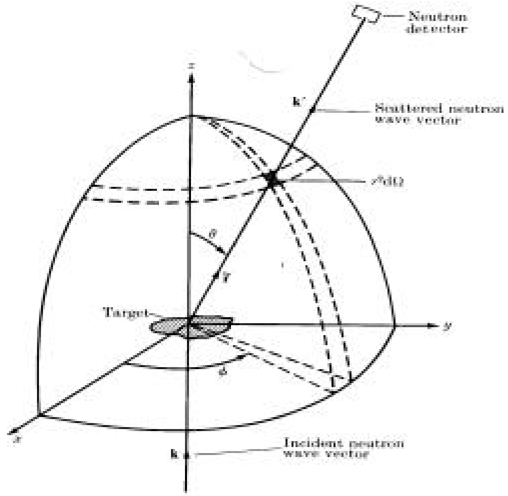
Number of final neutron states:

$$\rho(k_1) = \frac{L^3}{(2\pi)^3} d\mathbf{k}_1 = \frac{L^3}{(2\pi)^3} d\Omega\, k_1^2 dk_1 = \frac{L^3}{(2\pi)^3} \frac{m}{\hbar^2} k_1\, d\varepsilon_1 d\Omega$$

The transition probability (energy conservation):

$$w_{0\to 1} = \left|\langle 1|\hat{V}|0\rangle\right|^2 \frac{L^3}{(2\pi)^2}\frac{m}{\hbar^3} k_1 d\varepsilon_1\, d\Omega\, \delta\left(\varepsilon_0 + E_0 - \varepsilon_1 - E_1\right)$$

Scattering cross section (1)



Incident flux: 1 neutron, $[k_0, \varepsilon_0]$

$$\Phi(e_0) = r\, v_0 = \frac{1}{L^3}\frac{p_0}{m} = \frac{1}{L^3}\frac{\hbar k_0}{m}$$

$$\left[\frac{d^2 s}{d\Omega de}\right]_{0\to1} = \frac{1}{N}\frac{1}{\Phi(e_0)}\frac{dI_{0\to1}}{d\Omega de_1} = \frac{1}{N}\frac{mL^3}{\hbar k_0}\frac{w_{0\to1}}{d\Omega de_1}$$

... and the expression for the cross section becomes:

$$\left(\frac{d^2\sigma}{d\Omega\, d\varepsilon}\right)_{0\to1} = \frac{1}{N}\frac{k_1}{k_0}\left(\frac{mL^3}{2\pi\hbar^2}\right)^2 \left|\langle 1|\hat{V}|0\rangle\right|^2 \delta(\varepsilon + E_0 - E_1)$$

The matrix element

|0> and |1> are GLOBAL states of the system (target + neutron):

$$\langle 1|\hat{V}|0\rangle = \langle \mathbf{k}_1, \mathbf{s}_1; \Lambda_1, s_1|\hat{V}|\mathbf{k}_0, \mathbf{s}_0; \Lambda_0, s_0\rangle$$

If NO neutron polarization analysis is carried out:

$$\langle 1|\hat{V}|0\rangle = \langle \mathbf{k}_1; \Lambda_1, s_1|\hat{V}|\mathbf{k}_0; \Lambda_0, s_0\rangle$$

$$= \frac{1}{L^3}\int d\mathbf{r}\, e^{i\mathbf{k}_1\cdot\mathbf{r}}\langle \Lambda_1, s_1|\hat{V}|\Lambda_0, s_0\rangle e^{-i\mathbf{k}_0\cdot\mathbf{r}}$$

n-nucleus interaction Hamiltonian

- Thermal neutrons: l $\approx$ 2. Å = 2 x 10^{-10} m
- Nuclear size:
  (potential range) $r_0 \approx$ fm = 1 x 10^{-15} m

FERMI pseudo-potential:

$$\hat{V}_j(\boldsymbol{r}) = \frac{2p\,\hbar^2}{m}\,\hat{b}_j\; d(\boldsymbol{r} - \hat{\boldsymbol{R}}_j)$$

where:

$\boldsymbol{R}_j$ = position of j-th nucleus

b_j = scattering amplitude of j-th nucleus

Matrix element

$$\langle 1|\hat{V}|0\rangle = \frac{1}{L^3}\int d\mathbf{r}\; e^{i\mathbf{k}_1\cdot\mathbf{r}}\langle\Lambda_1, s_1|\sum_j \hat{V}_j(\mathbf{r})|\Lambda_0, s_0\rangle e^{-i\mathbf{k}_0\cdot\mathbf{r}}$$

$$= \frac{1}{L^3}\frac{2p\,\hbar^2}{m}\sum_j \int d\mathbf{r}\; e^{-i\mathbf{k}\cdot\mathbf{r}}\langle\Lambda_1, s_1|\hat{b}_j\, d(\mathbf{r}-\hat{\mathbf{R}}_j)|\Lambda_0, s_0\rangle$$

$$= \frac{1}{L^3}\frac{2p\,\hbar^2}{m}\sum_j \langle\Lambda_1, s_1|\hat{b}_j \int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}} d(\mathbf{r}-\hat{\mathbf{R}}_j)|\Lambda_0, s_0\rangle$$

$$= \frac{1}{L^3}\frac{2p\,\hbar^2}{m}\sum_j \langle\Lambda_1, s_1|\hat{b}_j\, e^{-i\mathbf{k}\cdot\mathbf{R}_j}|\Lambda_0, s_0\rangle$$

$$= \frac{1}{L^3}\frac{2p\,\hbar^2}{m}\sum_j \langle s_1|\hat{b}_j|s_0\rangle\langle\Lambda_1|e^{-i\mathbf{k}\cdot\mathbf{R}_j}|\Lambda_0\rangle = \sum_j f_{0\to 1}(\mathbf{k}, j)$$

Sum over N independent nuclear events

Scattering cross section (2)

$$\left[\frac{d^2 s}{d\Omega de}\right]_{0\to 1} = \frac{1}{N}\frac{k_1}{k_0}\left|\sum_j f_{0\to 1}(\mathbf{k}, j)\right|^2 d\left(e + E_0 - E_1\right)$$

where:

|0> and |1> now refer to the atomic states

j- labels the nuclei

MEMO

In general:

Initial state: |0> thermally populated

Final state: |1> not selected

Sum over states

Sum over final states:

$$\left[\frac{d^2 s}{d\Omega de}\right]_{0\to 1} = \frac{1}{N}\frac{k_1}{k_0}\sum_{\Lambda_1, s_1}\left|\sum_j f_{0\to 1}(\mathbf{k}, j)\right|^2 d\left(e + E_0 - E_1\right)$$

Thermal average over initial states:

$$\left[\frac{d^2\sigma}{d\Omega d\varepsilon}\right] = \frac{1}{N}\frac{k_1}{k_0}\sum_{\Lambda_0, \sigma_0} p(\Lambda_0)\, p(\sigma_0) \sum_{\Lambda_1, \sigma_1}\left|\sum_j f_{0\to 1}(\boldsymbol{k}, j)\right|^2 \delta(\varepsilon + E_0 - E_1)$$

where:

$$\sum_{\sigma_0} p(\sigma_0) = 1 \qquad \sum_{\Lambda_0} p(\Lambda_0) = 1$$

Dirac d-function

The Dirac δ-function writes:

$$\delta\left(\varepsilon + E_0 - E_1\right) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt\ \exp\left\{-\frac{it}{\hbar}\left(\varepsilon + E_0 - E_1\right)\right\}$$

... we take into account that:

$$E_0 = E(\Lambda_0) + E(\sigma_0)$$

$$E_1 = E(\Lambda_1) + E(\sigma_1)$$

$$d\left(e + E_0 - E_1\right) = \frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt$$

$$\exp\left\{-\frac{it}{\hbar}\left[e + E(\Lambda_0) + E(s_0) - E(\Lambda_1) - E(s_1)\right]\right\}$$

Scattering cross section (3)

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\sum_{j,l}\sum_{\Lambda_0,s_0} p(\Lambda_0)p(s_0)\sum_{\Lambda_1,s_1}$$

$$\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{\left\{-\frac{it}{\hbar}[e+E(\Lambda_0)+E(s_0)-E(\Lambda_1)-E(s_1)]\right\}}$$

$$\langle\Lambda_0|e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j}|\Lambda_1\rangle\langle s_0|\hat{b}_j^+|s_1\rangle$$

$$\langle\Lambda_1|e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l}|\Lambda_0\rangle\langle s_1|\hat{b}_l|s_0\rangle$$

Scattering cross section (4)

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\sum_{j,l}\sum_{\Lambda_0, s_0} p(\Lambda_0)p(s_0)\sum_{\Lambda_1, s_1}$$

$$\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{\left\{-\frac{ite}{\hbar}\right\}}$$

$$\left\langle \Lambda_0 \left| e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j} \right| \Lambda_1 \right\rangle \left\langle s_0 \left| \hat{b}_j^+ \right| s_1 \right\rangle$$

$$e^{\frac{it}{\hbar}E(\Lambda_1)} \left\langle \Lambda_1 \left| e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l} \right| \Lambda_0 \right\rangle e^{-\frac{it}{\hbar}E(\Lambda_0)}$$

$$e^{\frac{it}{\hbar}E(s_1)} \left\langle s_1 \left| \hat{b}_l \right| s_0 \right\rangle e^{-\frac{it}{\hbar}E(s_0)}$$

Energy terms are distributed close to the various |ket> and <bra| eigenstates where they belong

Initial and final states are eigenstates of the unperturbed Hamiltonian, H

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\sum_{j,l}\sum_{\Lambda_0,s_0} p(\Lambda_0)p(s_0)\sum_{\Lambda_1,s_1}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{\left\{-\frac{ite}{\hbar}\right\}}$$

$$\langle\Lambda_0|e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j}|\Lambda_1\rangle\langle s_0|\hat{b}_j^+|s_1\rangle$$

$$\langle\Lambda_1|e^{\frac{it}{\hbar}\hat{H}(\Lambda)}\, e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l}\, e^{-\frac{it}{\hbar}\hat{H}(\Lambda)}|\Lambda_0\rangle$$

$$\langle s_1|e^{\frac{it}{\hbar}\hat{H}(s)}\,\hat{b}_l\, e^{-\frac{it}{\hbar}\hat{H}(s)}|s_0\rangle$$

The Heisenberg operator

$$\hat{O}_H(t) = e^{i\frac{\hat{H}t}{\hbar}} \hat{O}_S e^{-i\frac{\hat{H}t}{\hbar}}$$

and the cross section becomes:

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\sum_{j,l}\sum_{\Lambda_0, s_0} p(\Lambda_0)p(s_0)\sum_{\Lambda_1, s_1}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{-iwt}$$

$$\left\langle \Lambda_0 \left| e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j(0)} \right| \Lambda_1 \right\rangle \left\langle \Lambda_1 \left| e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l(t)} \right| \Lambda_0 \right\rangle$$

$$\left\langle s_0 \left| \hat{b}_j^+(0) \right| s_1 \right\rangle \left\langle s_1 \left| \hat{b}_l(t) \right| s_0 \right\rangle$$

The representation of the final states is COMPLETE

$$\sum_{\Lambda_1} |\Lambda_1\rangle\langle\Lambda_1| = 1 \qquad \sum_{s_1} |s_1\rangle\langle s_1| = 1$$

and the double differential cross section becomes:

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\sum_{j,l}\sum_{\Lambda_0, s_0} p(\Lambda_0)\, p(s_0)\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{-iwt}$$

$$\langle\Lambda_0| e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j(0)} e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l(t)} |\Lambda_0\rangle$$

$$\langle s_0 | \hat{b}_j^+(0)\, \hat{b}_l(t) | s_0\rangle$$

Summarizing:

- The cross section is RIGOROUS within the 1st Born approximation
- The cross section is determined by:
  - Nuclear position dynamics $\Rightarrow$ R(t)
  - Nuclear spin dynamics $\Rightarrow$ b(t)
- Using unpolarized neutrons, the spin dynamics information is INCOMPLETE
- Within the same framework, we NEGLECT the nuclear spin dynamics $\Rightarrow$ b(t)=b(0)

Neglecting spin dynamics:

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{-iwt} \sum_{j,l} \sum_{s_0} p(s_0)\langle s_0 | \hat{b}_j^+ \hat{b}_l | s_0 \rangle$$

$$\sum_{\Lambda_0} p(\Lambda_0)\langle \Lambda_0 | e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j(0)} e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l(t)} | \Lambda_0 \rangle$$

Cross section determined by dynamics of nuclear pairs

We define the pair correlation function:

$$Y_{j,l}(\boldsymbol{k}, t) = \sum_{\Lambda_0} p(\Lambda_0)\langle \Lambda_0 | e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}_j} \; e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}_l(t)} | \Lambda_0 \rangle$$

$$= \left\langle e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}_j} \; e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{R}}_l(t)} \right\rangle$$

Double differential cross section

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{1}{N}\frac{k_1}{k_0}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{-iwt} \sum_{j,l}$$

$$\sum_{s_0} p(s_0)\langle s_0 | \hat{b}_j^+ \hat{b}_l | s_0 \rangle \left\langle e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j} e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l(t)} \right\rangle$$

MEMO:

Operators $\mathbf{R}_j(0)$ and $\mathbf{R}_l(t)$, taken at different times,

DO NOT COMMUTE !

