Lecture 7
Neutron Scattering Basics

October 2023

Francesco Piscitelli

Outline

WHY NEUTRONS

ELASTIC VS INELASTIC

COHERENT VS INCOHERENT

CONTRAST MATCHING – an example

Outline

Coherent	Incoherent
Elastic	Inelastic

WHY NEUTRONS

Why neutrons

Identity card

mass	$m = 1.675\ 10^{-27}$ kg
charge	$q = 0$
magnetic dipole moment	$\mu_n = -\ 1.913\ \mu_N$
spin	$s = ½$
de Broglie wavelength	$\lambda = h\ /\ mv$

Planck constant $h = 6.626\ 10^{-34}$ J s

Neutrons interact with nuclei
- Sensitive to light atoms
- Isotopic substitution

Uncharged
- Strongly penetrating
- Non-invasive probe

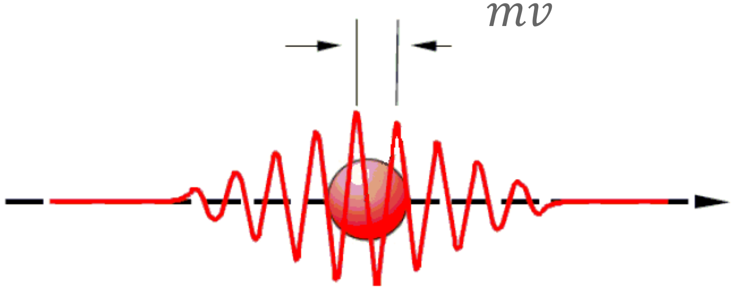
Magnetic
- Investigating magnetic strucutres microscopically
- Magnetic fluctuations
- Devel new magnetic materials

Spin
- Polarized beams
- Study of nuclear atomic orientation
- Coherent and incoherent scattering

Why neutrons

$$\lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega$$

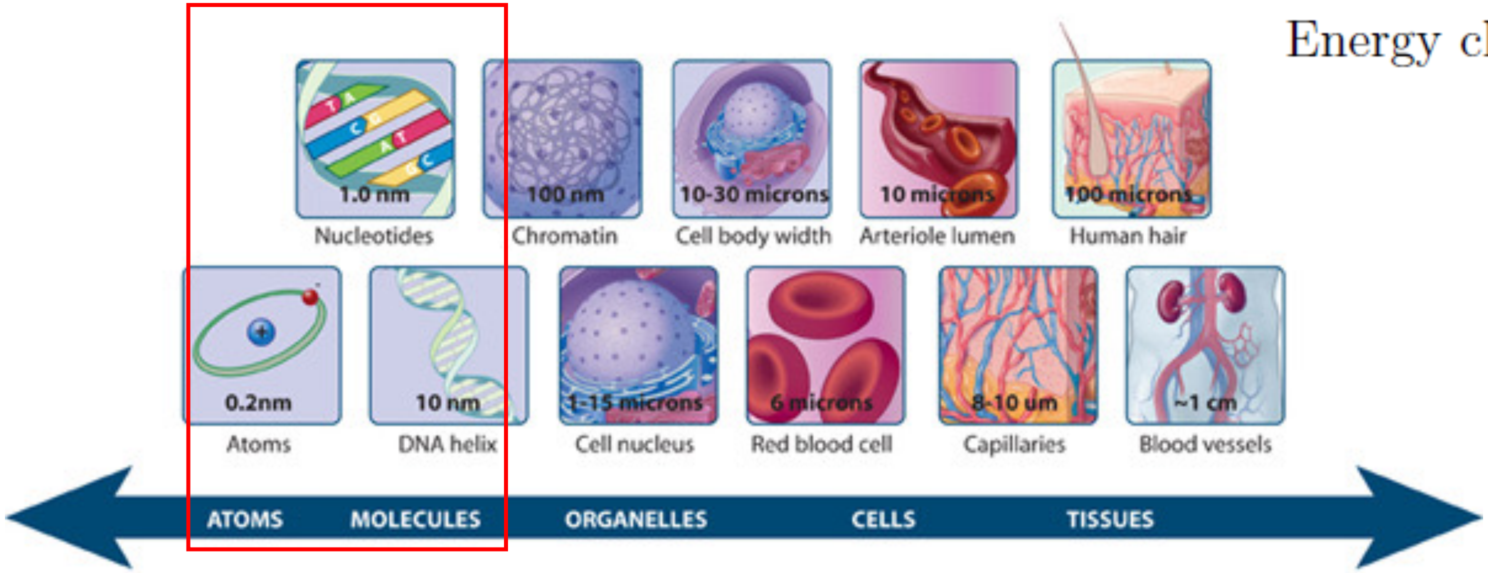


$$E_k = \frac{1}{2}mv^2 = 25meV \Rightarrow \lambda = \frac{h}{\sqrt{2mE_k}} \approx 1.8A$$

$$E_k = \frac{1}{2}mv^2 = 1MeV \Rightarrow \lambda = \frac{h}{\sqrt{2mE_k}} \approx 0.0003A$$

Energy classification	
slow (cold)	0 - 0.005 eV
thermal	0.005 - 0.5 eV
epithermal	0.5 - 1000 eV
intermediate	1 - 100 KeV
fast	0.1 - 10 MeV

Energy classification of neutrons



Why neutrons

$$E_k = \frac{1}{2}mv^2 = 25meV \Rightarrow \lambda = \frac{h}{\sqrt{2mE_k}} \approx 1.8A$$

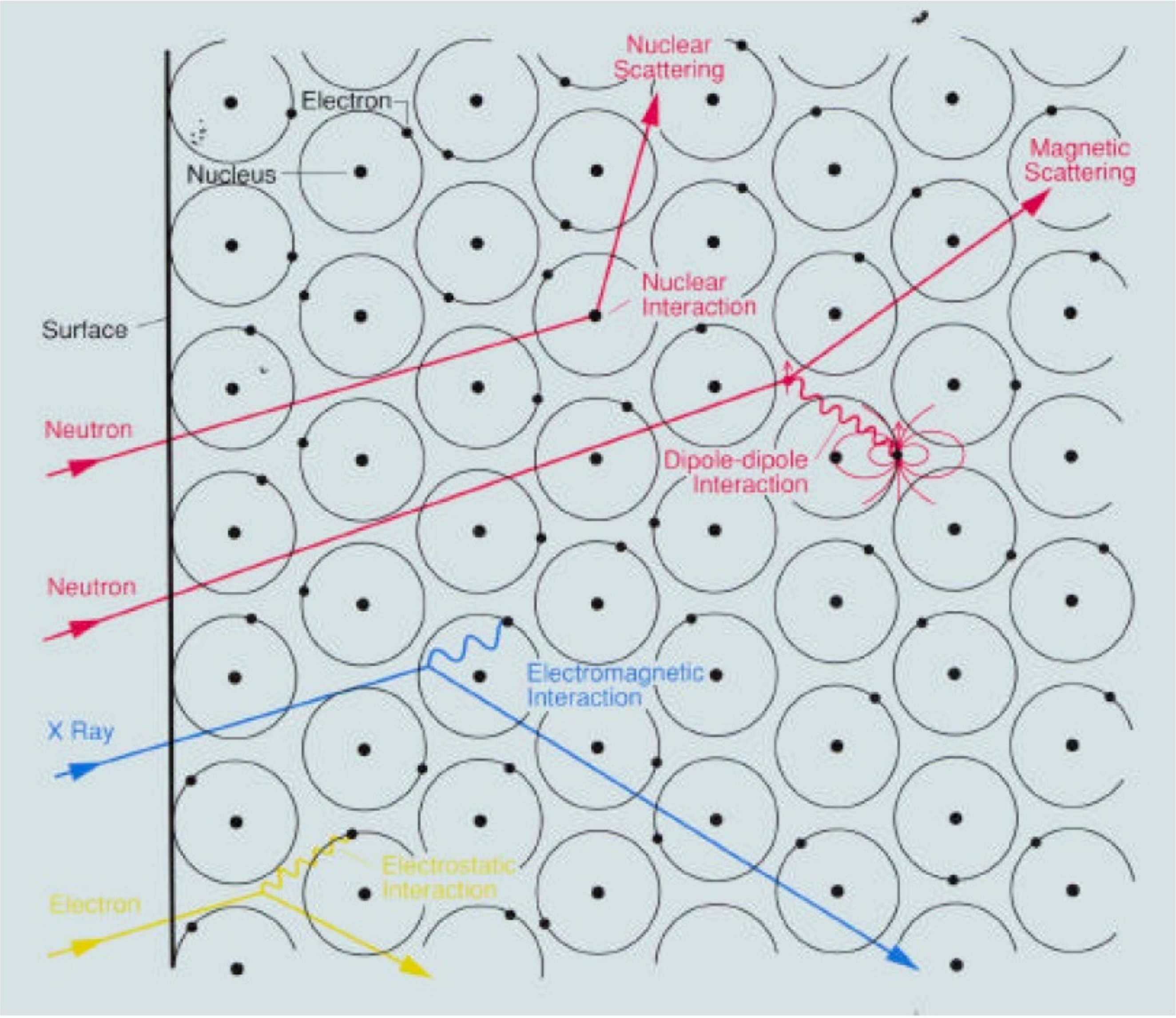
Wavelength similar to distances in condensed matter

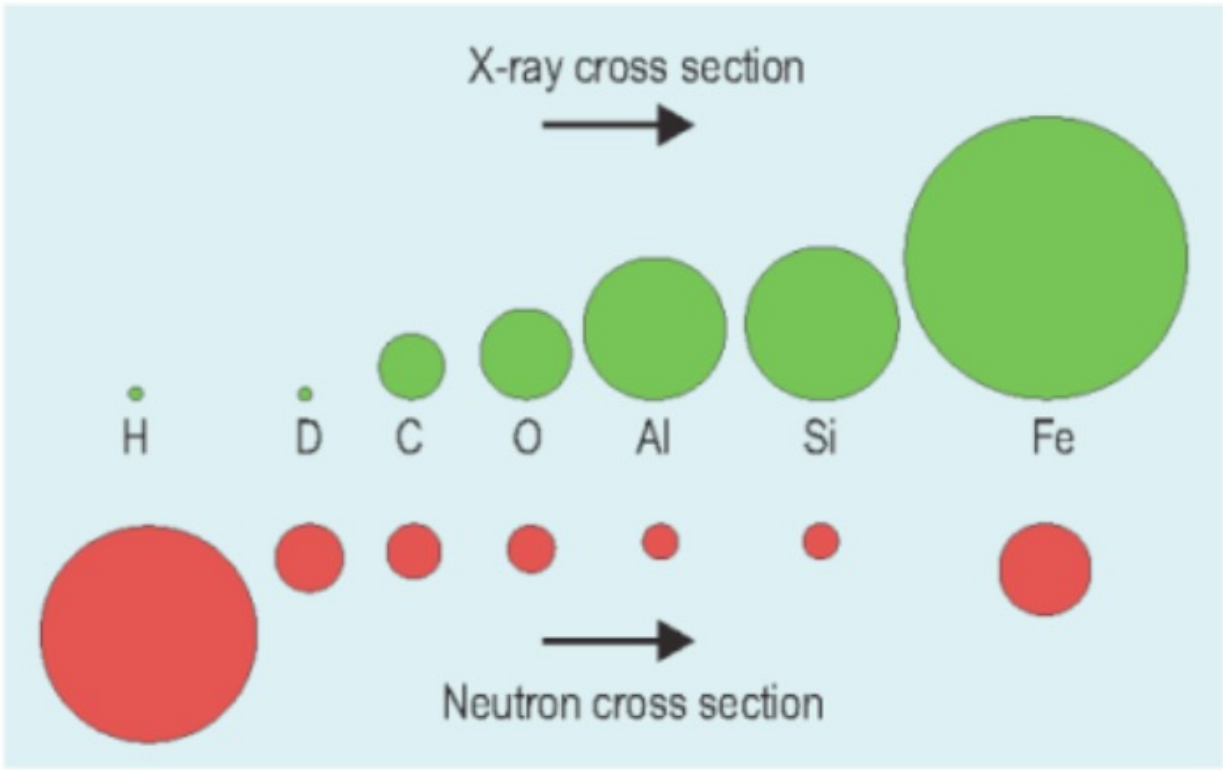
Energy similar to many excitations in solids and liquids:

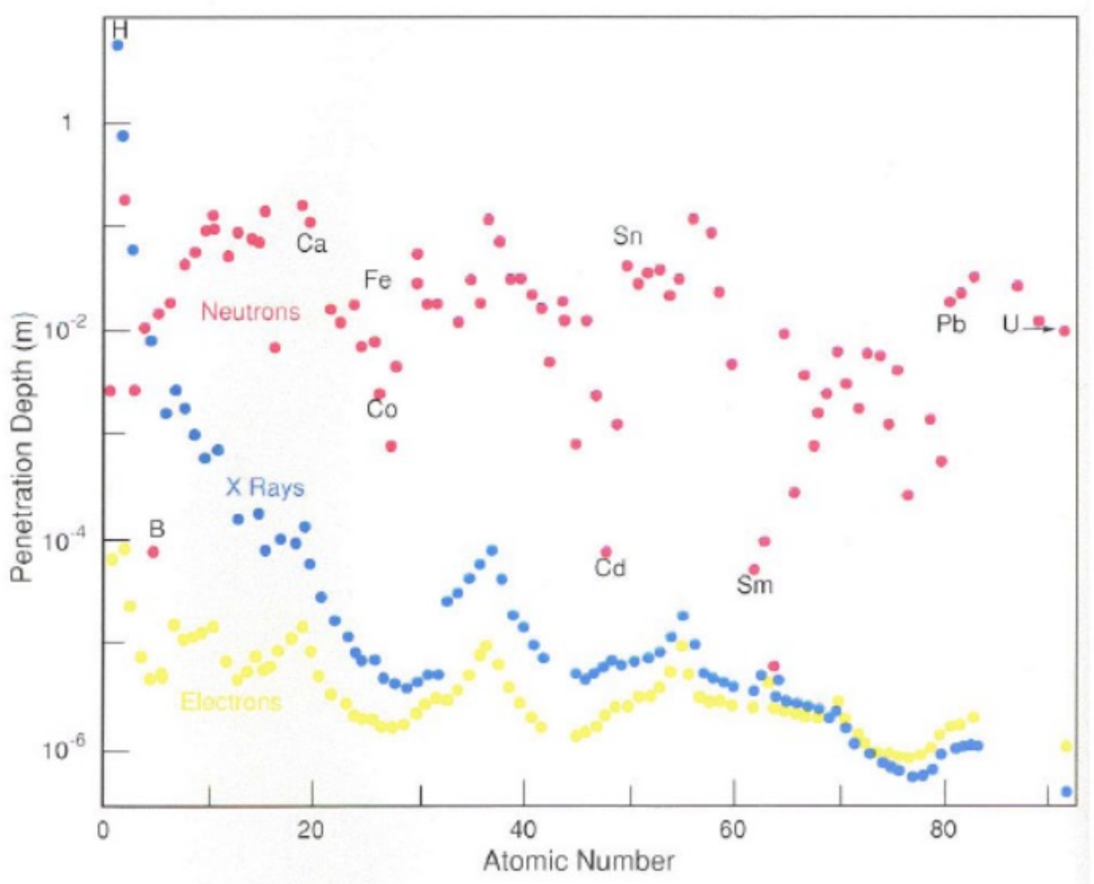
- Molecular vibrations
- Lattice modes
- Atomic dynamics

NOTE: X-rays for same wavelengths have keV energy so not suitable for these excitations

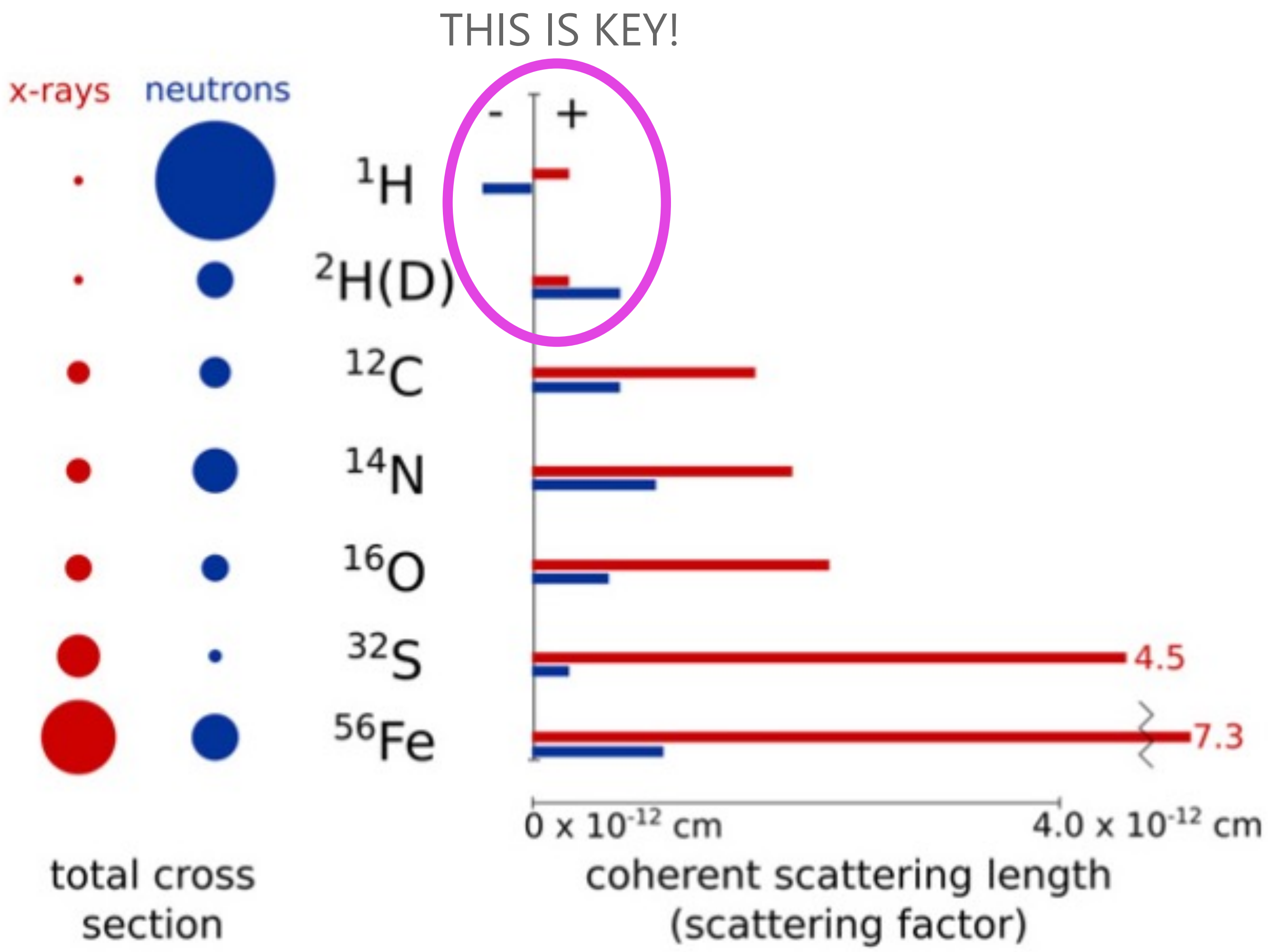
Neutrons' interactions




X-ray cross section
H
D
C
O
Al
Si
Fe
Neutron cross section

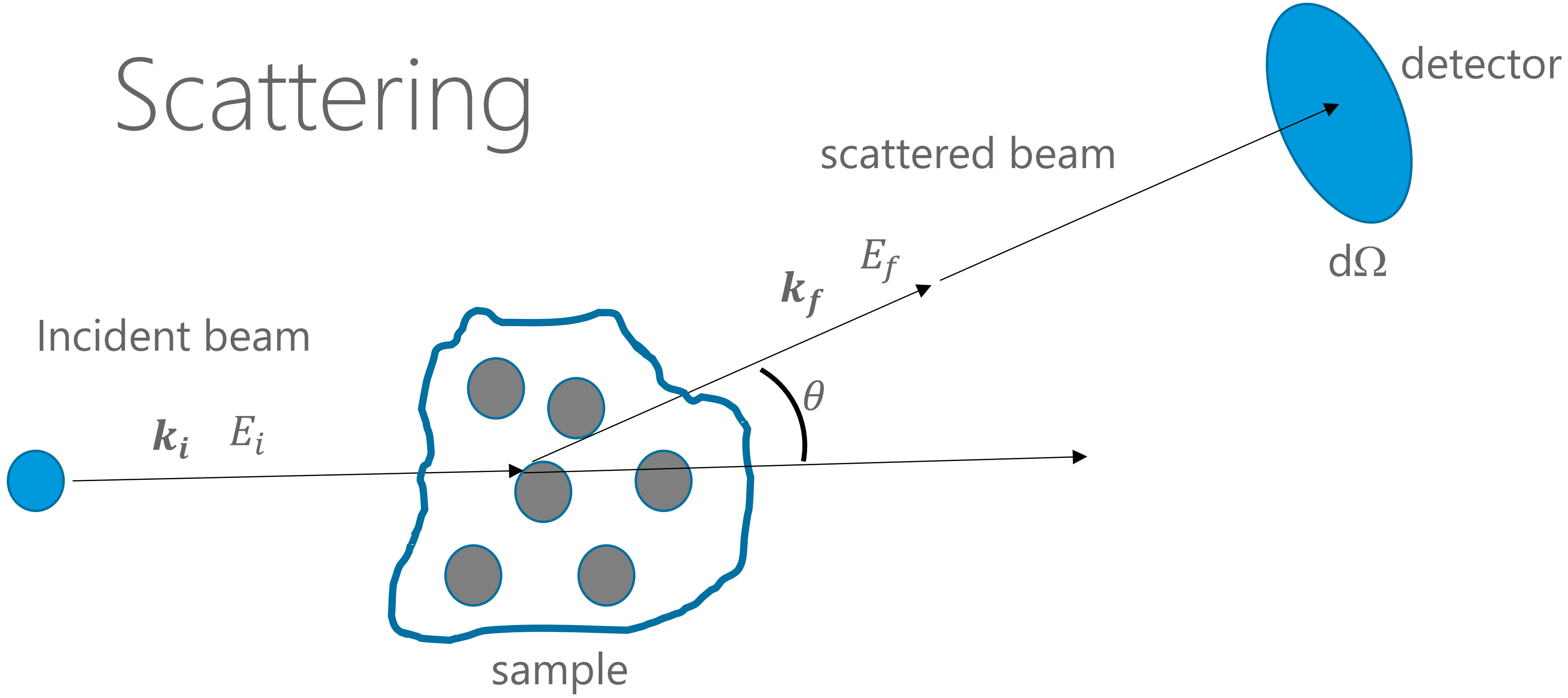

Penetration Depth (m)
1
10⁻²
10⁻⁴
10⁻⁶
Atomic Number
0
20
40
60
80
H
B
Ca
Fe
Co
Sn
Cd
Sm
Pb
U
Neutrons
X Rays
Electrons

Why neutrons



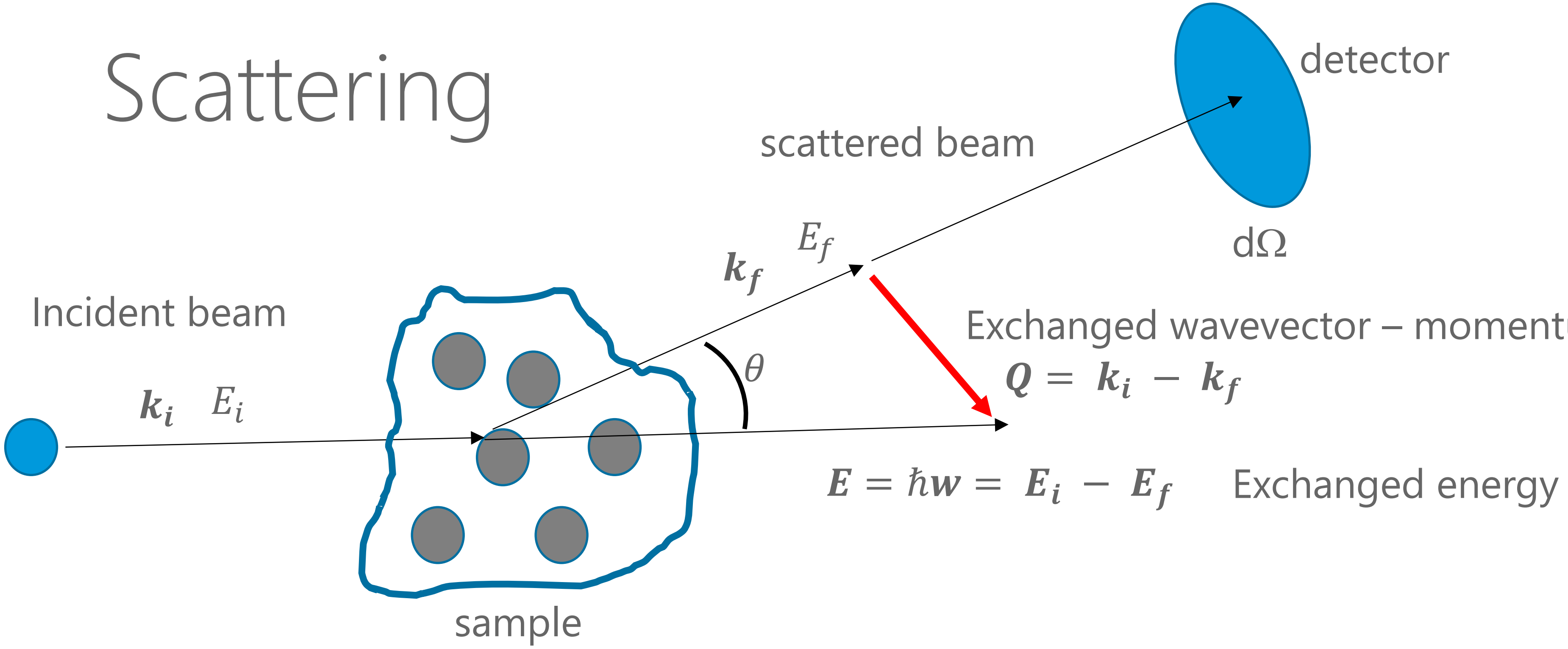
ELASTIC
VS
INELASTIC

Scattering



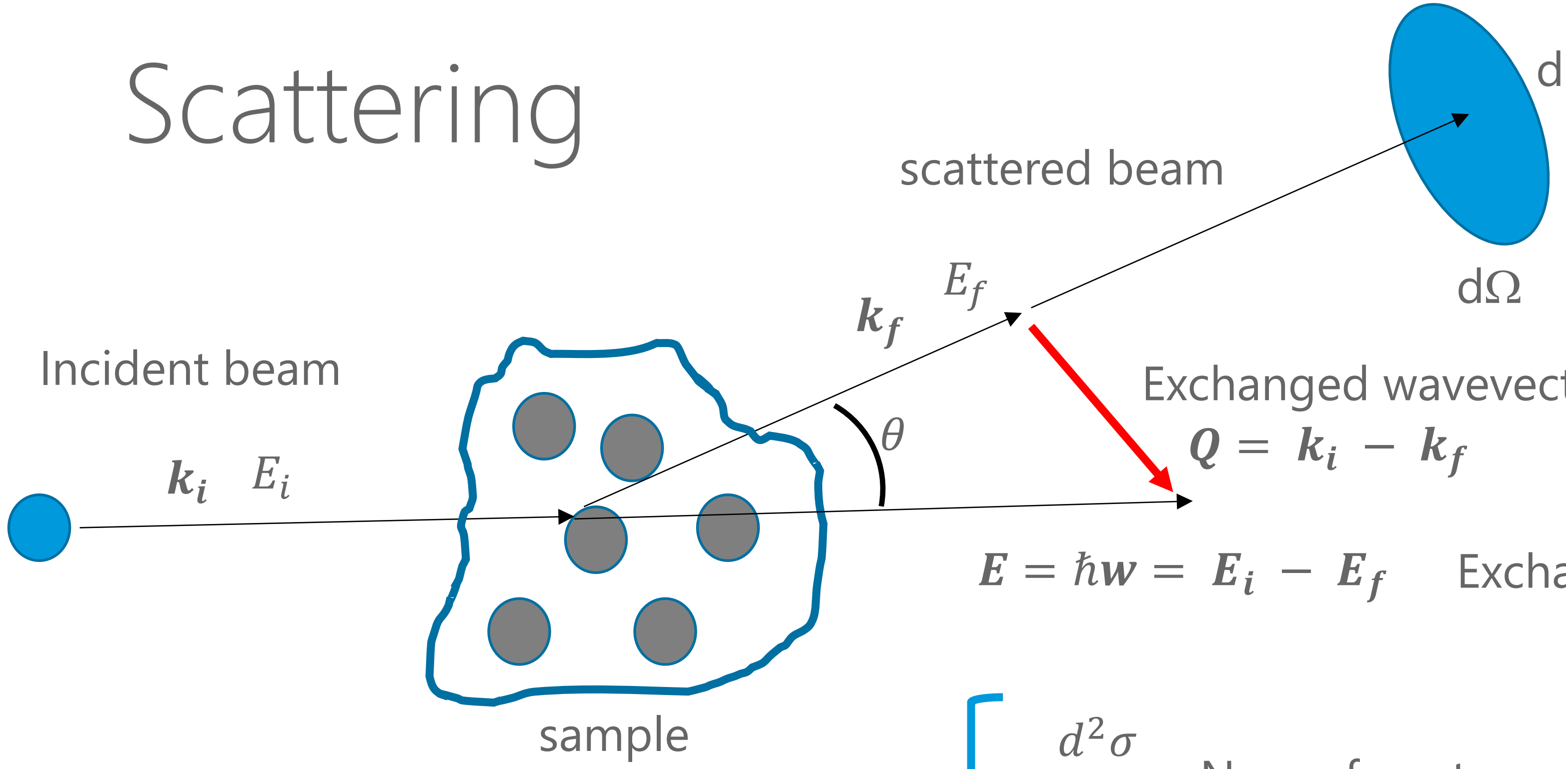
dΩ

Scattering



dΩ

Scattering



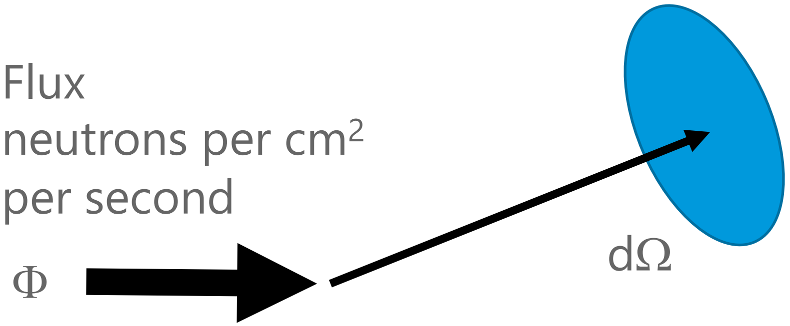
Exchanged wavevector – momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

$$\boldsymbol{E} = \hbar \boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$$ Exchanged energy

