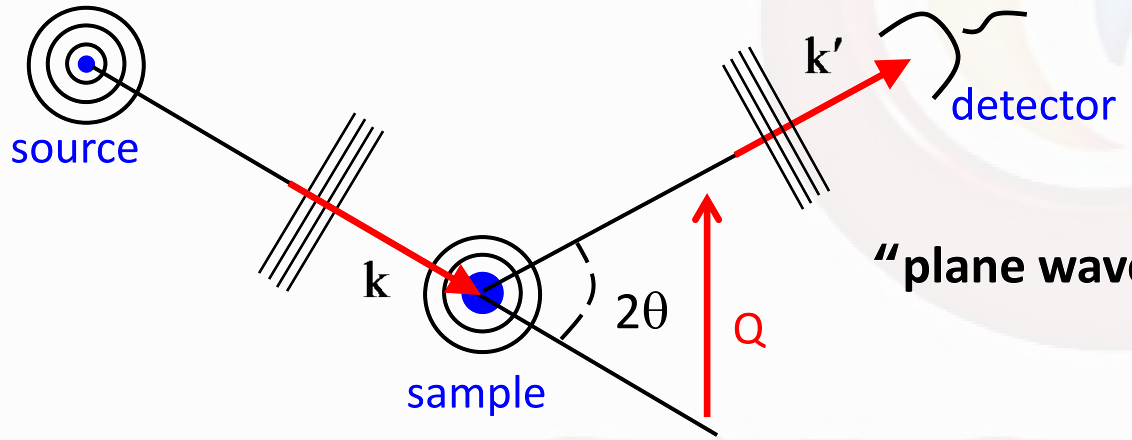
Scattering

- **Fraunhofer approximation:**

$\varnothing$ sample << { distance source, distance detector }



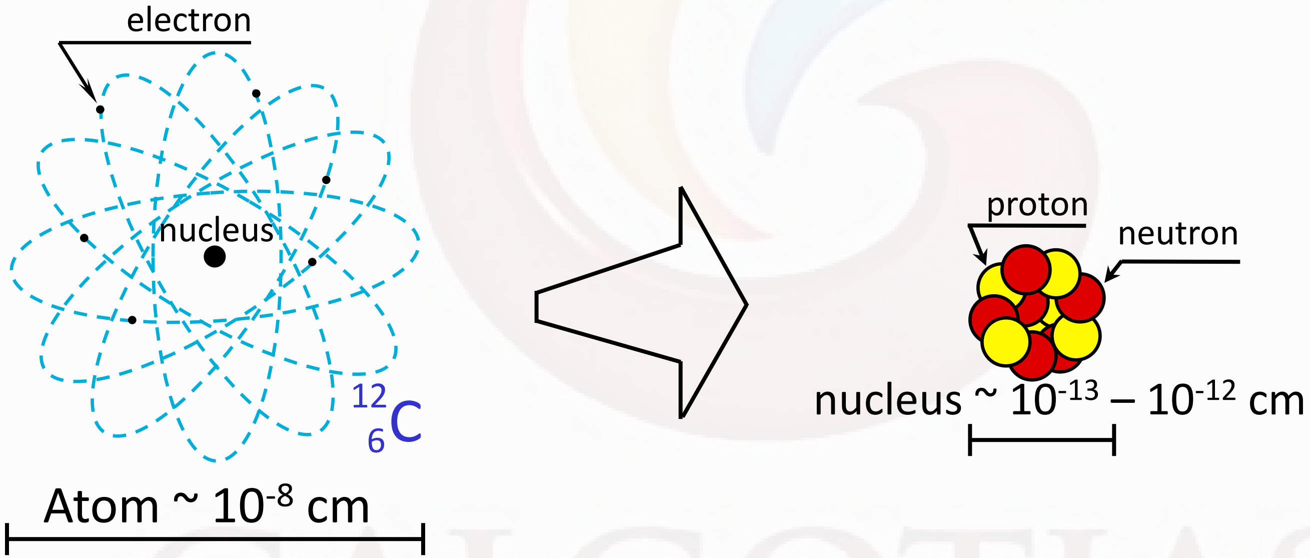
"plane wave" { wavelength λ, propagation direction }