The two exponentials can be combined
in the classical limit ONLY.

TWO possibilities for the sum over nucler positions

$\ell = j$ self term

$$\sum_{s_0} p_{s_0} \langle s_0 | \hat{b}_j^+ \hat{b}_j | s_0 \rangle = \langle \hat{b}_j^+ \hat{b}_j \rangle \equiv \overline{b_j^2}$$

$\ell \neq j$ distinct term

MEMO: We assume a negligible quantum correlation between different nuclei.

$$\sum_{s_0} p_{s_0} \langle s_0 | \hat{b}_j^+ \hat{b}_l | s_0 \rangle = \sum p_{s_0^1}^{(1)} \cdots p_{s_0^N}^{(N)} \langle s_0^{(1)} \cdots s_0^{(N)} | \hat{b}_j^+ \hat{b}_l | s_0^{(1)} \cdots s_0^{(N)} \rangle$$

$$= \sum p_{s_0^j}^{(j)} \langle s_0^{(j)} | \hat{b}_j^+ | s_0^{(j)} \rangle \sum p_{s_0^l}^{(l)} \langle s_0^{(l)} | \hat{b}_l | s_0^{(l)} \rangle$$

$$= \langle \hat{b}_j^+ \rangle \langle \hat{b}_l \rangle = \bar{b}_j^* \, \bar{b}_l$$

Decomposition in self & distinct terms

We define the self term: $$I_{self}(\mathbf{k},t)=\frac{1}{N}\sum_j \overline{b_j^2}\left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)}e^{i\mathbf{k}\cdot\mathbf{R}_j(t)}\right\rangle$$

... and the distinct term

$$I_{dist}(\mathbf{k},t)=\frac{1}{N}\sum_j\sum_{l\neq j} \bar{b}_j^* \, \bar{b}_l \left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} \, e^{i\mathbf{k}\cdot\mathbf{R}_l(t)}\right\rangle$$

The cross section becomes:

$$\left[\frac{d^2\sigma}{d\Omega d\varepsilon}\right]=\frac{k_1}{k_0}\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}dt\,\exp\{-i\omega t\}\left[I_{dist}(\boldsymbol{k},t)+I_{self}(\boldsymbol{k},t)\right]$$

Monatomic, monoisotopic sample

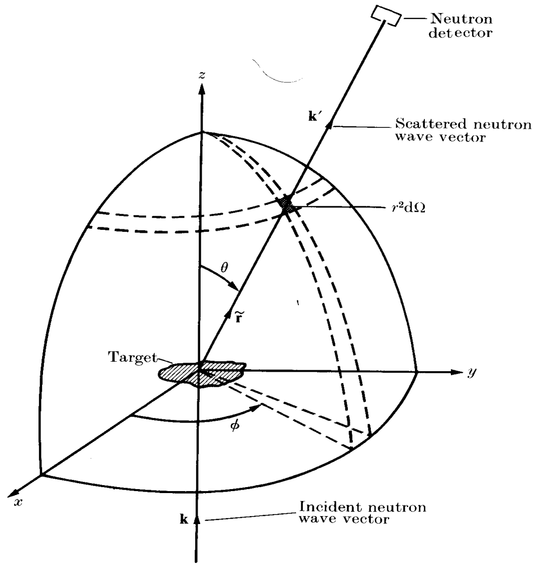
$$\hat{b}_j = \hat{b}_l = \hat{b}$$ ... as a consequence:

The self term: $$I_{self}(\mathbf{k},t) = \frac{\overline{b^2}}{N} \sum_j \left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} e^{i\mathbf{k}\cdot\mathbf{R}_j(t)} \right\rangle$$

The distinct term: $$I_{dist}(\mathbf{k},t) = \frac{\overline{b}^* \, \overline{b}}{N} \sum_j \sum_{l \neq j} \left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} \, e^{i\mathbf{k}\cdot\mathbf{R}_l(t)} \right\rangle$$

A neutron diffraction experiment:

integration over all final energies



the differential cross section is:

$$\frac{d\sigma}{d\Omega} = \int_{-\infty}^{+\infty} d\varepsilon \frac{d^2\sigma}{d\Omega d\varepsilon}$$

MEMO:

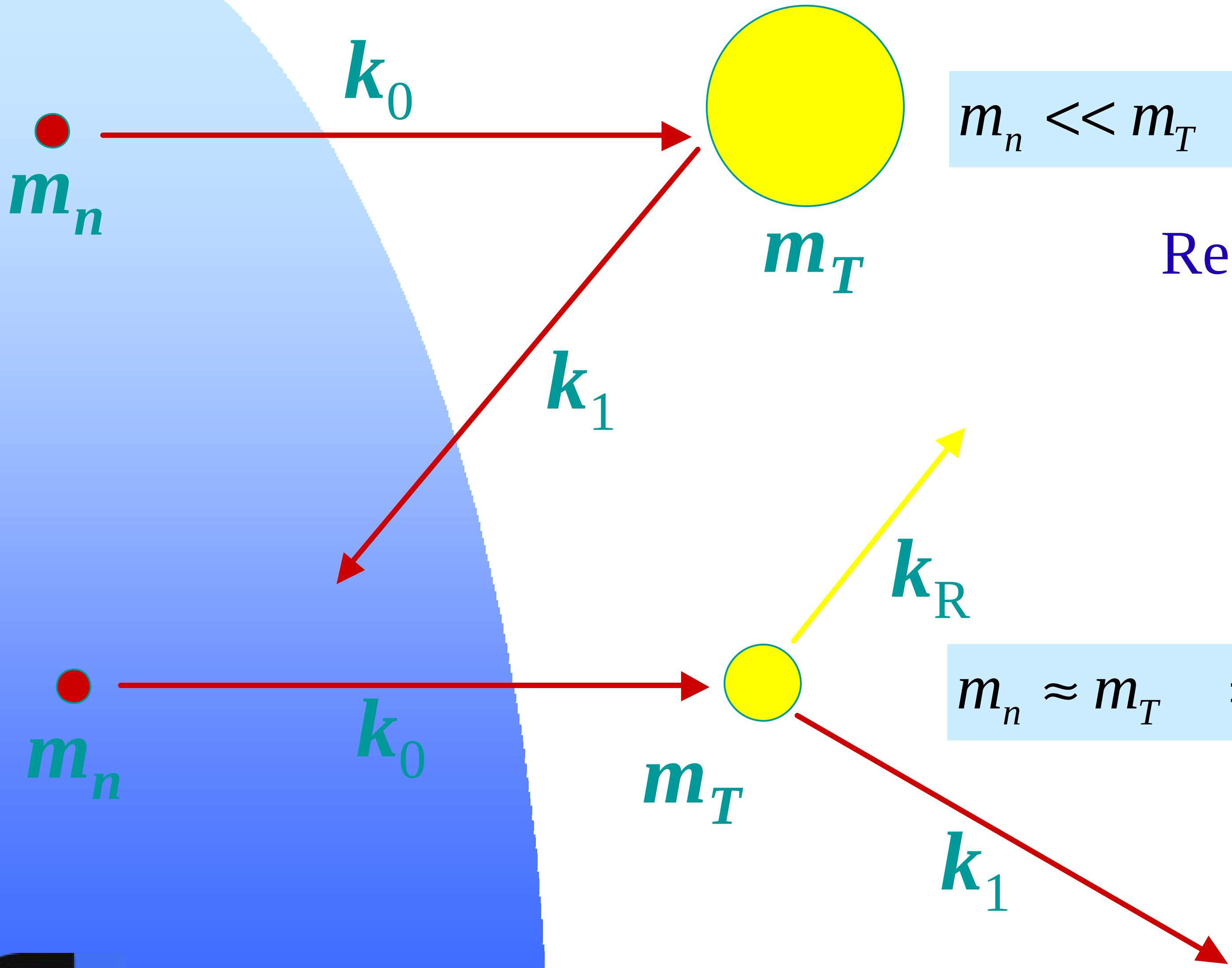
True IF $\varepsilon_0 \rightarrow \infty$

$$\frac{d\sigma}{d\Omega} = \int_{-\infty}^{+\infty} d\omega \cancel{\frac{k_1}{k_0}} \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \exp\{-i\omega t\}\left[I_{dist}(\mathbf{k},t) + I_{self}(\mathbf{k},t)\right]$$

In the same limit the static approximation holds: $k_1 \cong k_0$

$$\frac{d\sigma}{d\Omega} = I_{dist}(\mathbf{k},0) + I_{self}(\mathbf{k},0)$$

How good is the static approximation?
(thermal neutrons: atomic case)



$m_n << m_T \quad \Rightarrow \quad$ elastic scattering

Recoil negligible

$k_1 = k_0$

$m_n \approx m_T \quad \Rightarrow \quad$ inelastic scattering

Recoil consistent

$k_1 \neq k_0$

How good is the static approximation?
(thermal neutrons: molecular / crystal case)

- Molecular case:
  - M >> m, overall recoil negligible
  - $\varepsilon_0 < \Delta E$ (smallest molecular excitation)
- Crystal case:
  - $\varepsilon_0 < \Delta E$ (smallest phonon excitation)
- In practice:
  - Careful analysis, case by case.

The differential cross section

$$\frac{d\sigma}{d\Omega} = I_{dist}(\mathbf{k},0) + I_{self}(\mathbf{k},0)$$

where:

$$I_{self}(\mathbf{k},0) = \frac{\overline{b^2}}{N} \sum_j \left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} e^{i\mathbf{k}\cdot\mathbf{R}_j(0)} \right\rangle = \overline{b^2}$$

Operators $\mathbf{R}_j$ and $\mathbf{R}_l$, taken at the same time DO COMMUTE

The two exponentials can be combined:

$$I_{dist}(\mathbf{k},0) = \frac{\bar{b}^* \bar{b}}{N} \sum_j \sum_{l \neq j} \left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} \; e^{i\mathbf{k}\cdot\mathbf{R}_l(0)} \right\rangle = \frac{\left|\bar{b}\right|^2}{N} \sum_j \sum_{l \neq j} \left\langle e^{-i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_l)} \right\rangle$$

The structure factor

Definition:

$$S(\mathbf{k}) = \frac{1}{N} \sum_{j,l} \left\langle e^{-i\mathbf{k}\cdot\left(\mathbf{R}_l - \mathbf{R}_j\right)} \right\rangle$$

As a consequence:

$$\frac{1}{N} \sum_{j} \sum_{l \neq j} \left\langle e^{-i\mathbf{k}\cdot\left(\mathbf{R}_l - \mathbf{R}_j\right)} \right\rangle = S(\mathbf{k}) - 1$$

And the differential cross section becomes:

$$\frac{ds}{d\Omega} = \overline{b^2} + \left|\overline{b}\right|^2 \left[S(\mathbf{k}) - 1\right]$$

Basic expression for a diffraction experiment

The total scattering cross section

For an isotropic system:

$$\sigma(k) = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi \overline{b^2} + 4\pi \left|\overline{b}\right|^2 \left[S(k) - 1\right]$$

For a homogeneous system: S(k) = 1

$$\sigma(k) = 4\pi \overline{b^2} = \sigma_{tot}$$

Definition:

$$\sigma_{coh} = 4\pi \left|\overline{b}\right|^2$$

$$\sigma_{inc} = 4\pi \left[\overline{b^2} - \left|\overline{b}\right|^2\right]$$

$$\sigma_{tot} = \sigma_{coh} + \sigma_{inc} = 4\pi \overline{b^2}$$

- Coherent cross section
- Incoherent cross section
- Total cross section

back to the d.d. scattering c.s.

