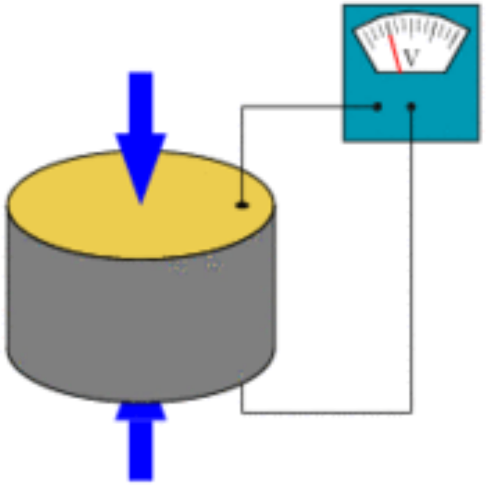
# PSI Master School 2017

## Introducing photons, neutrons and muons for materials characterization

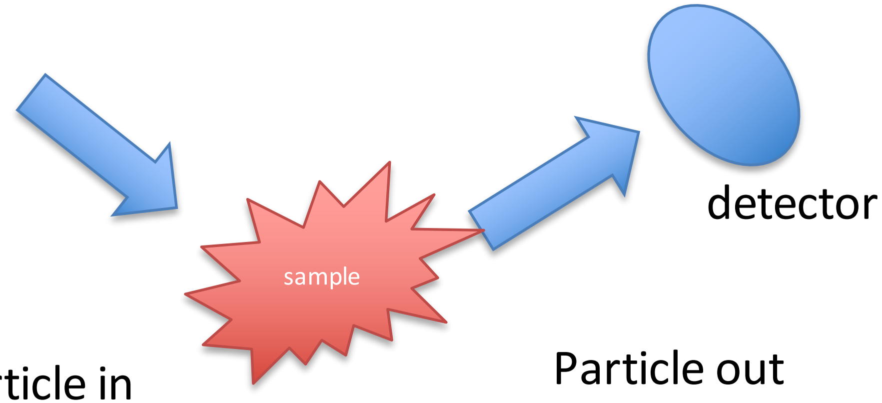
### Lecture 6: Neutron Cross Sections with Matter

# Sensor and particle probe measurements

Sensor measurement



Particle probes for measurements




Particle in
(energy, polarization,
direction

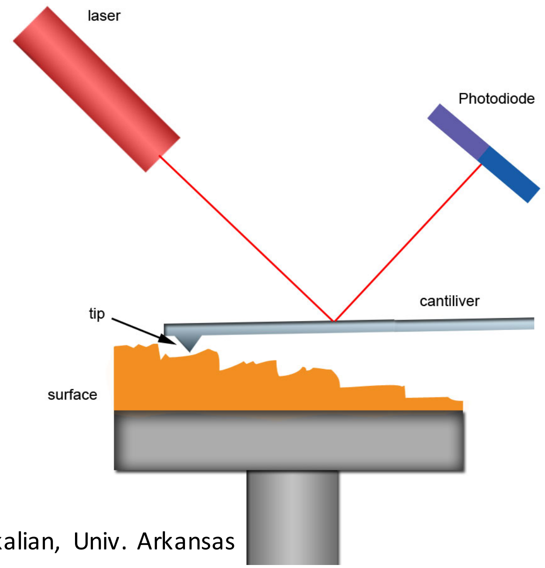
Particle out
(energy, pol,
direction etc)

Sensor experiments:
Sensor is sensitive to physical property and converts the signal to something observable

Particle probe experiments:
Particles injected and ejected in sample probe the materials properties of the material

# Examples: Sensor vs particle probe measurements

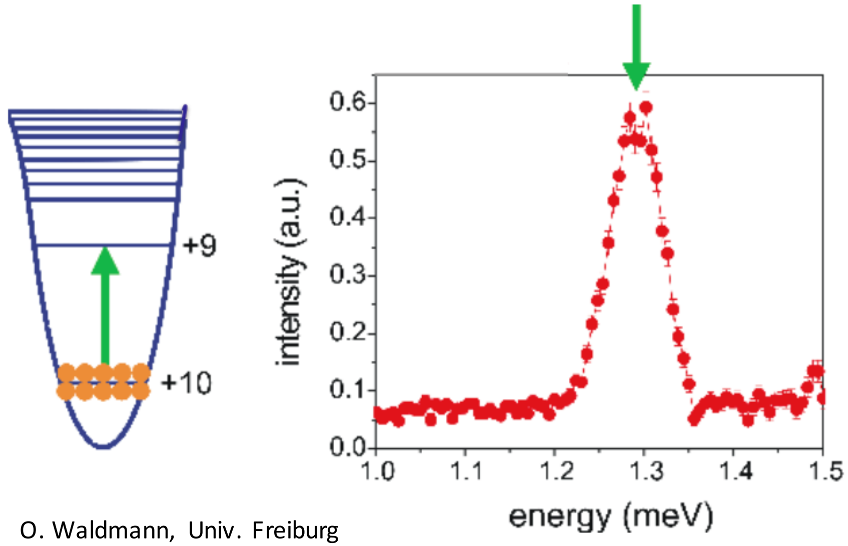
## Sensor measurement




J. Chakalian, Univ. Arkansas

Example: Atomic force microscopy
AFM acts as sensor, whose position can be measured with a laser

## Particle probes for measurements




O. Waldmann, Univ. Freiburg

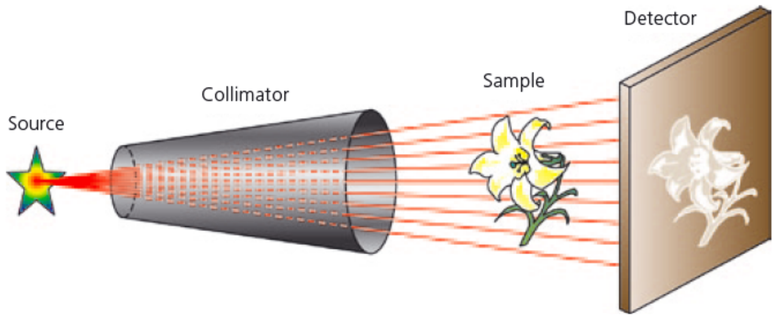
Example: Inelastic neutron scattering
Neutrons transfer momentum and energy to excitations in the material, these changes can be detected by the scattered neutron

# Types of Photon/Neutron Experiments

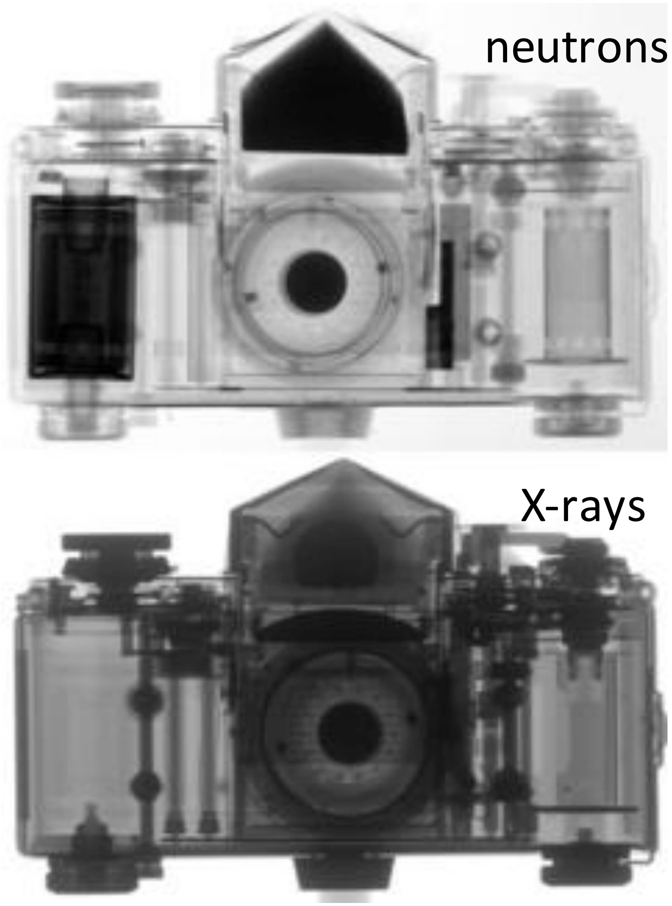
- Absorption: absorption of particles in transmission
  - Neutron and X-ray Imaging
  - X-ray absorption spectroscopy
- Scattering: radiation (light, particles) change direction is used to probe materials
  - Coherent scattering experiment
  - Reflection
- Emission experiments (Photon in-photon out, Neutron in-Photon out; Photon in-Electron out)
  - Neutron prompt gamma experiments
  - ARPES (angular resolved photoemssion)