- **Elastic scattering (diffraction):** $k = |\mathbf{k}| = |\mathbf{k}'| = k' = \dfrac{2\pi}{\lambda}$ -- (1) $Q = |\mathrm{Q}| = \sqrt{k^2 + k'^2 - 2kk'\cos 2\theta}$

- **Scattering vector:** $\mathrm{Q} = \mathrm{k}' - \mathrm{k}$

$$Q = \frac{2\pi}{\lambda}\sin\theta \quad ----- \quad (2)$$

Atom and Nucleus



Size of an atom:

(≈ 0.1 nm = 10^{-8} cm)

A neutron is about $1/10^5$(≈ 10^{-13} cm) as large as an atom.

Particle Nature of Neutron

Hadrons
- **Mesons (2 Quarks)**
- **Baryons (3 Quarks)**
  - **Proton**
  - **Neutron**

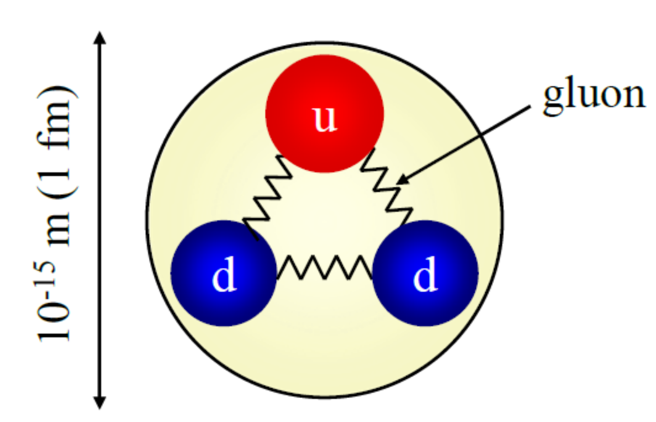
} **Nucleons**

Decay of free neutron:

$$n \xrightarrow[\text{week interaction}]{889s} p + e^{-} + \overline{\nu}$$

Neutron:

Bound state of 3 Quarks:



Mass : 1.675 x 10^{-27} kg (nearly equal to that of proton)

Charge: 10^{-18} e (substantially zero)

Spin : 1/2

Magnetic dipole moment ⇒ $\mu_n = -1.913\mu_N$

$$\mu_N = \frac{e\hbar}{2m_p}$$ "nuclear magneton"

Particle as a Wave

$E = k_B T$ **(From classical physics)**

$E = \hbar\omega$ **(Plank's hypothesis)**

$$p = \frac{E}{c} = \frac{\hbar\omega}{c}$$ **(Plank-Einstein relation)**

$$\vec{p} = \hbar\vec{k} \Rightarrow p = \frac{h}{\lambda}$$ **(de Broglie hypothesis)**

(here, ω=ck and the fact that the momentum and wave vector point in the same direction)

To calculate the interference effect during the scattering process, a particle has to be described as a matter wave.

Kinetic energy of neutron: $$E_n = \frac{p^2}{2m_n} = \frac{h^2}{2m_n\lambda^2} \equiv k_B T_{eq} \Rightarrow p = mv = \sqrt{2m_n k_B T}$$

Wave length of neutron: $$\lambda = \frac{h}{\sqrt{2m_n k_B T}}$$

Scattering

Internal structure:

what are the relevant building blocks (atoms, molecules, colloidal particles, ...) and how are they arranged?

Microscopic dynamics:

How do these building blocks move (atomic movements) and what are their internal degrees of freedom?