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{k_1}{k_0}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, \exp\{-iwt\}\left[I_{dist}(\mathbf{k},t) + I_{self}(\mathbf{k},t)\right]$$

For a monatomic, mono-isotopic system:

$$I_{dist}(\mathbf{k},t) = \left|\overline{b}\right|^2 \frac{1}{N}\sum_j \sum_{l\neq j}\left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)}\; e^{i\mathbf{k}\cdot\mathbf{R}_l(t)}\right\rangle = \left|\overline{b}\right|^2 F_{dist}(\mathbf{k},t)$$

$$I_{self}(\mathbf{k},t) = \overline{b^2}\,\frac{1}{N}\sum_j \left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} e^{i\mathbf{k}\cdot\mathbf{R}_j(t)}\right\rangle = \overline{b^2}\, F_{self}(\mathbf{k},t)$$

F_{self}(k,t) = F_{dist}(k,t) = intermediate scattering functions

The classical formula for the double differential scattering cross section:

[L. Van Howe, Phys. Rev. **95**, 249, (1954)]

$$\left(\frac{d^2\sigma}{d\Omega\, d\omega}\right) = \left(\frac{k_1}{k_0}\right)\left(\frac{\sigma_{coh}}{4\pi} S(k,\omega) + \frac{\sigma_{inc}}{4\pi} S_{self}(k,\omega)\right)$$

Where the dynamic structure factors are defined as:

$$S(k,\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\tau\, \exp\left[-i\omega\tau\right] F(k,\tau)$$

$$S_{self}(k,\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\tau\, \exp\left[-i\omega\tau\right] F_{self}(k,\tau)$$

General considerations
on the distinct term (classical limit)

The distinct term: $$I_{dist}(\mathbf{k},t) = \frac{1}{N}\sum_{j}\sum_{l\neq j} \bar{b}_j^* \, \bar{b}_l \left\langle e^{-i\mathbf{k}\cdot\left[\mathbf{R}_j(0)-\mathbf{R}_l(t)\right]}\right\rangle$$

$[R_j - R_l] >$ internuclear distance (≈1 A)

when $k >> 1\ A^{-1}$

then, fast phase oscillations impose: $I_{dist}(k,t) \cong 0$

when $k << 1\ A^{-1}$

$I_{dist}(k,t)$ probes long-wavelength collective (phonon) modes

General considerations
on the self term (classical limit)

The self term

$$I_{self}(\mathbf{k},t)=\frac{1}{N}\sum_j \overline{b_j^2}\left\langle e^{-i\mathbf{k}\cdot[\mathbf{R}_j(0)-\mathbf{R}_j(t)]}\right\rangle$$

Large k probe the short-time self dynamics.

Small k probe the long-time diffusive motion [exp $\rightarrow$ 1, in a crystal (NO diffusion)].

Self term is the only surviving at large k.

Very large k $\Rightarrow$ very short-time dynamics

$[R_j(t) - R_j(0)] \cong v_j\, t$ (impulse approximation)

coherent / incoherent scattering

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{k_1}{k_0}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{-iwt}\,\frac{1}{N}\sum_{j,l}\left\langle \hat{b}_j^{+}\,\hat{b}_l\right\rangle\left\langle e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_j}\,e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_l(t)}\right\rangle$$

by writing:

$$\left\langle \hat{b}_j^{+}\,\hat{b}_l\right\rangle = \left\langle \hat{b}_j^{+}\,\hat{b}_l\right\rangle_{l\neq j} + d_{j,l}\left\langle \hat{b}_j^{+}\,\hat{b}_j\right\rangle$$

$$= \left\langle \hat{b}_j^{+}\right\rangle\left\langle \hat{b}_l\right\rangle_{l\neq j} + d_{j,l}\left\langle b_j^2\right\rangle \pm d_{j,l}\left\langle \hat{b}_j^{+}\right\rangle\left\langle \hat{b}_j\right\rangle$$

$$= \left\langle \hat{b}_j\right\rangle^{*}\left\langle \hat{b}_l\right\rangle + d_{j,l}\left[\left\langle b_j^2\right\rangle - \left\langle \hat{b}_j\right\rangle^{*}\left\langle \hat{b}_j\right\rangle\right]$$

For a monatomic, mono-isotopic system:

$$\left\langle \hat{b}_j^{+}\,\hat{b}_l\right\rangle = \left|\overline{b}\right|^2 + d_{j,l}\left[\overline{b^2} - \left|\overline{b}\right|^2\right] = \frac{1}{4p}\left[s_{coh} + d_{j,l}\, s_{inc}\right]$$

Scattering cross section (5)

$$\left[\frac{d^2 s}{d\Omega de}\right] = \frac{k_1}{k_0}\frac{1}{2p\hbar}\int_{-\infty}^{+\infty} dt\, e^{-iwt}\, I(\mathbf{k},t)$$

where:

$$I(\mathbf{k},t) = I_{coh}(\mathbf{k},t) + I_{inc}(\mathbf{k},t)$$

with:

$$I_{coh}(\mathbf{k},t) = \frac{s_{coh}}{4p} F(\mathbf{k},t)$$

$$I_{inc}(\mathbf{k},t) = \frac{s_{inc}}{4p} F_{self}(\mathbf{k},t)$$

and:

$$F(\mathbf{k},t) = \frac{1}{N}\sum_{j,l}\left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} e^{i\mathbf{k}\cdot\mathbf{R}_l(t)}\right\rangle$$

$$F_{self}(\mathbf{k},t) = \frac{1}{N}\sum_{j}\left\langle e^{-i\mathbf{k}\cdot\mathbf{R}_j(0)} e^{i\mathbf{k}\cdot\mathbf{R}_j(t)}\right\rangle$$

Origin of incoherence in elastic neutron scattering

Monatomic mono-isotopic system:

- **Nuclear spin ^{1} 0:** the spin transition introduces a random term in the phase of the scattered neutron wave
(constructive interference NOT possible).
$\Rightarrow$ incoherent scattering (es.: Vanadium 51)
- **Nuclear spin = 0:** NO spin transition allowed (constructive interference IS possible)
$\Rightarrow$ coherent scattering (es.: Argon 36)

Monatomic isotopic mixture

- Incoherence is induced by different scattering lenghts of different isotopes

Origin of incoherence in neutron inelastic scattering

Collective excitations (phonons)

- The scattering event on the single nucleus is (substantially) elastic:
- $\Rightarrow$ constructive interference IS possible

Molecular transitions are excited:

- The intra-molecular transition introduces a random phase in the scattered neutron propagator:
- $\Rightarrow$ NO constructive interference possible.

Summing up:

- Neutron features
- How neutrons are produced
- Thermal and pulsed neutron sources
- General theory of a neutron inelastic scattering experiment
- Integration over the final energy (diffraction)
- General considerations on D.D. cross section:
  - High k limit
  - Low k limit
  - origin of the incoherence in neutron scattering

THE END

- ... of part 1
- to be continued ....

Plan of module N.2
(discussing the Born approximation)

1. Scattering from a central potential
2. General solution
   (Green function method)
3. Perturbative solution
4. 1st order solution (Born approximation)
5. Validity Criterion
6. Failure of the Born approximation
   (wow!)
7. Fermi conjecture
8. Fermi pseudo-potential

Particle scattering problem in Quantum Mechanics (A. Messiah, Ch.XIX)

Problem: scattering from a central potential V(r).

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r})$$

Schrödinger Equation

A known Eigensolution (with the correct asymptotic behaviour) is:

$$\Psi(\mathbf{r}) \approx e^{i\mathbf{k}_0\cdot\mathbf{r}} + f(\Omega)\frac{e^{ik_1 r}}{r}$$

with

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

Solution of Schrödinger equation

we define: $$U(r) = \frac{2m}{\hbar^2} V(r)$$

$$\left(\nabla^2 + k^2\right)\Psi(r) = U(r)\Psi(r)$$ Schrödinger equation

General Solution of the inhomogeneous equation:

$$\Psi(\mathbf{r}) = \Psi_{\text{homogeneous}}(\mathbf{r}) + \Psi_{\text{particular}}(\mathbf{r})$$

Solution of the homogeneous equation:

$$\left(\nabla^2 + k^2\right)\Phi(\mathbf{r}) = 0 \quad \Rightarrow \quad \Phi(\mathbf{r}) = e^{i\mathbf{k}_0 \cdot \mathbf{r}}$$

the Green function method
for the particular solution

Definition of the Green function:

$$\left(\nabla^2 + k^2\right) G(\mathbf{r} - \mathbf{r}') = d(\mathbf{r} - \mathbf{r}')$$

Particular solution:

$$\Psi(\mathbf{r}) = \int d\mathbf{r}' \, G(\mathbf{r} - \mathbf{r}') \, U(r') \, \Psi(\mathbf{r}')$$

Formal general solution of Schrödinger equation:

$$\Psi(\mathbf{r}) = \Phi(\mathbf{r}) - \int d\mathbf{r}' \, G(\mathbf{r} - \mathbf{r}') \, U(r') \, \Psi(\mathbf{r}')$$

soution of the Green equation:

$$\left(\nabla^2 + k^2\right)G(\mathbf{r}) = -d(\mathbf{r})$$

We define the Fourier transform:

$$F(\mathbf{q}) = \int d\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}} G(\mathbf{r})$$

the differential equation becomes:

$$\left(-q^2 + k^2\right)F(\mathbf{q}) = -1$$

... and the solution is:

$$F(q) = \frac{1}{q^2 - k^2}$$

From which, using the inverse Fourier transform:

$$G(\mathbf{r}) = \frac{1}{(2p)^3}\int d\mathbf{q}\, e^{i\mathbf{q}\cdot\mathbf{r}} F(\mathbf{q})$$

the Fourier integral (angular part):

$$G(\mathbf{r}) = \frac{1}{(2\pi)^3}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin(\theta)\int_0^{\infty} dq\, q^2\, e^{iqr\cos(\theta)} F(q)$$

$$= \frac{2\pi}{(2\pi)^3}\int_{-1}^{1} dx \int_0^{\infty} dq\, q^2\, e^{iqrx} F(q)$$

$$= \frac{1}{(2\pi)^2}\int_0^{\infty} dq\, q^2\, F(q) \int_{-1}^{1} dx\, e^{iqrx}$$

$$= \frac{1}{(2\pi)^2}\int_0^{\infty} dq\, q^2\, F(q) \frac{2\sin(qr)}{qr}$$

$$= \frac{1}{2\pi^2 r}\int_0^{\infty} dq\, q \sin(qr) F(q)$$

the Fourier integral (radial term):

$$G(\mathbf{r}) = \frac{1}{2p^2 r}\int_0^{\infty} dq\, q \sin(qr) \frac{1}{q^2 - k^2}$$

- integrand EVEN in κ

$$= \frac{1}{4p^2 r}\int_{-\infty}^{+\infty} dq\, \sin(qr) \frac{1}{q^2 - k^2}$$

- exp. form of sin(κr)

$$= \frac{1}{4p^2 r}\int_{-\infty}^{+\infty} dq\, q \frac{e^{iqr} - e^{-iqr}}{2i} \frac{1}{q^2 - k^2}$$