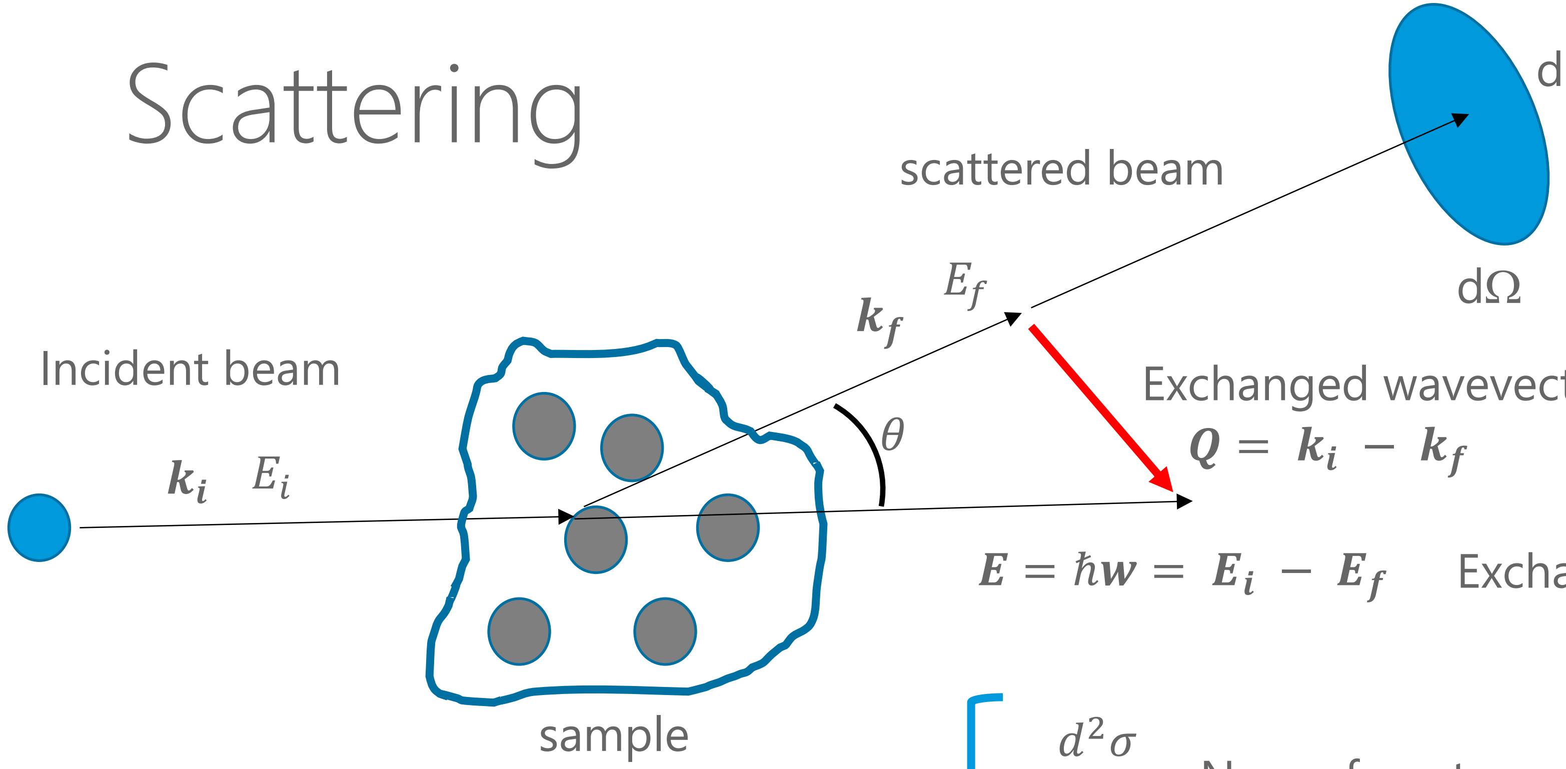
$\frac{d^2\sigma}{d\Omega dE}$ Num of neutrons scattered into $d\Omega$ and dE per second

Flux
neutrons per cm^2
per second



The cross-sect are the measured quantities

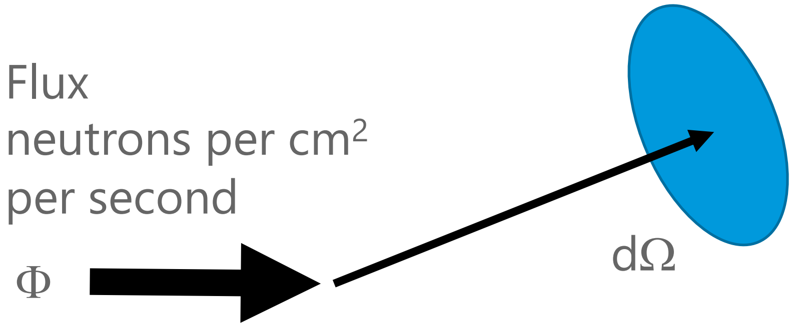
Scattering



Exchanged wavevector – momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

$$\boldsymbol{E} = \hbar \boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$$ Exchanged energy



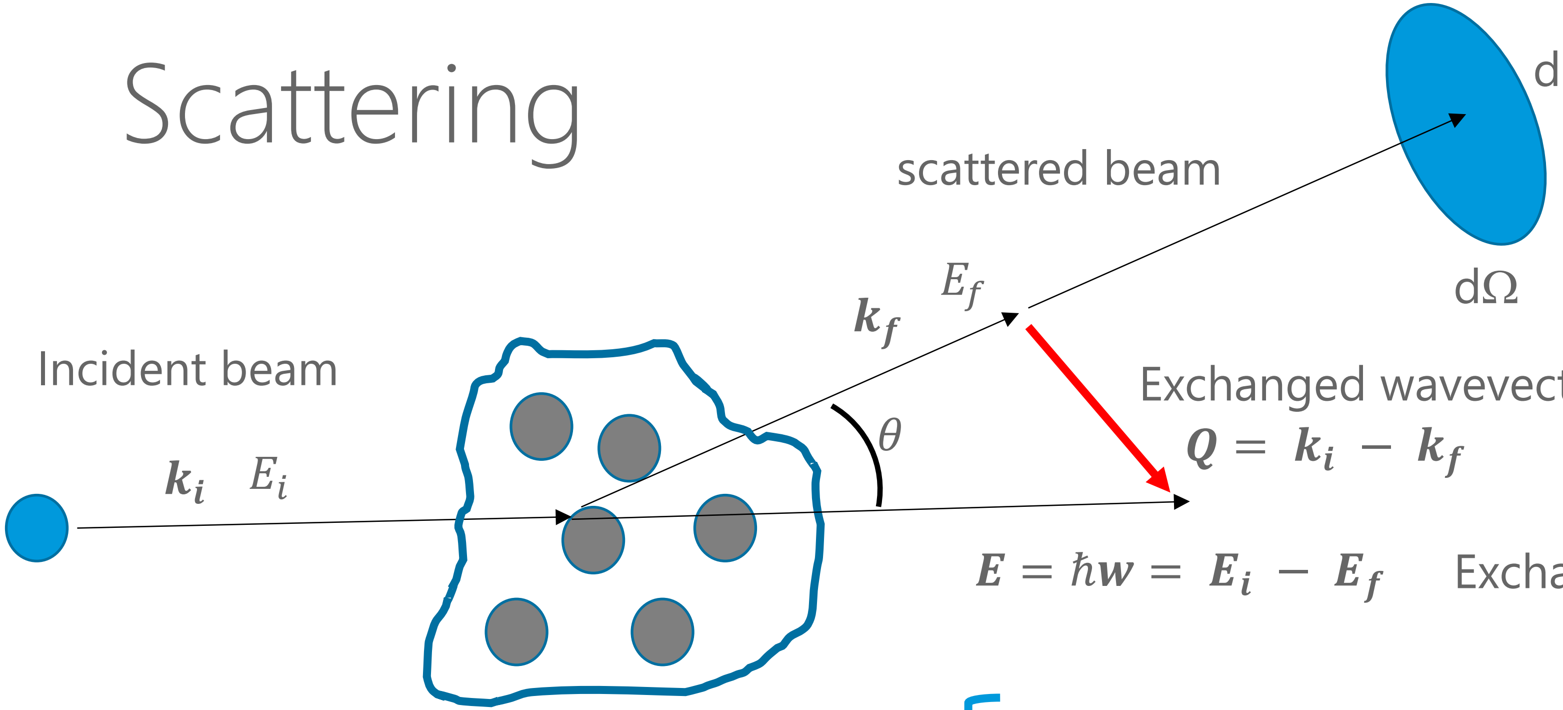
$$\frac{d^2\sigma}{d\Omega dE}$$ Num of neutrons scattered into $d\Omega$ and dE per second

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$ Num of neutrons scattered into $d\Omega$ per second

$$\sigma_{tot} = \int_{4\pi} \left(\frac{d\sigma}{d\Omega} \right) d\Omega$$ Num of neutrons scattered into 4π per second

The cross-sect are the measured quantities

Scattering

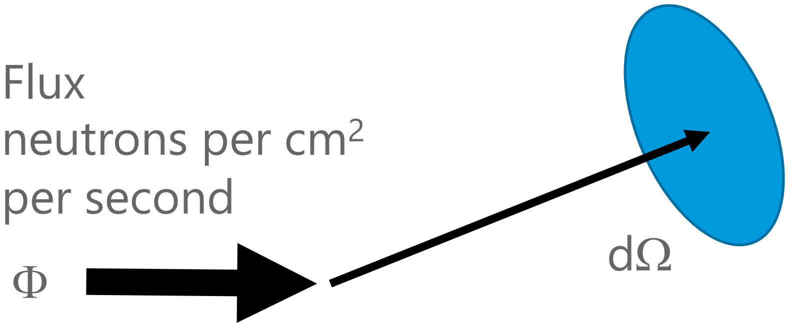


Exchanged wavevector – momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

$$\boldsymbol{E} = \hbar \boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$$ Exchanged energy

Flux
neutrons per cm^2
per second



$\frac{d^2\sigma}{d\Omega dE}$ Num of neutrons scattered into $d\Omega$ and dE per second

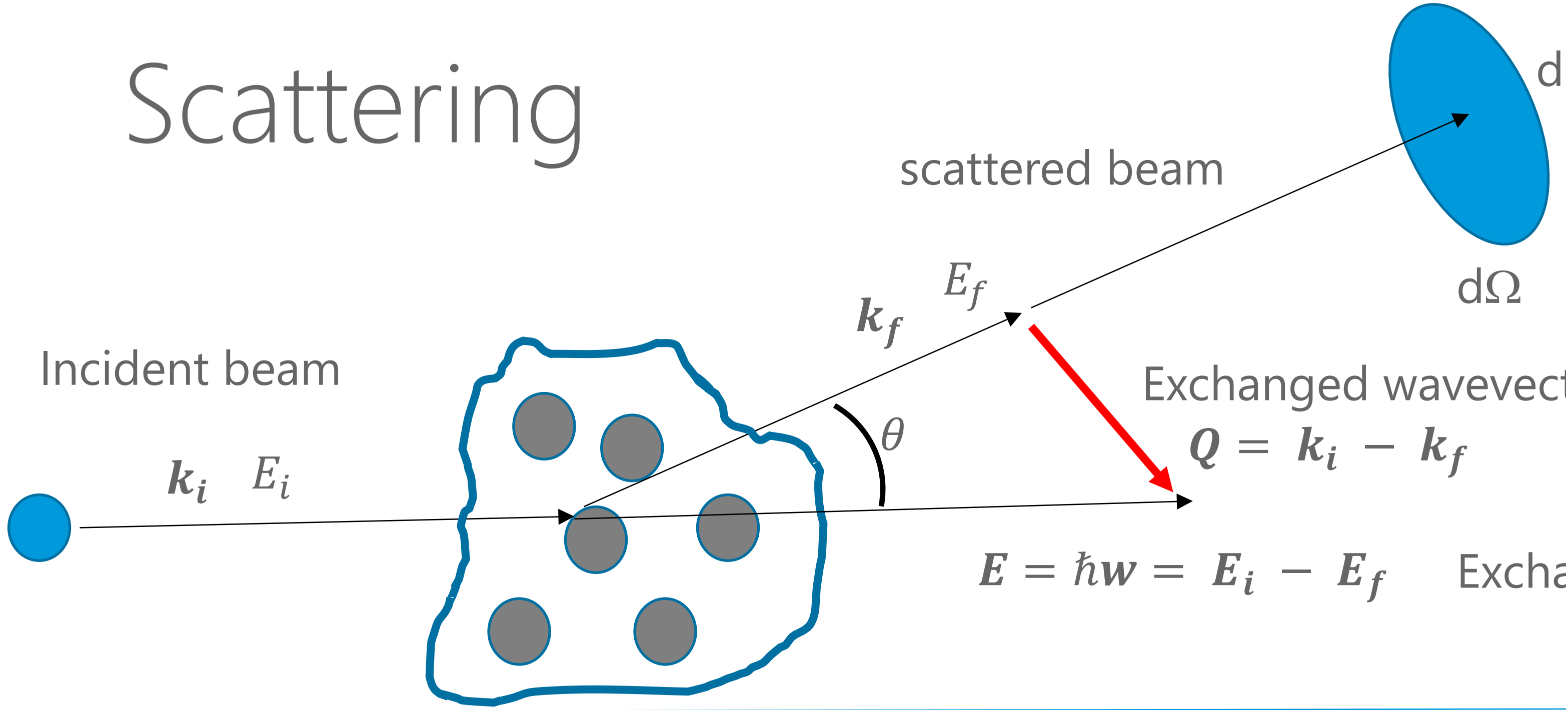
diffraction spectroscopy

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$ Num of neutrons scattered into $d\Omega$ per second

$$\sigma_{tot} = \int_{4\pi} \left(\frac{d\sigma}{d\Omega} \right) d\Omega$$ Num of neutrons scattered into 4π per second

The cross-sect are the measured quantities

Scattering

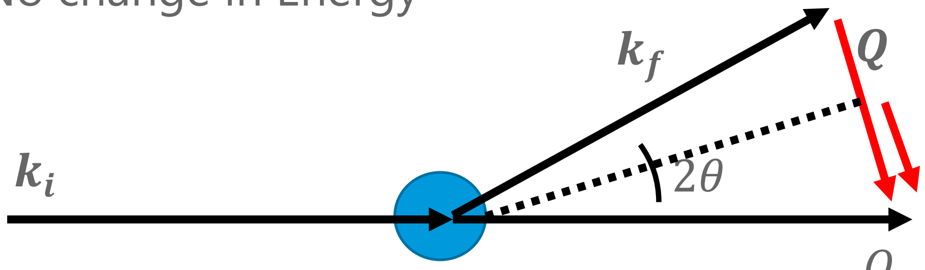


Exchanged wavevector – momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

$$\boldsymbol{E} = \hbar \boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$$ Exchanged energy

No change in Energy



$$\frac{Q}{2} = k_i \sin\theta$$

$$E_i = \frac{\hbar^2 {k_i}^2}{2m}$$

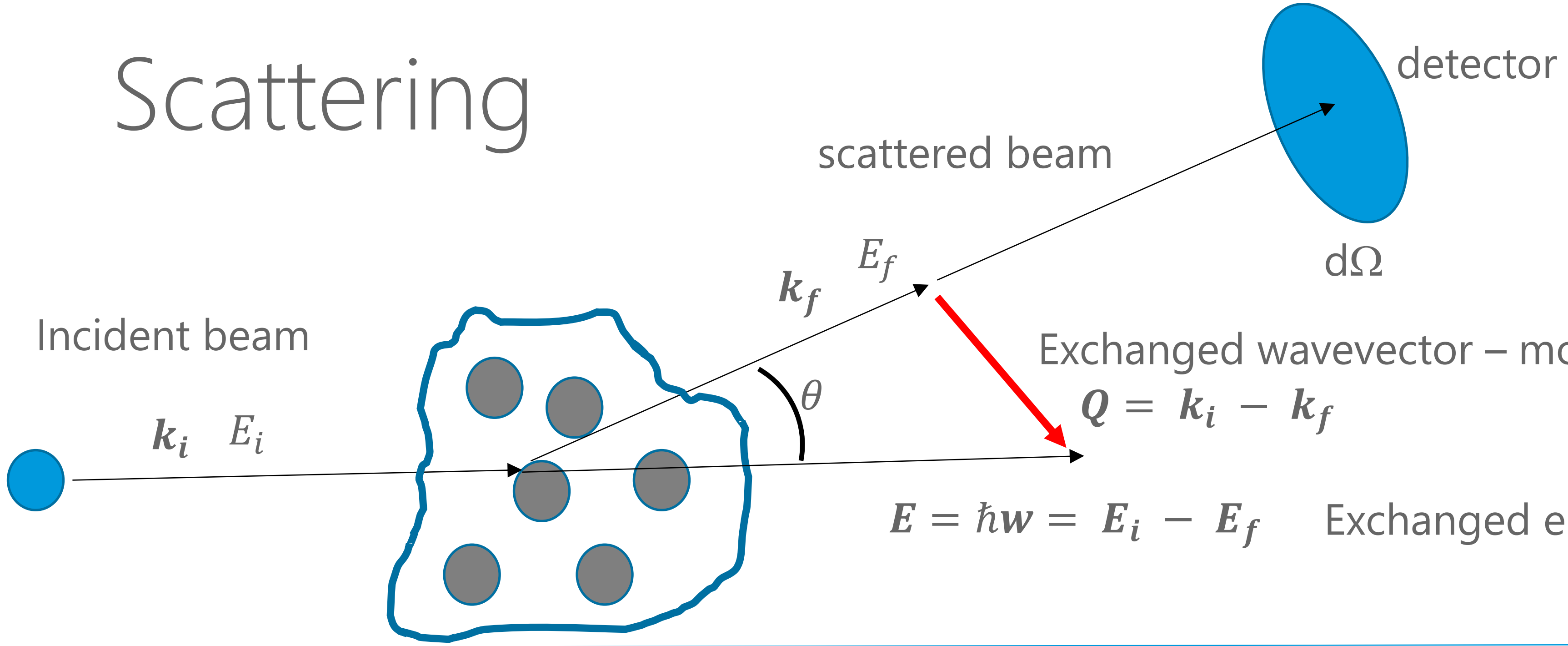
$$E_f = E_i$$

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

$$k_i = k_f$$

$$Q = 2k_i \sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

Scattering

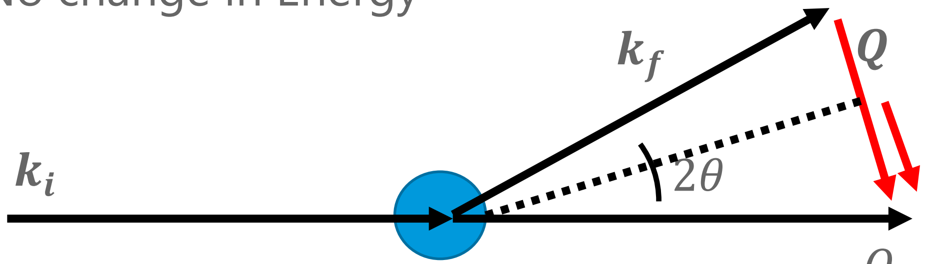


Exchanged wavevector – momentum transfer

$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$

$\boldsymbol{E} = \hbar \boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$ Exchanged energy

No change in Energy



$$E_i = \frac{\hbar^2 {k_i}^2}{2m}$$

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

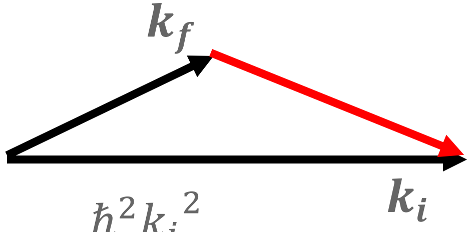
$$Q = 2k_i \sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

$$E_f = E_i$$

$$k_i = k_f$$

$$\frac{Q}{2} = k_i \sin\theta$$

N loses energy



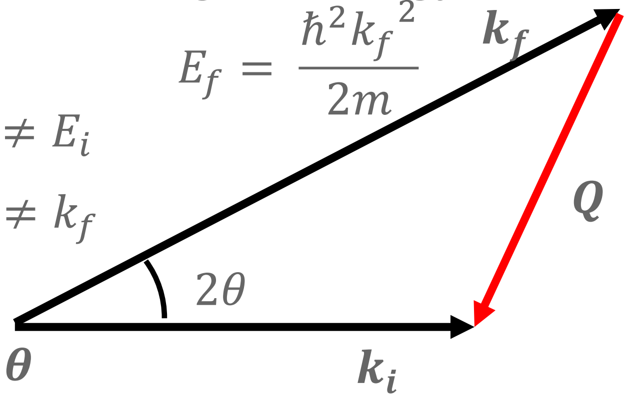
$$E_i = \frac{\hbar^2 {k_i}^2}{2m}$$

$$E_f \neq E_i$$

$$k_i \neq k_f$$

N gains energy

$$E_f = \frac{\hbar^2 {k_f}^2}{2m}$$

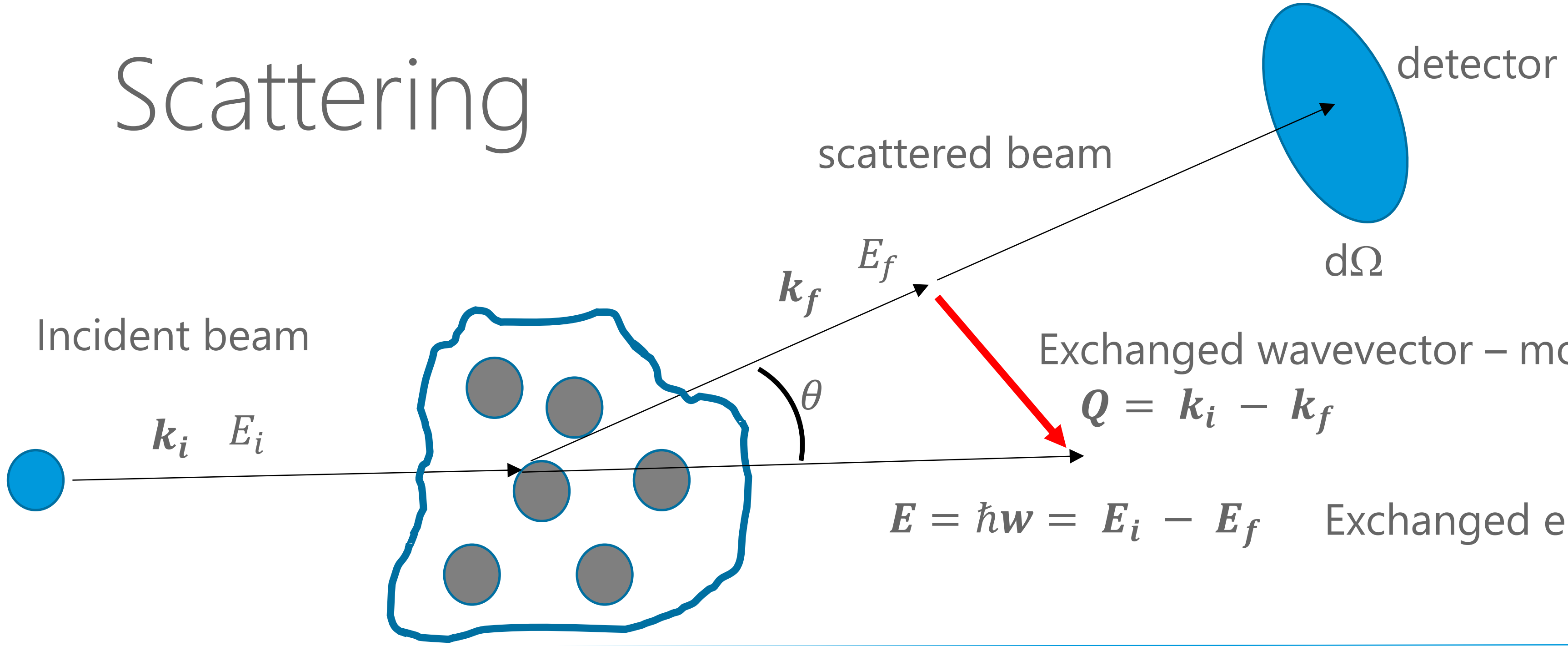


$$\boldsymbol{Q}^2 = \boldsymbol{k_i}^2 + \boldsymbol{k_f}^2 - 2\boldsymbol{k_i}\boldsymbol{k_f}\cos 2\boldsymbol{\theta}$$

$\omega = E_i - E_f$ Energy transfer

$$\boldsymbol{Q}^2 = \boldsymbol{k_i}^2\left(\boldsymbol{1} + \left(\boldsymbol{1} - \frac{\boldsymbol{\omega}}{\boldsymbol{E_i}}\right) - \boldsymbol{2}\cos 2\boldsymbol{\theta}\sqrt{\boldsymbol{1} - \frac{\boldsymbol{\omega}}{\boldsymbol{E_i}}}\right)$$