# Photons vs neutrons

Example of neutron imaging



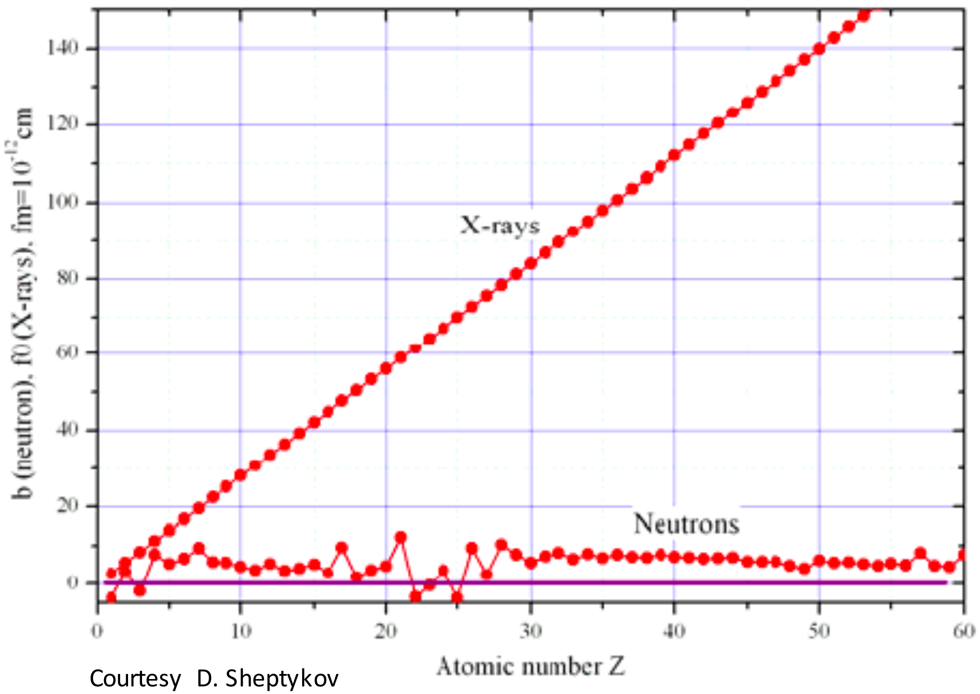

X-rays and neutrons have different cross-sections with matter




www.psi.ch

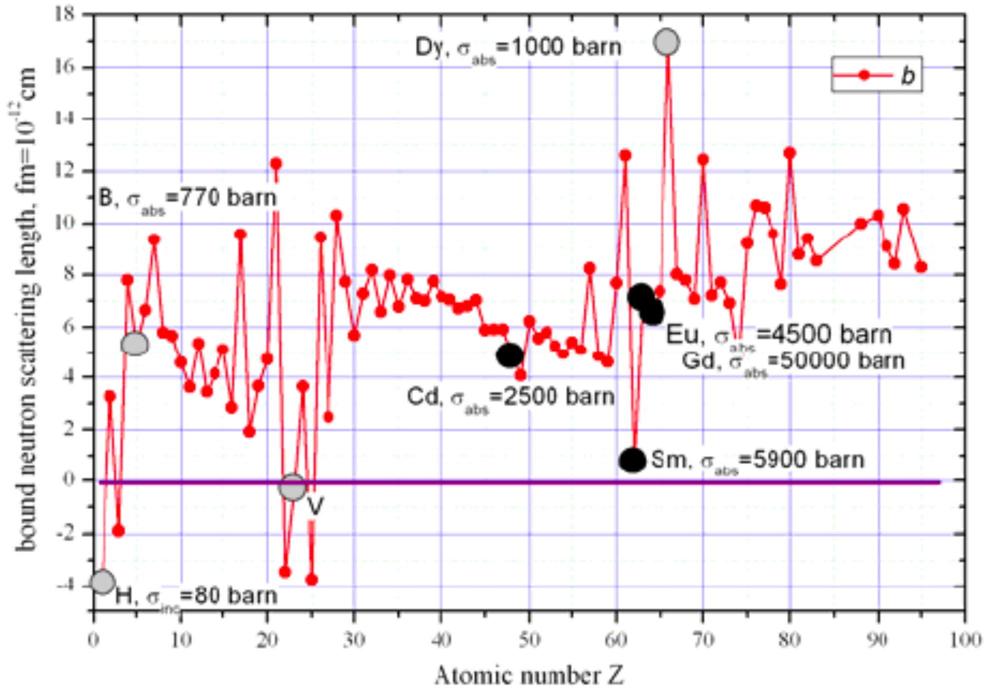
# Cross-sections photons and neutrons

***X-ray scattering amplitudes and neutron scattering lengths:***



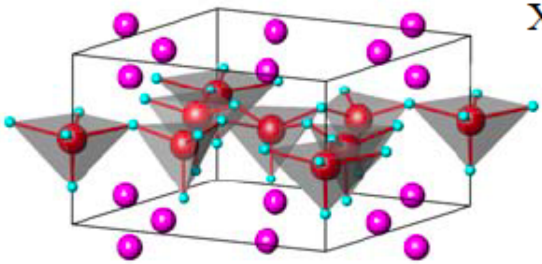

Courtesy D. Sheptykov

***(Coherent, elastic) bound neutron scattering lengths for the natural occurrences of the elements:***

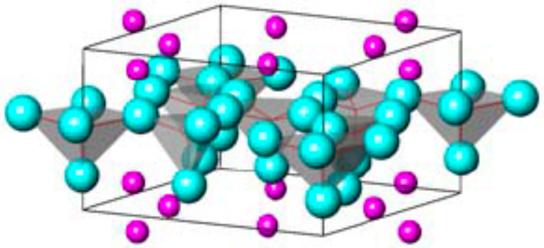



X-rays interact with electron shell, nuclear neutron scattering interacts with the nuclei

# Example: X-ray vs. neutron diffraction

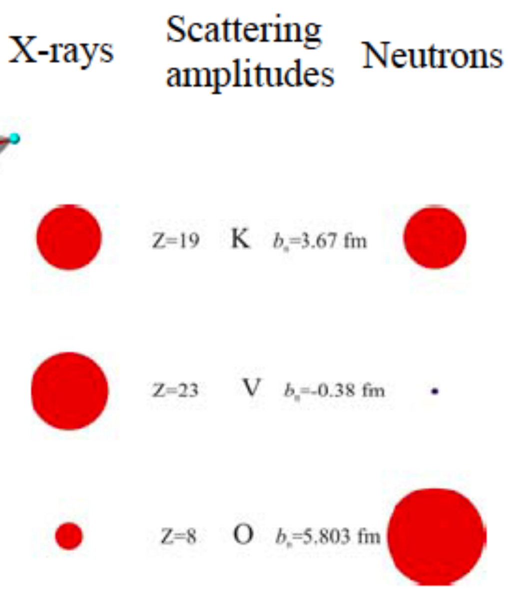


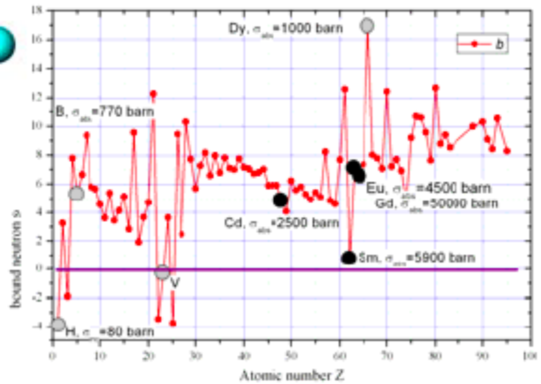
X-rays

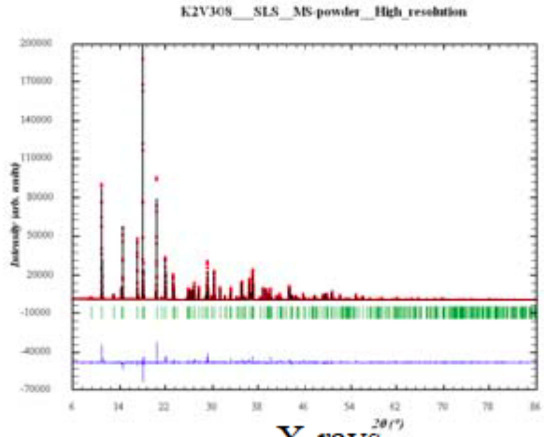


Neutrons

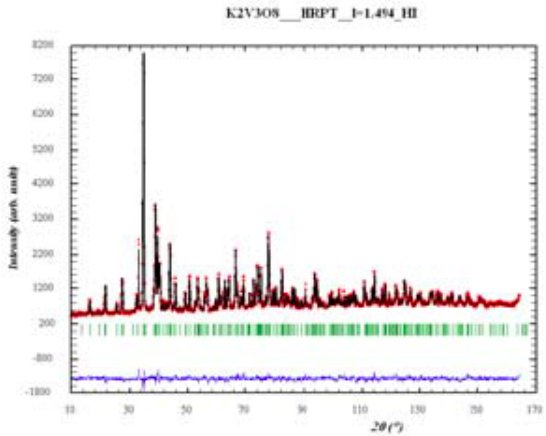
Courtesy D. Sheptykov



X-rays



Neutrons

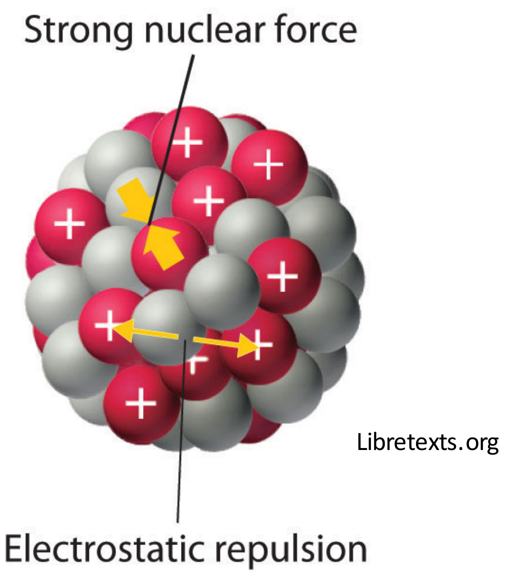
# Neutron interactions with matter

- Strong nuclear interaction

  length scale 10fm

  → scattering

  → absorption




- Magnetic interaction

  power law decay

Write potentials for two interactions

$$V(\mathbf{R}) = -\boldsymbol{\mu}_n \cdot \mathbf{B}(\mathbf{R})$$

# Nuclear scattering length

- Origin of nuclear scattering
    - Strong interaction of neutron with nuclei is complex
    - Wave-length of thermal neutrons is ~ 0.1nm >> $10^{-6}$ nm of nuclear force
    - Nuclear interactions can be approximated by point like potential

$$V(\mathbf{r}) = \frac{2\pi\hbar^2}{m_N} b\delta(\mathbf{r})$$

- b is nuclear scattering length (units of a length)
- b depends on nuclei and isotope
- Cross section (units of barn or $cm^2$)

$$\sigma_{\text{tot}} = 4\pi b^2$$

# Nuclear spin scattering

- Some nuclei possess nuclear spin
- This lead to additional cross-section, and a change of the scattering length

$$b = b_c + \frac{2b_i}{\sqrt{I(I+1)}}\mathbf{s} \cdot \mathbf{I}$$

- Very anisotropic scattering length
- Nuclear spin is not ordered, so in average scattering is isotropic
- Because scattering length can be different on same atomic position, this can lead to incoherent scattering