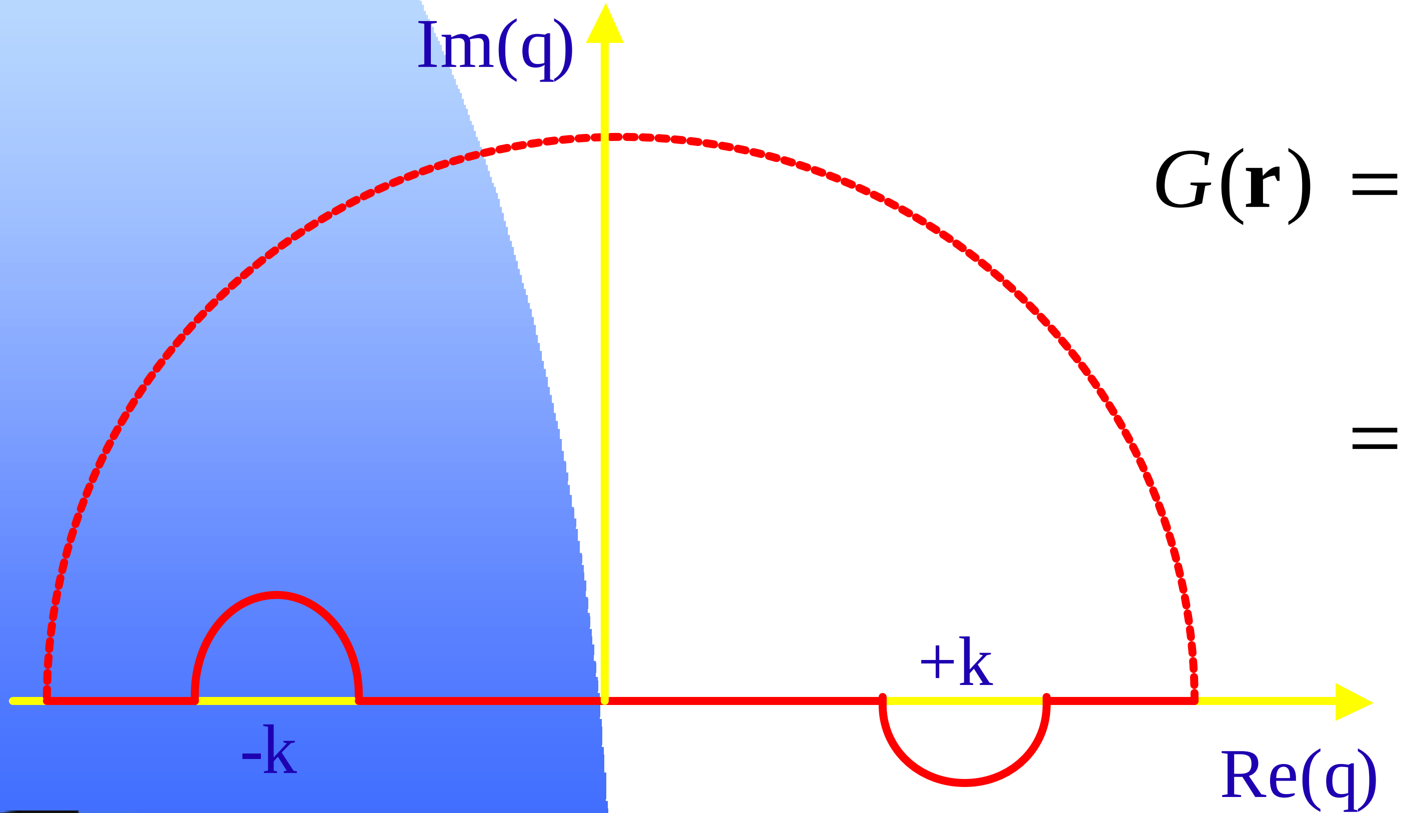
- combining the 2 exp.

$$= \frac{1}{4ip^2 r}\int_{-\infty}^{+\infty} dq\, q \frac{e^{iqr}}{q^2 - k^2}$$

- contour integral in the complex plane

the contour integral:

$$G(\mathbf{r}) = \frac{1}{4ip^2 r}\int_{-\infty}^{+\infty} dq\, q \frac{e^{iqr}}{(q-k)(q+k)}$$



$$G(\mathbf{r}) = \frac{1}{4ip^2 r} 2p\, i\, k \frac{e^{ikr}}{2k}$$

$$= \frac{e^{ikr}}{4p\, r}$$

the Green function:

The final result for the Green function is:

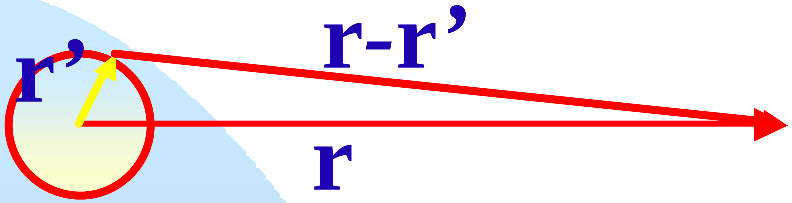
$$G(\mathbf{r}-\mathbf{r}') = \frac{e^{ik_1|\mathbf{r}-\mathbf{r}'|}}{4p\,|\mathbf{r}-\mathbf{r}'|}$$

And the formal solution of the Schrödinger equation becomes:

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \int d\mathbf{r}'\,\frac{e^{ik_1|\mathbf{r}-\mathbf{r}'|}}{4p\,|\mathbf{r}-\mathbf{r}'|}\,U(r')\,\Psi(\mathbf{r}')$$

The result is RIGOROUS: no approximation made

Approximation N. 1: *far field*



We are looking for a solution far from the potential centre.

r_0= range of U(r) << r

$$|\mathbf{r}-\mathbf{r}'| \cong r - \mathbf{r}'\cdot\hat{\mathbf{r}}$$

Thus the formal solution becomes ($\mathbf{k}_1$ directed as **r**):

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{e^{ik_1 r}}{4\pi\, r}\int d\mathbf{r}'\; e^{-i\mathbf{k}_1\cdot\mathbf{r}'}\,U(r')\,\Psi(\mathbf{r}')$$

Perturbative solution:

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{e^{ik_1 r}}{4p\ r}\int d\mathbf{r}'\ e^{-ik_1(\mathbf{r}'\cdot\hat{\mathbf{r}})}U(r')\,\Psi(\mathbf{r}')$$

Equation can be solved iteratively
[provided U(r) is small]

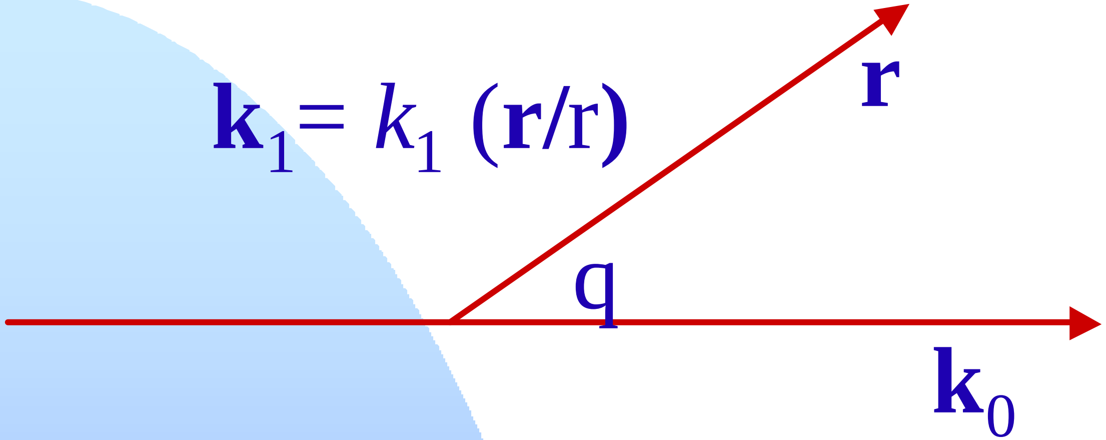
$$\Psi^{(0)}(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}}$$

0-th order solution !

1-st order solution !

$$\Psi^{(1)}(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{e^{ik_1 r}}{4p\ r}\int d\mathbf{r}'\ e^{-i\mathbf{k}_1\cdot\mathbf{r}'}\ U(r')\,\Psi^{(0)}(\mathbf{r}')$$

1st order solution (Born approximation):



$$\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_0$$

$$\Psi^{(1)}(\mathbf{r}) = e^{i\mathbf{k}_0 \cdot \mathbf{r}} - \frac{e^{ik_1 r}}{4p\ r} \int d\mathbf{r}'\ e^{-i(\mathbf{k}_1 - \mathbf{k}_0)\cdot \mathbf{r}'}\, U(r')$$

The solution, in Born approximation, becomes:

$$f(\Omega) = \frac{-1}{4p} \int d\mathbf{r}'\ e^{-i\mathbf{k}\cdot\mathbf{r}'}\, U(r') = \frac{-2m}{4p\ \hbar^2} \int d\mathbf{r}'\ e^{-i\mathbf{k}\cdot\mathbf{r}'}\, V(r')$$

validity condition of the Born approximation

1st order solution:

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \int d\mathbf{r}' \frac{e^{ik_1|\mathbf{r}-\mathbf{r}'|}}{4p|\mathbf{r}-\mathbf{r}'|} U(r')\, e^{i\mathbf{k}_0\cdot\mathbf{r}'}$$

The 2nd term (spherical wave) SHOULD be smaller than the 1st (plane wave).

$$\left| \frac{2m}{\hbar^2} \int d\mathbf{r}' \frac{e^{ik_1|\mathbf{r}-\mathbf{r}'|}}{4p\,|\mathbf{r}-\mathbf{r}'|} V(r')\, e^{i\mathbf{k}_0\cdot\mathbf{r}'} \right| << 1$$

This condition should be valid in any point **r**, where the interaction potential is ≠ 0

check on the validity condition

Without loss in generality, we assume:

- square well potential (depth V_0 and range r_0)
- $\mathbf{r} \cong 0$

$$\Delta = \left| \frac{2m}{\hbar^2} \int d\mathbf{r}' \, \frac{e^{ik_1 r'}}{4p \; r'} V(r') \, e^{i\mathbf{k}_0 \cdot \mathbf{r}'} \right| << 1$$

Moreover:

- We take the the z-axis along $\mathbf{k}_0$
- We assume $k_1 \sim k_0$

angular integration

$$\Delta = \left| \frac{2m}{\hbar^2} \, 2\pi \int_0^{\pi} d\theta \sin\theta \int_0^{r_0} dr \, r^2 \, \frac{e^{ik_0 r}}{4\pi \, r} V(r) \, e^{ik_0 r \cos\theta} \right|$$

$$= \left| \frac{m}{\hbar^2} \int_0^{r_0} dr \, r^2 \, \frac{e^{ik_0 r}}{r} V(r) \int_{-1}^{1} dx \, e^{ik_0 r x} \right|$$

$$= \left| \frac{m}{\hbar^2} \int_0^{r_0} dr \, r^2 \, \frac{e^{ik_0 r}}{r} V(r') \, \frac{1}{ik_0 r} \left[e^{ik_0 r} - e^{-ik_0 r} \right] \right|$$

$$= \left| \frac{mV_0}{ik_0 \hbar^2} \int_0^{r_0} dr \left[e^{2ik_0 r} - 1 \right] \right|$$

radial integration

$$\Delta = \left| \frac{mV_0}{ik_0\hbar^2} \int_0^{r_0} dr \left[e^{2ik_0 r} - 1 \right] \right|$$

$$= \left| \frac{mV_0}{ik_0\hbar^2} \left[\frac{1}{2ik_0} \left(e^{2ik_0 r_0} - 1 \right) - r_0 \right] \right|$$

We define: $y = 2\, k_0\, r_0$

$$\Delta = \frac{mV_0}{2k_0^2\hbar^2} \left| e^{iy} - iy - 1 \right|$$

$$= \frac{mV_0}{2k_0^2\hbar^2} \left[\left(e^{iy} - iy - 1 \right)\left(e^{-iy} + iy - 1 \right) \right]^{\frac{1}{2}}$$

$$= \frac{mV_0}{2k_0^2\hbar^2} \left[y^2 + 2 + 2y \sin y - 2\cos y \right]^{\frac{1}{2}}$$

failure of the Born approximation !

Assuming: $\lambda_0 \cong 10^{-8}$ cm, $r_0 = 2 \times 10^{-13}$ cm

$y = 2\, k_0\, r_0 = 2.5 \times 10^{-4} << 1$

$$\Delta = \frac{mV_0}{2k_0^2\hbar^2}\left[y^2 + 2 - 2y\sin y - 2\cos y\right]^{1/2} = \frac{mV_0}{2k_0^2\hbar^2}\left[\frac{y^4}{4} + \cdots\right]^{1/2}$$

and the condition becomes: $\Delta \cong \frac{mV_0 r_0^2}{\hbar^2} << 1$

Assuming (n-p interaction): $V_0 \cong 36$ MeV

$$\Delta \cong \frac{mV_0 r_0^2}{\hbar^2} = \frac{(1.6\times10^{-24})\cdot(36\times10^6\cdot1.6\times10^{-12})\cdot 4\times10^{-26}}{10^{-54}} \cong 3.7$$

Definitely Δ is NOT << 1 !!!