Scattering



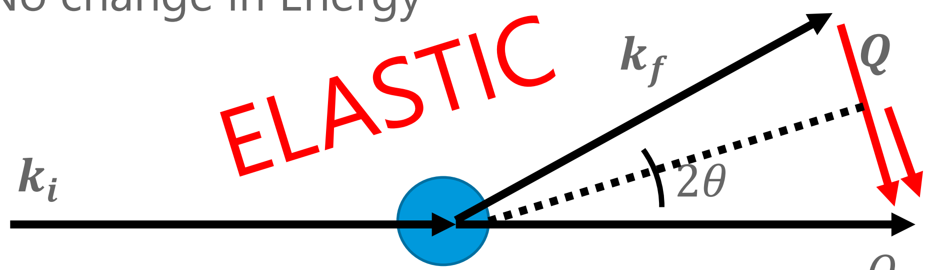
Exchanged wavevector – momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

$$\boldsymbol{E} = \hbar\boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$$ Exchanged energy

No change in Energy

ELASTIC



$$\frac{Q}{2} = k_i \sin\theta$$

$$E_i = \frac{\hbar^2 k_i^{\ 2}}{2m}$$

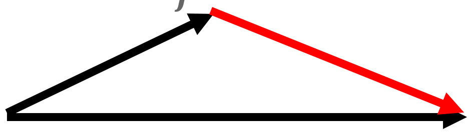
$$E_f = E_i$$

$$k_i = k_f$$

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$$

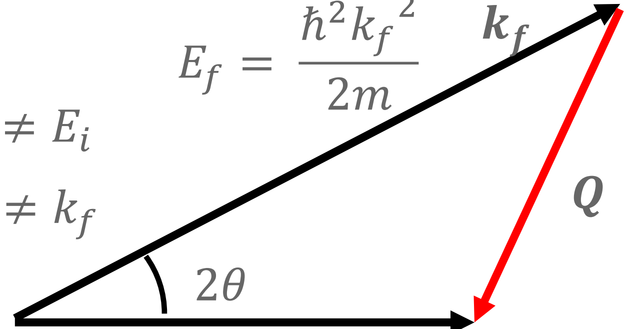
$$Q = 2k_i \sin\theta = \frac{4\pi}{\lambda}\sin\theta$$

N loses energy



N gains energy

$$E_f = \frac{\hbar^2 k_f^{\ 2}}{2m}$$



$$E_f \neq E_i$$

$$k_i \neq k_f$$

$$E_i = \frac{\hbar^2 k_i^{\ 2}}{2m}$$

$$\boldsymbol{Q^2} = \boldsymbol{k_i}^2 + \boldsymbol{k_f}^2 - \boldsymbol{2k_ik_f}\cos\boldsymbol{2\theta}$$

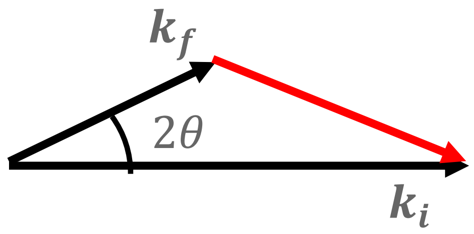
$\omega = E_i - E_f$ Energy transfer

INELASTIC

$$\boldsymbol{Q^2} = \boldsymbol{k_i}^2\left(\boldsymbol{1} + \left(\boldsymbol{1} - \frac{\boldsymbol{\omega}}{\boldsymbol{E_i}}\right) - \boldsymbol{2}\cos 2\boldsymbol{\theta}\sqrt{\boldsymbol{1} - \frac{\boldsymbol{\omega}}{\boldsymbol{E_i}}}\right)$$

Q-E equation

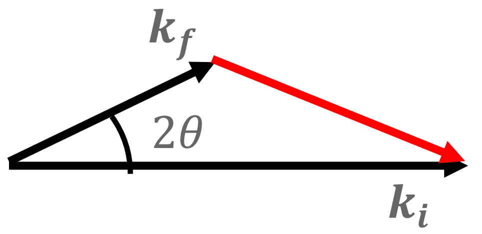
$$Q^2 = k_i{}^2\left(1 + \left(1 - \frac{\omega}{E_i}\right) - 2\cos 2\theta \sqrt{1 - \frac{\omega}{E_i}}\right)$$



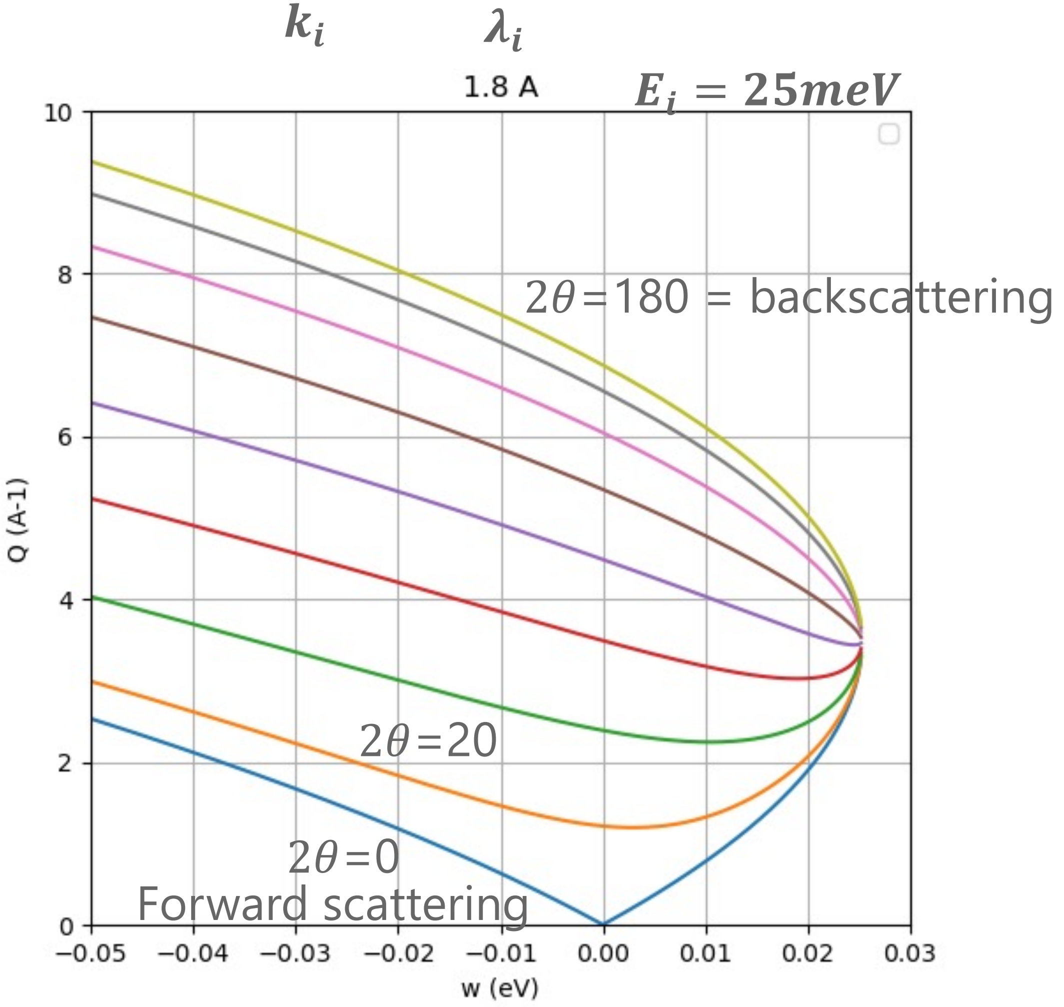
Q is a function of the energy transfer!

Q-E equation

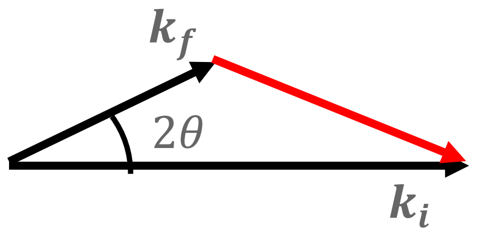
$$Q^2 = k_i^{\,2}\left(1 + \left(1 - \frac{\omega}{E_i}\right) - 2\cos 2\theta \sqrt{1 - \frac{\omega}{E_i}}\right)$$



Q is a function of the energy transfer!

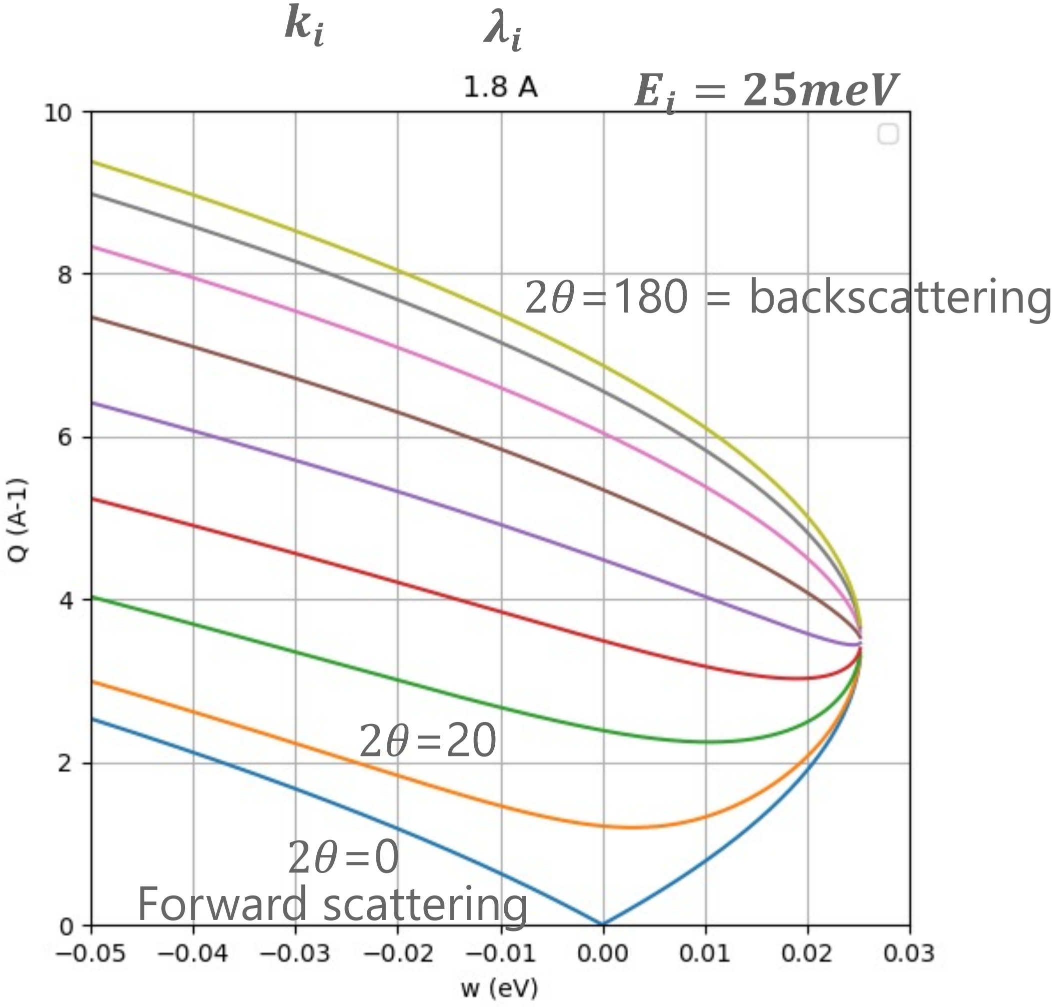


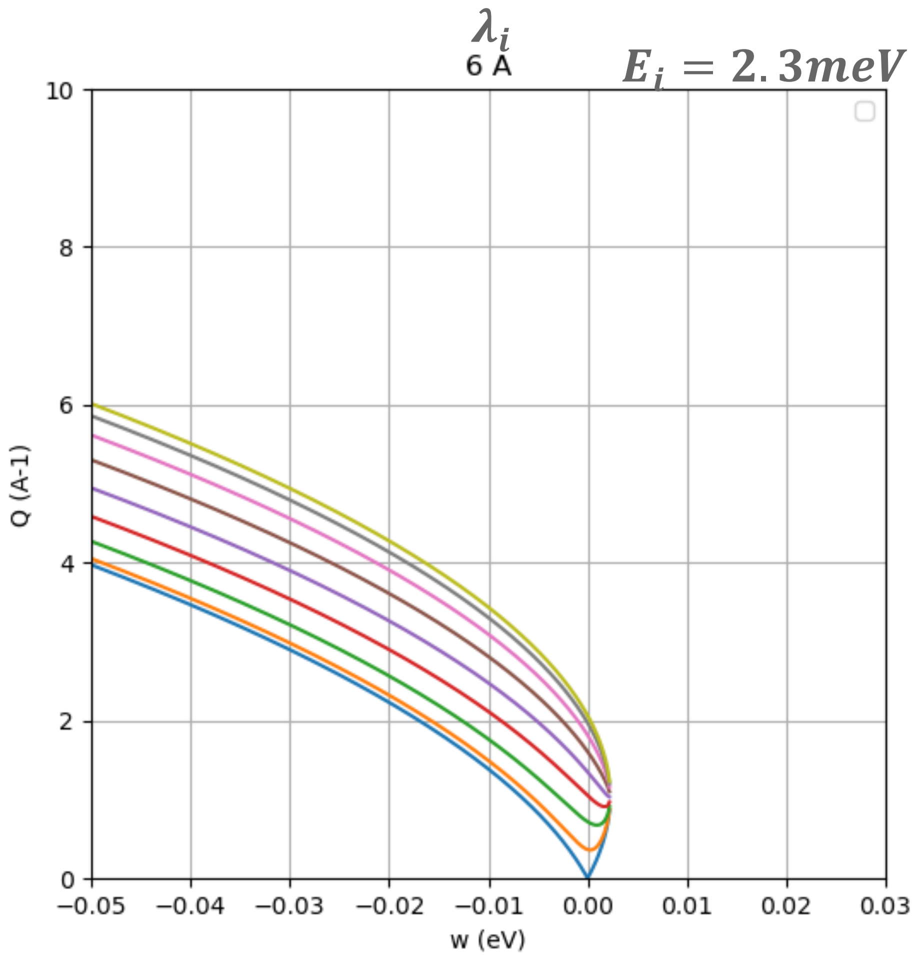
Q-E equation



$$Q^2 = k_i^2\left(1+\left(1-\frac{\omega}{E_i}\right) - 2\cos 2\theta \sqrt{1-\frac{\omega}{E_i}}\right)$$

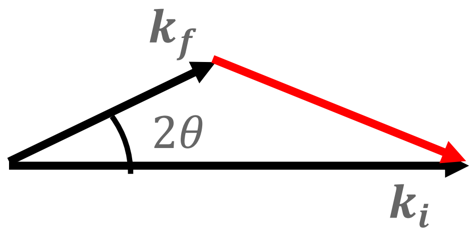
Q is a function of the energy transfer!





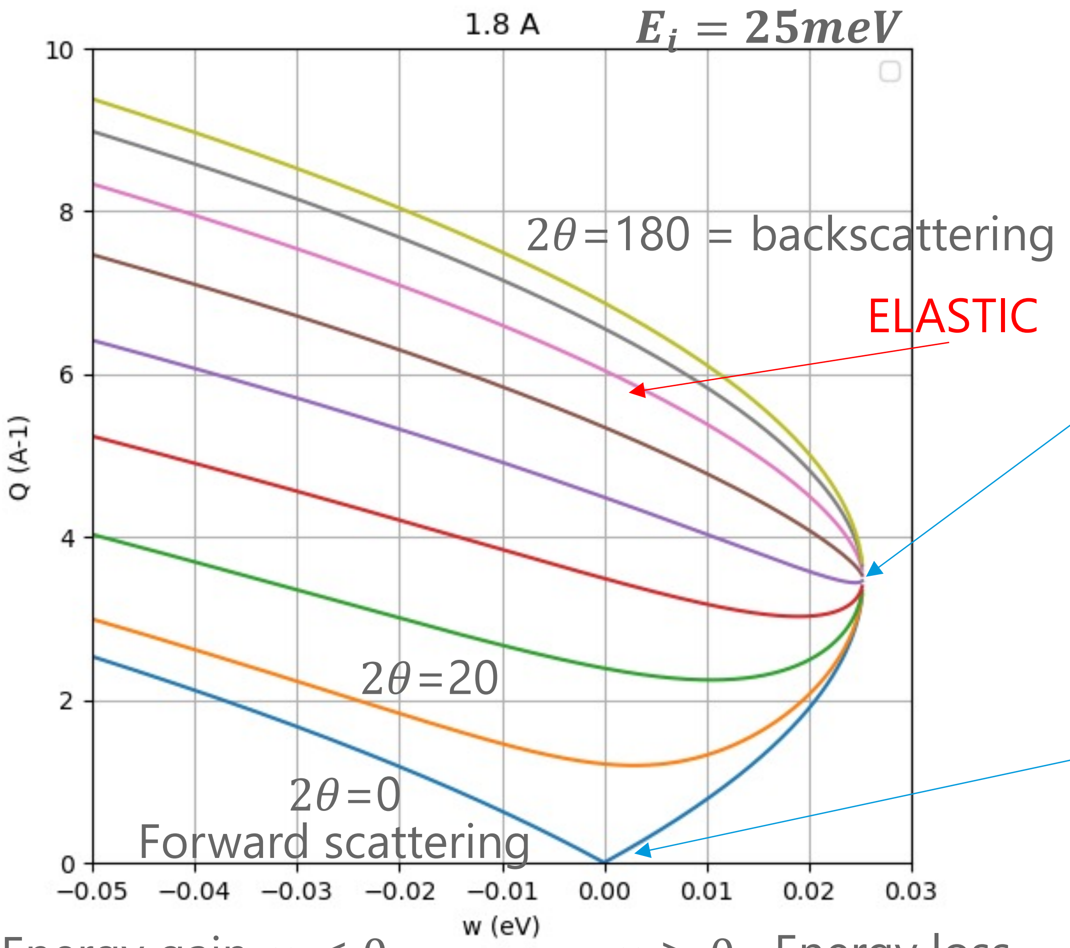
Q-E equation

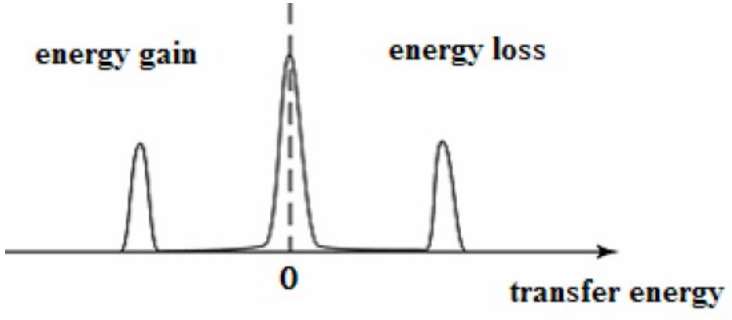
$$Q^2 = k_i^{\,2}\left(1 + \left(1 - \frac{\omega}{E_i}\right) - 2\cos 2\theta \sqrt{1 - \frac{\omega}{E_i}}\right)$$



Q is a function of the energy transfer!

λ_i





$E_i = 25meV$

$2\theta = 0$

$\omega = 0$

$Q = 0$

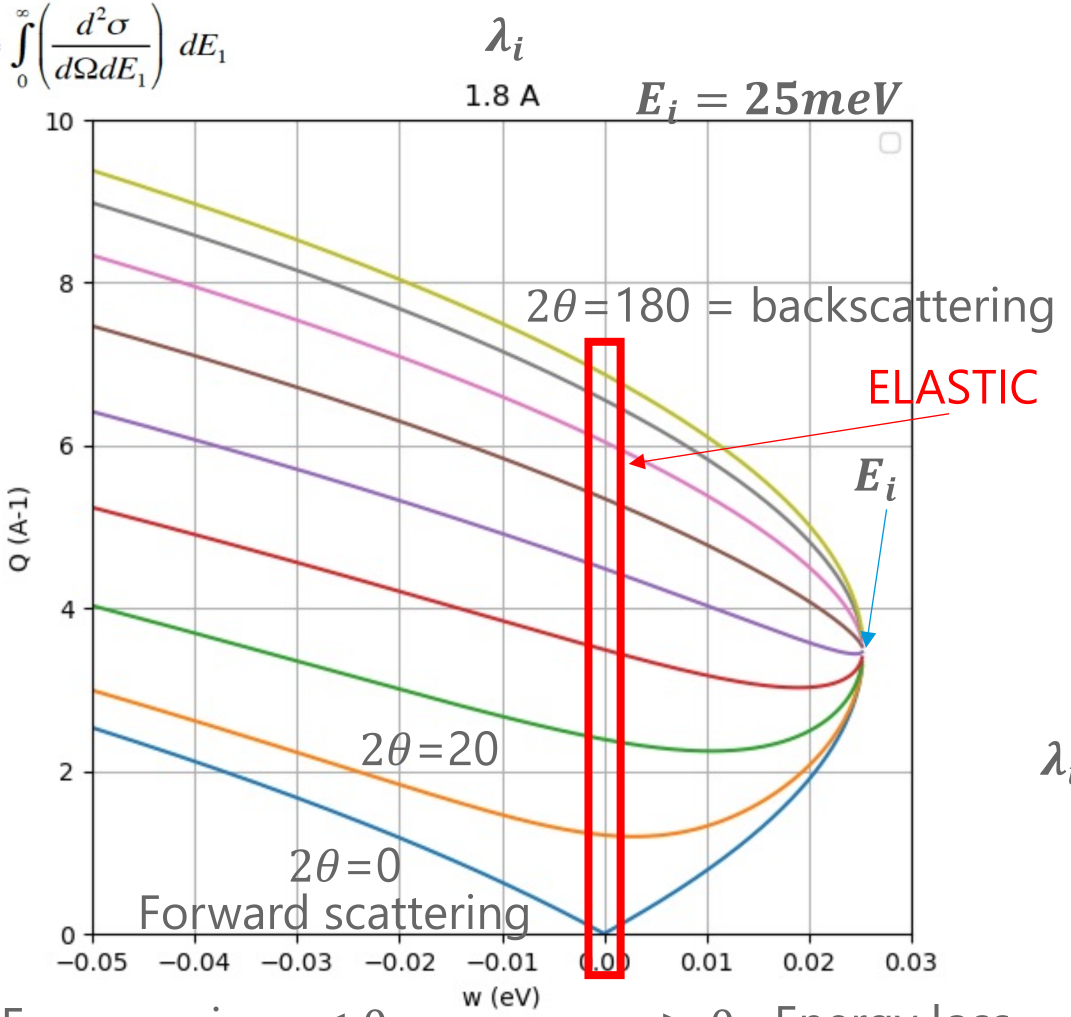
Transmitted beam

Energy gain $\omega < 0$ $\omega > 0$ Energy loss $\omega = E_i - E_f$

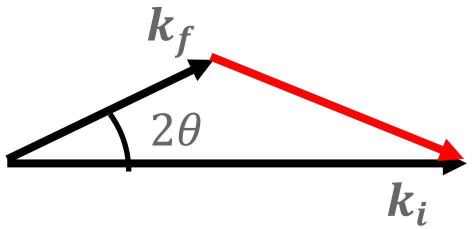
Q-E equation - INELASTIC

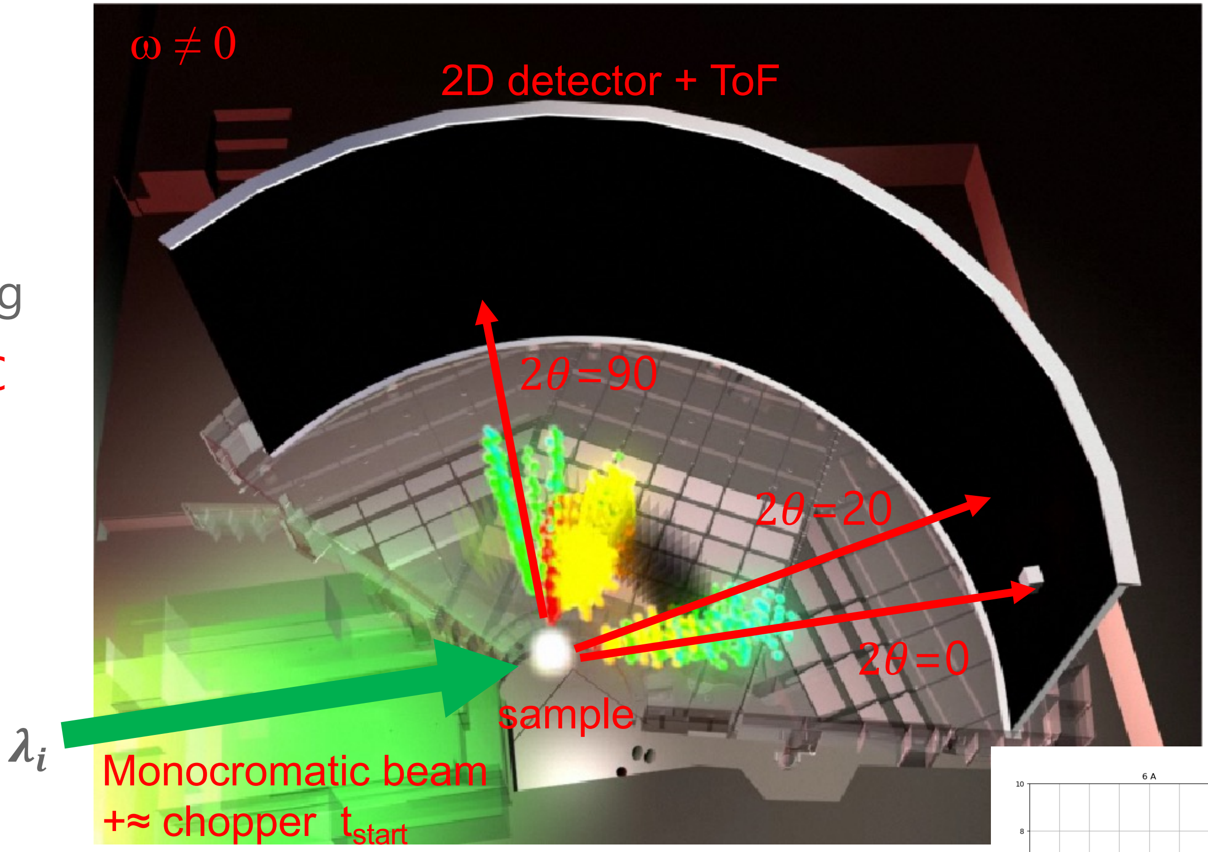
diffraction — spectroscopy

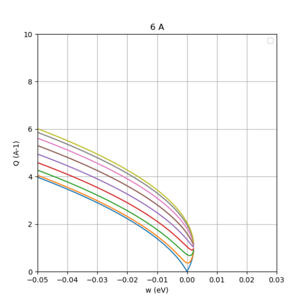
$$\frac{d\sigma}{d\Omega} = \int_0^{\infty} \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$