# Nuclear length from different isotopes

- Atoms are stable with different number of neutrons
  → isotopes
- Interactions between neutron and nuclei depends on number of neutrons
- Neutron scattering length depends on isotope

Example: H

| Isotope | conc | Coh b | Inc b |
|---|---|---|---|
| H | --- | -3.7390 | --- |
| 1H | 99.985 | -3.7406 | 25.274 |
| 2H | 0.015 | 6.671 | 4.04 |
| 3H | (12.32 a) | 4.792 | -1.04 |

Example: He

| Isotope | conc | Coh b | Inc b |
|---|---|---|---|
| He | --- | 3.26(3) | --- |
| 3He | 0.00014 | 5.74-1.483*i* | -2.5+2.568*i* |
| 4He | 99.99986 | 3.26 | 0 |

# Example: Isotope with different nuclear spin

Case: nucleus with one isotope with nuclear spin $I$

Two states: $I$+1/2, $I$-1/2

| | | | | |
|---|---|---|---|---|
| Examples: | hydrogen $I$=1/2 | : | $b^+$=10.85 fm, | $b^-$=-47.50 fm |
| | deuterium $I$=1 | : | $b^+$=9.53 fm, | $b^-$=0.98 fm |

How to calculate the incoherent scattering?

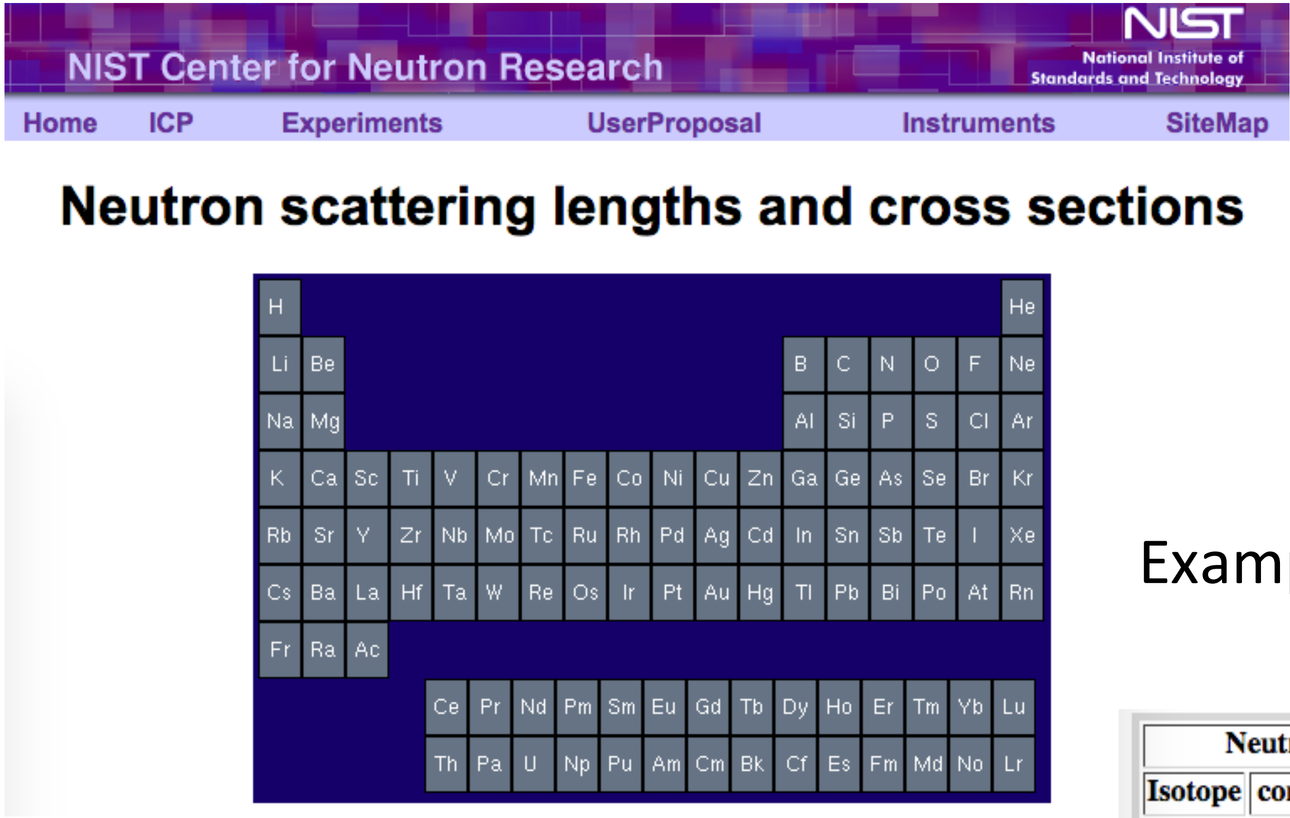
The number of states are:
For $I$+1/2 : $2I+2$
For $I$-1/2 : $2I$

$$f^+ = \frac{2I+2}{4I+2}$$
$$f^- = \frac{2I}{4I+2}$$

Total states: 4I+2

$$\overline{b} = \frac{1}{2I+1}\left((I+1)b^+ + Ib^-\right)$$

# Neutron scattering length and cross sections




Example Cu

**Neutron scattering lengths and cross sections**

| Isotope | conc | Coh b | Inc b | Coh xs | Inc xs | Scatt xs | Abs xs |
|---|---|---|---|---|---|---|---|
| Cu | --- | 7.718 | --- | 7.485 | 0.55 | 8.03 | 3.78 |
| 63Cu | 69.17 | 6.43 | 0.22 | 5.2 | 0.006 | 5.2 | 4.5 |
| 65Cu | 30.83 | 10.61 | 1.79 | 14.1 | 0.4 | 14.5 | 2.17 |

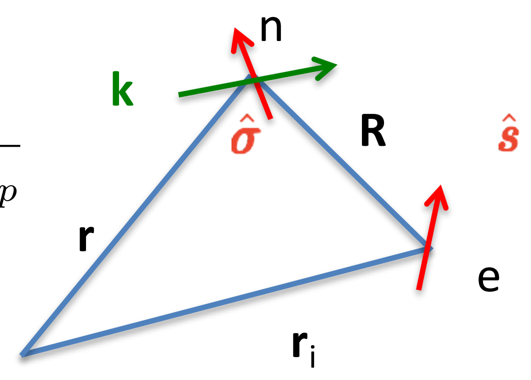
https://www.ncnr.nist.gov/resources/n-lengths/

Scattering length (fm units)
Cross sections (barn=$10^{-24}$cm$^2$ units)

# Magnetic neutron scattering

$$\boldsymbol{\mu}_n = 2\gamma\mu_n\frac{\hat{\boldsymbol{\sigma}}}{2} \qquad \mu_N = \frac{e\hbar}{2m_p}$$