Fermi conjecture

(La Ricerca Scientifica, v.7, p.13, 1936)

$$f(\Omega) \approx \frac{m}{\hbar^2}\int d\mathbf{r}' \; e^{-i\mathbf{k}\cdot\mathbf{r}'} V(r') \approx \frac{m}{\hbar^2} V_0 r_0^3$$

= scattering amplitude (can be measured)

- Decrease V_0 and increase r_0 in such a way that $V_0\ r_0^3$ remains ≅ constant
- For example:
  - $V_0^* = V_0 \times 10^{-6}$
  - $r_0^* = r_0 \times 10^2$
- $k_0\ r_0^* = 2.5\ 10^{-2} << 1$

$$\Delta \cong \frac{m V_0^* (r_0^*)^2}{\hbar^2} \cong 3.7\times10^{-6}\times10^4 = 3.7\times10^{-2}$$

In other words:

- Collision theory for thermal neutrons can be reformulated in such a way that the 1st Born approximation can be safely applied.
- Thermal neutron wavelength is long enough, that we may extend the range of the neutron-nucleon potential by two orders of magnitude, still considering the scattering event as happening in a point.
- This allows to decrease the effective amplitude of the potential by six orders of magnitude, without changing the scattering length

Definition of Fermi pseudo-potential

$$\hat{V}_j(\boldsymbol{r}) = \frac{2\pi\hbar^2}{m}\hat{b}_j\,\delta(\boldsymbol{r} - \hat{\boldsymbol{R}}_j)$$

- It contains only the (measurable) scattering length ...
- ... and some fundamental constants (neutron mass and $\hbar$)

Summing up:

- Scattering Problem in Q.M.
- Solution of Schrödinger equation (using the Green function method)
- The 1-st order solution (Born approximation)
- Failure of the Born Approximation
- Fermi conjecture
- Fermi pseudo-potential

Plan of module N.3
(dealing with recoil)

1. Recalling some basic QM relations
2. Intermediate scattering functions
3. Evidencing the recoil factor

Some basic QM relations (1)

$$\left[R_{j,\alpha}, P_{l,\beta}\right] = i\hbar\, \delta_{jl}\, \delta_{\alpha,\beta}$$

j,l label the nuclei

α, β label the Cartesian components

As a consequence:

$$\left[P_{j,\alpha}, A(r,p)\right] = -i\hbar \frac{\partial}{\partial R_{j,\alpha}} A(r,p) \qquad \left[R_{j,\alpha}, A(r,p)\right] = i\hbar \frac{\partial}{\partial P_{j,\alpha}} A(r,p)$$

in particular:

$$\left[P_{j,\alpha}, \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_l\right)\right] = \hbar\, k_\alpha\, \delta_{jl}\, \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_l\right)$$

from which:

$$P_{j,\alpha} \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_l\right) = \exp\left(i\boldsymbol{k}\cdot\boldsymbol{R}_l\right)\left(\hbar\, k_\alpha\, \delta_{j,l} + P_{j,\alpha}\right)$$

Some basic QM relations (2)

The procedure can be iterated:

$$(P_{j,a})^n \exp[i\mathbf{k}\cdot\mathbf{R}_l] = \exp[i\mathbf{k}\cdot\mathbf{R}_l](\hbar k_a \delta_{j,l} + P_{j,a})^n$$

and we arrive to the general expression:

$$A(r,p)\exp\{i\mathbf{k}\cdot\mathbf{R}_j\} = \exp\{i\mathbf{k}\cdot\mathbf{R}_j\}A\left[r;\mathbf{P}_1,\mathbf{P}_2,\ldots,(\mathbf{P}_j+\hbar\mathbf{k}),\ldots,\mathbf{P}_N\right]$$

Thus, for any function of operators A(r,p) we have:

$$\exp\{+i\mathbf{k}\cdot\mathbf{R}_j\}A(r,p)\exp[-i\mathbf{k}\cdot\mathbf{R}_l] =$$
$$= \exp\{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_l)\}A(r;\mathbf{P}_1,\mathbf{P}_2,\cdots,\mathbf{P}_l-\hbar\mathbf{k},\cdots,\mathbf{P}_N)$$

Application to the Hamiltonian

$$e^{i\mathbf{k}\cdot\mathbf{R}_l} e^{\frac{it}{\hbar}\mathrm{H}} e^{-i\mathbf{k}\cdot\mathbf{R}_l} = e^{\frac{it}{\hbar}\mathrm{H}\left(r;\mathbf{P}_1,\cdots,\mathbf{P}_l-\hbar\mathbf{k},\cdots,\mathbf{P}_N\right)}$$

If the Hamiltonian has the standard form:

$$\mathrm{H}(r,p)=\frac{p^2}{2M}+\Phi(r)$$

... then we have:

$$\mathrm{H}\left(r;\mathbf{P}_1,\cdots,\mathbf{P}_l-\hbar\mathbf{k},\cdots,\mathbf{P}_N\right)=\mathrm{H}(r,p)-\frac{\hbar}{M}\left(\mathbf{P}_l\cdot\mathbf{k}\right)+\frac{\hbar^2k^2}{2M}$$

Recall the intermediate scattering functions

$$F(\mathbf{k},t) = \frac{1}{N}\sum_{j,l} \left\langle e^{i\mathbf{k}\cdot\mathbf{R}_j} e^{-i\mathbf{k}\cdot\mathbf{R}_l(t)} \right\rangle$$

$$= \frac{1}{N}\sum_{j,l} \left\langle e^{i\mathbf{k}\cdot\mathbf{R}_j} e^{-i\mathbf{k}\cdot\mathbf{R}_l} e^{i\mathbf{k}\cdot\mathbf{R}_l} e^{-i\mathbf{k}\cdot\mathbf{R}_l(t)} \right\rangle$$

$$= \frac{1}{N}\sum_{j,l} \left\langle e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_l)} e^{i\mathbf{k}\cdot\mathbf{R}_l} e^{\frac{it}{\hbar}\mathrm{H}} e^{-i\mathbf{k}\cdot\mathbf{R}_l} e^{-\frac{it}{\hbar}\mathrm{H}} \right\rangle$$

$$F_{self}(\mathbf{k},t) = \frac{1}{N}\sum_{j} \left\langle e^{i\mathbf{k}\cdot\mathbf{R}_j} e^{\frac{it}{\hbar}\mathrm{H}} e^{-i\mathbf{k}\cdot\mathbf{R}_j} e^{-\frac{it}{\hbar}\mathrm{H}} \right\rangle$$

They become:

$$F(\mathbf{k},t) = e^{\frac{it}{\hbar}\frac{\hbar^2 k^2}{2M}} \frac{1}{N} \sum_{j,l} \left\langle e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_l)} e^{\frac{it}{\hbar}\left[\mathrm{H} - \frac{\hbar}{M}(\mathbf{P}_l \cdot \mathbf{k})\right]} e^{-\frac{it}{\hbar}\mathrm{H}} \right\rangle$$

coherent term

$$F_{self}(\mathbf{k},t) = e^{\frac{it}{\hbar}\frac{\hbar^2 k^2}{2M}} \frac{1}{N} \sum_{j} \left\langle e^{\frac{it}{\hbar}\left[\mathrm{H} - \frac{\hbar}{M}(\mathbf{P}_j \cdot \mathbf{k})\right]} e^{-\frac{it}{\hbar}\mathrm{H}} \right\rangle$$

incoherent (self) term

define the operator $A_j(k,t)$

$$A_j(\mathbf{k},t) = e^{\frac{it}{\hbar}\mathrm{H}'_j(r,p)}\, e^{-\frac{it}{\hbar}\mathrm{H}(r,p)}$$

where: $$\mathrm{H}'_j(r,p) = \left[\mathrm{H}(r,p) - \frac{\hbar}{M}\left(\mathbf{P}_j \cdot \mathbf{k}\right)\right] = \left[\mathrm{H}(r,p) - \hbar\, \mathbf{v}_j \cdot \mathbf{k}\right]$$

its equation of motion is:

$$\frac{d}{dt}A_j(\mathbf{k},t) = \left(\frac{i\mathrm{H}'}{\hbar}\right) e^{\frac{it}{\hbar}\mathrm{H}'} e^{-\frac{it}{\hbar}\mathrm{H}} + e^{\frac{it}{\hbar}\mathrm{H}'}\left(\frac{-i\mathrm{H}}{\hbar}\right) e^{-\frac{it}{\hbar}\mathrm{H}}$$

$$= e^{\frac{it}{\hbar}\mathrm{H}'}\left(i\,\frac{\mathrm{H}' - \mathrm{H}}{\hbar}\right) e^{-\frac{it}{\hbar}\mathrm{H}}$$

$$= e^{\frac{it}{\hbar}\mathrm{H}'}\left(-i\, \mathbf{v}_j \cdot \mathbf{k}\right) e^{-\frac{it}{\hbar}\mathrm{H}}$$

Choosing the reference system

- Origin ≡ position of j-th particle at t=0
- $\Phi(r)=\Phi(R_1, \ldots, R_{j-1}, R_{j+1}, \ldots, , R_N)$ (independent of R_j)

As a consequence:

- $[P_j, H(r,p)] = 0$
- the Eq. of motion reduces to:

$$\frac{d}{dt} A_j(\mathbf{k},t) = \left[-i\, \mathbf{v}_j(t) \cdot \mathbf{k}\right] A_j(\mathbf{k},t)$$

whose solution is:

$$A_j(\mathbf{k},t) = A_j(\mathbf{k},0) - i \int_0^t dt_1 \left[\mathbf{v}_j(t_1) \cdot \mathbf{k}\right] A_j(\mathbf{k},t_1)$$

Iterative solution of Operator $A_j(k,t)$

$$A_j(\mathbf{k},t) = 1 - ik\int_0^t dt_1 v_{j,k}(t_1)\ A_j(\mathbf{k},t_1)$$

1-th order solution:

$$A_j^{(1)}(\mathbf{k},t) = 1 - ik\int_0^t dt_1\ v_{j,k}(t_1)$$

2-nd order solution:

$$A_j^{(2)}(\mathbf{k},t) = 1 - ik\int_0^t dt_1\ v_{j,k}(t_1)\ A^{(1)}(\mathbf{k},t_1)$$

$$= 1 - ik\int_0^t dt_1\ v_{j,k}(t_1)\left[1 - ik\int_0^{t_1} dt_2\ v_{j,k}(t_2)\right]$$

$$= 1 + (-ik)\int_0^t dt_1 v_{j,k}(t_1) + (-ik)^2\int_0^t dt_1\int_0^{t_1} dt_2\ v_{j,k}(t_1)\, v_{j,k}(t_2)$$

Formal solution of $A_j(k,t)$

$$A_j(\mathbf{k},t) = \sum_{n=0}^{\infty} (-ik)^n \int_0^t dt_1 \cdots \int_0^{t_{n-1}} dt_n v_{j,k}(t_1) \cdots v_{j,k}(t_n)$$

Introducing the Dyson (Time Ordering) ***T*** operator:

$$A_j(\mathbf{k},t) = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \int_0^t dt_1 \cdots \int_0^t dt_n \mathrm{T}\left\{v_{j,k}(t_1) \cdots v_{j,k}(t_n)\right\}$$

and the formal solution becomes:

$$A_j(\mathbf{k},t) = \mathrm{T} e^{-ik \int_0^t dt_1 \, v_{j,k}(t_1)}$$

Introducing atomic displacement

Atomic motion: $$\mathbf{R}_j(t) = \mathbf{R}_j(0) + \int_0^t dt'\, \mathbf{v}_j(t')$$

projecting along **k**: $$R_{j,k}(t) = R_{j,k}(0) + \int_0^t dt'\, v_{j,k}(t')$$

$$A_j(\mathbf{k},t) = \mathrm{T}e^{ik\left\{R_{j,k}(0) - R_{j,k}(t)\right\}}$$ = formal solution.