Scattering

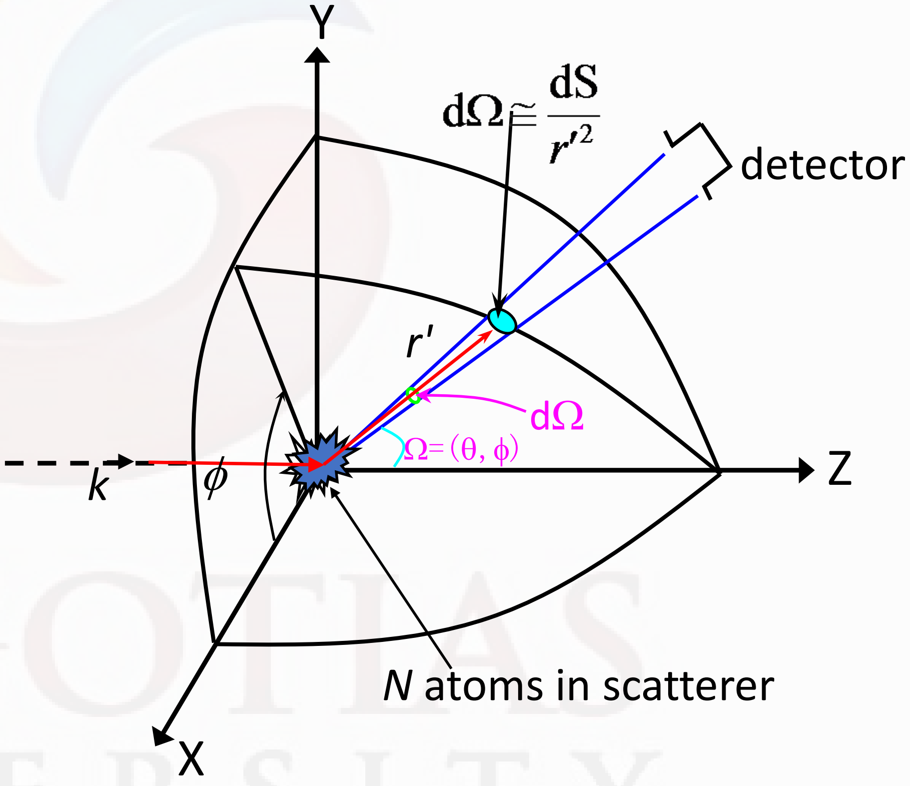
For magnetic systems, we need to know the arrangement of the microscopic magnetic moments due to spin and orbital angular momentum and their excitation spectra.

- The macroscopic response and transport properties, such as specific heat, thermal conductivity, elasticity, viscosity, susceptibility, magnetization etc., which are the quantities of interest for applications, result from the microscopic structure and dynamics.

Differential Scattering Cross Section

The number of particles $\Delta N(\Omega)$ per unit time per unit target volume that have undergone a collision and are recorded by the detector is proportional to

i) The flux I_0 of incident particles
ii) The density n_t, of the target particle
iii) The solid angle $d\Omega$ the detector subtends as seen from the target