$$\boldsymbol{\mu}_e = -2\mu_B\hat{\mathbf{s}}$$

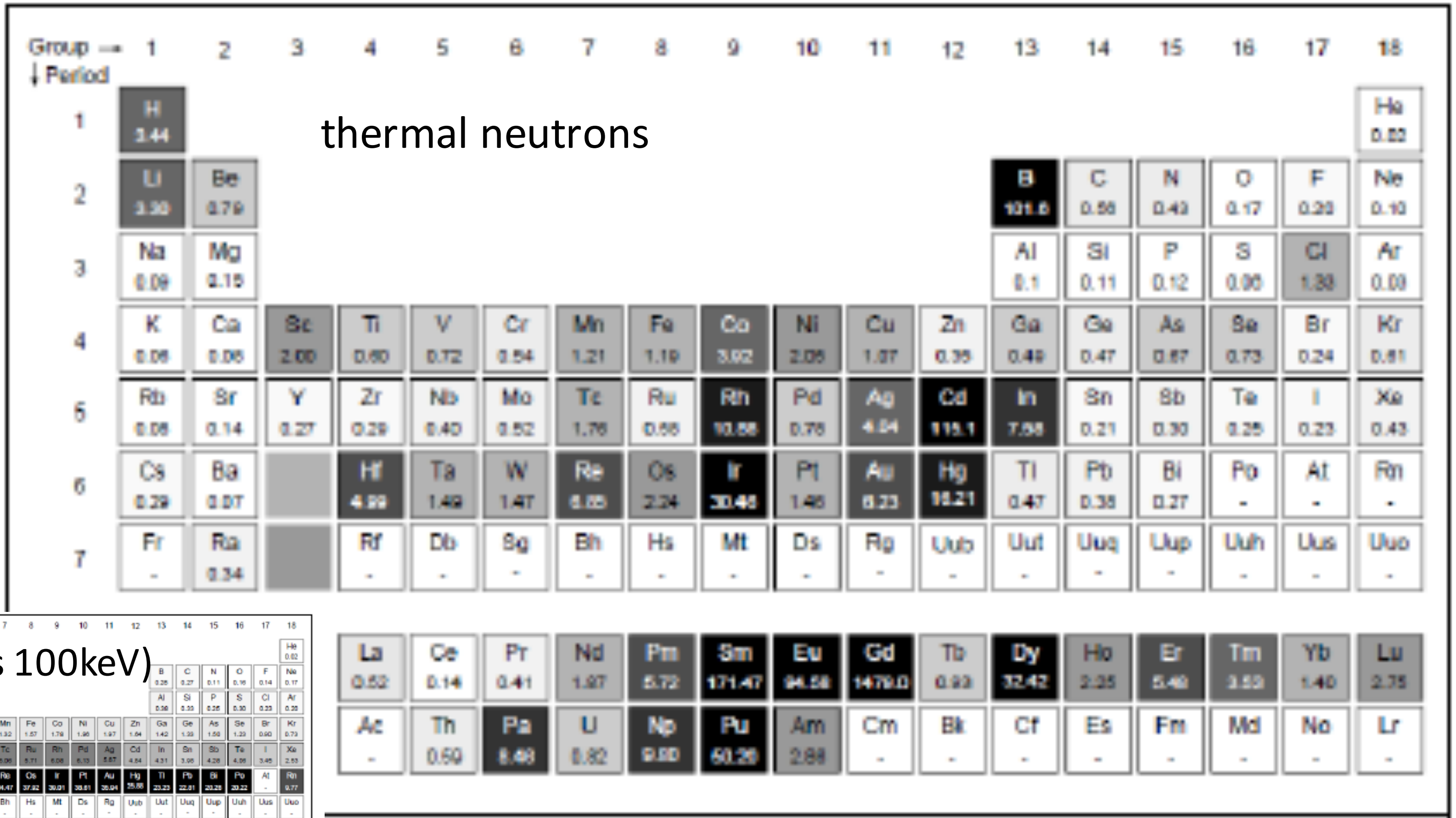


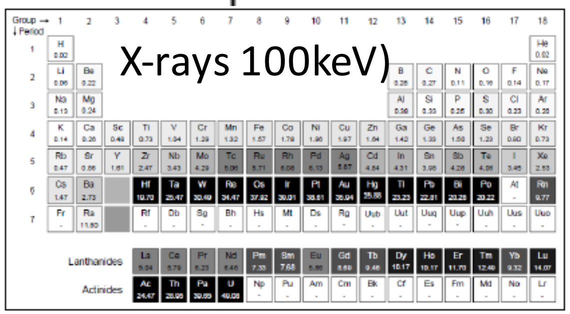

Magnetic field from electron: $\mathbf{B}(\mathbf{R}) = \boldsymbol{\nabla} \times \left(\frac{\mu_0}{4\pi}\frac{\boldsymbol{\mu}_e \times \hat{\mathbf{R}}}{R^2}\right)$

Neutron-electron interaction: $V(\mathbf{R}) = -\boldsymbol{\mu}_n \cdot \mathbf{B}(\mathbf{R})$

# Absorption cross-section

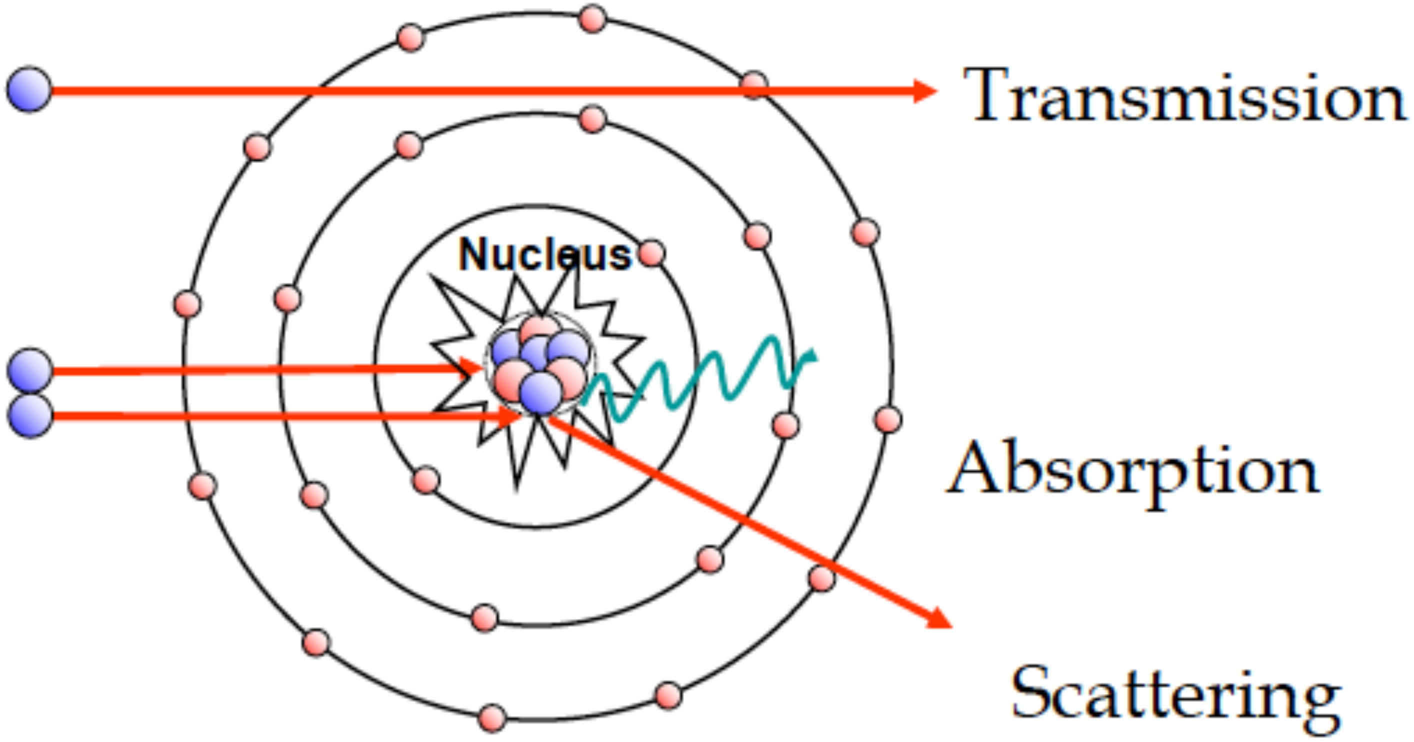
- Neutrons can be absorbed by nuclei (neutron capture)
- Very different absorption length than X-rays (for 100keV)