Energy gain $\omega < 0$ — $\omega > 0$ Energy loss







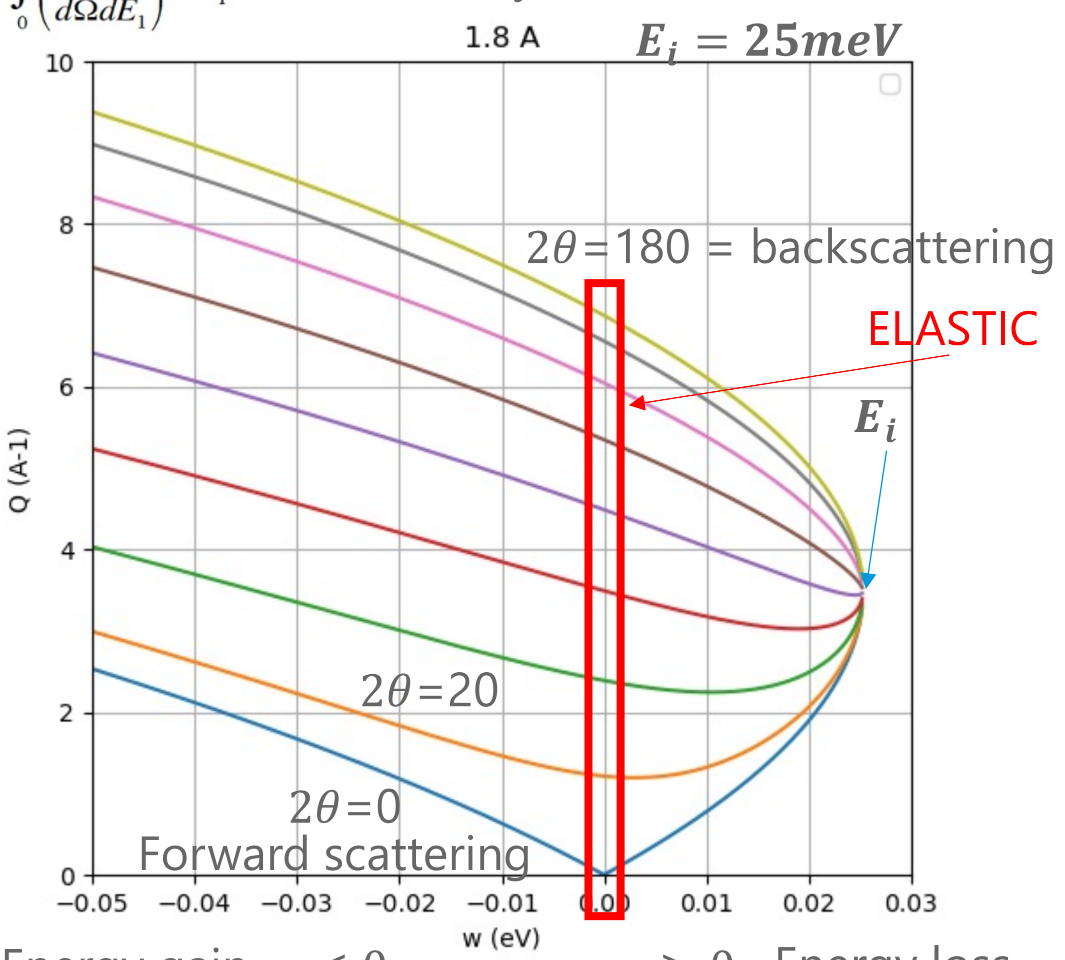
Q-E equation - ELASTIC

diffraction

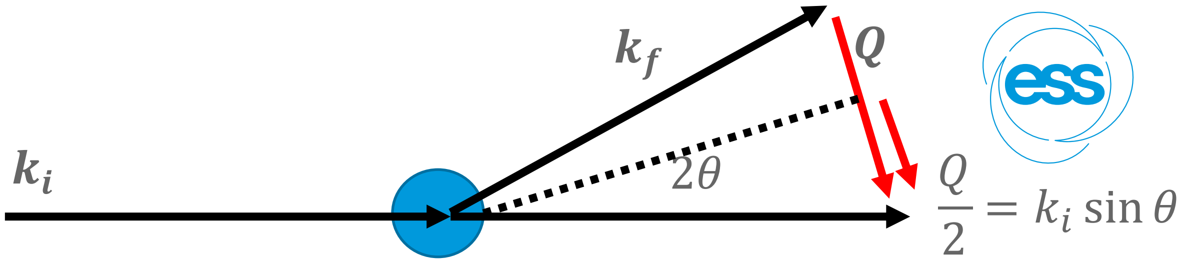
spectroscopy

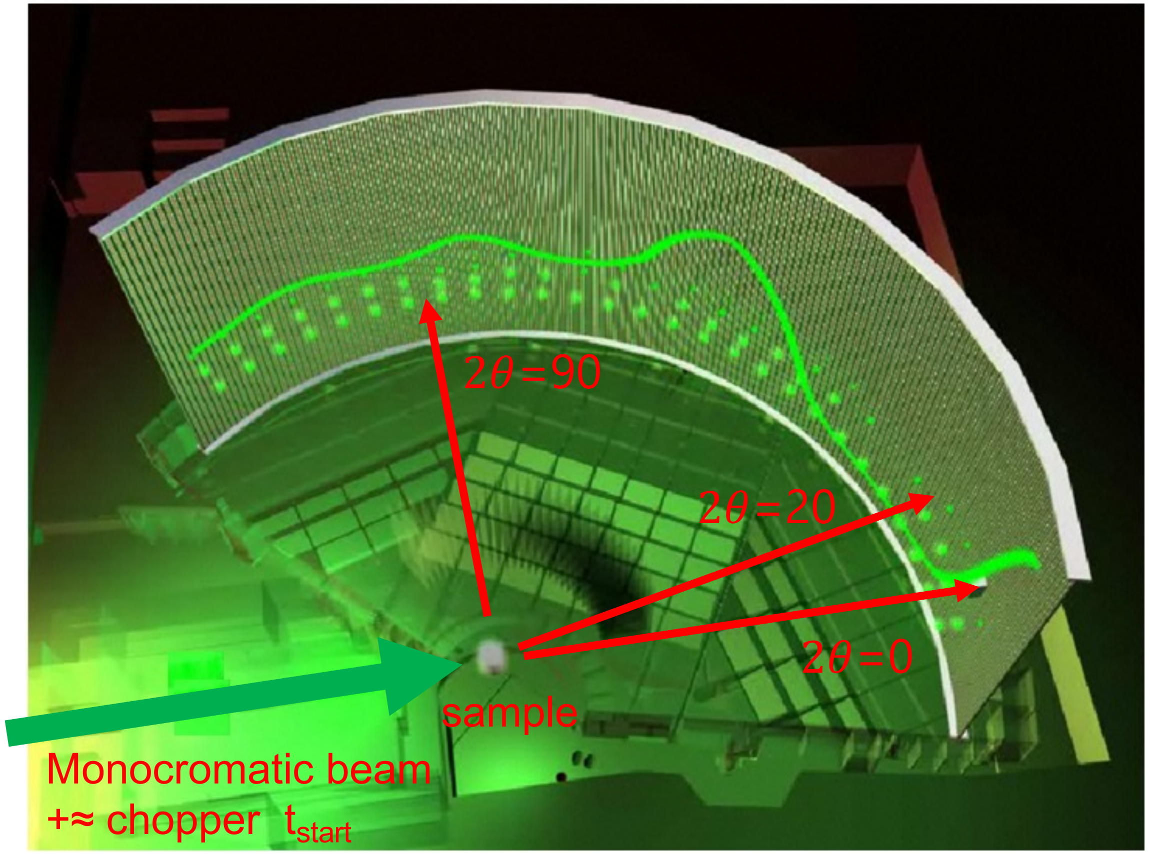
$$\frac{Q}{2} = k_i \sin\theta$$

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$



Energy gain $\omega < 0$ $\omega > 0$ Energy loss





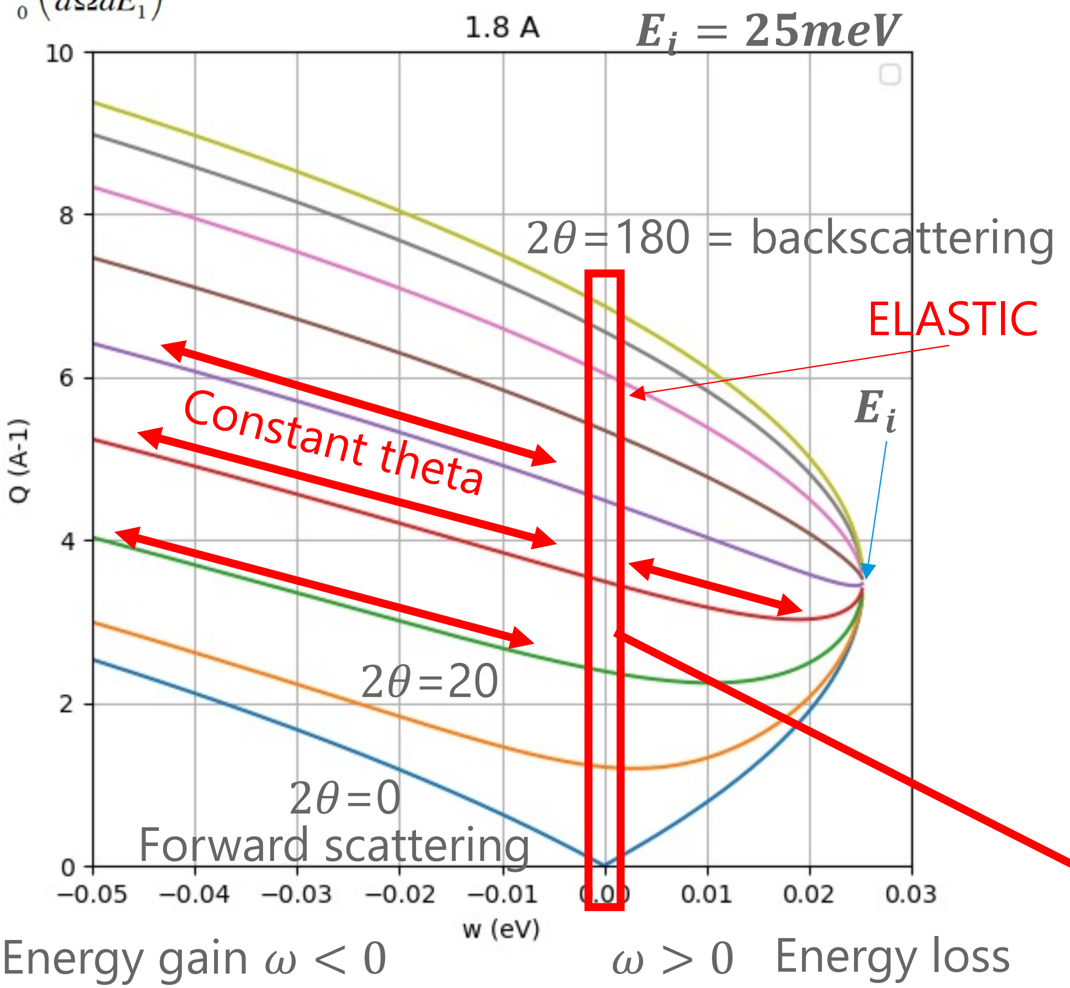
Q-E equation - ELASTIC

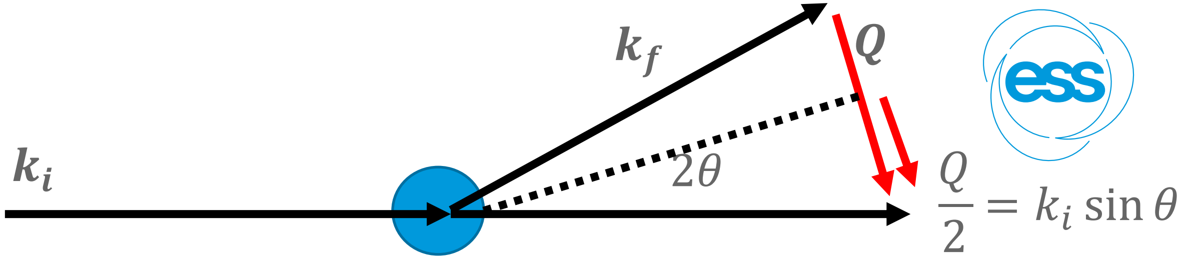
diffraction

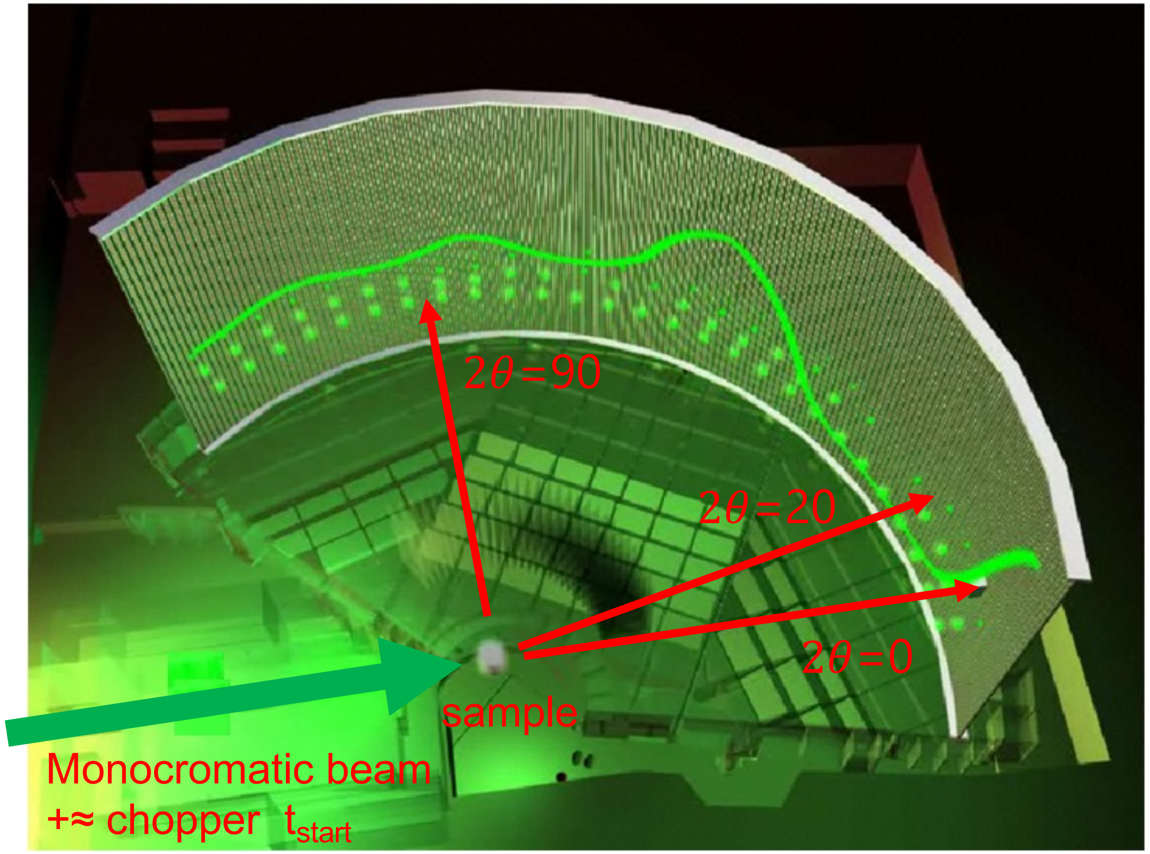
spectroscopy

$$\frac{Q}{2} = k_i \sin\theta$$

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$







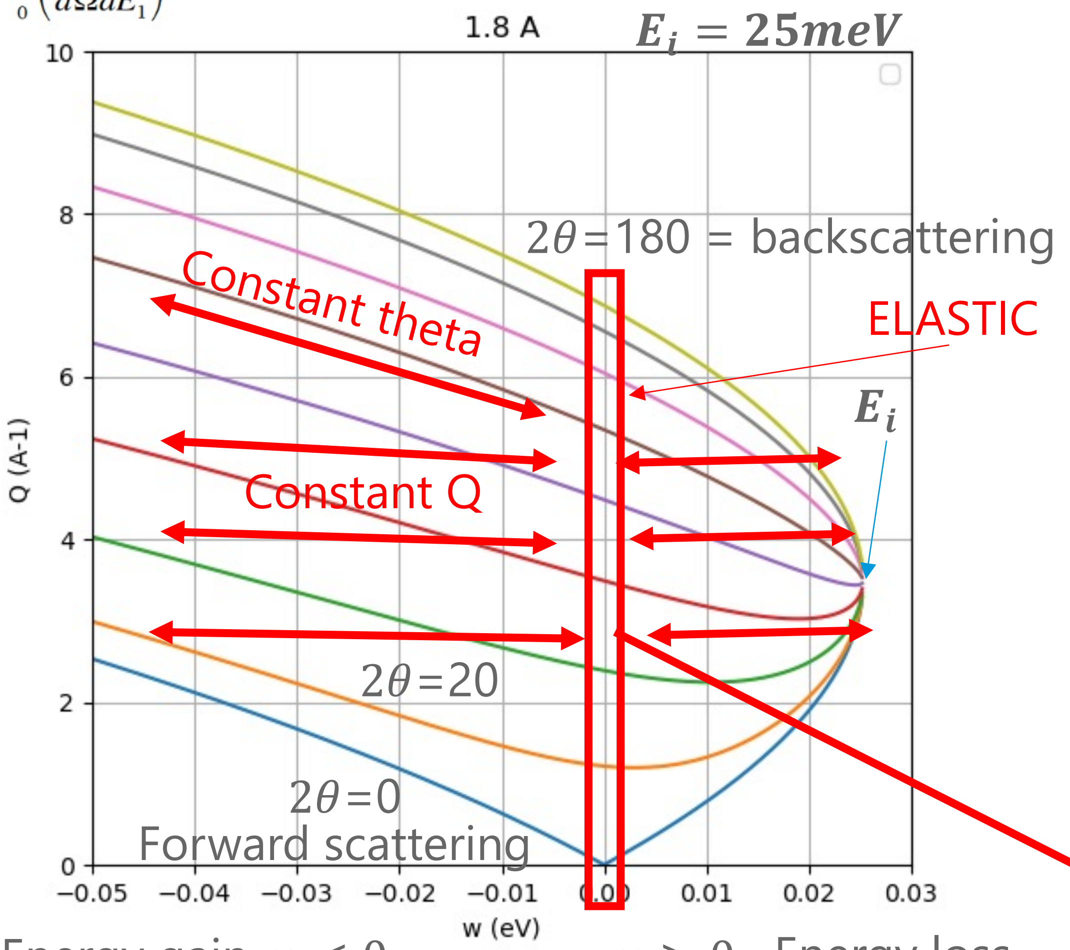
Q-E equation - ELASTIC

diffraction

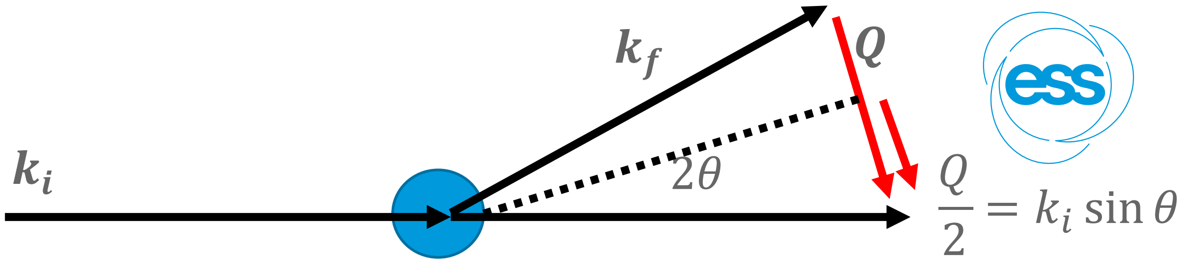
spectroscopy

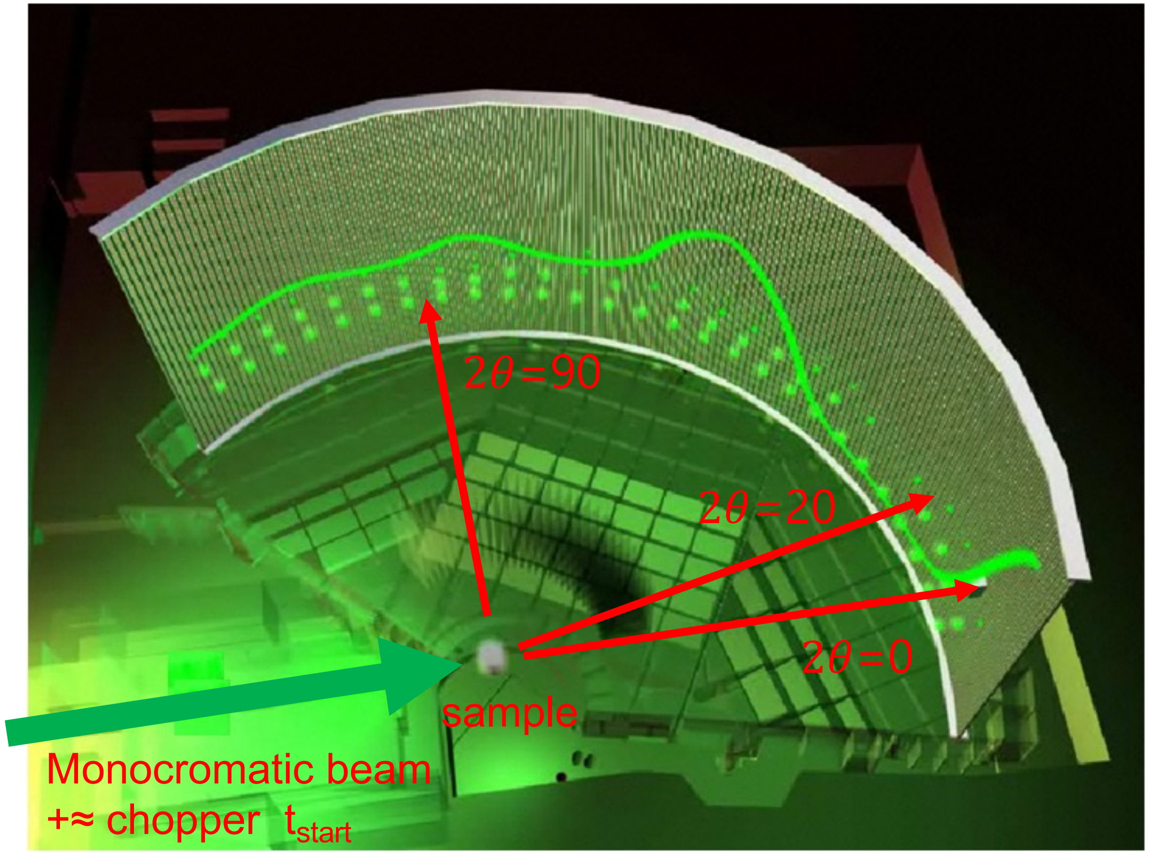
$$\frac{Q}{2} = k_i \sin\theta$$

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$



Energy gain $\omega < 0$ $\omega > 0$ Energy loss

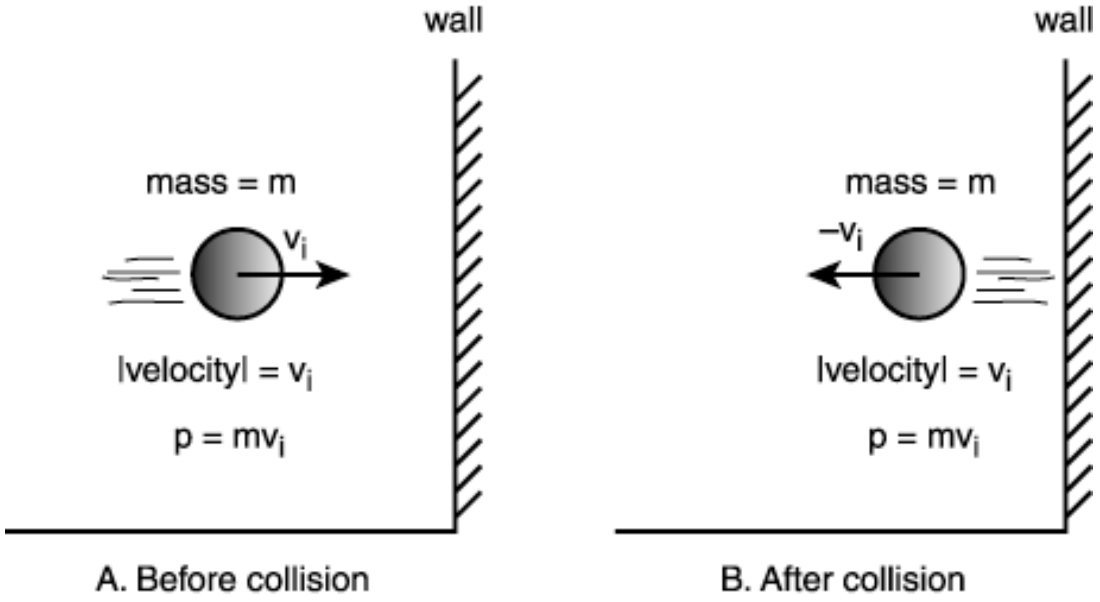




Momentum and Energy transfer

$$|\bar{Q}| = p_{fin} - p_{in} = 2mv$$

$$ELASTIC \rightarrow vin = vout$$



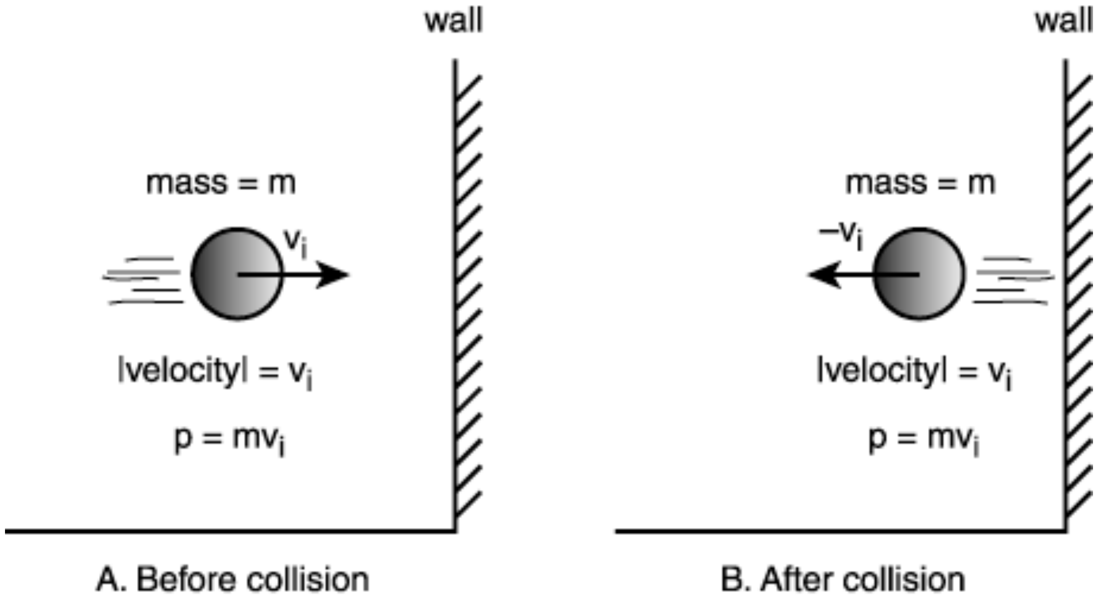
$$2\theta = 180$$

It tells you there is a wall

Momentum and Energy transfer

$|\bar{Q}| = p_{fin} - p_{in} = 2mv$

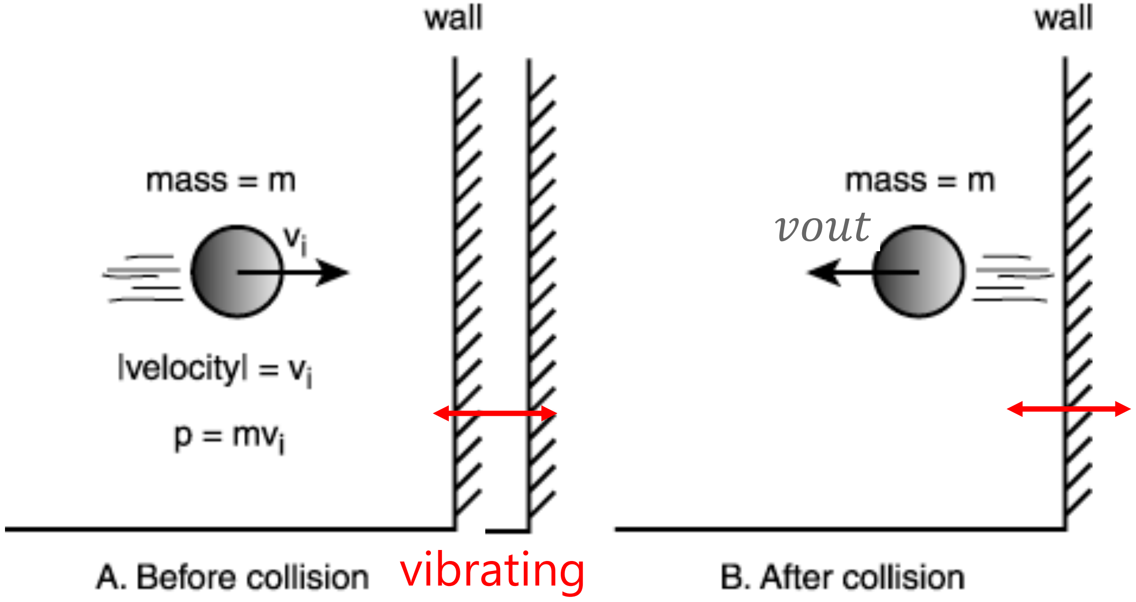
$ELASTIC \rightarrow vin = vout$



$2\theta = 180$

It tells you there is a wall

$INELASTIC \rightarrow vin \neq vout$



$2\theta = 180$

It tells you there is a wall and it is vibrating

INSTRUMENTS

NEUTRON SCATTERING

SPECTROSCOPY
WHERE THEY ARE AND HOW THEY MOVE

DIRECT
Fix Ei
CSPEC

INDIRECT
Fix Ef
BIFROST

SPIN-ECHO
Spin precession

DIFFRACTION
WHERE THEY ARE

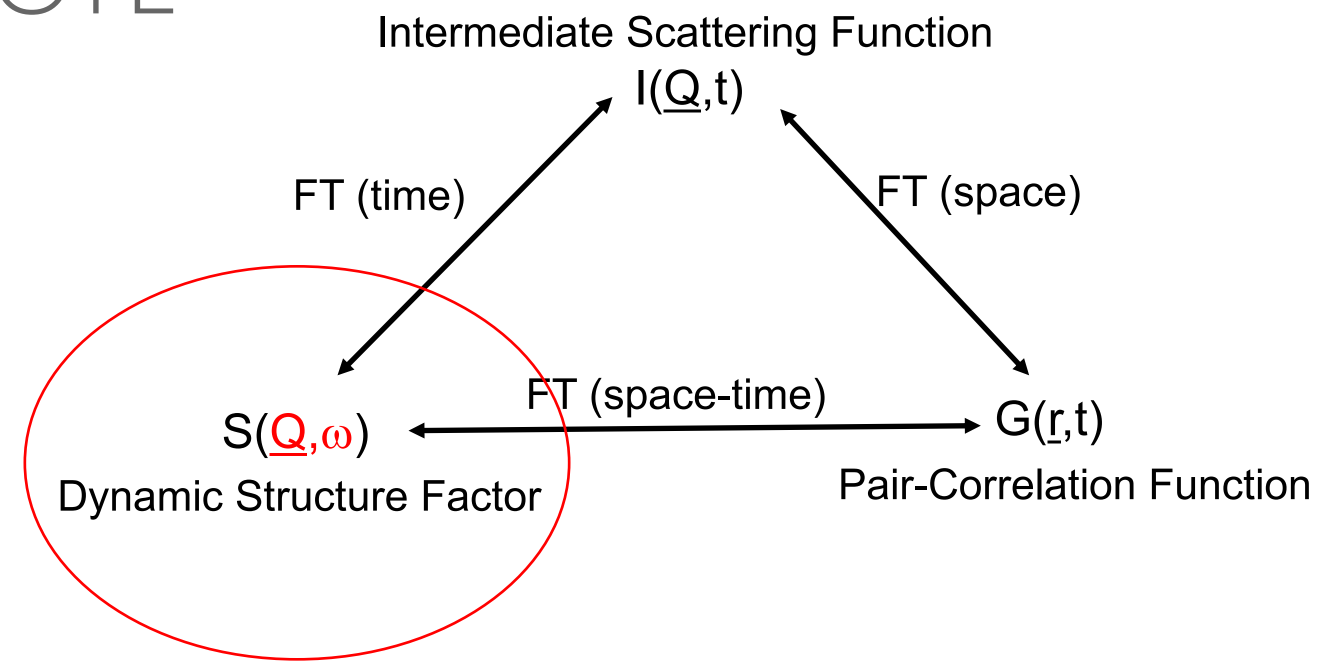
DIFFRACTION
DREAM

LSS

SANS
LOKI

REFL
ESTIA

NOTE



S(Q,ω) is proportional to the measured intensity I(θ,T)

diffraction

spectroscopy

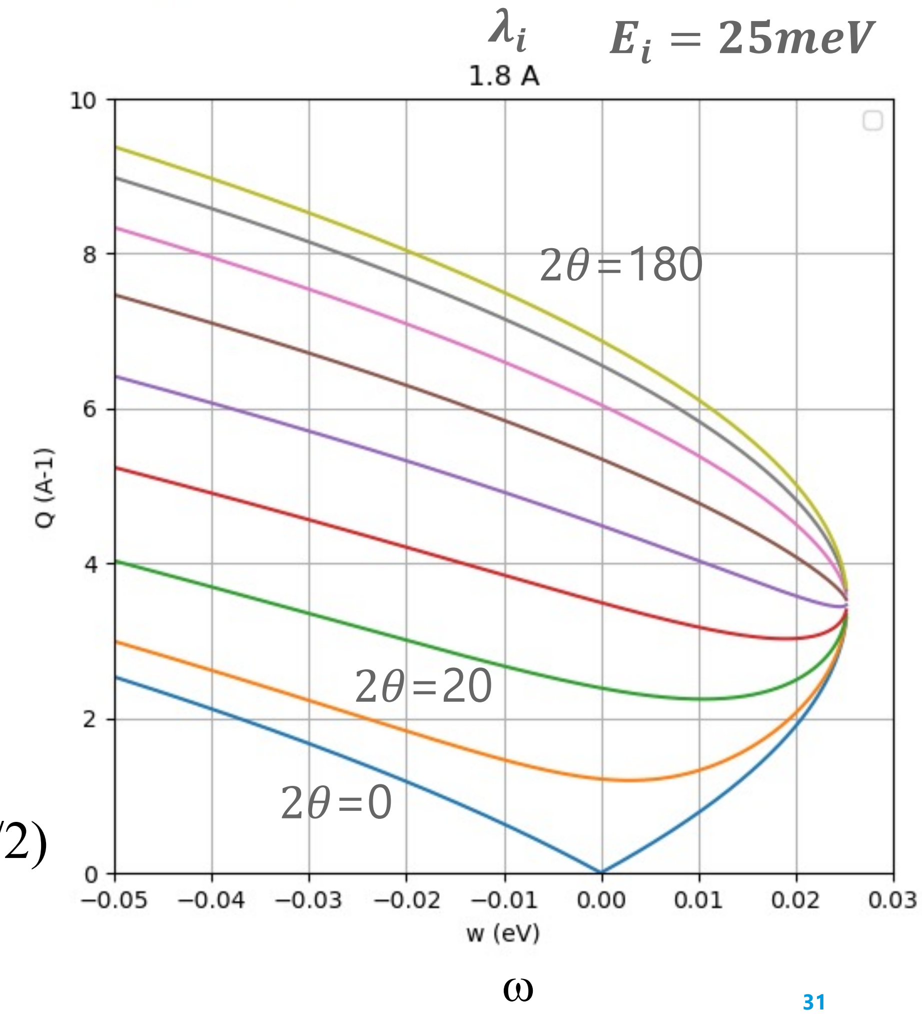
$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$

- Spectroscopy:

$$I(\theta,T) \propto S(Q,\omega) \qquad \text{with } Q = f(\theta, \lambda_i, \lambda_f)\,, \quad \omega = \omega_i - \omega_f$$

- Diffraction:

$$I(\theta,T) \propto \int_{-\infty}^{+\infty} S(Q,\omega)d\omega = S(Q) \qquad \text{with } Q_{el} = (4\pi / \lambda_i)\ \text{sen}(\theta/2)$$



NOTE

A detector has to give us information about the ***single*** neutron (not always!):

"Where" (diffraction) (1D, 2D) (Q)

"Where and when" (spectroscopy)(Q,E)

diffraction

spectroscopy

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1} \right) dE_1$$

Note: ToF is needed in both diffraction and spectroscopy

- Spectroscopy:

  $I(\theta,T) \propto S(\underline{Q},\omega)$ with $Q = f(\theta, \lambda_i, \lambda_f)$, $\omega = \omega_i - \omega_f$

- Diffraction:

  $I(\theta,T) \propto \int_{-\infty}^{+\infty} S(Q,\omega) = S(Q)$ with $Q_{el} = (4\pi / \lambda_i)\, \mathrm{sen}(\theta/2)$

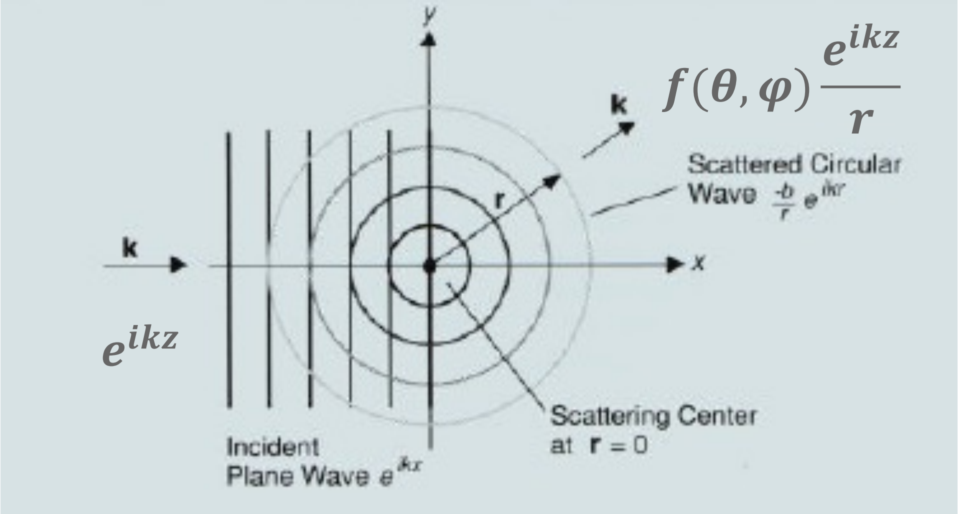
COHERENT VS INCOHERENT

Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$

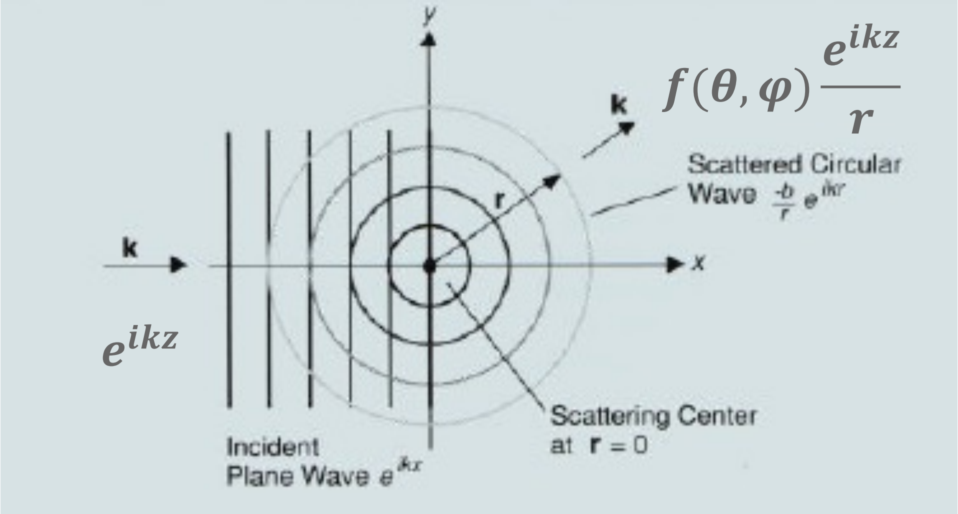
Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$

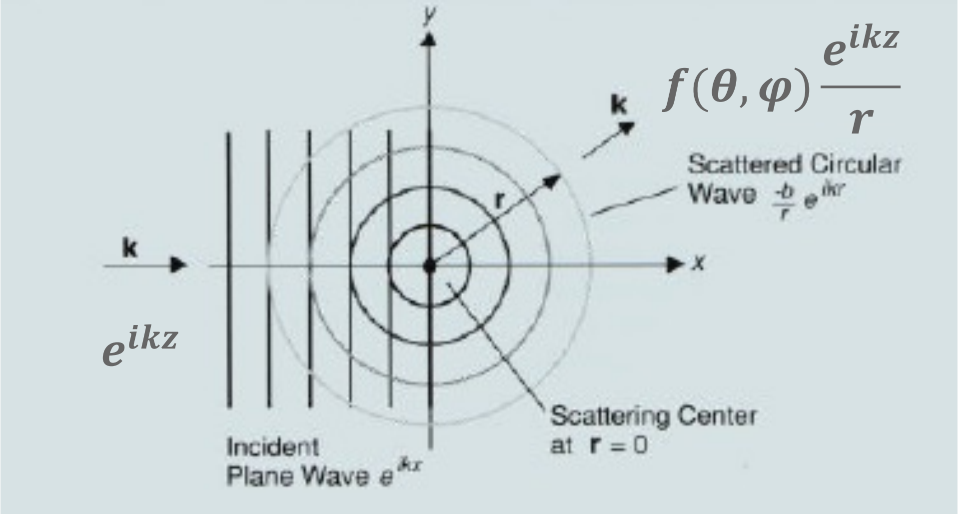


$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

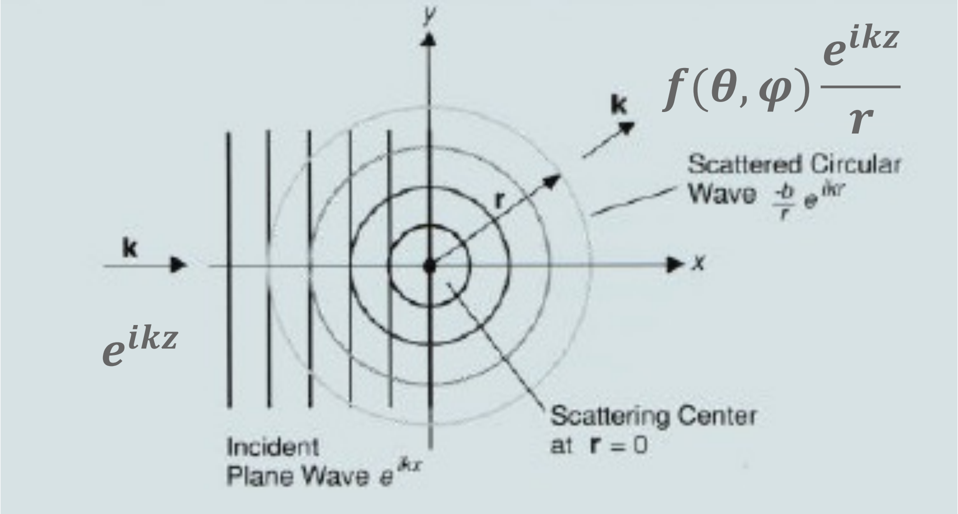
$$\bar{J}(\bar{r},t) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{d\Psi}{d\bar{r}} - \Psi\frac{d\Psi^*}{d\bar{r}}\right)$$ Probability current

$$\bar{J}_i = \frac{\hbar k}{m}\hat{u}_z, \qquad \bar{J}_s = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,\hat{u}_r$$

$$d\sigma = \frac{\frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2 r^2 d\Omega}{\frac{\hbar k}{m}} = |f(\theta,\phi)|^2\,d\Omega \quad \Rightarrow \quad \boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2}$$

Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



Thermal neutron cannot change the internal energy of the nucleus

$E = 25meV \longrightarrow \boldsymbol{k_f} = \boldsymbol{k_i} = \mathbf{k}$

Single neutron to single nucleus scattering IS ELASTIC

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

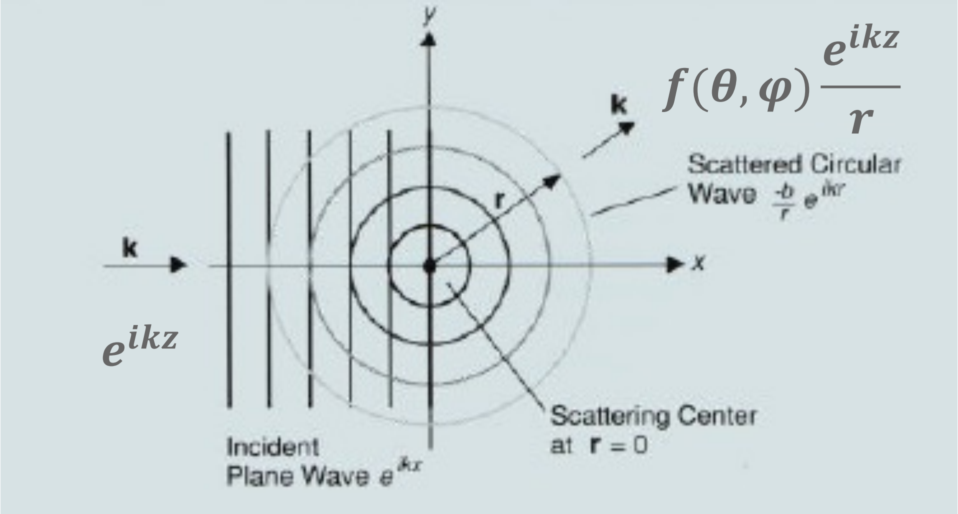
$$\bar{J}(\bar{r},t) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{d\Psi}{d\bar{r}} - \Psi\frac{d\Psi^*}{d\bar{r}}\right)$$ Probability current