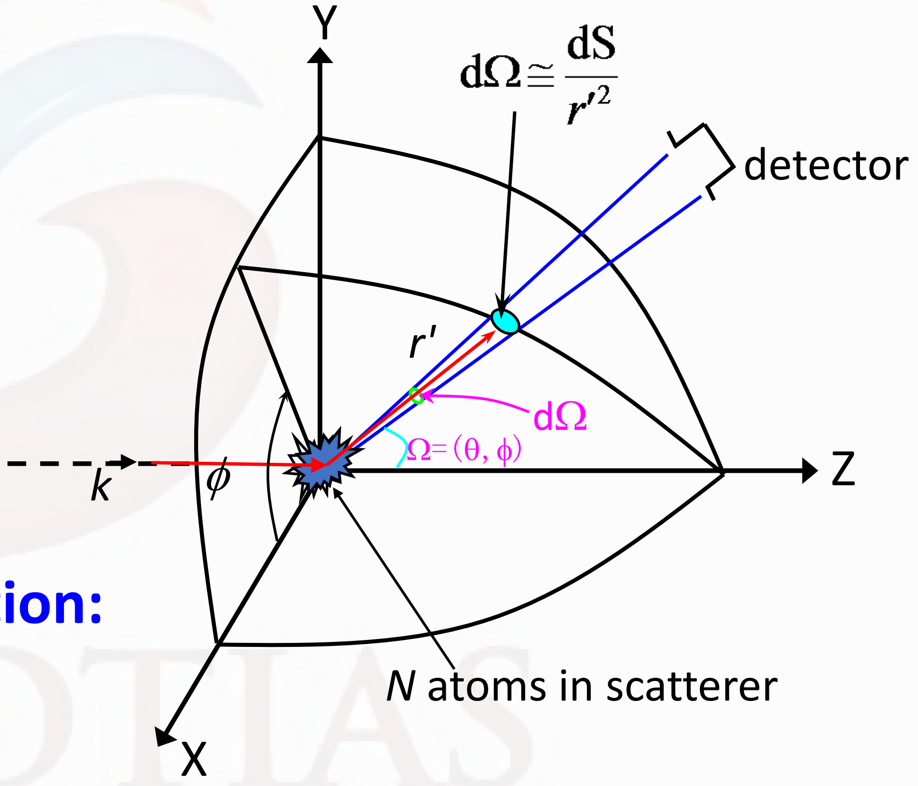


Differential Scattering Cross Section

We then have:

$$dN(\Omega) = I_0 n_t \frac{d\sigma}{d\Omega} d\Omega \quad \text{-----} \quad (3)$$

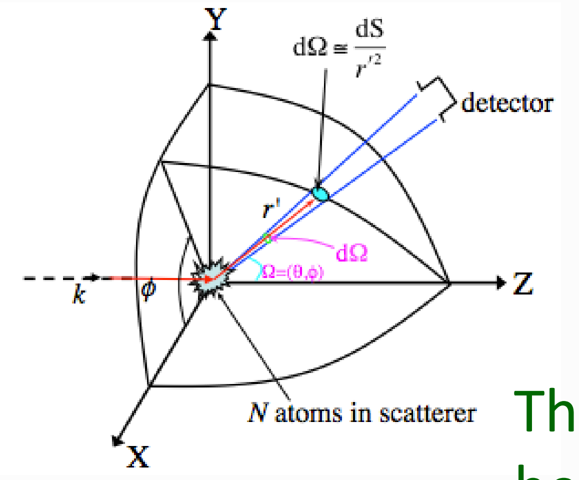
Differential scattering cross section



Integrating over Ω we obtain the total cross section:

$$\sigma_t = \int \frac{d\sigma}{d\Omega} d\Omega \quad \text{-----} \quad (4)$$

Scattering From a Static System



A quantum mechanical wave function can be describe by:

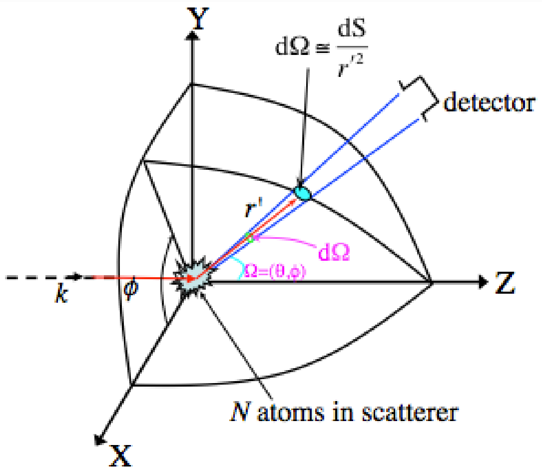
$$\psi(\mathrm{r},t) = A\exp(i(\varpi t - \mathrm{k}\cdot\mathrm{r})) \quad ------ \quad (5)$$

where, $\varpi = 2\pi f, \quad k = 2\pi/\lambda$

The probability of the observation of a particle can be described by:

$$I = |\psi(\mathrm{r},t)|^2 \quad ----- \quad (6)$$

Scattering From a Static System



The wave scattered by a single scattering center is given by:

$$\psi(\mathrm{r}',t) = \frac{\exp(-i(k|\mathrm{r}'-\mathrm{r}_j|))}{|\mathrm{r}'-\mathrm{r}_j|} b_j \psi(\mathrm{r},t) \quad \text{-----} \quad (7)$$