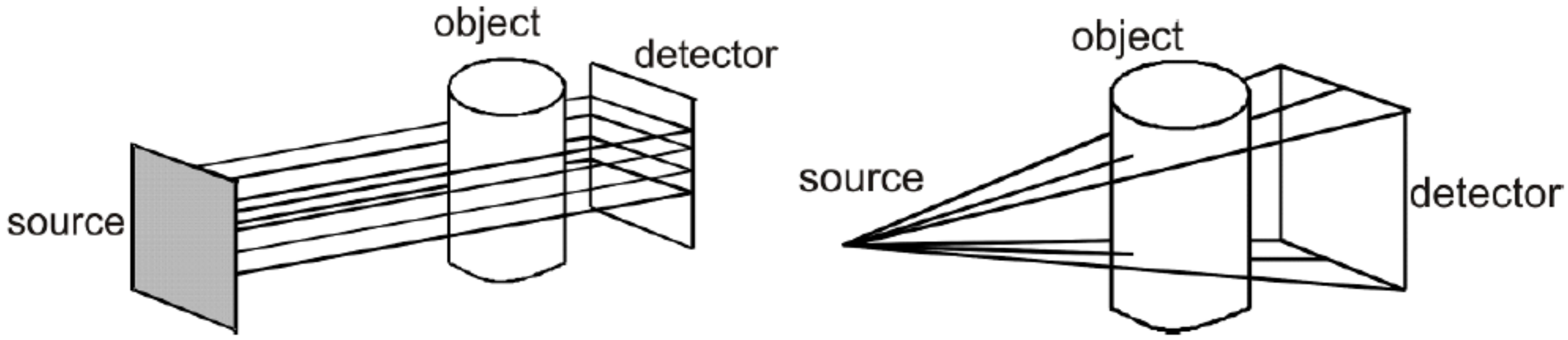



# Neutrons and matter

- Very weak interaction
- Many neutrons are transmitted



# Neutron Imaging (neutron radiography)

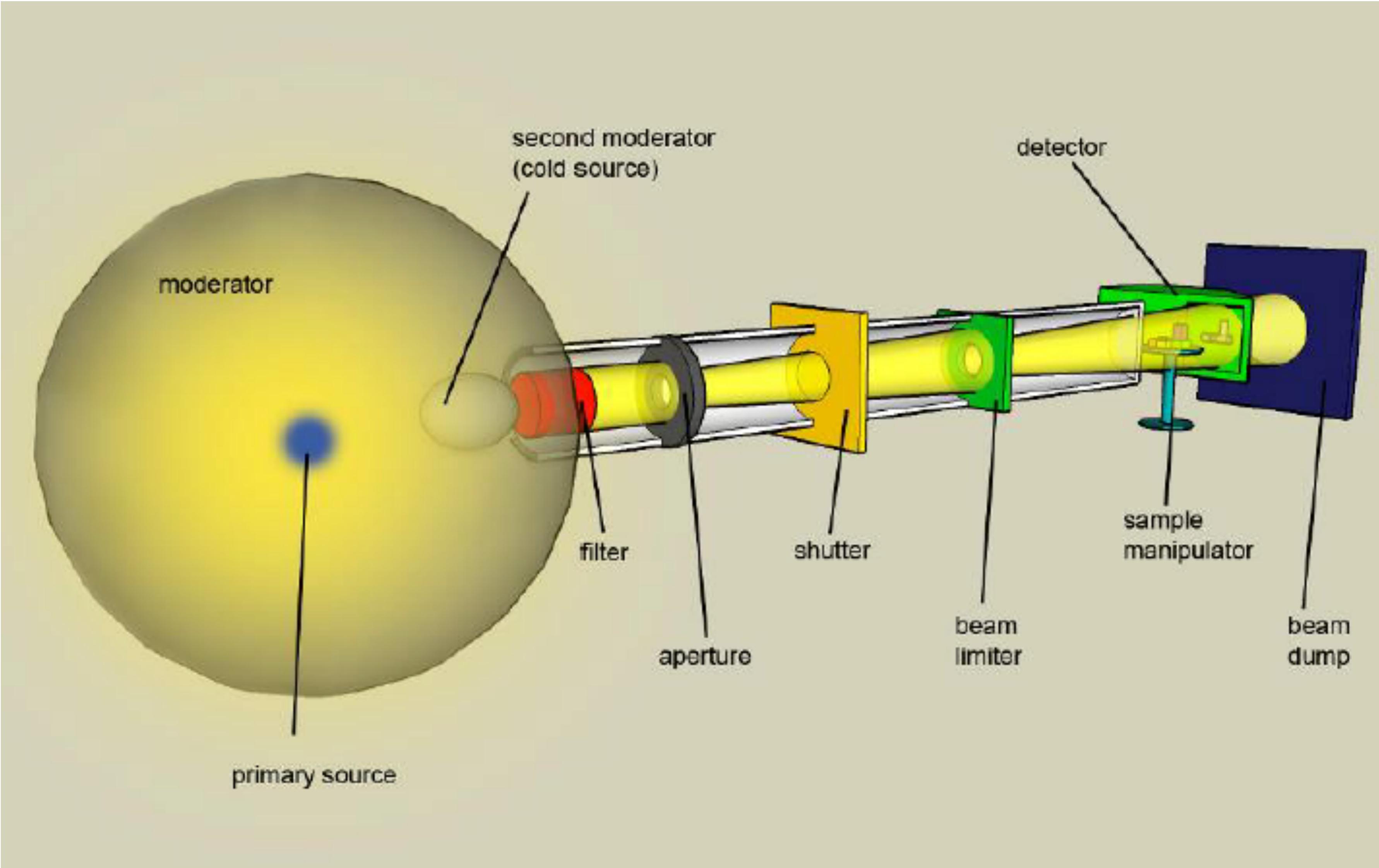



- Objects or materials can be imaged quantitiavely by using neutron transmission pictures
- Intensity decreases exponentially with thickness d of the sample

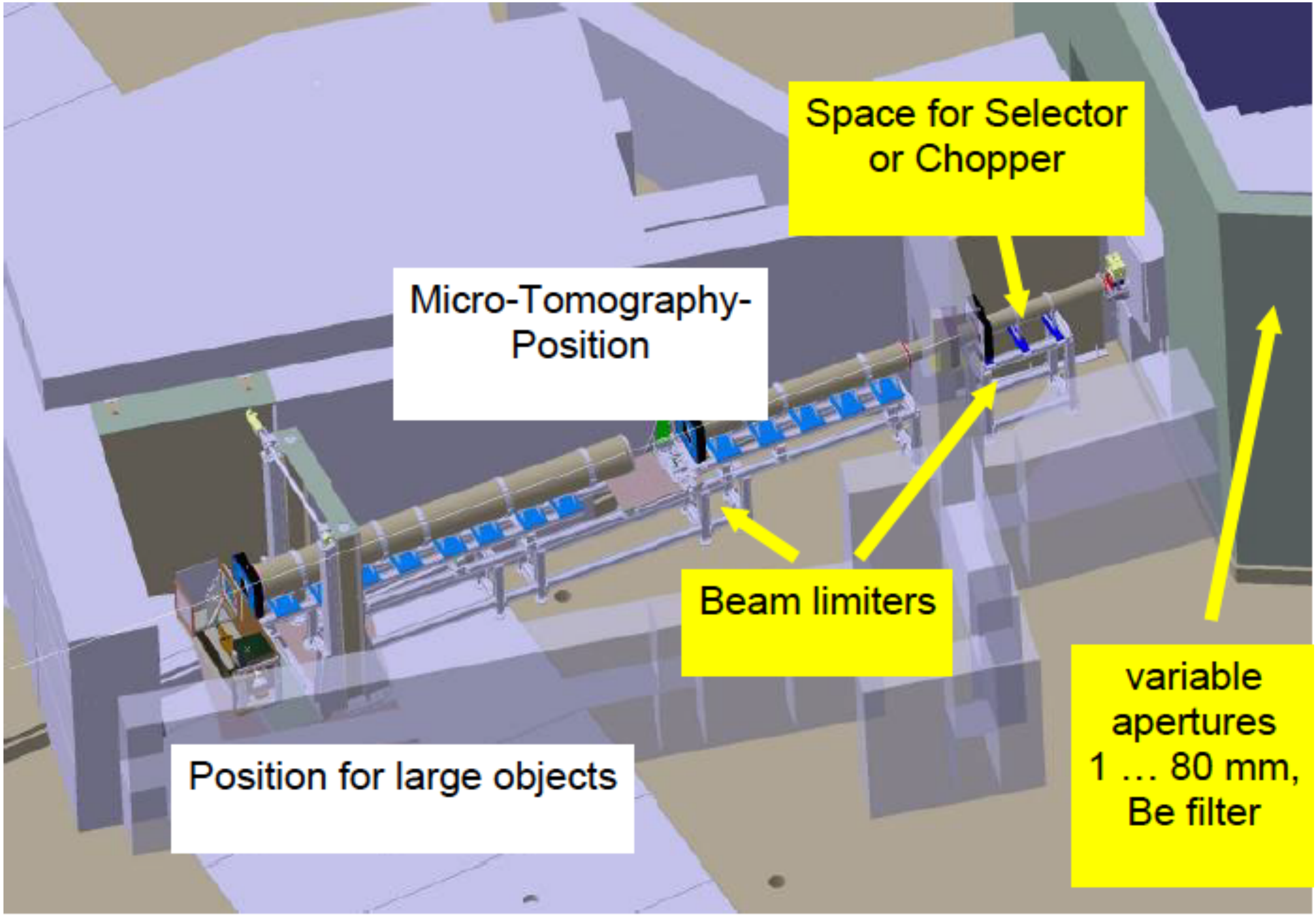
$$I(x,y,E) = I_0(x,y,E) \cdot e^{-\Sigma(x,y,E) \cdot d(x,y)}$$