In vector form:

$$A_j(\mathbf{k},t) = \mathrm{T}e^{i\mathbf{k}\cdot\left[\mathbf{R}_j(0) - \mathbf{R}_j(t)\right]} = \mathrm{T}e^{-i\mathbf{k}\cdot\left[\mathbf{R}_j(t) - \mathbf{R}_j(0)\right]}$$

$$= e^{-i\mathbf{k}\cdot\left[\mathbf{R}_j(t) - \mathbf{R}_j(0)\right]} = e^{-i\mathbf{k}\cdot d\mathbf{R}_j(t)}$$

Back to intermediate sc. functions

$$F(\mathbf{k},t) = e^{\frac{it}{\hbar}E_R} \frac{1}{N} \sum_{j,l} \left\langle e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_l)} A_l(\mathbf{k},t) \right\rangle$$

$$F_{self}(\mathbf{k},t) = e^{\frac{it}{\hbar}E_R} \frac{1}{N} \sum_{j} \left\langle A_j(\mathbf{k},t) \right\rangle = e^{\frac{it}{\hbar}E_R} \left\langle A(\mathbf{k},t) \right\rangle$$

$$= e^{\frac{it}{\hbar}E_R} \left\langle e^{-i\mathbf{k}\cdot d\,\mathbf{R}(t)} \right\rangle$$

Having defined the recoil energy: $E_R = \dfrac{\hbar^2 k^2}{2M}$

Summing up:

- Very general Q.M. relations
- Applied to the intermediate scattering functions $F(k,t)$ and $F_{dist}(k,t)$
- Explicit derivation of recoil term

Thank you for your attention!

INES
Italian Neutron Experimental Station

Scuola di Spettroscopia Neutronica “F.P. Ricci”
S. Margherita di Pula (CA)
25 Sept. - 6 Oct., 2006

Marco Zoppi

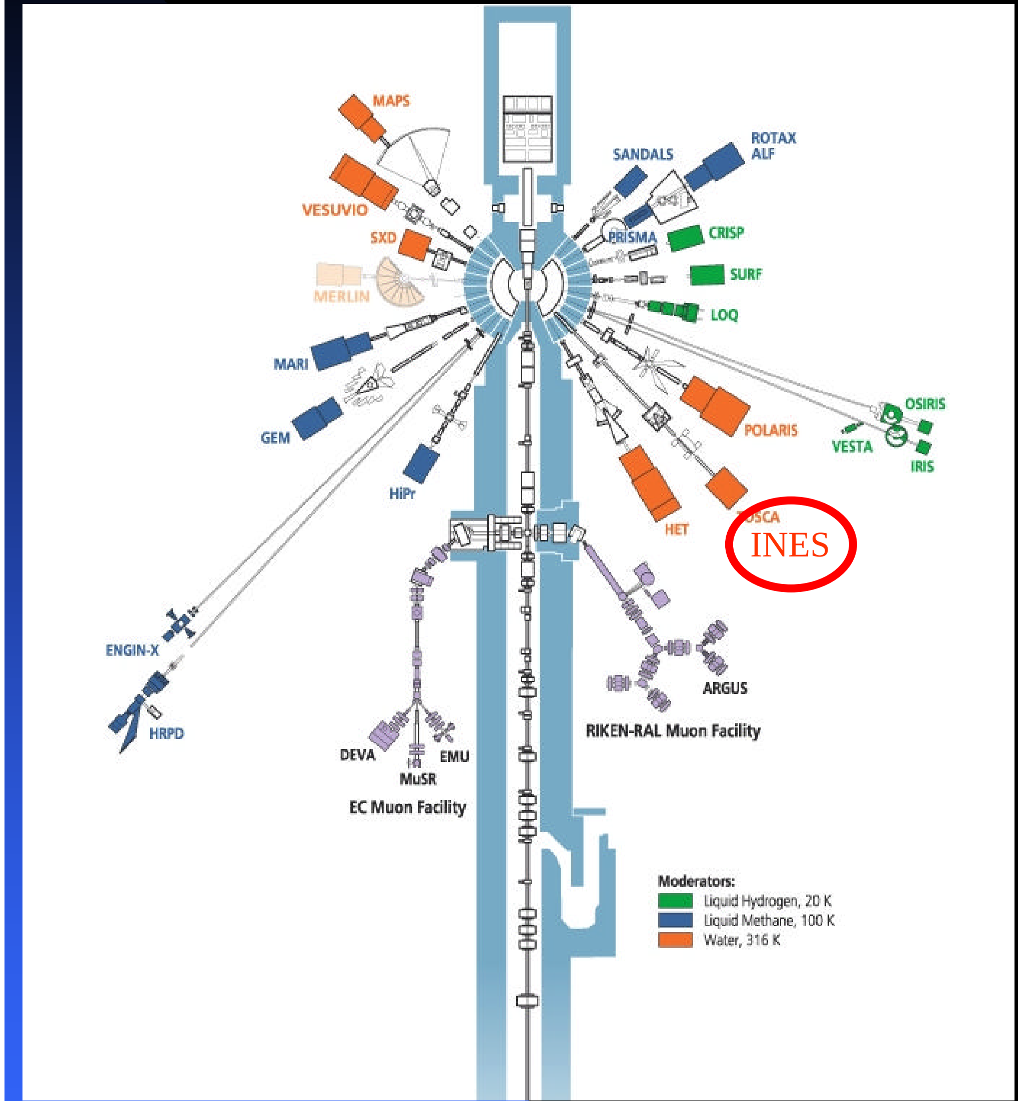
Istituto dei Sistemi Complessi

Consiglio Nazionale delle Ricerche

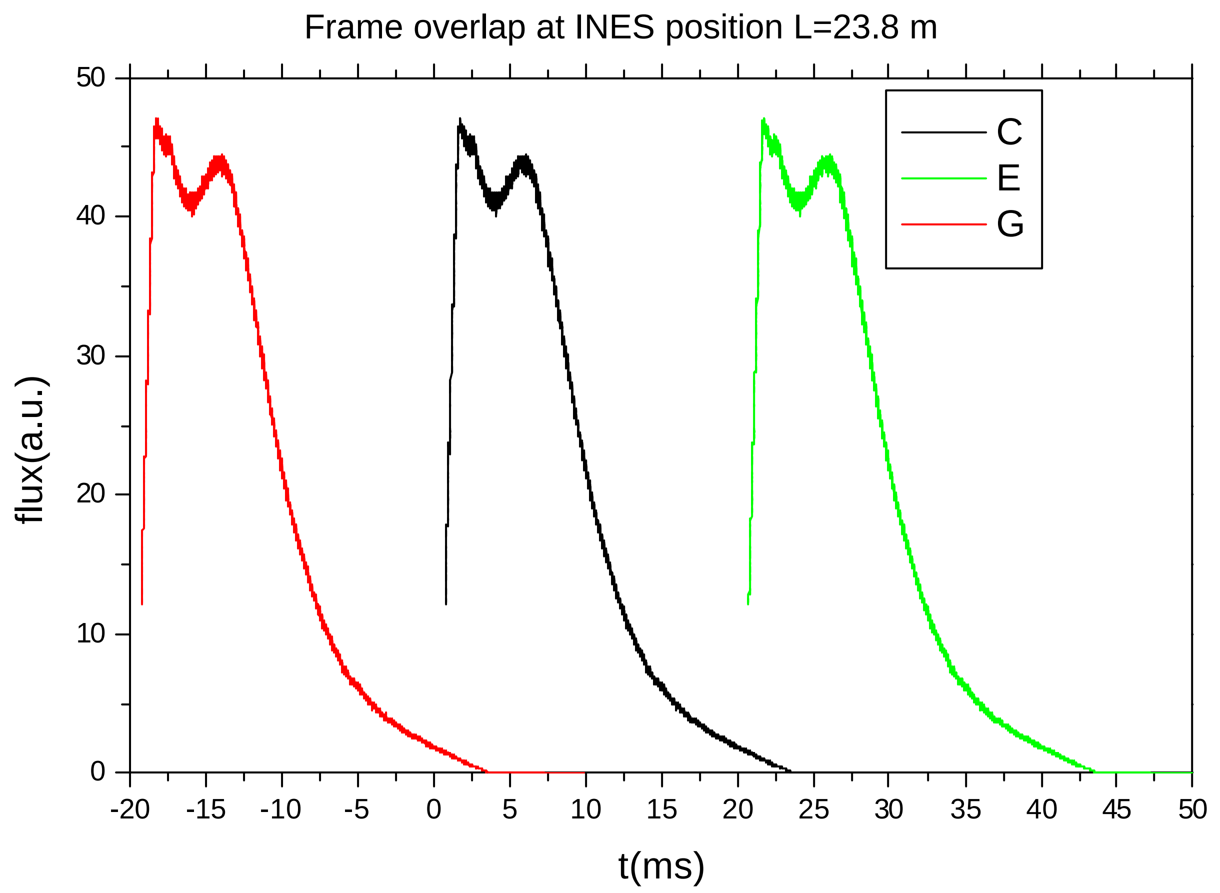
INES: W. W. W. W. & W.

- WHO:
  - Italian CNR Neutron Spettroscopy Committe
- WHY:
  - Italy has NO national source for neutron scattering
- WHAT:
  - Multi-purpose powder diffractometer
- WHERE:
  - ISIS (the moste powerful pulsed neutron source)
  - Beamline N-8, downstream TOSCA spectrometer
- WHEN:
  - 2003 - Official start of project
  - 2005 - End of Commissioning
  - 2006 - Beginning of user program

Location of INES@ISIS



Frame overlap on INES



We assume as an acceptable limit:

Slow neutron flux < 0.001 Fast neutron flux

INES features

- L_0 = 22.80 m.
- L_1 = 1.00 m.
- λ_{min} = 0.17 Å λ_{max} = 3.24 Å
- θ_{min} = 11.6°

  Q_{min} = 0.4 $Å^{-1}$ d_{max} = 16.1 Å

  Q_{max} = 17. $Å^{-1}$ d_{min} = 0.4 Å
- θ_{max} = 170.6°

  Q_{min} = 3.8 $Å^{-1}$ d_{max} = 1.65 Å

  Q_{max} = 75. $Å^{-1}$ d_{min} = 0.08 Å

Diffraction resolving power
(pulsed neutrons)

In general: $$\left(\frac{\Delta d}{d}\right)^2 = \left(\frac{\Delta Q}{Q}\right)^2 = \left(\frac{\Delta t}{t}\right)^2 + \left(\frac{\Delta L}{L}\right)^2 + \left(\frac{\Delta J}{\tan J}\right)^2$$