Here,

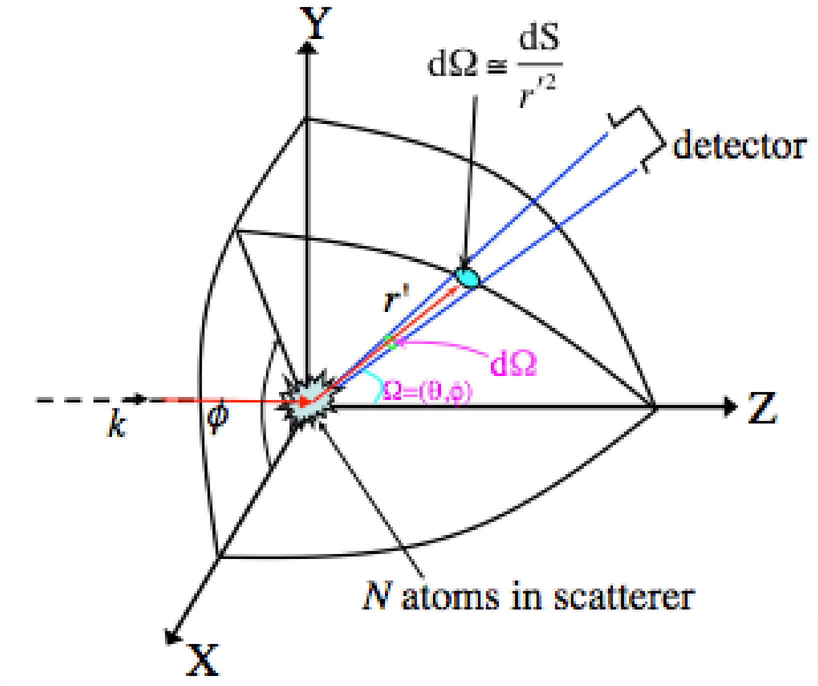
r′⇒ point of observation of the scattered wave

r_j ⇒position of the scattering center

b_j ⇒ property of this scattering center, the scattering length

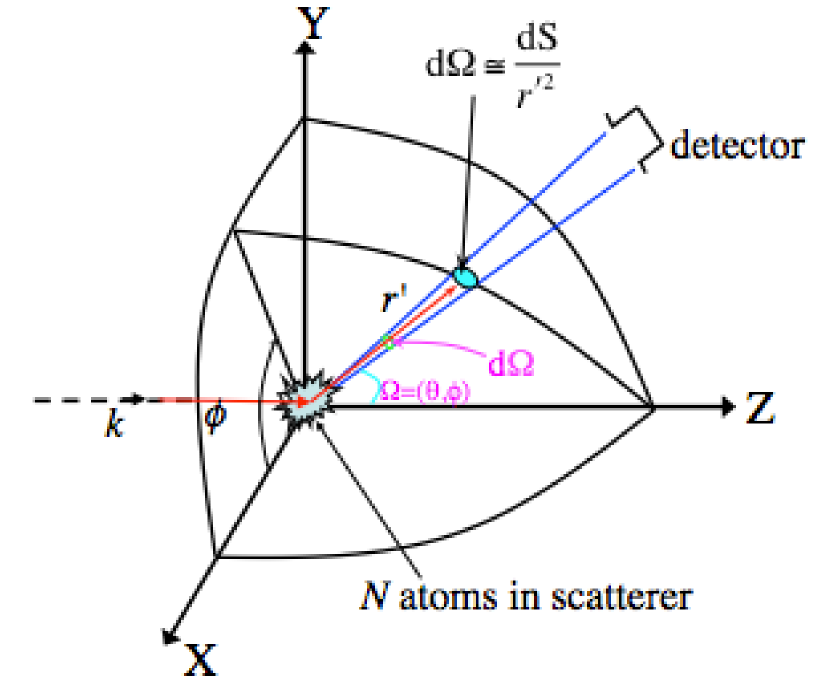
exp(-i(k|r′-r_j|))⇒additional oscillations between the scattering process and detection

Scattering From a Static System



Now we assumed that the scattering centres are fixed points in space described by coordinates $r_j(t)$=const. = r_j. In this case the scattering is elastic so that before and after the scattering process energy will not change.