$\Sigma(x,y,E)$ is the effective attenuation coefficient at x,y and for E

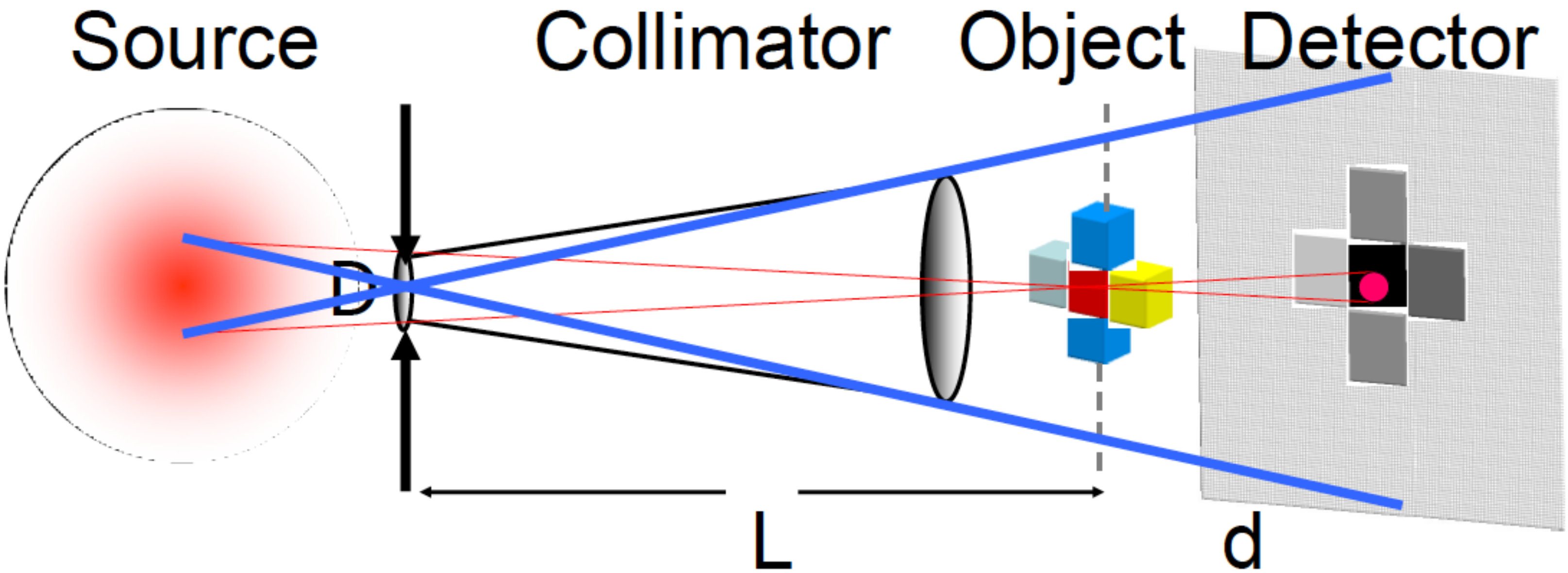
# Neutron imaging instrument



# ICON neutron imaging beamline



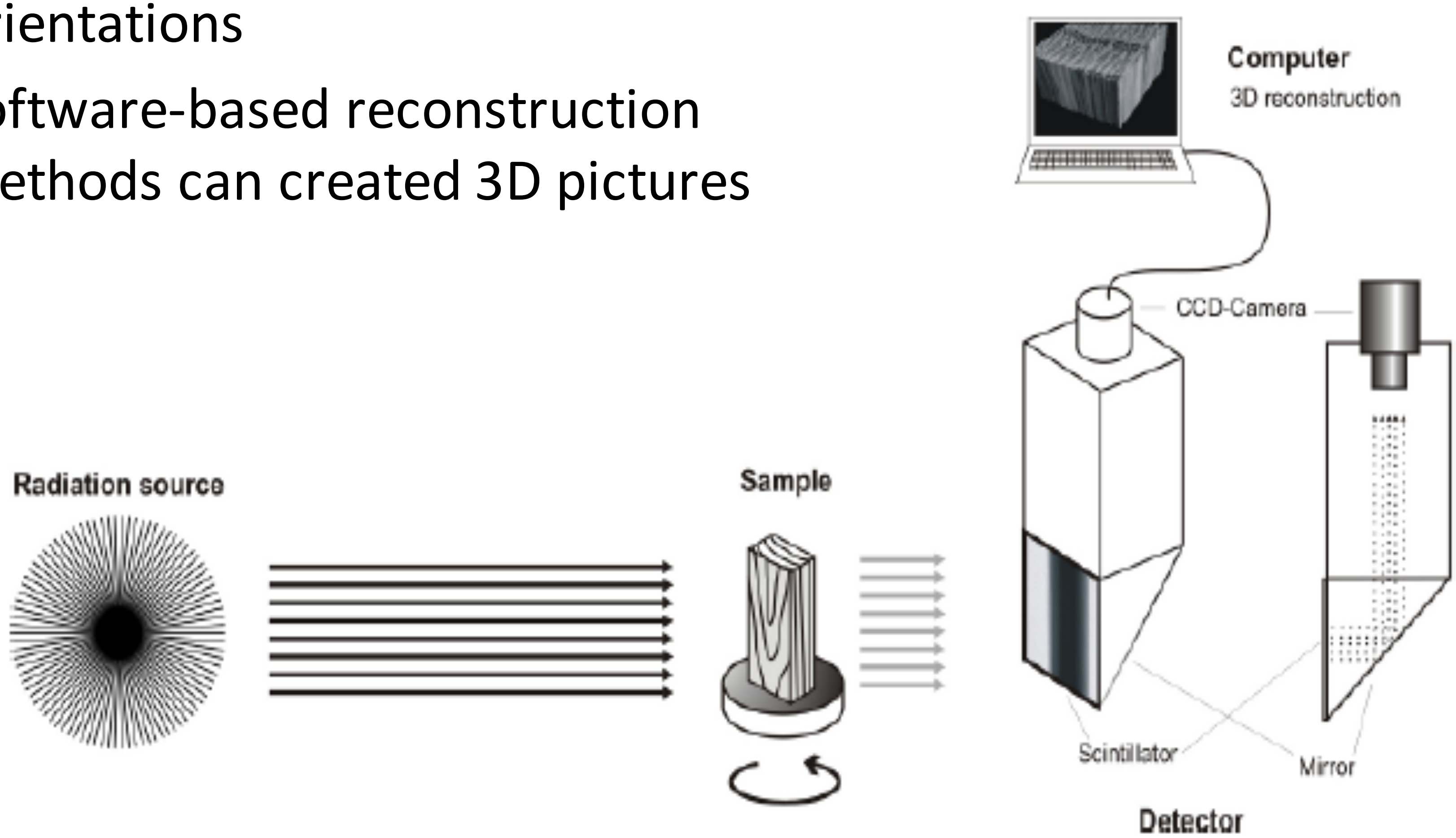
# Imaging: spatial resolution



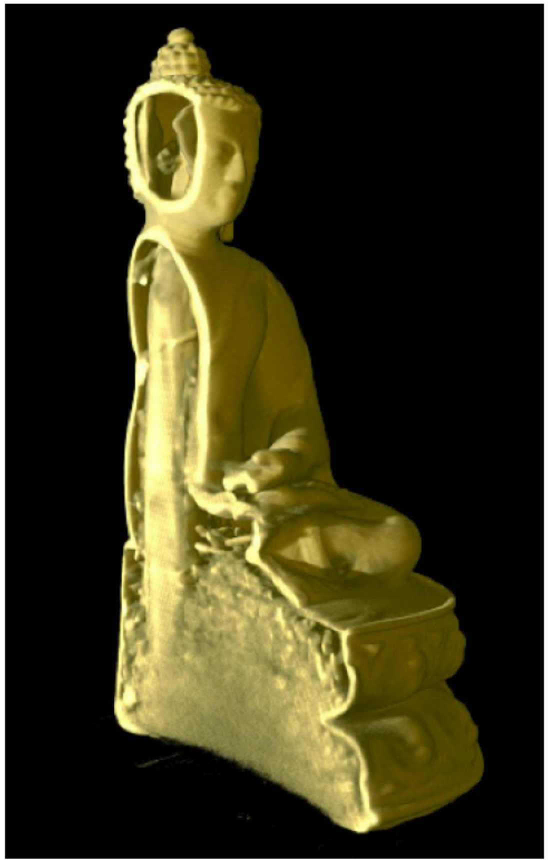

- Collimation ratio C = L/D
  - L: collimator length
  - D: primary aperture opening
- Geometric blurring u = d/C

# Tomography Imaging

- neutron radiography in different orientations
- Software-based reconstruction methods can created 3D pictures



# Example: neutron imaging

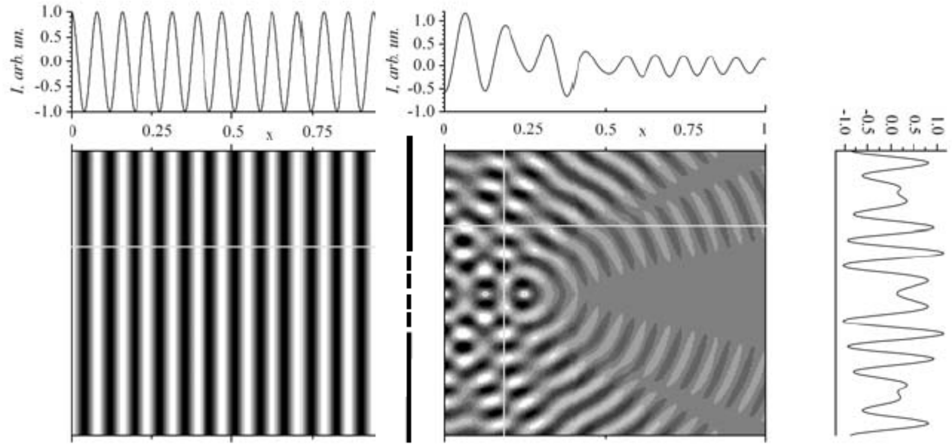
| Object | Neutron radiography | Neutron tomography |
| --- | --- | --- |
|  |  |  |