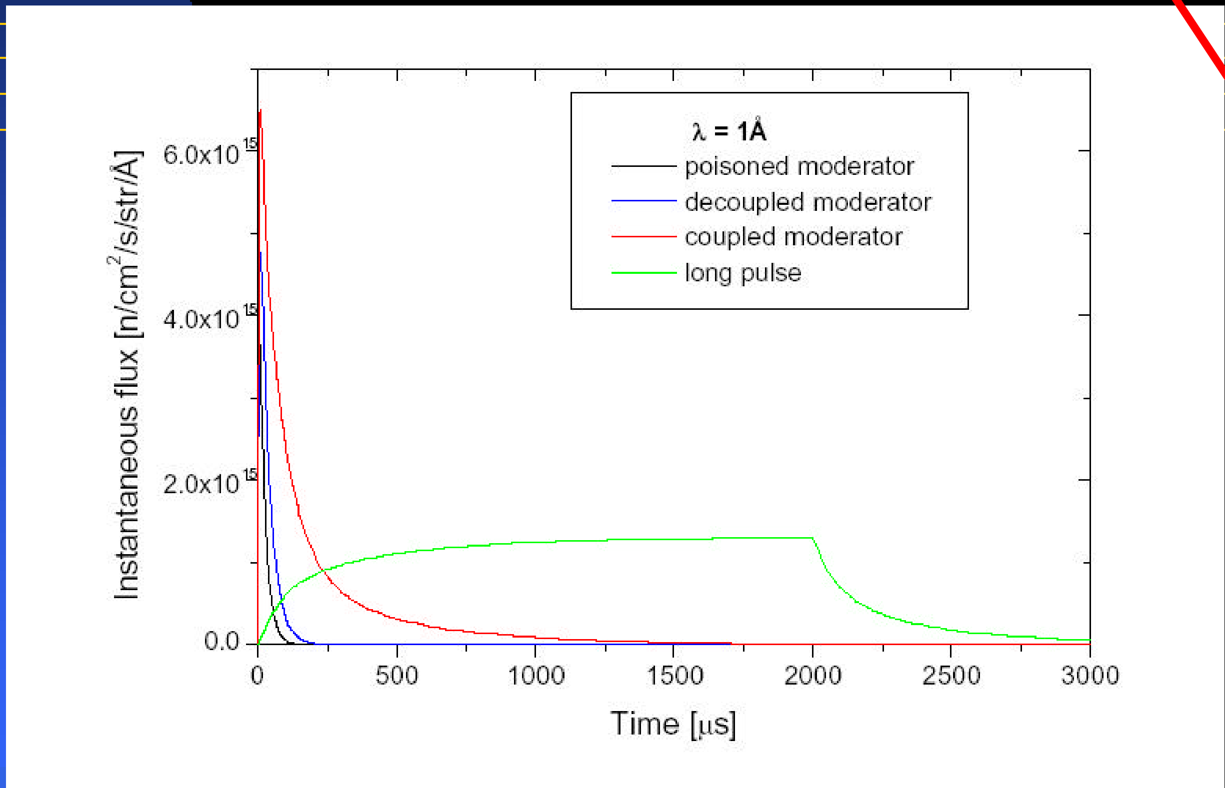
Shape and size of moderator

Shape and size of sample and detector

Relative angular size of sample and detector

Moderator effect

$$\left(\frac{\Delta d}{d}\right)^2 = \left(\frac{\Delta Q}{Q}\right)^2 + \left(\frac{\Delta t}{t}\right)^2 + \left(\frac{\Delta L}{L}\right)^2 + \left(\frac{\Delta J}{\tan J}\right)^2$$



sample

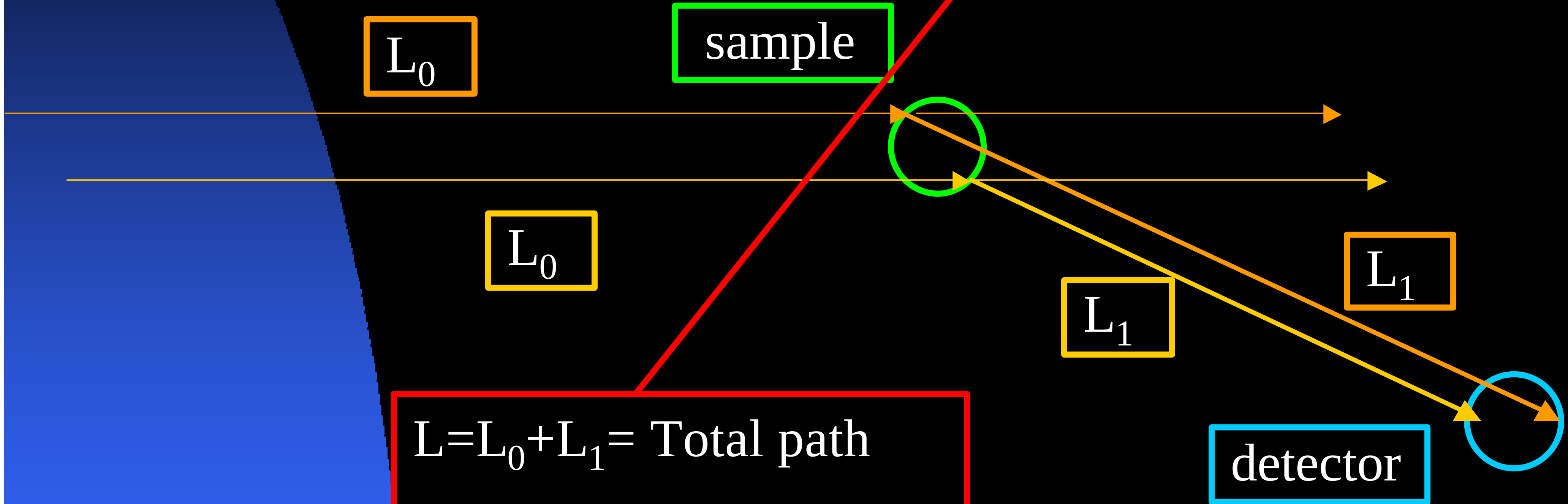
Different λ

⇓

Different time distributions

sample & detector size-effect

$$\left(\frac{\Delta d}{d}\right)^2 = \left(\frac{\Delta Q}{Q}\right)^2 = \left(\frac{\Delta t}{t}\right)^2 + \left(\frac{\Delta L}{L}\right)^2 + \left(\frac{\Delta J}{\tan J}\right)^2$$

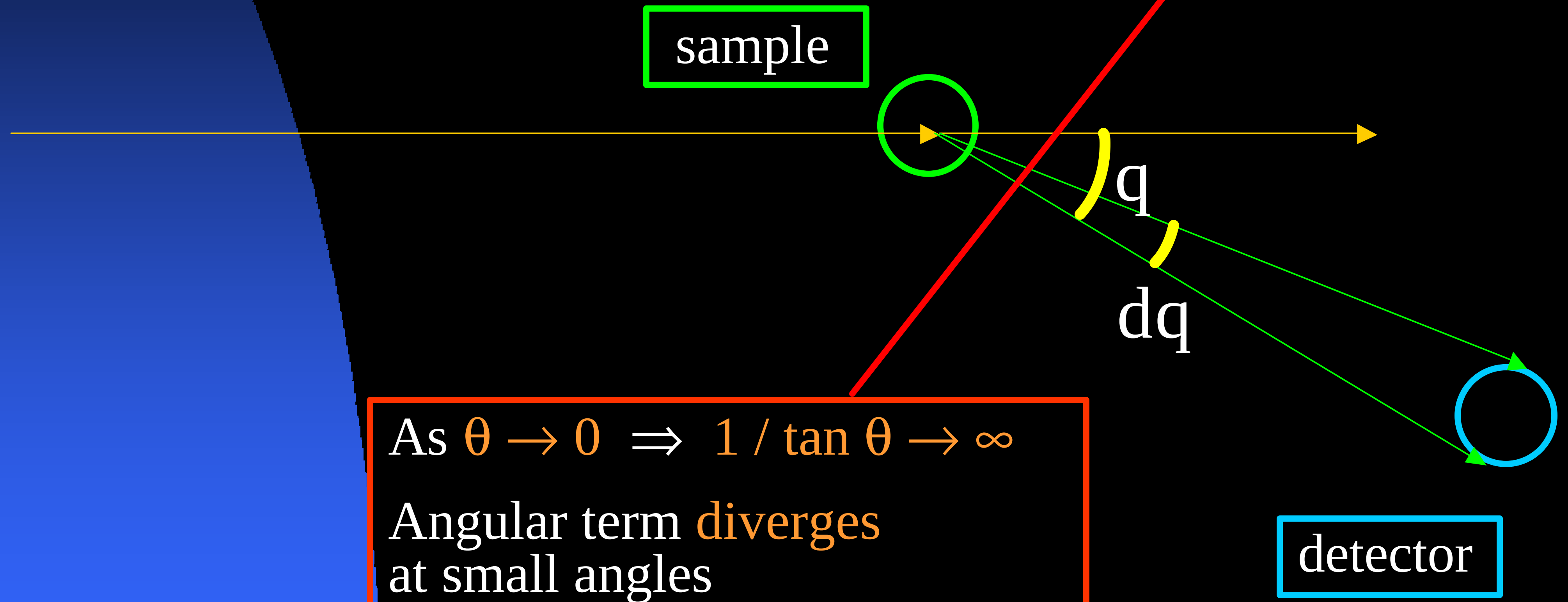


$L = L_0 + L_1 =$ Total path

Different in the 2 cases !

Angular size effect

$$\left(\frac{\Delta d}{d}\right)^2 = \left(\frac{\Delta Q}{Q}\right)^2 = \left(\frac{\Delta t}{t}\right)^2 + \left(\frac{\Delta L}{L}\right)^2 + \left(\frac{\Delta J}{\tan J}\right)^2$$



As $\theta \to 0 \Rightarrow 1/\tan\theta \to \infty$

Angular term diverges at small angles

Neutron diffraction resolving power

In general: $$\left(\frac{\Delta d}{d}\right)^2 = \left(\frac{\Delta Q}{Q}\right)^2 = \left(\frac{\Delta t}{t}\right)^2 + \cancel{\left(\frac{\Delta L}{L}\right)^2} + \left(\frac{\Delta J}{\tan J}\right)^2$$

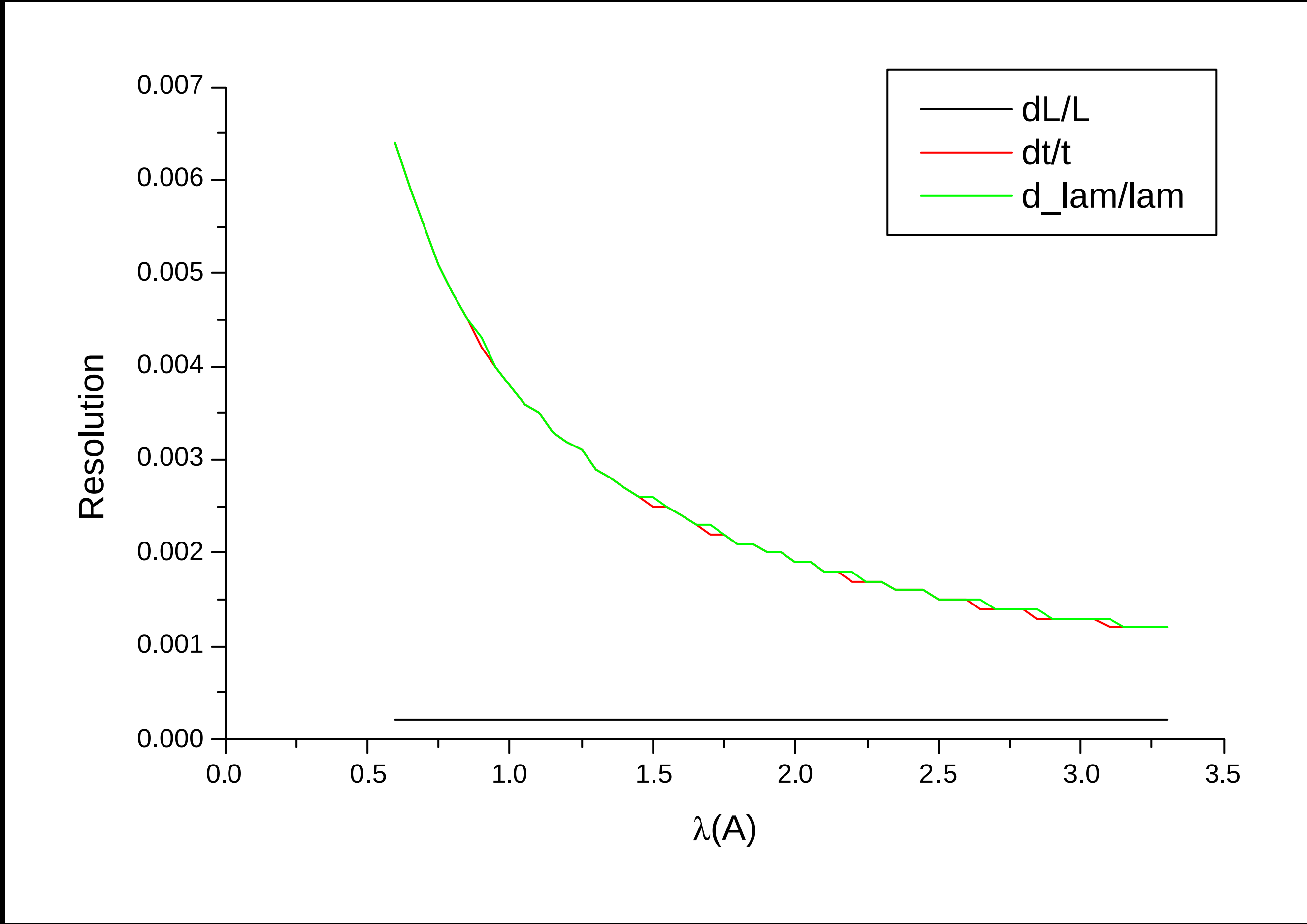
Using squashed detectors

Decreasing efficiency?