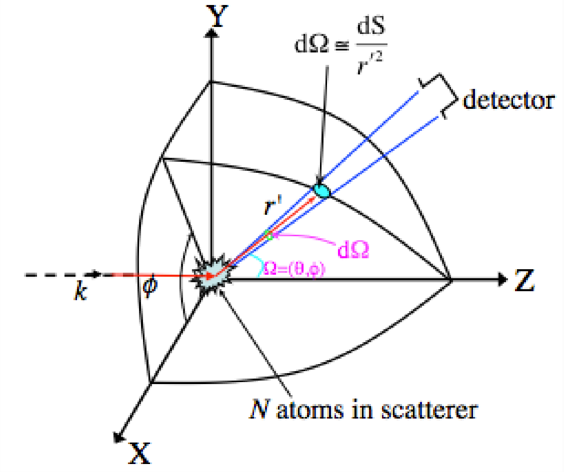
Scattering From a Static System



Without loss of generality one can define the direction of the incident beam as the z direction: k=(0,0,*k*). By using eq. 5 and eq. 7, the wave scattered by particle j into the detector can be expressed as

$$\psi(\mathrm{r}',t) = \frac{\exp(-i(k|\mathrm{r}'-\mathrm{r}_j|))}{|\mathrm{r}'-\mathrm{r}_j|} A b_j \exp(i(\varpi t - \mathrm{k}\cdot\mathrm{r})) \quad \text{------} \quad (8)$$

Scattering From a Static System



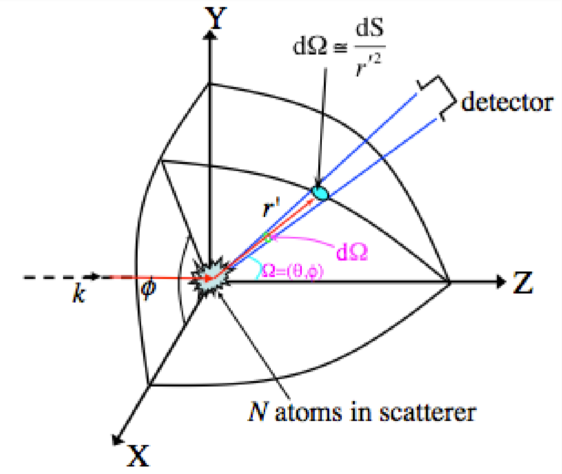
Now, we assumed that SDD, R, is large compared to the size of the sample (Fraunhofer diffraction). Then an expression to 1st order in the scatterer's position yields:

$$\psi(\mathrm{r}',t) = \frac{A}{R} e^{i\varpi t} e^{ik(R+L)} b_j \exp(i\mathrm{Q}\cdot\mathrm{r_j}) \quad ----- \quad (9)$$

Then the intensity:

$$I = \psi\cdot\psi^* = \frac{A^2}{R^2}\left|\sum_{j=1}^{N} b_j \exp(i\mathrm{Q}\cdot\mathrm{r_j})\right|^2 \quad ----- \quad (10)$$

Scattering From a Static System



The differential scattering cross section can be written as:

$$\frac{d\sigma}{d\Omega} = \left\langle \left| \sum_{j=1}^{N} b_j \exp(iQ \cdot r_j) \right|^2 \right\rangle = \left\langle |A(Q)|^2 \right\rangle \quad \text{-----} \quad (11)$$

Where, $A(Q) = \sum_j b_j \exp(iQ \cdot r_j)$ ----- (11a)

is the superposition of the individual scattering amplitudes.