$$\bar{J}_i = \frac{\hbar k}{m}\hat{u}_z, \qquad \bar{J}_s = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,\hat{u}_r$$

$$d\sigma = \frac{\frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2 r^2 d\Omega}{\frac{\hbar k}{m}} = |f(\theta,\phi)|^2\,d\Omega \quad \Rightarrow \quad \boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2}$$

Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

$$\bar{J}(\bar{r},t) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{d\Psi}{d\bar{r}} - \Psi\frac{d\Psi^*}{d\bar{r}}\right)$$ Probability current

$$\bar{J}_i = \frac{\hbar k}{m}\hat{u}_z, \qquad \bar{J}_s = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,\hat{u}_r$$

$$d\sigma = \frac{\frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,r^2 d\Omega}{\frac{\hbar k}{m}} = |f(\theta,\phi)|^2\,d\Omega \quad \Rightarrow \quad \boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2}$$

Thermal neutron cannot change the internal energy of the nucleus

$E = 25meV \longrightarrow \boldsymbol{k_f = k_i = \mathbf{k}}$

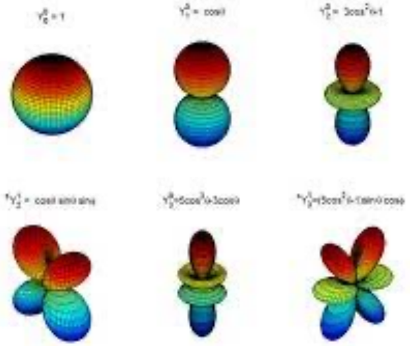
Single neutron to single nucleus scattering IS ELASTIC

$\boldsymbol{f(\theta,\varphi)}$ Means that the scattering depends on the direction! BUT…

$$e^{ikz} = \sum_{l=0}^{\infty} i^l\sqrt{4\pi\,(2l+1)}\,j_l(kr)Y_l^0(\theta)$$

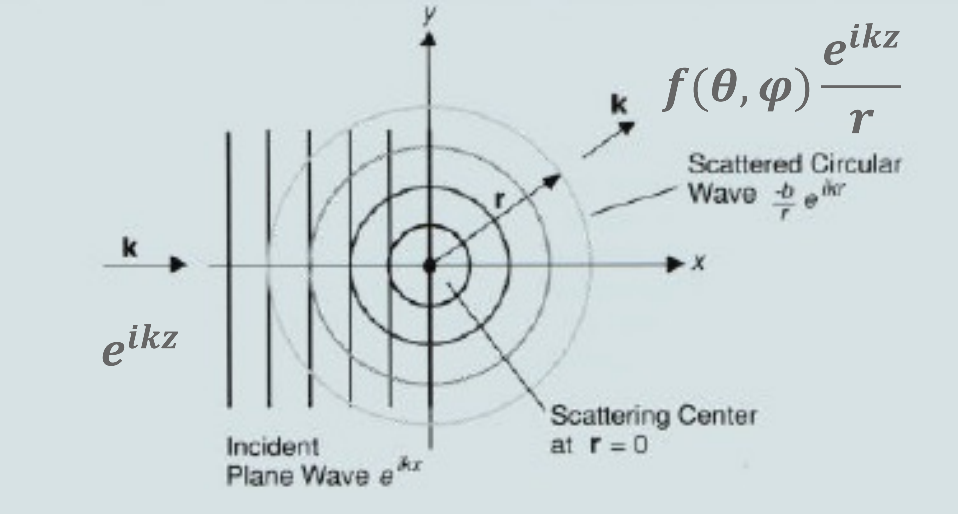
Bessel funct

Spherical harmonics



Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_B T = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



Thermal neutron cannot change the internal energy of the nucleus

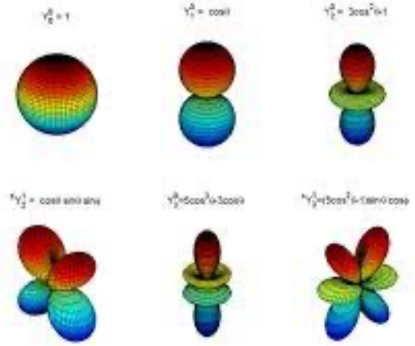
$E = 25meV \longrightarrow \boldsymbol{k_f} = \boldsymbol{k_i} = \mathbf{k}$

Single neutron to single nucleus scattering IS ELASTIC

$f(\theta,\varphi)$ Means that the scattering depends on the direction! BUT…

$$e^{ikz} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi\,(2l+1)}\, j_l(kr) Y_l^0(\theta)$$

Bessel funct — Spherical harmonics



$\lambda = 1.8\text{Å} \approx 10^{-10}m$

Nuclear interaction $10^{-15}m$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

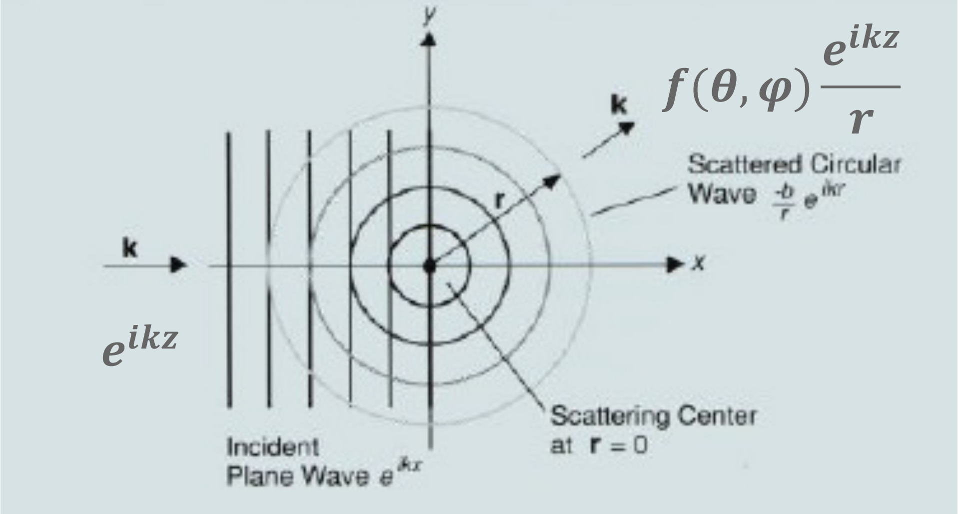
$$\bar{J}(\bar{r},t) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{d\Psi}{d\bar{r}} - \Psi\frac{d\Psi^*}{d\bar{r}}\right)$$ Probability current

$$\bar{J}_i = \frac{\hbar k}{m}\hat{u}_z, \qquad \bar{J}_s = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,\hat{u}_r$$

$$d\sigma = \frac{\frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2 r^2 d\Omega}{\frac{\hbar k}{m}} = |f(\theta,\phi)|^2\,d\Omega \quad \Rightarrow \quad \boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2}$$

Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_BT = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



Thermal neutron cannot change the internal energy of the nucleus

$E = 25meV$ ⟶ $\boldsymbol{k_f = k_i = k}$

Single neutron to single nucleus scattering IS ELASTIC

$\boldsymbol{f(\theta,\varphi)}$ Means that the scattering depends on the direction! BUT…

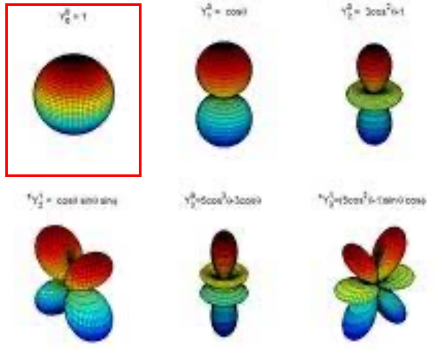
$$e^{ikz} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi\,(2l+1)}\, j_l(kr) Y_l^0(\theta)$$

Bessel funct — Spherical harmonics

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\lambda = 1.8\text{Å} \approx 10^{-10}m$$

Nuclear interaction $10^{-15}m$



$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

Expansion only first term S=0 (spherical wave)

$Y_{l=0}^{0} = cost$

spherical symmetric no dependence on angles

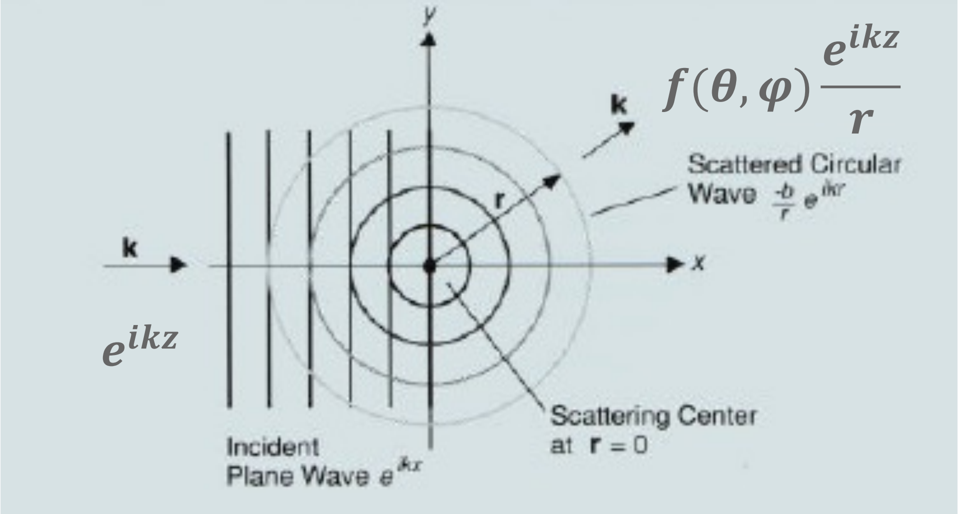
$$\bar{J}(\bar{r},t) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{d\Psi}{d\bar{r}} - \Psi\frac{d\Psi^*}{d\bar{r}}\right)$$ Probability current

$$\bar{J}_i = \frac{\hbar k}{m}\hat{u}_z, \qquad \bar{J}_s = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\,\hat{u}_r$$

$$d\sigma = \frac{\frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2 r^2 d\Omega}{\frac{\hbar k}{m}} = |f(\theta,\phi)|^2\,d\Omega \quad \Rightarrow \quad \frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2$$

Scattering by a SINGLE nucleus

$$E = \frac{1}{2}mv^2 = k_BT = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \lambda = \frac{h}{mv} \qquad k = \frac{2\pi}{\lambda}$$