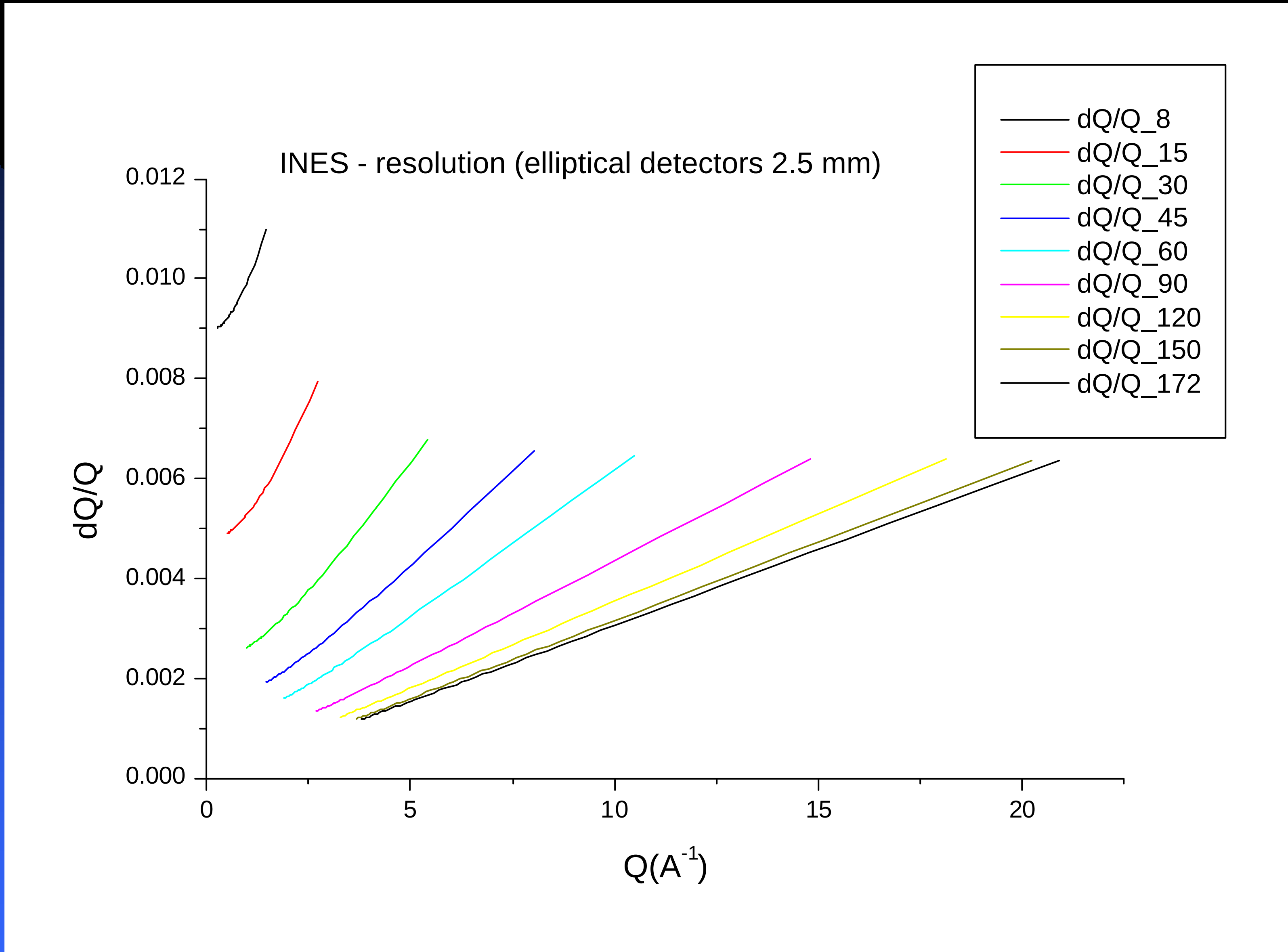
NO PROBLEM

⇒ High pressure ^{3}He detectors

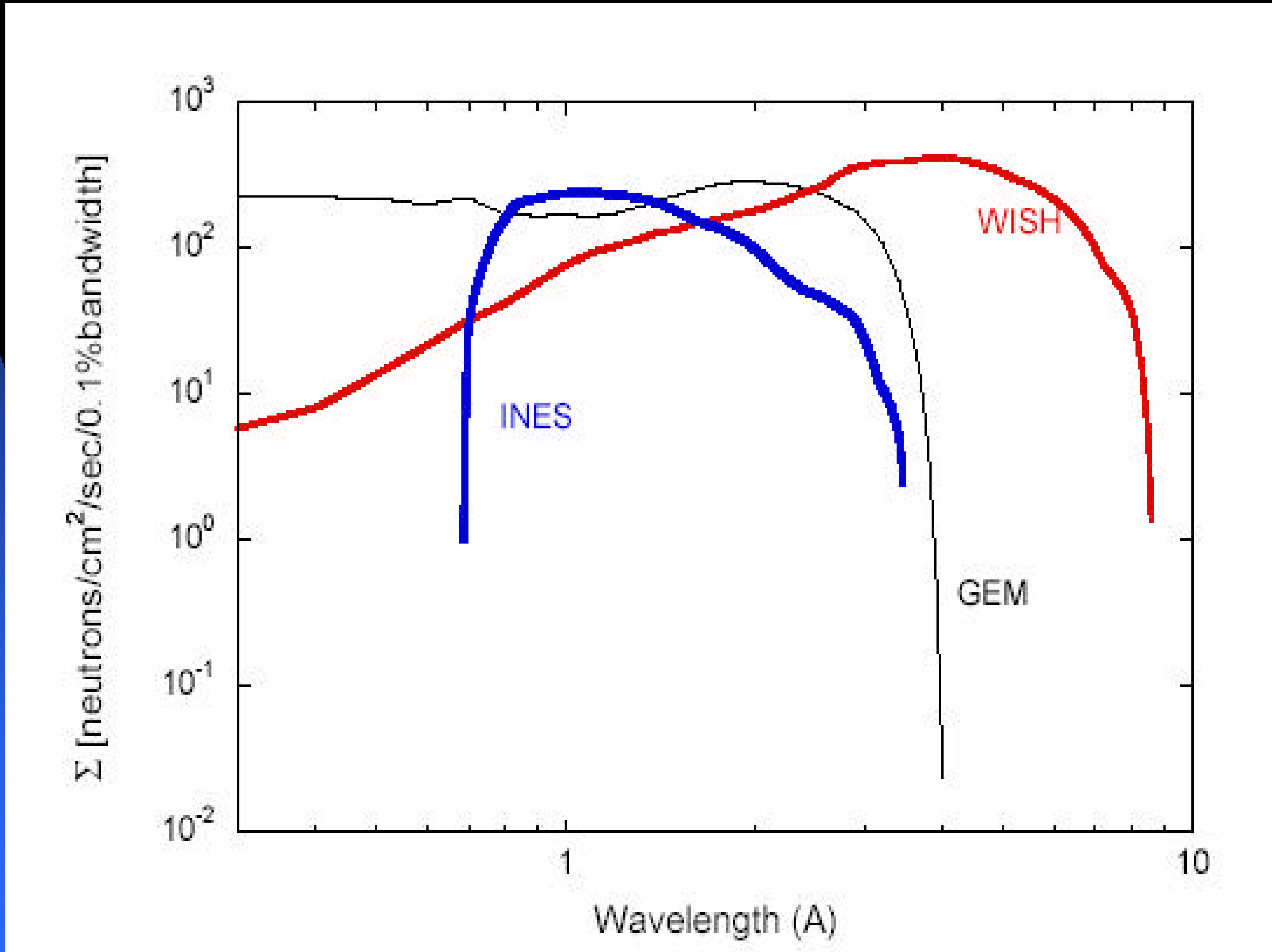
INES resolving power
(no angular contribution)



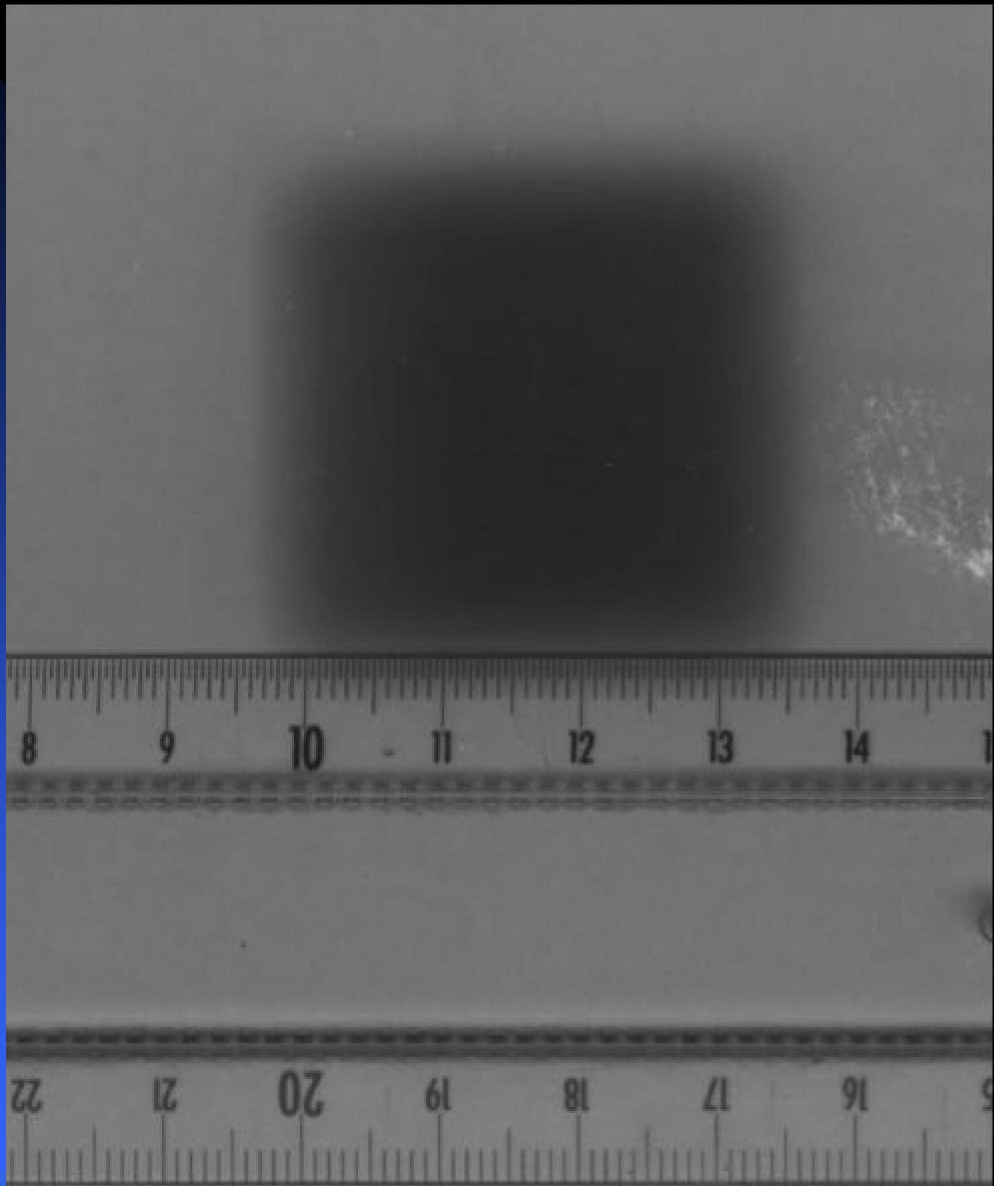
INES resolving power (total)



What about the neutron flux?
(courtesy of P.G. Radaelli)



INES: the actual instrument



Beam size: 34x34 mm^2

Uniform flux

Limited penumbra

goto ⇒ slides