Coherent and Incoherent Scattering

Since, the individual scattering lengths are independent, then, we can write:

$$\langle b_i b_j \rangle = \langle b \rangle^2 + \left(\langle b^2 \rangle - \langle b \rangle^2 \right) \delta_{ij} \quad \text{-----} \quad (12)$$

Where, δ_{ij} is the delta function

The macroscopic differential scattering cross section can be written as:

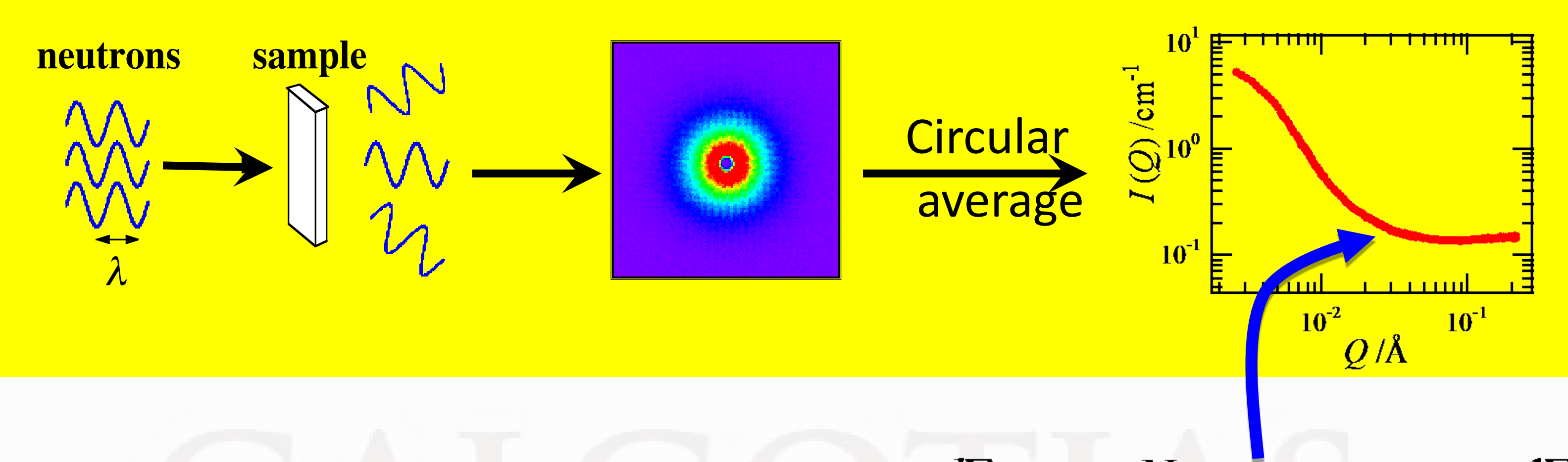
$$\frac{d\Sigma}{d\Omega} = \frac{1}{V_s} \frac{d\sigma}{d\Omega}$$

Coherent and Incoherent Scattering

$$\frac{d\Sigma}{d\Omega}(Q) = \underbrace{\frac{1}{V_s}\langle b\rangle^2 \sum_{j=1}^{N}\left\langle \left|\exp(iQ\cdot r_j)\right|^2\right\rangle}_{} + \underbrace{\frac{N}{V_s}\left(\langle b^2\rangle - \langle b\rangle^2\right)}_{} \qquad \text{-----} \quad (13)$$

$$\Rightarrow \quad \frac{d\Sigma}{d\Omega}(Q) = \frac{d\Sigma}{d\Omega_{Coh}}(Q) + \frac{d\Sigma}{d\Omega_{Incoh}}$$

Coherent and Incoherent Scattering



$P(\vec{Q}) \Rightarrow$ Form factor

$S(\vec{Q}) \Rightarrow$ Structure factor

$$\frac{d\Sigma}{d\Omega}(Q) = \frac{N_m}{V_S} P(\vec{Q}) S(\vec{Q}) + \frac{d\Sigma}{d\Omega_{Incoh}}$$