Thermal neutron cannot change the internal energy of the nucleus

$E = 25meV \longrightarrow \mathbf{k}_f = \mathbf{k}_i = \mathbf{k}$

Single neutron to single nucleus scattering IS ELASTIC

$f(\theta,\varphi)$ Means that the scattering depends on the direction! BUT…

$$e^{ikz} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi\,(2l+1)}\, j_l(kr) Y_l^0(\theta)$$

Bessel funct — Spherical harmonics

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi_{(\bar{r}\to\infty)} \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$ Solution

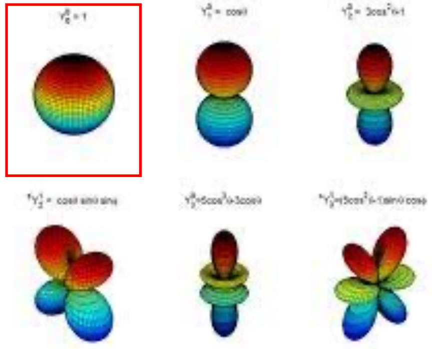
$$\bar{J}(\bar{r},t) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{d\Psi}{d\bar{r}} - \Psi\frac{d\Psi^*}{d\bar{r}}\right)$$

$$\bar{J}_i = \frac{\hbar k}{m}\hat{u}_z, \qquad \bar{J}_s = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2\hat{u}_r$$

$$d\sigma = \frac{\frac{\hbar k}{m}\frac{1}{r^2}|f(\theta,\phi)|^2 r^2 d\Omega}{\frac{\hbar k}{m}} = |f(\theta,\phi)|^2 d\Omega \Rightarrow \frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2$$

$\lambda = 1.8\text{Å} \approx 10^{-10}m$

Nuclear interaction $10^{-15}m$



Expansion only first term S=0 (spherical wave)

$Y_{l=0}^0 = cost$

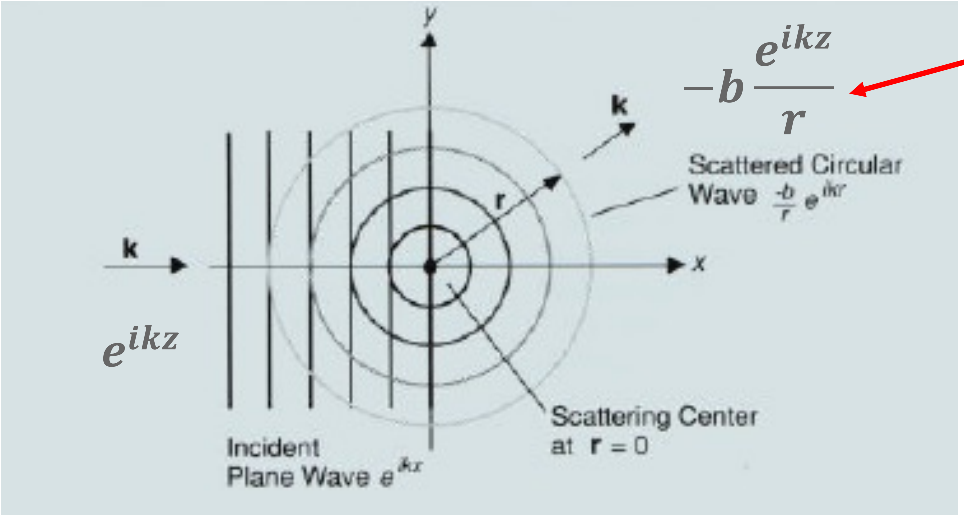
spherical symmetric no dependence on angles

$$\Psi^{scatt.}_{(\bar{r}\to\infty)} \sim e^{ikz} - b\frac{e^{ikr}}{r}$$

$$\frac{d\sigma}{d\Omega} = |b|^2 \longrightarrow \sigma_{tot} = 4\pi|b|^2$$

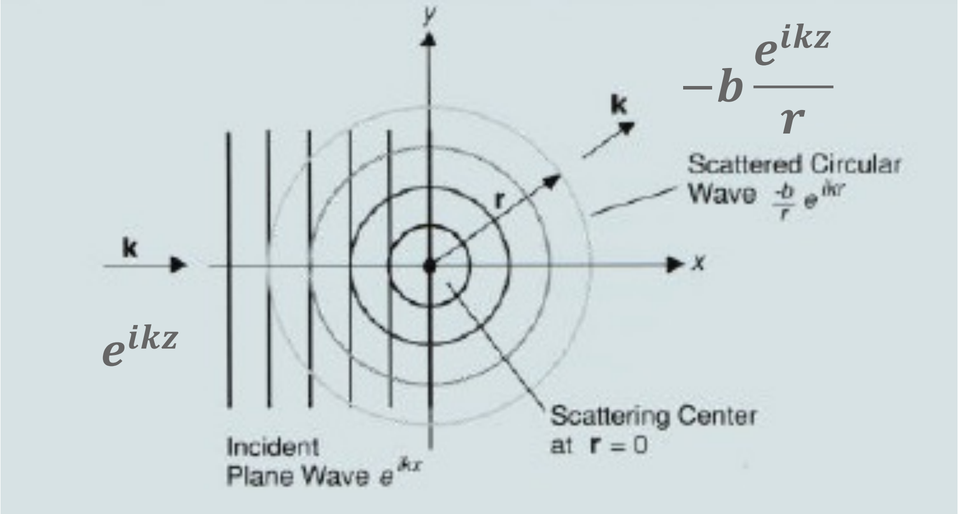
Scattering by a SINGLE nucleus

Fermi pseudo-potential



$$f(\theta,\varphi)\frac{e^{ikz}}{r}$$

Scattering by a SINGLE nucleus   Fermi pseudo-potential



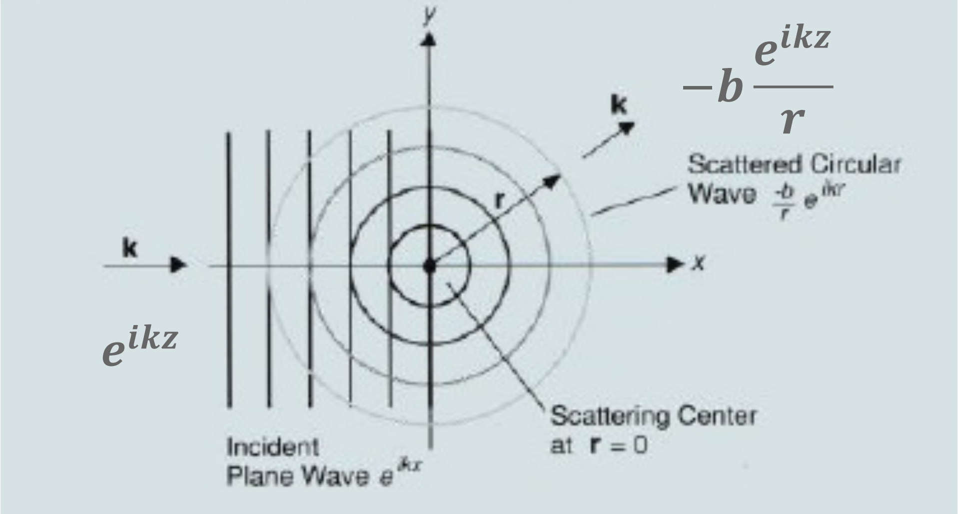
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi^{scatt.}_{(\bar{r}\to\infty)} \sim e^{ikz} - b\frac{e^{ikr}}{r}$$

$$V(\bar{r}) = a\,\delta(\bar{r}) \longrightarrow V(\bar{r}) = \frac{2\pi\hbar^2}{m_n}b\,\delta(\bar{r})$$

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

Scattering by a SINGLE nucleus — Fermi pseudo-potential



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\Psi = E\Psi$$ Schrodinger

$$\Psi^{scatt.}_{(\bar{r}\to\infty)} \sim e^{ikz} - b\frac{e^{ikr}}{r}$$

$$V(\bar{r}) = a\,\delta(\bar{r}) \longrightarrow V(\bar{r}) = \frac{2\pi\hbar^2}{m_n}\,b\,\delta(\bar{r})$$

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

$-b\frac{e^{ikz}}{r} \longrightarrow$ $b > 0 \longrightarrow$ repulsive; $b < 0 \longrightarrow$ attractive

Or scattered wave in phase or out of phase with incoming wave

b is independent from the neutron Energy

b is in general a complex quantity $b = b' - ib''$

$$\sigma_{tot} = 4\pi|b|^2 \qquad \sigma_{abs} = \frac{4\pi}{k} Im\{b\}$$

Scattering by a SINGLE nucleus

b is independent from the neutron Energy

b is in general a complex quantity $b = b' - ib''$ $\sigma_{tot} = 4\pi|b|^2$ $\sigma_{abs} = \frac{4\pi}{k} Im\{b\}$

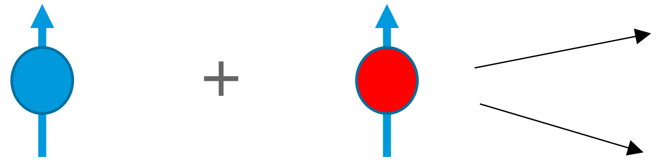
b depends on the neutron-nucleus system spin state (combined spin $I - \frac{1}{2}$ or $I + \frac{1}{2}$),

Scattering by a SINGLE nucleus

b is independent from the neutron Energy

b is in general a complex quantity $b = b' - ib''$ $\sigma_{tot} = 4\pi|b|^2$ $\sigma_{abs} = \frac{4\pi}{k} Im\{b\}$

b depends on the neutron-nucleus system spin state (combined spin $I - \frac{1}{2}$ or $I + \frac{1}{2}$),



Combined spin = 0 b = -47.50 fm

Combined spin = 1 b = 10.85 fm

Neutron
spin S = 1/2

Proton (^1H)
spin I = 1/2

Scattering by a SINGLE nucleus

b is independent from the neutron Energy

b is in general a complex quantity $b = b' - ib''$ $\sigma_{tot} = 4\pi|b|^2$ $\sigma_{abs} = \frac{4\pi}{k} Im\{b\}$

b depends on the neutron-nucleus system spin state (combined spin $I - \frac{1}{2}$ or $I + \frac{1}{2}$),

Neutron
spin S = 1/2

Proton (^{1}H)
spin I = 1/2

Combined spin = 0 b = -47.50 fm

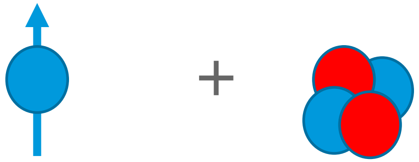
Combined spin = 1 b = 10.85 fm

Neutron
spin S = 1/2

D (^{2}H)
spin I = 1

Combined spin = 1/2 b = 0.98 fm

Combined spin = 3/2 b = 9.53 fm



Neutron
spin S = 1/2

alpha
(^{4}He)
spin I = 0

Combined spin = 1/2 b = 3.26 fm Only one value for b!!!

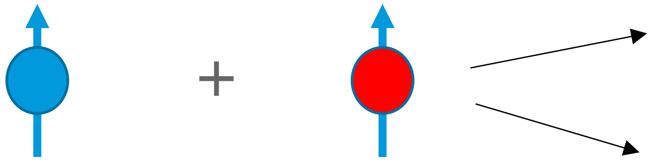
Coherent and Incoherent scattering has a meaning only when we consider a group of nuclei not a single nucleus

Scattering by a SINGLE nucleus

b is independent from the neutron Energy

b is in general a complex quantity $b = b' - ib''$ $\sigma_{tot} = 4\pi|b|^2$ $\sigma_{abs} = \frac{4\pi}{k} Im\{b\}$

b depends on the neutron-nucleus system spin state (combined spin $I - \frac{1}{2}$ or $I + \frac{1}{2}$),

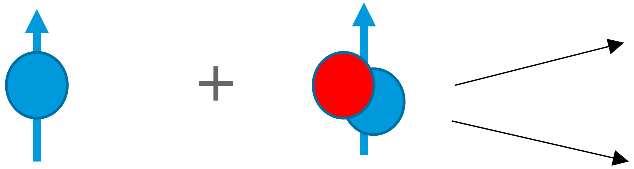


Neutron
spin S = 1/2

Proton (^{1}H)
spin I = 1/2

Combined spin = 0 b = -47.50 fm

Combined spin = 1 b = 10.85 fm

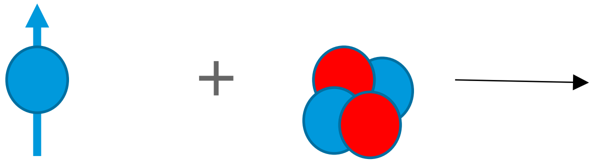


Neutron
spin S = 1/2

D (^{2}H)
spin I = 1

Combined spin = 1/2 b = 0.98 fm

Combined spin = 3/2 b = 9.53 fm



Neutron
spin S = 1/2

alpha
(^{4}He)
spin I = 0

Combined spin = 1/2 b = 3.26 fm Only one value for b!!!

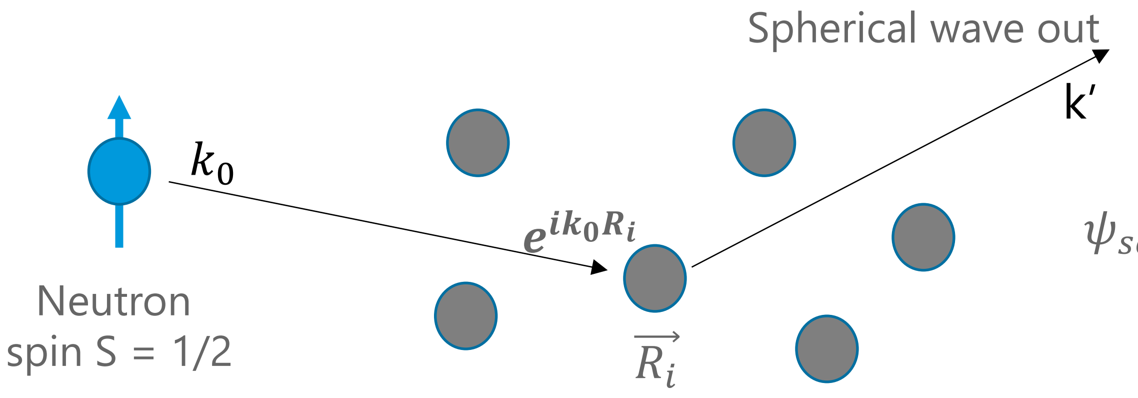
Coherent and Incoherent scattering has a meaning only when we consider a group of nuclei not a single nucleus

Scattering by a MANY nuclei

NOTE: we do the math for no exchange of energy

Scattering by a MANY nuclei Even from the same type !!!

Very simplified math! Just enough to understand the principle.

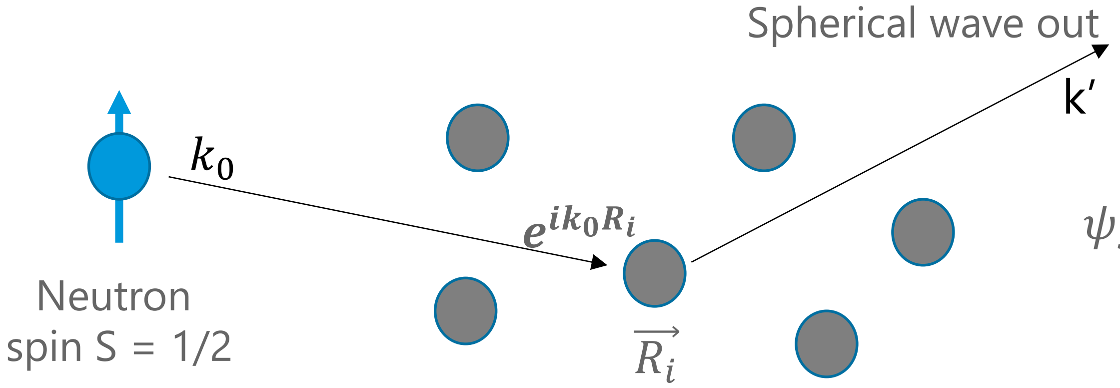


$$\psi_{scatt} = \sum e^{ik_0R_i}\left[\frac{-b_i}{|r-R_i|}e^{ik'(r-R_i)}\right]$$

Many nuclei so now this is a sum !

Scattering by a MANY nuclei Even from the same type !!!

Very simplified math! Just enough to understand the principle.



$$\psi_{scatt} = \sum e^{ik_0R_i}\left[\frac{-b_i}{|r-R_i|}e^{ik'(r-R_i)}\right]$$

Many nuclei so now this is a sum !

Assuming r >> R_i

$$\frac{d\sigma}{d\Omega} \propto |\psi|^2 = \sum_{i,j} b_i b_j e^{i(k_0-k')(R_i-R_j)} = \sum_{i,j} b_i b_j e^{-iQ(R_i-R_j)}$$

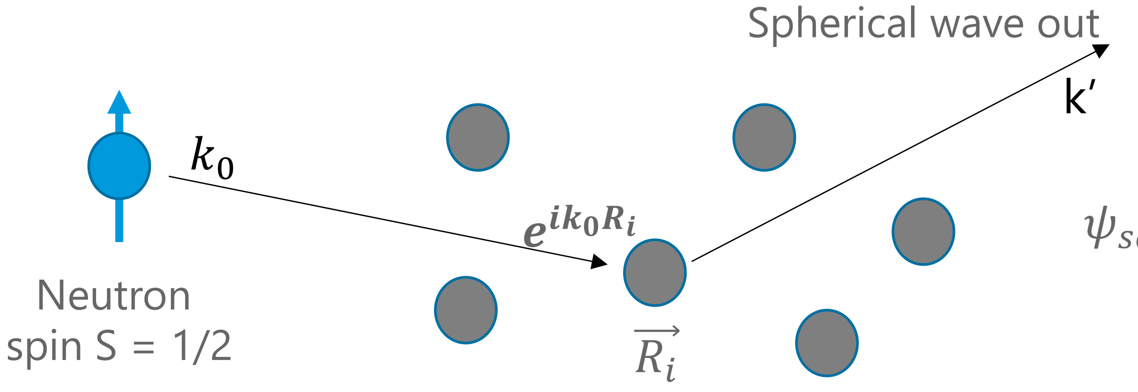
Momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k'} - \boldsymbol{k_0}$$

Note: N = number of atoms in scattering system

Scattering by a MANY nuclei   Even from the same type !!!

Very simplified math! Just enough to understand the principle.



$$\psi_{scatt} = \sum e^{ik_0 R_i}\left[\frac{-b_i}{|r-R_i|} e^{ik'(r-R_i)}\right]$$

Many nuclei so now this is a sum !

Assuming r >> R_i

$$\frac{d\sigma}{d\Omega} \propto |\psi|^2 = \sum_{i,j} b_i b_j e^{i(k_0-k')(R_i-R_j)} = \sum_{i,j} b_i b_j e^{-iQ(R_i-R_j)}$$

Momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k'} - \boldsymbol{k_0}$$

Note: N = number of atoms in scattering system

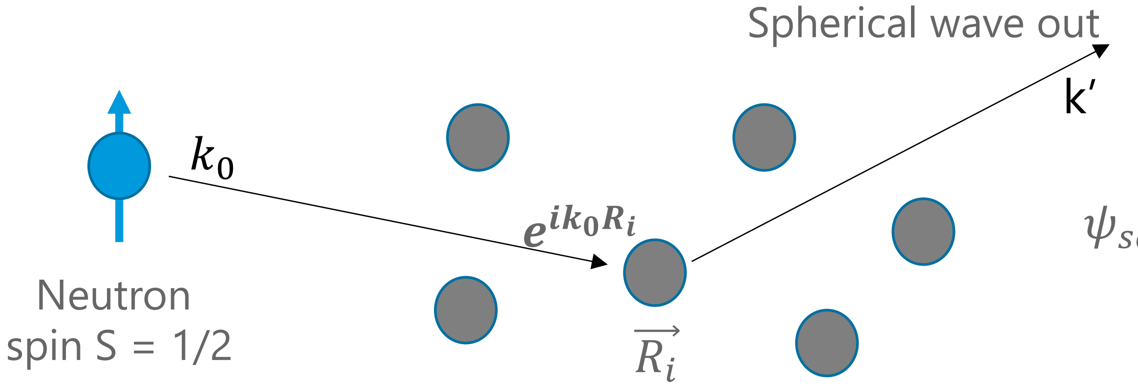
$$= \sum_{i=j} b_i b_j e^{-iQ(R_i-R_j)} + \sum_{i\neq j} b_i b_j e^{-iQ(R_i-R_j)} = \cdots = (\langle b^2\rangle - \langle b\rangle^2)\,N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}$$

$$= \sum_{i=j} b_i b_i e^{-iQ(R_i-R_i)}$$

$$= \sum_{i=j} b_i b_i e^0 = \sum_{i=j} b_i b_i 1$$

Scattering by a MANY nuclei Even from the same type !!!

Very simplified math! Just enough to understand the principle.



$$\psi_{scatt} = \sum e^{ik_0R_i}\left[\frac{-b_i}{|r-R_i|}e^{ik'(r-R_i)}\right]$$

Many nuclei so now this is a sum !

Assuming r >> R_i

$$\frac{d\sigma}{d\Omega} \propto |\psi|^2 = \sum_{i,j} b_i b_j e^{i(k_0-k')(R_i-R_j)} = \sum_{i,j} b_i b_j e^{-iQ(R_i-R_j)}$$

Momentum transfer

$$\boldsymbol{Q} = \boldsymbol{k'} - \boldsymbol{k_0}$$

Note: N = number of atoms in scattering system

$$= \sum_{i=j} b_i b_j e^{-iQ(R_i-R_j)} + \sum_{i\neq j} b_i b_j e^{-iQ(R_i-R_j)} = \cdots = (\langle b^2\rangle - \langle b\rangle^2)\,N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}$$

Incoherent Scattering
Uniform in all directions

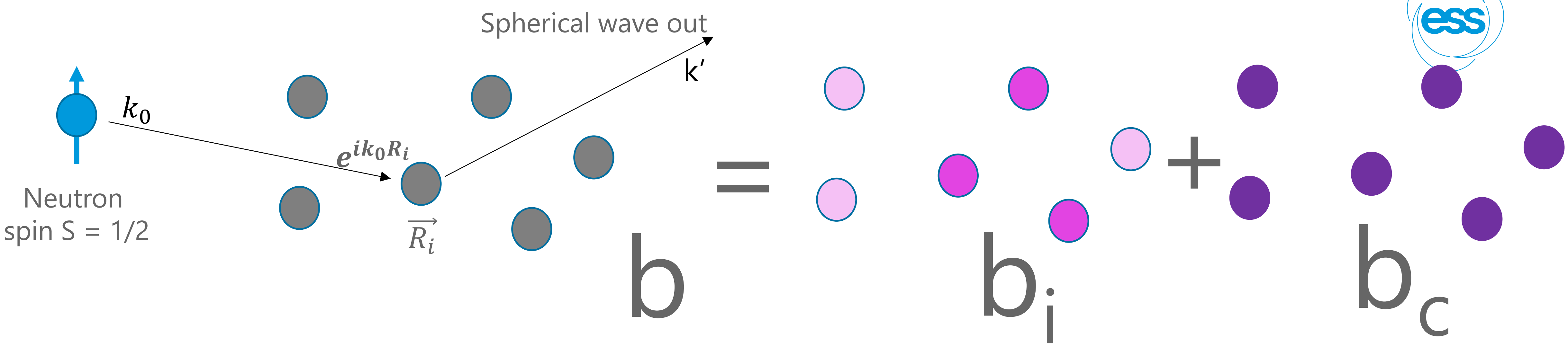
Coherent Scattering
Depends on the direction of Q

$$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2) = 4\pi|b_i|^2 \qquad \sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$$

$$\sigma_{tot} = \sigma_c + \sigma_i = 4\pi|b|^2 \qquad \sigma_{abs} = \frac{4\pi}{k} Im\{b\}$$

Scattering by a MANY nuclei Even from the same type !!!

Very simplified math! Just enough to understand the princip



$$= \sum_{i=j} b_i b_j e^{-iQ(R_i-R_j)} + \sum_{i\neq j} b_i b_j e^{-iQ(R_i-R_j)} = \cdots = (\langle b^2\rangle - \langle b\rangle^2)\, N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}$$

Incoherent Scattering
Uniform in all directions

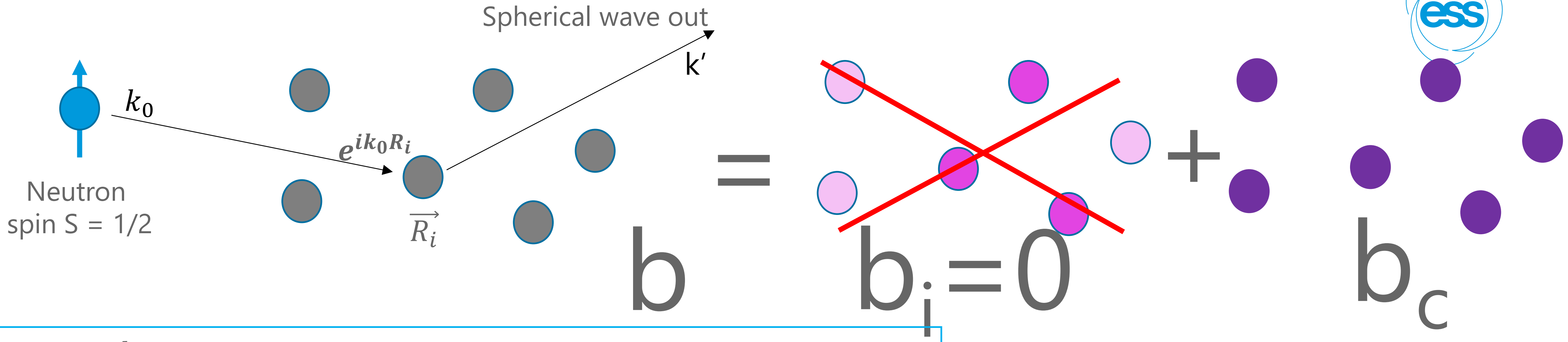
Coherent Scattering
Depends on the direction of Q

$$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2) = 4\pi|b_i|^2 \qquad \sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$$

$$\sigma_{tot} = \sigma_c + \sigma_i = 4\pi|b|^2 \qquad \sigma_{abs} = \frac{4\pi}{k} Im\{b\}$$

Scattering by a MANY nuclei   Even from the same type !!!

Very simplified math! Just enough to understand the princip



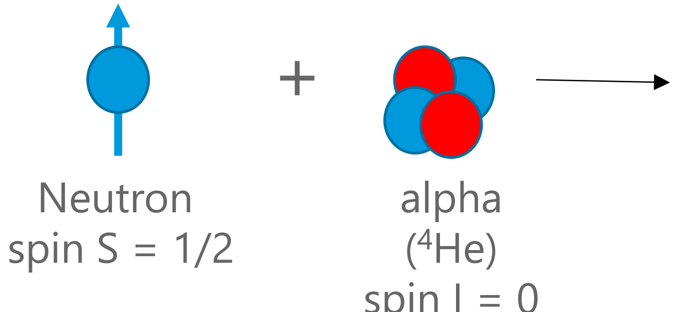
$$\frac{d\sigma}{d\Omega} \propto \left(\langle b^2\rangle - \langle b\rangle^2\right) N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}$$

Incoherent Scattering
Uniform in all directions

Coherent Scattering
Depends on the direction of Q

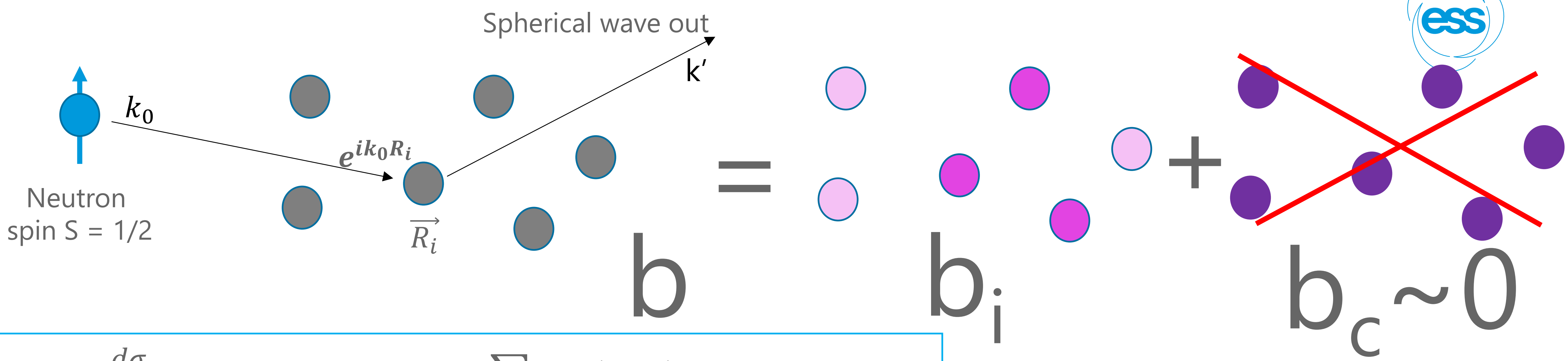
$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2) = 4\pi|b_i|^2$ $\sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$

$\sigma_{tot} = \sigma_c + \sigma_i = 4\pi|b|^2$ $\sigma_{abs} = \frac{4\pi}{k} Im\{b\}$



Combined spin = 1/2   b = 3.26 fm   Only one value for b!!!