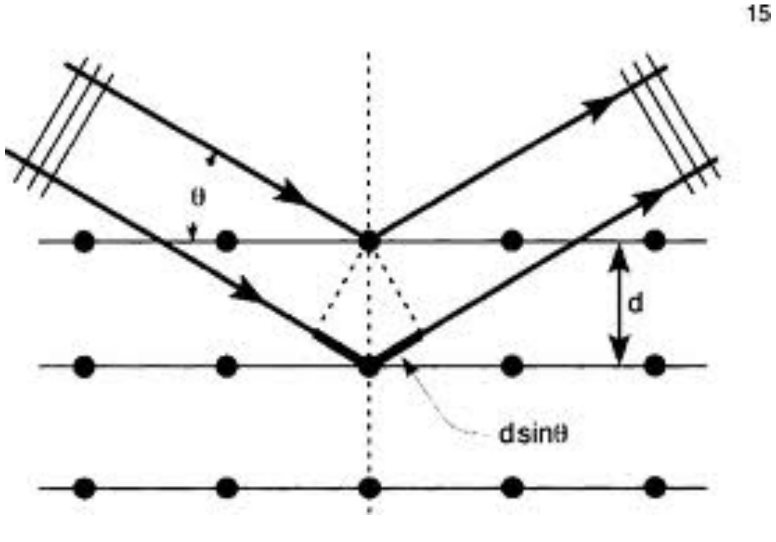
# Principle of scattering

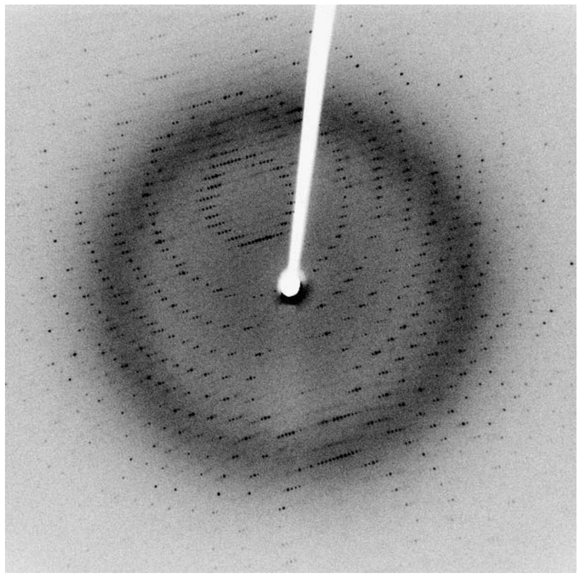
Interference of waves at objects

Constructive and destructive interference at two slit object

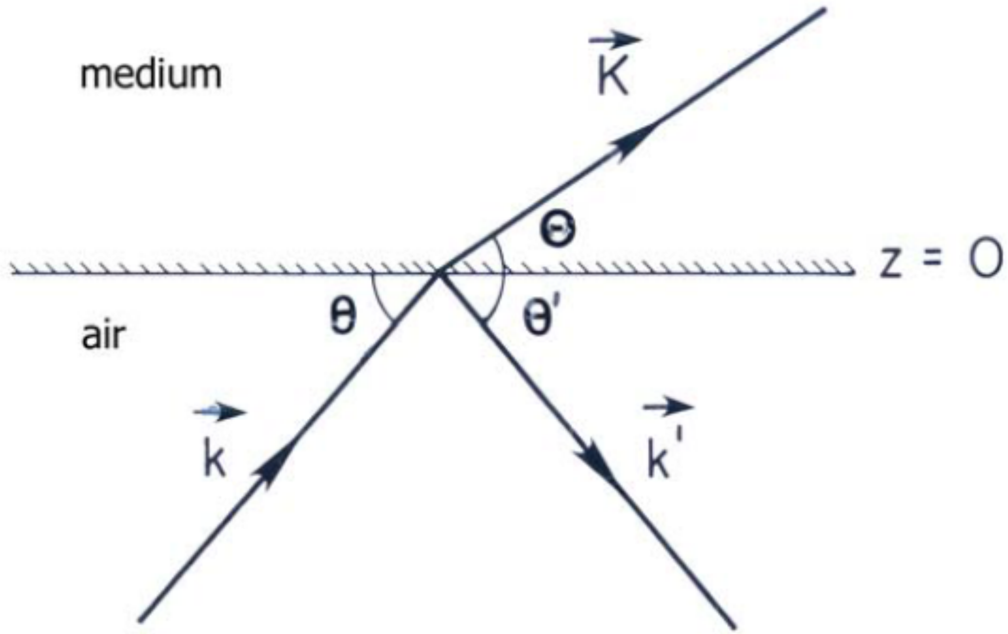
Bragg's law in crystals
→ Constructive interference at reciprocal wave-vectors



# Wave-function and matter

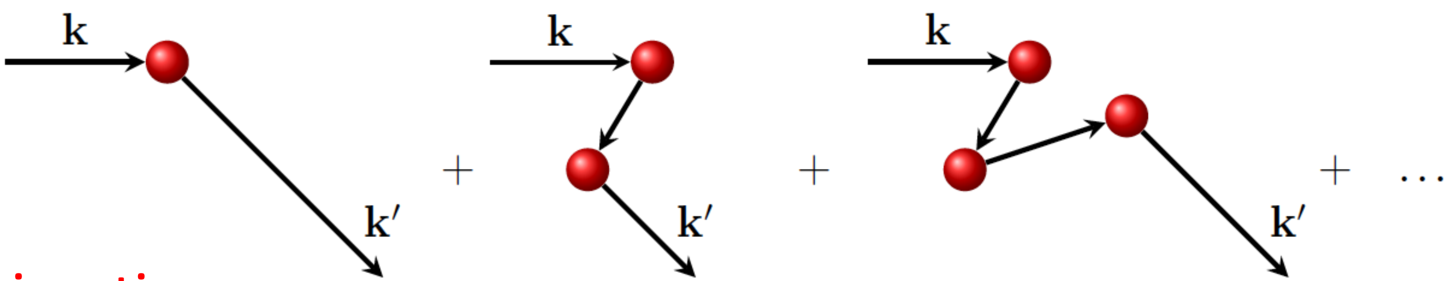



- Wave-function describing neutron particles can change when entering a material
- This can affect the overall interaction of neutron with materials

→ Refraction
→ Total reflection

# Kinematic or Born approximation

- Interaction between neutron and matter is very weak
- Often only one scattering even in the material
- the incident wave is in many cases only very weakly affected by the material




Approximation:

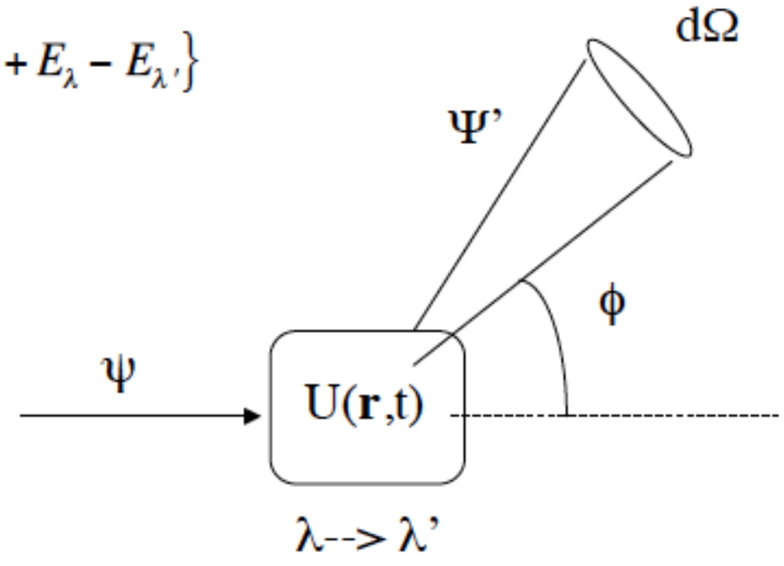
- Only one scattering event
- Wave-function in vacuum and in material are the same

# Fermi Golden Rule

- Single scattering event
- Incident wave k, interaction potential U, scattered wave k’

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 \sum_{\lambda} p_\lambda \sum_{\lambda'} \left|\langle \mathbf{k}'\lambda' | \hat{U} | \mathbf{k}\lambda \rangle\right|^2 \delta\{\hbar\omega + E_\lambda - E_{\lambda'}\}$$

$$\hat{U}(\mathbf{r}) = \frac{2\pi\hbar^2}{m} \sum_j b_j \delta\{\mathbf{r} - \mathbf{R}_j\}$$




$b_i \approx 10^{-12}$ cm --> $\dfrac{d^2\sigma}{d\Omega d\omega} \approx 10^{-24}\, cm^2$ = 1 barn

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

# Calculation of correlation function

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{\lambda} p_{\lambda}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \langle \lambda | e^{-i\hat{\mathbf{Q}}\hat{\mathbf{R}}_{j'}(0)} e^{i\hat{\mathbf{Q}}\hat{\mathbf{R}}_j(t)} | \lambda \rangle e^{-i\omega t} dt$$

$$\langle \hat{A} \rangle = \sum_{\lambda} p_{\lambda} \langle \lambda | \hat{A} | \lambda \rangle \qquad \mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i$$

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \left\langle e^{-i\hat{\mathbf{Q}}\hat{\mathbf{R}}_{j'}(0)} e^{i\hat{\mathbf{Q}}\hat{\mathbf{R}}_j(t)} \right\rangle e^{-i\omega t} dt$$

# Correlation functions

Intermediate correlation function: $$I(\mathbf{Q},t) = \frac{1}{N}\sum_{j,j'}\left\langle e^{-i\mathbf{QR}_{j}'(0)} e^{i\mathbf{QR}_{j}(t)}\right\rangle$$

Pair correlation function: $$G(\mathbf{R},t) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} I(\mathbf{Q},t)e^{-i\mathbf{QR}}d\mathbf{Q}$$

Dynamical structure factor: $$S(\mathbf{Q},\omega) = \frac{1}{(2\pi\hbar)}\int_{-\infty}^{\infty} I(\mathbf{Q},t)e^{-i\omega t}dt$$

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}NS(\mathbf{q},\omega) \qquad \sigma_{coh} = 4\pi b^2$$

# Elastic Scattering

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_j b_{j'} \int_{-\infty}^{\infty} \langle e^{-\imath \boldsymbol{Q}\cdot\hat{\boldsymbol{R}}_{j'}(0)} e^{\imath \boldsymbol{Q}\cdot\hat{\boldsymbol{R}}_j(t)} \rangle e^{-\imath\omega t}\mathrm{d}t$$

assume there is no time operator time dependence, and integrate over time

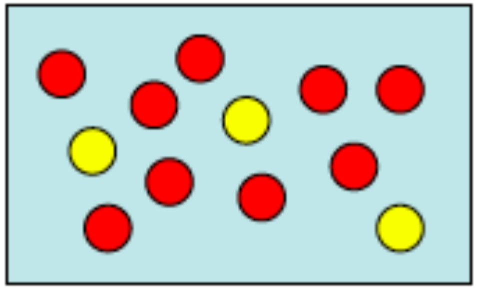
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \int_{-\infty}^{\infty} \left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega}\right) \mathrm{d}(\hbar\omega) = \sum_{j,j'} b_j b_{j'} \langle e^{-\imath \boldsymbol{Q}\cdot\hat{\boldsymbol{R}}_{j'}} e^{\imath \boldsymbol{Q}\cdot\hat{\boldsymbol{R}}_j} \rangle$$

Assume fixed atomic positions (replace operators with atomic positions)

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh}} = \langle b\rangle^2 \sum_{j,j'} e^{-\imath \boldsymbol{Q}\cdot(\boldsymbol{R}_{j'}-\boldsymbol{R}_j)},$$