Scattering by a MANY nuclei



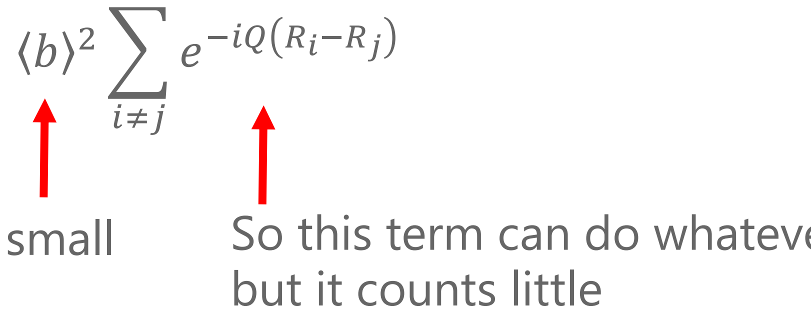
$$\frac{d\sigma}{d\Omega} \propto (\langle b^2\rangle - \langle b\rangle^2)\,N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i - R_j)}$$

Incoherent Scattering
Uniform in all directions

Coherent Scattering
Depends on the direction of Q

$$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2) = 4\pi|b_i|^2 \qquad \sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$$

$$\sigma_{tot} = \sigma_c + \sigma_i = 4\pi|b|^2 \qquad \sigma_{abs} = \frac{4\pi}{k} Im\{b\}$$



b_c

V	23			−0.3824(12)	
	50	6(+)	0.250	7.6(6)	
	51	7/2(−)	99.750	−0.402(2)	6.35(4)

VANADIUM

$$\frac{d\sigma}{d\Omega} \propto \left(\langle b^2\rangle - \langle b\rangle^2\right) N + \langle b\rangle^2 \sum_{i \neq j} e^{-iQ(R_i - R_j)}$$

Incoherent Scattering
Uniform in all directions

Coherent Scattering
Depends on the direction of Q

$$\sigma_i = 4\pi\left(\langle b^2\rangle - \langle b\rangle^2\right) = 4\pi|b_i|^2 \qquad \sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$$

$$\sigma_{tot} = \sigma_c + \sigma_i = 4\pi|b|^2 \qquad \sigma_{abs} = \frac{4\pi}{k} Im\{b\}$$

Sears

	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
H	1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
		3	1/2(+)	(12.32 a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0
He	2				3.26(3)		1.34(2)	0	1.34(2)	0.00747(1)
		3	1/2(+)	0.00014	5.74(7) −1.483(2)i	−2.5(6) +2.568(3)i	4.42(10)	1.6(4)	6.0(4)	5333.(7.)
		4	0(+)	99.99986	3.26(3)	0	1.34(2)	0	1.34(2)	0
Li	3				−1.90(2)		0.454(10)	0.92(3)	1.37(3)	70.5(3)
		6	1(+)	7.5	2.00(11) −0.261(1)i	−1.89(10) +0.26(1)i	0.51(5)	0.46(5)	0.97(7)	940.(4.)
		7	3/2(−)	92.5	−2.22(2)	−2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
Be	4	9	3/2(−)	100	7.79(1)	0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076(8)
B	5				5.30(4) −0.213(2)i		3.54(5)	1.70(12)	5.24(11)	767.(8.)
		10	3(+)	20.0	−0.1(3) −1.066(3)i	−4.7(3) +1.231(3)i	0.144(8)	3.0(4)	3.1(4)	3835.(9.)
		11	3/2(−)	80.0	6.65(4)	−1.3(2)	5.56(7)	0.21(7)	5.77(10)	0.0055(33)

Equivalently instead of b_i

$$I + \frac{1}{2} \quad \text{combined spin} \quad I - \frac{1}{2}$$

$$g_+ = \frac{I+1}{2I+1} \qquad g_- = \frac{I}{2I+1}$$

$$b_c = g_+ b_+ + g_- b_-$$

$$b_i{}^2 = g_+ g_- (b_+ - b_-)^2$$

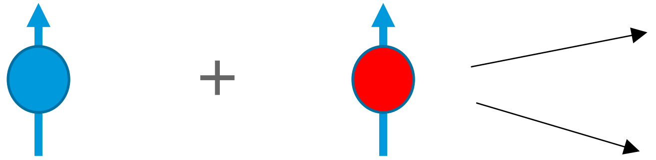
$$\frac{d\sigma}{d\Omega} \propto (\langle b^2\rangle - \langle b\rangle^2)\, N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i - R_j)}$$

Incoherent Scattering
Uniform in all directions

Coherent Scattering
Depends on the direction of Q

$$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2) = 4\pi|b_i|^2 \qquad \sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$$

$$\sigma_{tot} = \sigma_c + \sigma_i = 4\pi|b|^2 \qquad \sigma_{abs} = \frac{4\pi}{k} Im\{b\}$$



Combined spin = 0 b = -47.50 fm

Combined spin = 1 b = 10.85 fm

Neutron
spin S = 1/2

Proton ([1]H)
spin I = 1/2

$$g_+ = 3/4 \qquad g_- = 1/4$$

$$b_c = \frac{3}{4}10.8 - \frac{1}{4}47.4 = -3.7fm$$

$$b_i = \sqrt{\frac{3}{4}\frac{1}{4}(10.8 + 47.4)^2} = 25.2fm$$

ILL blue book

ZSymbA	p or $T_{1/2}$	I	b_c	b_+	b_-	c	σcoh	σ inc	σscatt	σabs
0-N-1	10.3 MIN	1/2	-37.0(6)	0	-37.0(6)		43.01(2)		43.01(2)	0
1-H			-3.7409(11)				1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
1-H-1	99.985	1/2	-3.7423(12)	10.817(5)	-47.420(14)	+/-	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)

Sears

	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
H	1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
		3	1/2(+)	(12.32 a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0

ILL blue book

ZSymbA	p or $T_{1/2}$	I	b_c	b_+	b_-	c	σ_{coh}	σ_{inc}	σ_{scatt}	σ_{abs}
0-N-1	**10.3 MIN**	**1/2**	**-37.0(6)**	**0**	**-37.0(6)**		**43.01(2)**		**43.01(2)**	**0**
1-H			**-3.7409(11)**				**1.7568(10)**	**80.26(6)**	**82.02(6)**	**0.3326(7)**
1-H-1	99.985	1/2	-3.7423(12)	10.817(5)	-47.420(14)	+/-	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
1-H-2	0.0149	1	6.674(6)	9.53(3)	0.975(60)		5.592(7)	2.05(3)	7.64(3)	0.000519(7)
1-H-3	12.26 Y	1/2	4.792(27)	4.18(15)	6.56(37)		2.89(3)	0.14(4)	3.03(5)	< 6.0E-6
2-He			**3.26(3)**				**1.34(2)**	**0**	**1.34(2)**	**0.00747(1)**
2-He-3	0.00013	1/2	5.74(7)	4.374(70)	9.835(77)	E	4.42(10)	1.532(20)	6.0(4)	5333.0(7.0)
2-He-4	0.99987	0	3.26(3)				1.34(2)	0	1.34(2)	0
3-Li			**-1.90(3)**				**0.454(10)**	**0.92(3)**	**1.37(3)**	**70.5(3)**
3-Li-6	7.5	1	2.0(1)	0.67(14)	4.67(17)	+/-	0.51(5)	0.46(5)	0.97(7)	940.0(4.0)
3-Li-7	92.5	3/2	-2.22(2)	-4.15(6)	1.00(8)	+/-	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
4-Be-9	**100**	**3/2**	**7.79(1)**				**7.63(2)**	**0.0018(9)**	**7.63(2)**	**0.0076(8)**
5-B			**5.30(4)**				**3.54(5)**	**1.70(12)**	**5.24(11)**	**767.0(8.0)**
5-B-10	19.4	3	-0.2(4)	-4.2(4)	5.2(4)		0.144(6)	3.0(4)	3.1(4)	3835.0(9.0)
5-B-11	80.2	3/2	6.65(4)	5.6(3)	8.3(3)		5.56(7)	0.21(7)	5.77(10)	0.0055(33)
6-C			**6.6484(13)**				**5.551(2)**	**0.001(4)**	**5.551(3)**	**0.00350(7)**
6-C-12	98.89	0	6.6535(14)				5.559(3)	0	5.559(3)	0.00353(7)
6-C-13	1.11	1/2	6.19(9)	5.6(5)	6.2(5)	+/-	4.81(14)	0.034(11)	4.84(14)	0.00137(4)
7-N			**9.36(2)**				**11.01(5)**	**0.50(12)**	**11.51(11)**	**1.90(3)**
7-N-14	99.635	1	9.37(2)	10.7(2)	6.2(3)		11.03(5)	0.50(12)	11.53(11)	1.91(3)
7-N-15	0.365	1/2	6.44(3)	6.77(10)	6.21(10)		5.21(5)	0.00005(10)	5.21(5)	0.000024(8)
8-O			**5.805(4)**				**4.232(6)**	**0.000(8)**	**4.232(6)**	**0.00019(2)**
8-O-16	99.75	0	5.805(5)				4.232(6)	0	4.232(6)	0.00010(2)
8-O-17	0.039	5/2	5.6(5)	5.52(20)	5.17(20)		4.20(22)	0.004(3)	4.20(22	0.236(10)
8-O-18	0.208	0	5.84(7)				4.29(10)	0	4.29(10)	0.00016(1)
9-F-19	**100**	**1/2**	**5.654(12)**	**5.632(10)**	**5.767(10)**	**+/-**	**4.017(14)**	**0.0008(2)**	**4.018(14)**	**0.0096(5)**
10-Ne			**4.566(6)**				**2.620(7)**	**0.008(9)**	**2.628(6)**	**0.039(4)**
10-Ne-20	90.5	0	4.631(6)				2.695(7)	0	2.695(7)	0.036(4)
10-Ne-21	0.27	3/2	6.66(19)				5.6(3)	0.05(2)	5.7(3)	0.67(11)
10-Ne-22	9.2	0	3.87(1)				1.88(1)	0	1.88(1)	0.046(6)

Sears

Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
	1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
	2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
	3	1/2(+)	(12.32 a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0
2				3.26(3)		1.34(2)	0	1.34(2)	0.00747(1)
	3	1/2(+)	0.00014	5.74(7)	−2.5(6)	4.42(10)	1.6(4)	6.0(4)	5333.(7.)
				−1.483(2)i	+2.568(3)i				
	4	0(+)	99.99986	3.26(3)	0	1.34(2)	0	1.34(2)	0
3				−1.90(2)		0.454(10)	0.92(3)	1.37(3)	70.5(3)
	6	1(+)	7.5	2.00(11)	−1.89(10)	0.51(5)	0.46(5)	0.97(7)	940.(4.)
				−0.261(1)i	+0.26(1)i				
	7	3/2(−)	92.5	−2.22(2)	−2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
4	9	3/2(−)	100	7.79(1)	0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076(8)
5				5.30(4)		3.54(5)	1.70(12)	5.24(11)	767.(8.)
				−0.213(2)i					
	10	3(+)	20.0	−0.1(3)	−4.7(3)	0.144(8)	3.0(4)	3.1(4)	3835.(9.)
				−1.066(3)i	+1.231(3)i				
	11	3/2(−)	80.0	6.65(4)	−1.3(2)	5.56(7)	0.21(7)	5.77(10)	0.0055(33)

Scattering by a MANY nuclei: NOTE

$$\frac{d\sigma}{d\Omega} \propto \underbrace{\left(\langle b^2\rangle - \langle b\rangle^2\right) N}_{\text{Incoherent Scattering}} + \underbrace{\langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i - R_j)}}_{\text{Coherent Scattering}}$$

Incoherent Scattering b_i

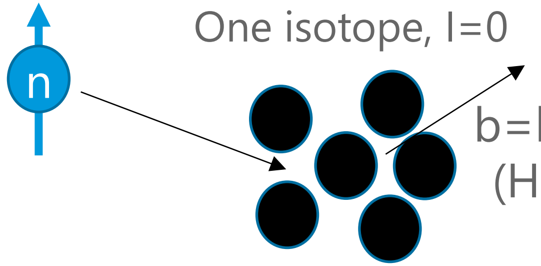
Coherent Scattering b_c

Scattering by a MANY nuclei: NOTE

$$\frac{d\sigma}{d\Omega} \propto \left(\langle b^2\rangle - \langle b\rangle^2\right) N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}$$

Incoherent Scattering — Coherent Scattering

One isotope, I=0



$b=b_+=b_-=b_c$
(Helium-4)

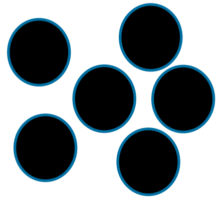
=

b_i

X

+

b_c



Only one spin-spin interaction possible

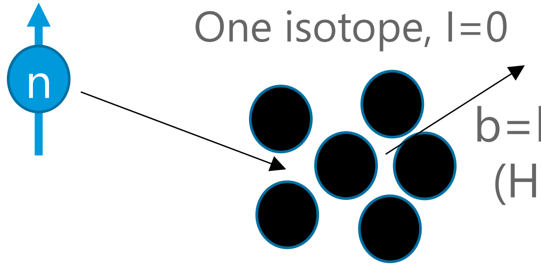
Scattering by a MANY nuclei: NOTE

$$\frac{d\sigma}{d\Omega} \propto \left(\langle b^2\rangle - \langle b\rangle^2\right) N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i - R_j)}$$

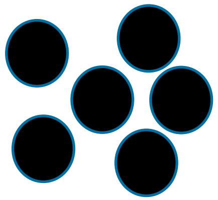
Incoherent Scattering | Coherent Scattering

b_i | b_c

One isotope, I=0

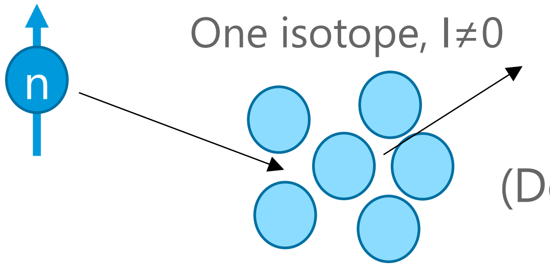


$b=b_+=b_-=b_c$ (Helium-4) = X +

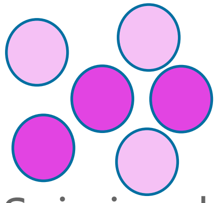


Only one spin-spin interaction possible

One isotope, I≠0

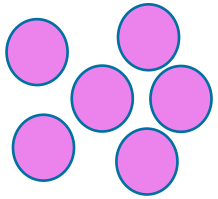


$b_+ \neq b_-$ (Deuterium) =



Spin incoh

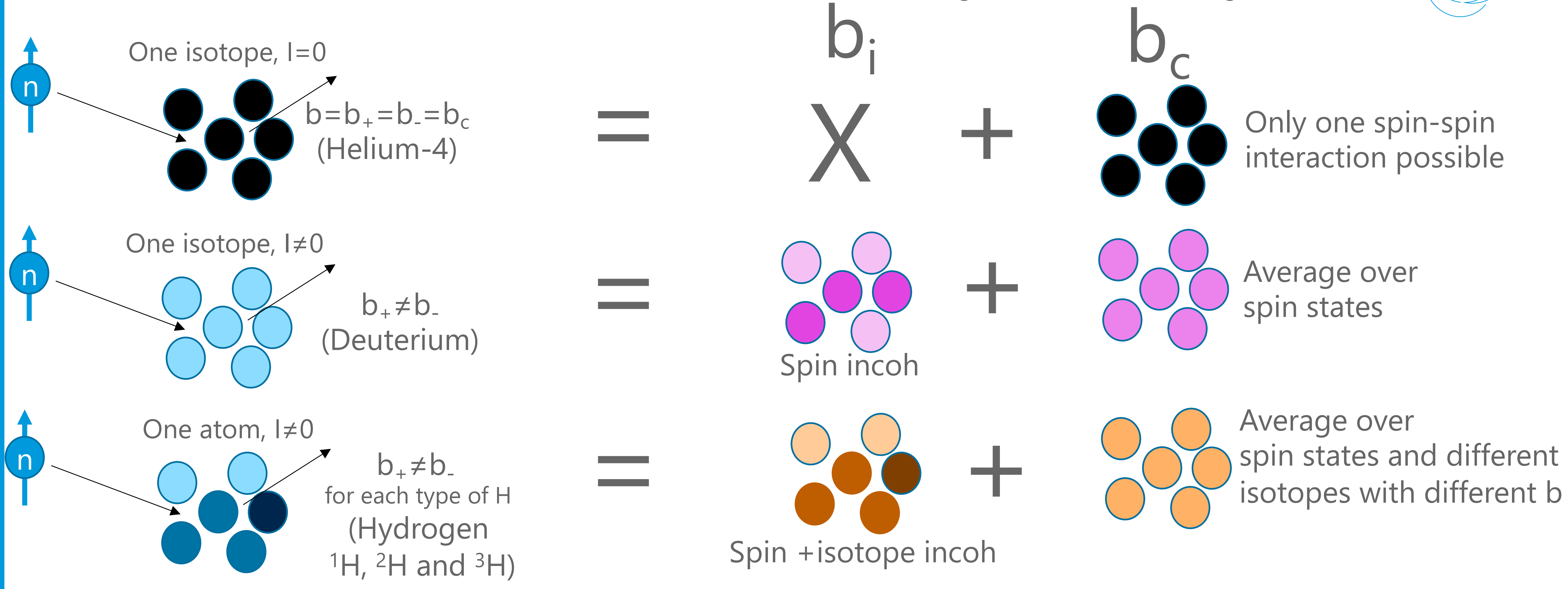
+



Average over spin states

Scattering by a MANY nuclei: NOTE

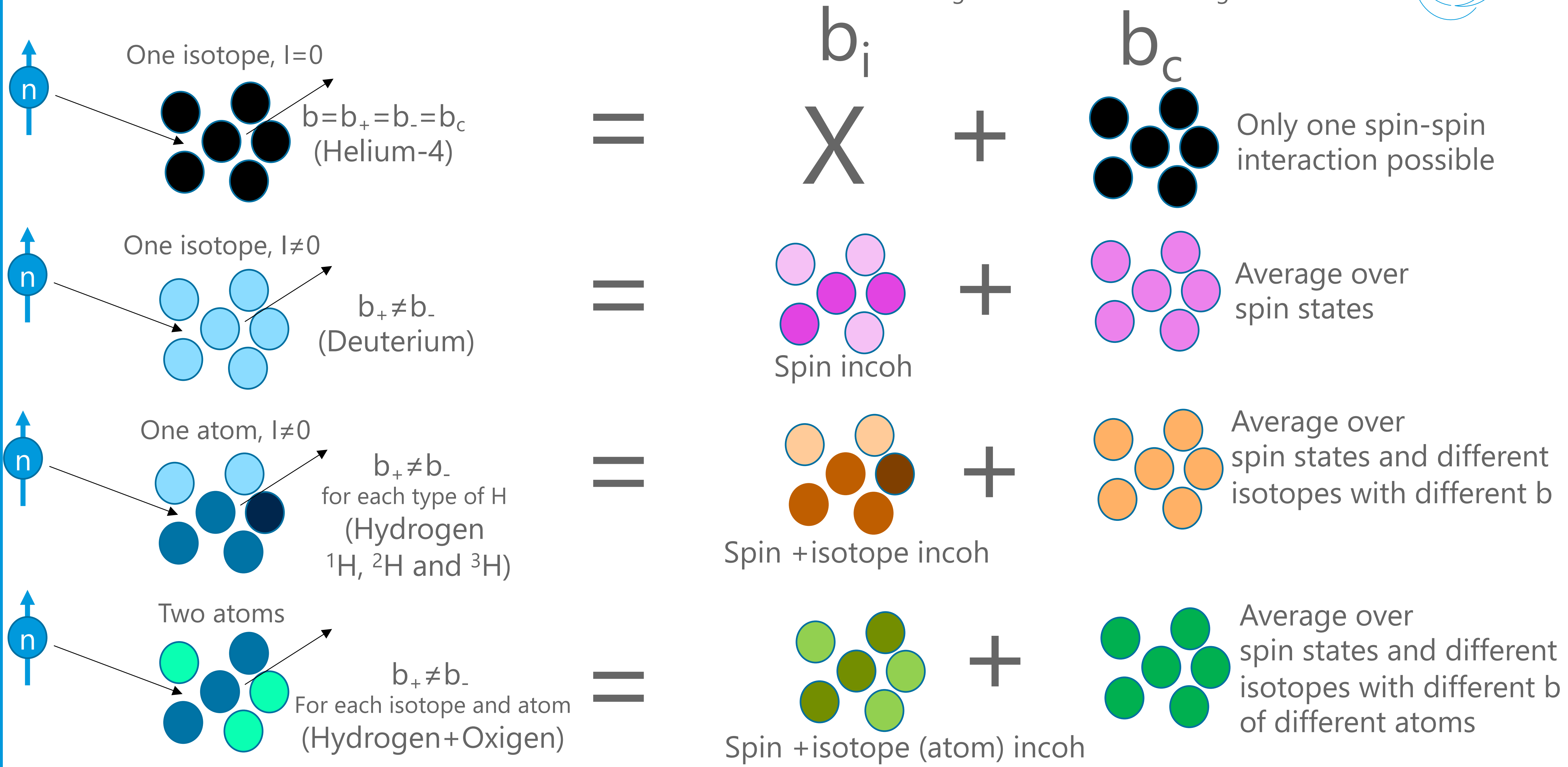
$$\frac{d\sigma}{d\Omega} \propto \underbrace{\left(\langle b^2\rangle - \langle b\rangle^2\right) N}_{\text{Incoherent Scattering}} + \underbrace{\langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}}_{\text{Coherent Scattering}}$$



Scattering by a MANY nuclei: NOTE

$$\frac{d\sigma}{d\Omega} \propto \left(\langle b^2\rangle - \langle b\rangle^2\right) N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i-R_j)}$$

Incoherent Scattering — Coherent Scattering



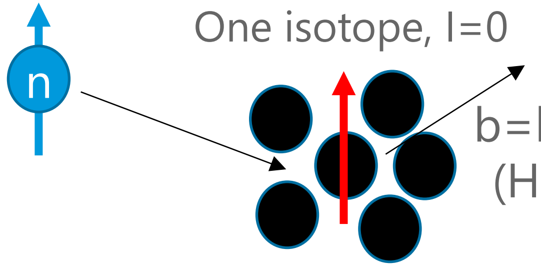
Scattering by a MANY nuclei: NOTE

$$\frac{d\sigma}{d\Omega} \propto \left(\langle b^2\rangle - \langle b\rangle^2\right) N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i - R_j)}$$

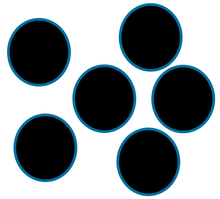
Incoherent Scattering — b_i

Coherent Scattering — b_c

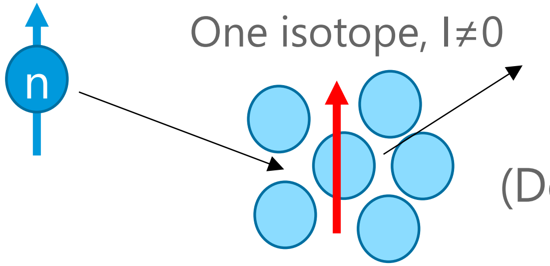
POLARIZED beam and sample (both need to be!!!)



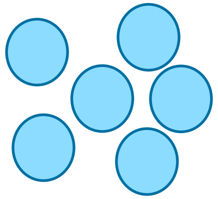
$b = b_+ = b_- = b_c$ (Helium-4)

= X + 

Only one spin-spin interaction possible

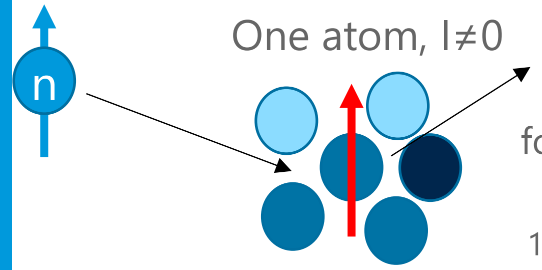


b_+ (Deuterium)

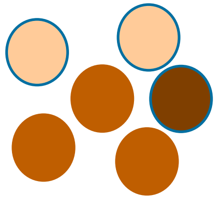
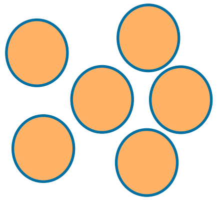
= X + 

Average over spin states only b+

These now are different averages!