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{inc}} = \left(\langle b^2\rangle - \langle b\rangle^2\right) \sum_{j=j'} e^{-\imath \boldsymbol{Q}\cdot(\boldsymbol{R}_{j'}-\boldsymbol{R}_j)} = N\left(\langle b^2\rangle - \langle b\rangle^2\right)$$

# Incoherent Scattering



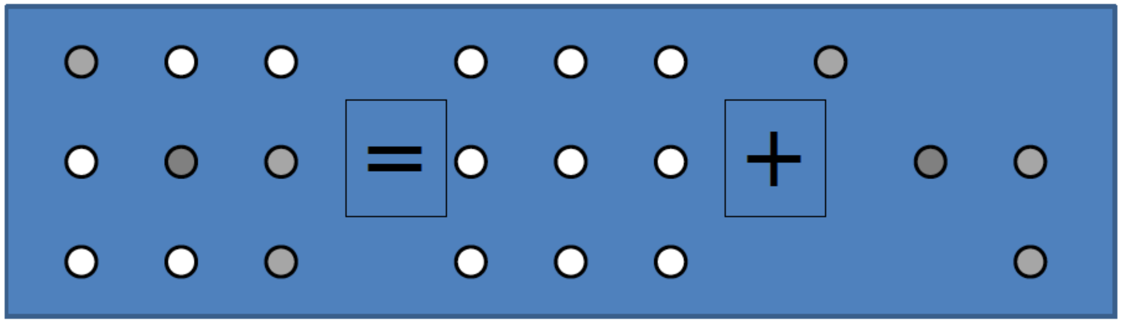
$P_\alpha$ : relative probability for isotope

$$\sum_\alpha P_\alpha = 1$$

$$\langle b \rangle = \sum_\alpha P_\alpha b_\alpha \qquad \langle b^2 \rangle = \sum_\alpha P_\alpha b_\alpha^2$$

$$\sigma_{coh} = 4\pi \langle b \rangle^2$$

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



# Dynamical scattering theory

- Multiple scattering was previously ignored because these effects are often weak
- Below an critical angle of incidence neutrons are completely reflected, this scattering is not weak

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_{\mathbf{k}}(\mathbf{r}) = E\psi_{\mathbf{k}}(\mathbf{r}) \qquad V(\mathbf{r}) = 0 \qquad \text{except } \mathbf{r} \in \text{ target region } \mathbb{T}$$

$$\psi'_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) + \int_{\mathbb{T}} d^3r' G_\circ(\mathbf{r}, \mathbf{r}'|E)\, V(\mathbf{r}')\, \psi'_{\mathbf{k}}(\mathbf{r}')$$

$$G_\circ(\mathbf{r}, \mathbf{r}'|E) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \qquad \text{with} \qquad k = \sqrt{\frac{2m}{\hbar^2}E}$$

# Dynamical scattering theory

- The wave-vector can change when a wave enters a medium

$$\left[\nabla^2 + 2m(E-\overline{V})/\hbar^2\right]\psi(r) = 0$$

incident wave: $\psi(r) = e^{i\vec{k}_o.\vec{r}}$ $\qquad \overline{V} = \frac{2\pi\hbar^2}{m}\rho$

- Vacuum : $k_0^2 = 2mE/\hbar^2$

- Medium: $k^2 = 2m(E-\overline{V})/\hbar^2 = k_0^2 - 4\pi\rho$

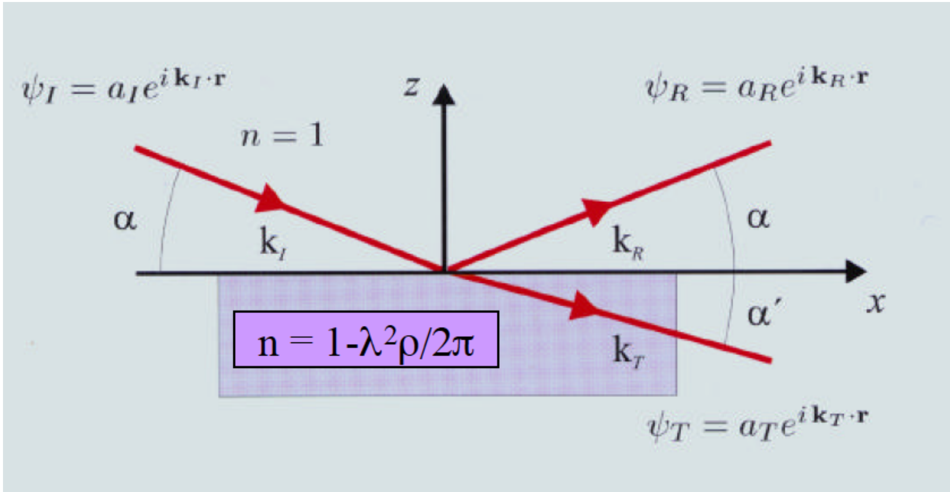
- Refractive index $n=k/k_0$: $n = 1\text{-}\lambda^2\rho/2\pi$

# Snell's and Fresnel's Law

- Continuity of Ψ and Ψ' at surface

$$a_I + a_R = a_T \qquad (1)$$
$$a_I\vec{k}_I + a_R\vec{k}_R = a_T\vec{k}_T$$

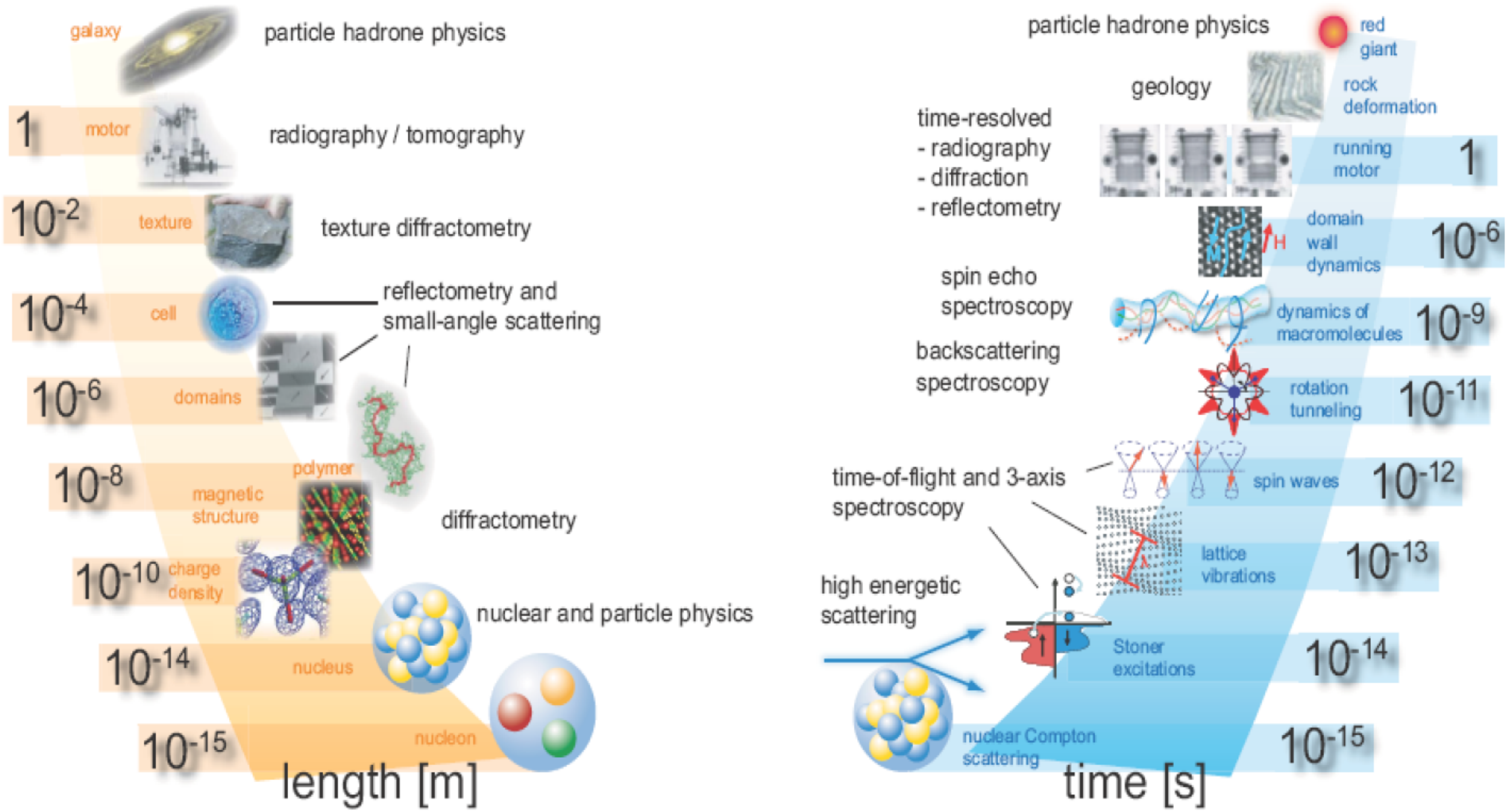
$$a_I k\cos\alpha + a_R k\cos\alpha = a_T nk\cos\alpha'$$
$$-(a_I - a_R)k\sin\alpha = -a_T nk\sin\alpha'$$




- Snell's law: $\boxed{\cos\alpha = n\cos\alpha'}$

- Fresnel's law: $\boxed{r = a_R / a_I = (k_{Iz} - k_{Tz})/(k_{Iz} + k_{Tz})}$

# Energy/time scales and length scales




T. Brückel, Jülich