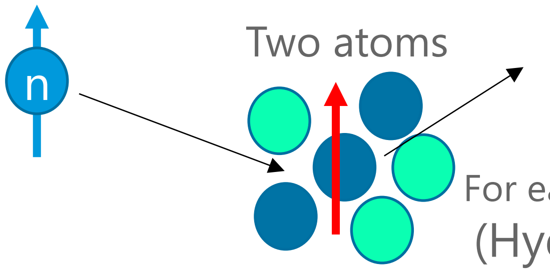


$b_+ \neq b_-$ for each type of H (Hydrogen ^1H, ^2H and ^3H)

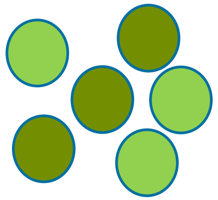
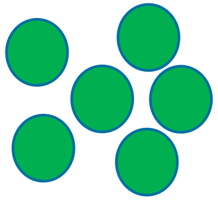
=  + 

~~Spin~~ +isotope incoh

Average over ~~spin states and~~ different isotopes with different b+



$b_+ \neq b_-$ For each isotope and atom (Hydrogen+Oxigen)

=  + 

~~Spin~~ +isotope (atom) incoh

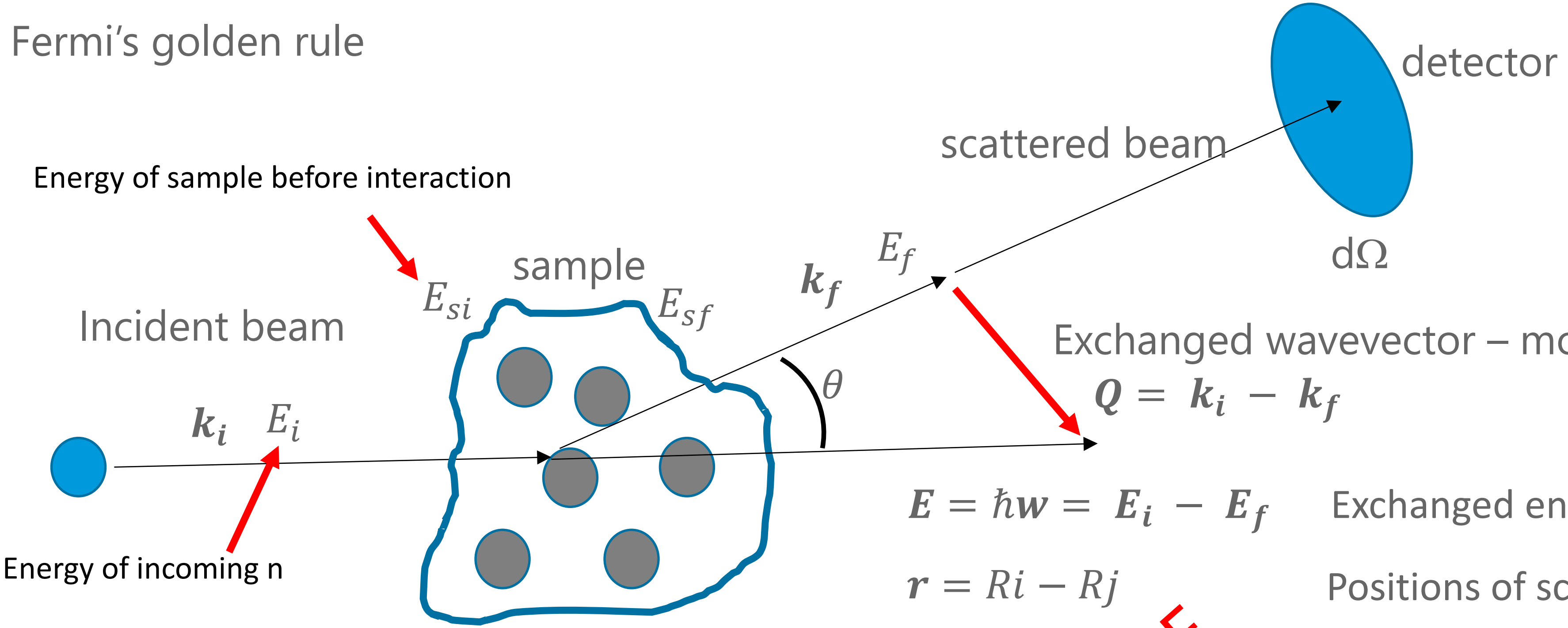
Average over ~~spin states and~~ different isotopes with different b+ of different atoms

GENERALIZATION

NOTE: we did the math for no exchange of energy

This is the math with energy exchange …

Fermi's golden rule



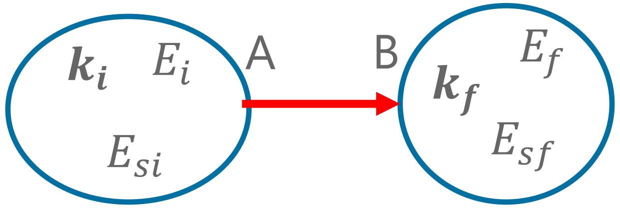
Exchanged wavevector – momentum transfer

$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$

$\boldsymbol{E} = \hbar \boldsymbol{w} = \boldsymbol{E_i} - \boldsymbol{E_f}$ Exchanged energy

$\boldsymbol{r} = Ri - Rj$ Positions of scattering centres

Fermi's golden rule: the cross-section represents all the processes in which the state of the scattering system changes from A to B



Conservation of energy implies:

$E_i + E_{si} - E_f - E_{sf} = 0 \longrightarrow \int \delta(E_i + E_{si} - E_f + E_{sf})\, dE = 1$

$$\frac{d^2\sigma}{d\Omega dE}_{A\to B} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\,j} b_l b_j \int_{-\infty}^{+\infty} \langle A|e^{-i\bar{Q}\cdot\bar{r}}|B\rangle \langle B|e^{iHt/\hbar}e^{i\bar{Q}\cdot\bar{r}}e^{-iHt/\hbar}|A\rangle e^{-i\omega t/\hbar} dt$$

UNFINISHED SLIDE

Sum over all possible A and B

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\,j} b_l b_j \int_{-\infty}^{+\infty} \langle e^{-i\bar{Q}\cdot\bar{r}(0)}|e^{i\bar{Q}\cdot\bar{r}(t)}\rangle e^{-i\omega t} dt$$

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\,j} b_l b_j \int_{-\infty}^{+\infty} \langle e^{-i\bar{Q}\cdot\bar{r}(0)}|e^{i\bar{Q}\cdot\bar{r}(t)}\rangle e^{-i\omega t} dt$$

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\,j} b_l b_j \int_{-\infty}^{+\infty} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle e^{-i\omega t} dt$$

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\neq j} b_l b_j \int_{-\infty}^{+\infty} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle e^{-i\omega t} dt + \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l=j} b_l b_j \int_{-\infty}^{+\infty} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle e^{-i\omega t} dt =$$

Add and subtract the l=j term

$$= \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\neq j} \langle b\rangle^2 \int_{-\infty}^{+\infty} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle e^{-i\omega t} dt + \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l=j} (\langle b^2\rangle - \langle b\rangle^2) \int_{-\infty}^{+\infty} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle e^{-i\omega t} dt =$$

UNFINISHED SLIDE

Coherent Scattering

Depends on the direction of Q

$$\sigma_c = 4\pi\langle b\rangle^2 = 4\pi|b_c|^2$$

$$\sum_{l\neq j} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle$$

Same nucleus at different times,
and correlation of different nuclei at different times
-> interference

Incoherent Scattering

Uniform in all directions

$$\sigma_i = 4\pi(\langle b^2\rangle - \langle b\rangle^2) = 4\pi|b_i|^2$$

$$\sum_{l=j} \left\langle e^{-i\bar{Q}\cdot\overline{rl}(0)} \middle| e^{i\bar{Q}\cdot\overline{rj}(t)} \right\rangle$$

Correlation of Same nucleus at different times
-> NO interference

$$\frac{d^2\sigma}{d\Omega dE} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\neq j} b_l b_j \int_{-\infty}^{+\infty}\langle e^{-i\bar{Q}\cdot\bar{rl}(0)}|e^{i\bar{Q}\cdot\overline{rj}(t)}\rangle\, e^{-i\omega t}dt + \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l=j} b_l b_j \int_{-\infty}^{+\infty}\langle e^{-i\bar{Q}\cdot\bar{rl}(0)}|e^{i\bar{Q}\cdot\overline{rj}(t)}\rangle\, e^{-i\omega t}dt =$$

$$=\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l\neq j}\langle b\rangle^2 \int_{-\infty}^{+\infty}\langle e^{-i\bar{Q}\cdot\bar{rl}(0)}|e^{i\bar{Q}\cdot\overline{rj}(t)}\rangle\, e^{-i\omega t}dt + \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{l=j}(\langle b^2\rangle - \langle b\rangle^2) \int_{-\infty}^{+\infty}\langle e^{-i\bar{Q}\cdot\bar{rl}(0)}|e^{i\bar{Q}\cdot\overline{rj}(t)}\rangle\, e^{-i\omega t}dt =$$

diff

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \left(\frac{d^2\sigma}{d\Omega dE_1}\right) dE_1$$

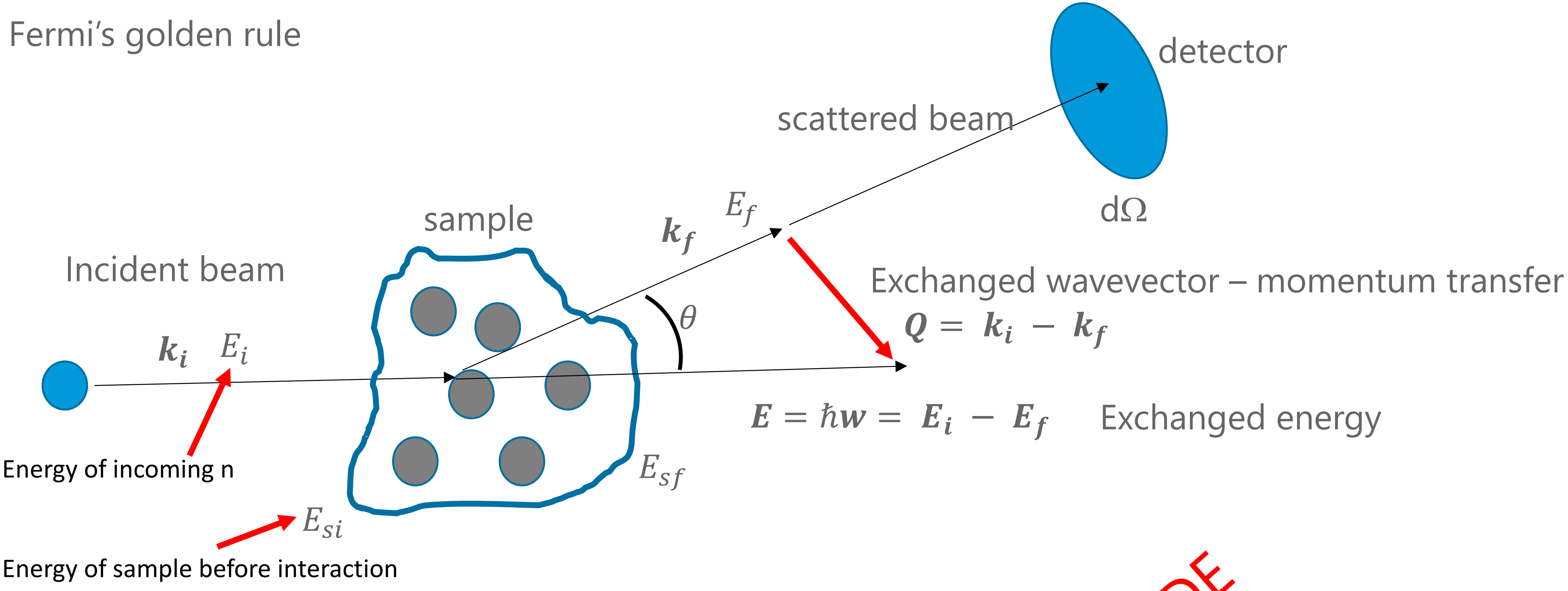
Squires chapt 2

$$\sigma_{tot} = \int_{4\pi}\left(\frac{d\sigma}{d\Omega}\right) d\Omega$$

$$\frac{d\sigma}{d\Omega} \propto (\langle b^2\rangle - \langle b\rangle^2)\, N + \langle b\rangle^2 \sum_{i\neq j} e^{-iQ(R_i - R_j)}$$

UNFINISHED SLIDE

Fermi's golden rule

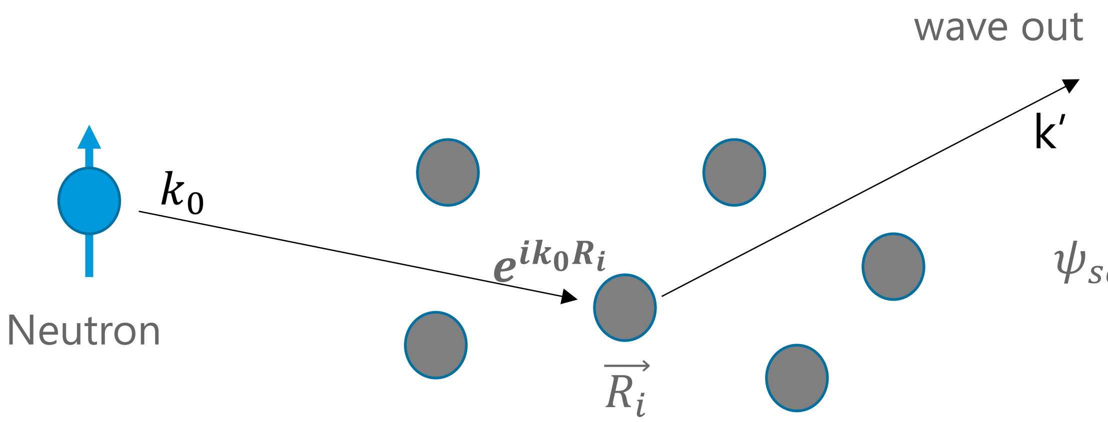


Conservation of energy implies:

$E_i + E_{si} - E_f - E_{sf} = 0 \longrightarrow \int \delta\left(E_i + E_{si} - E_f + E_{sf}\right) dE \;\; = 1$

$$\frac{d^2\sigma}{d\Omega dE}$$

UNFINISHED SLIDE



$$\psi_{scatt} = \sum e^{ik_0R_i}\left[\frac{-b_i}{|r-R_i|}e^{ik'(r-R_i)}\right]$$

$$\frac{d\sigma}{d\Omega} \propto |\psi|^2 = \sum_{i,j} b_i b_j e^{i(k_0-k')(R_i-R_j)} = \sum_{i,j} b_i b_j e^{-iQ(R_i-R_j)}$$

Momentum transfer

$$\boldsymbol{Q = k' - k_0}$$

Exchange in energy

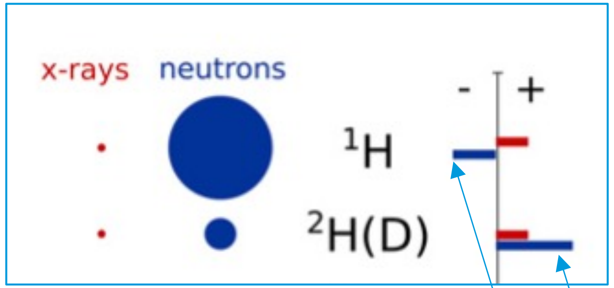
$$\boldsymbol{E = \hbar w = E_i - E_f}$$

UNFINISHED SLIDE

CONTRAST MATCHING

Contrast Matching

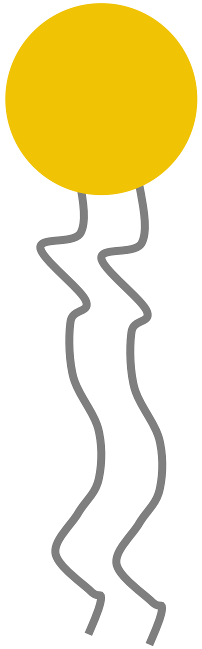
Isotopic substitution – Reflectometry example

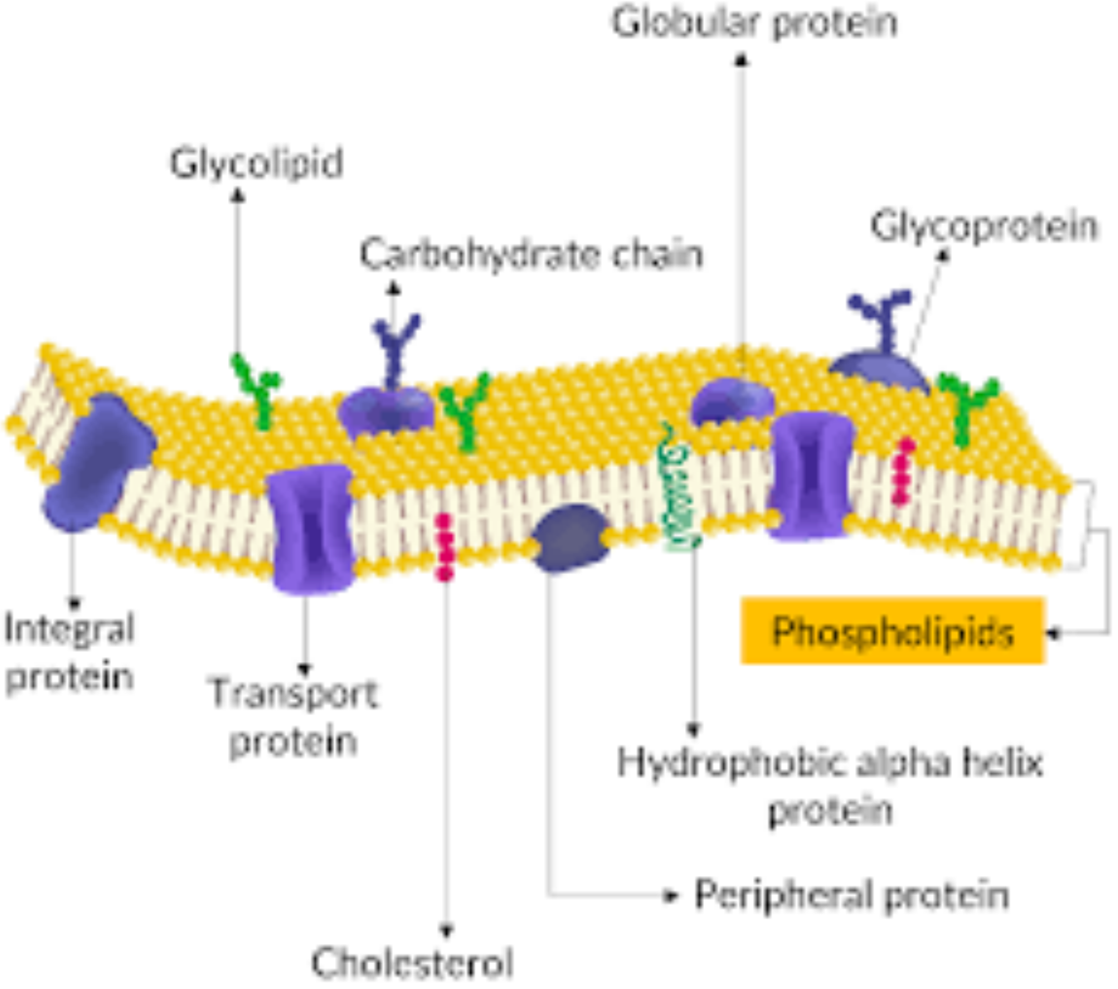


ZSymbA	p or $T_{1/2}$	I	b_c	b_+	b_-	c	σ_{coh}	σ_{inc}	σ_{scatt}	σ_{abs}
0-N-1	**10.3 MIN**	**1/2**	**-37.0(6)**	**0**	**-37.0(6)**		**43.01(2)**		**43.01(2)**	**0**
1-H			**-3.7409(11)**				**1.7568(10)**	**80.26(6)**	**82.02(6)**	**0.3326(7)**
1-H-1	99.985	1/2	-3.7423(12)	10.817(5)	-47.420(14)	+/-	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
1-H-2	0.0149	1	6.674(6)	9.53(3)	0.975(60)		5.592(7)	2.05(3)	7.64(3)	0.000519(7)

Isotopic substitution – Reflectometry example

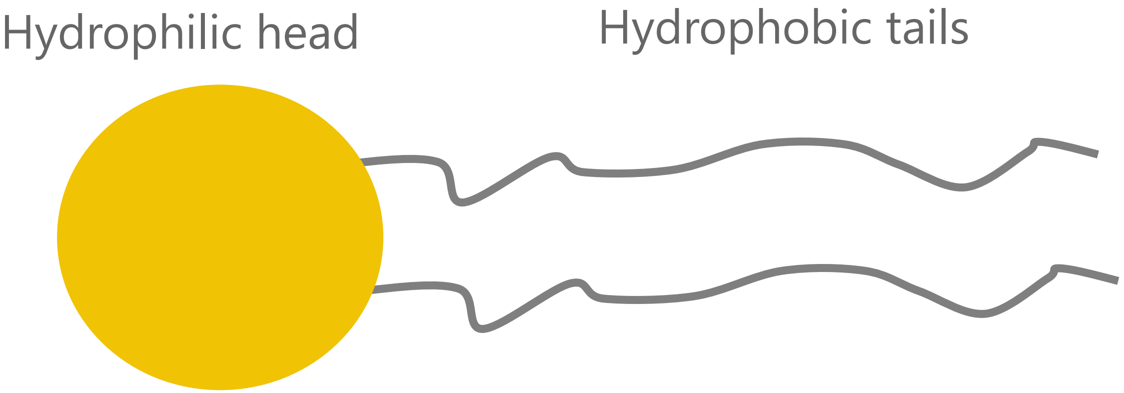
Phospholipids

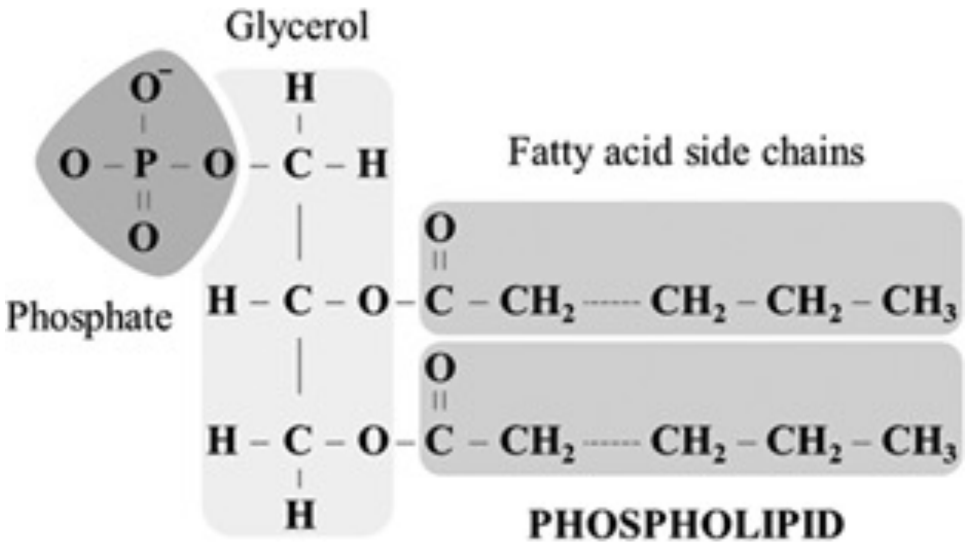




Isotopic substitution – Reflectometry example

Phospholipids



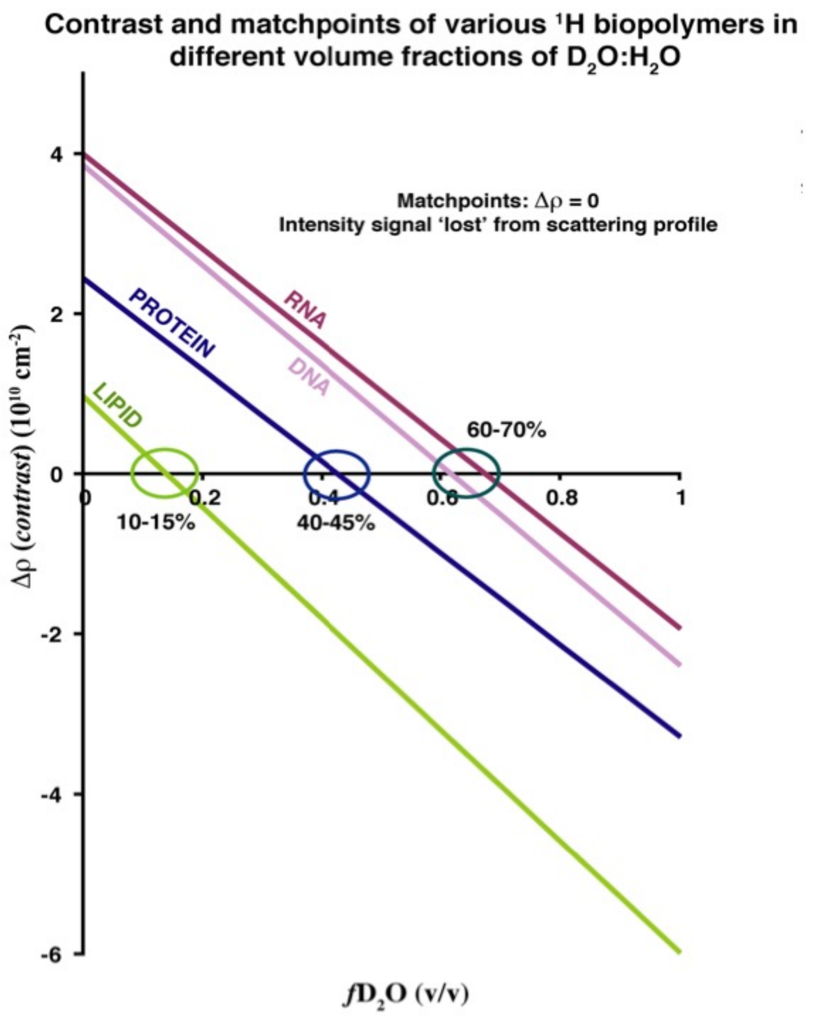


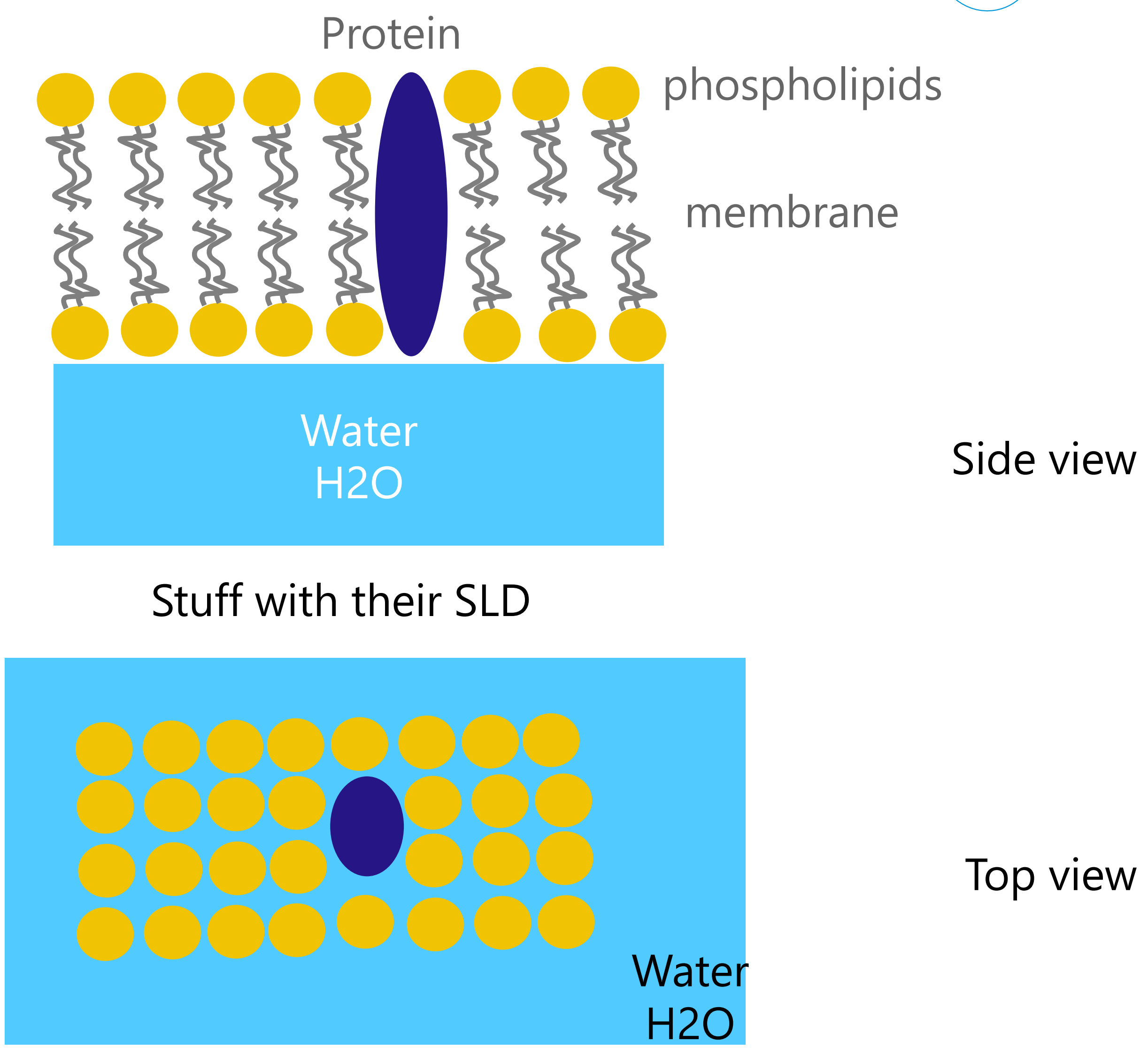
Isotopic substitution – Reflectometry example

$$SLD = \frac{\sum_{i=1}^{N} b_{ci}}{V_m}$$

Coherent scattering length of ith atom

Molecular volume



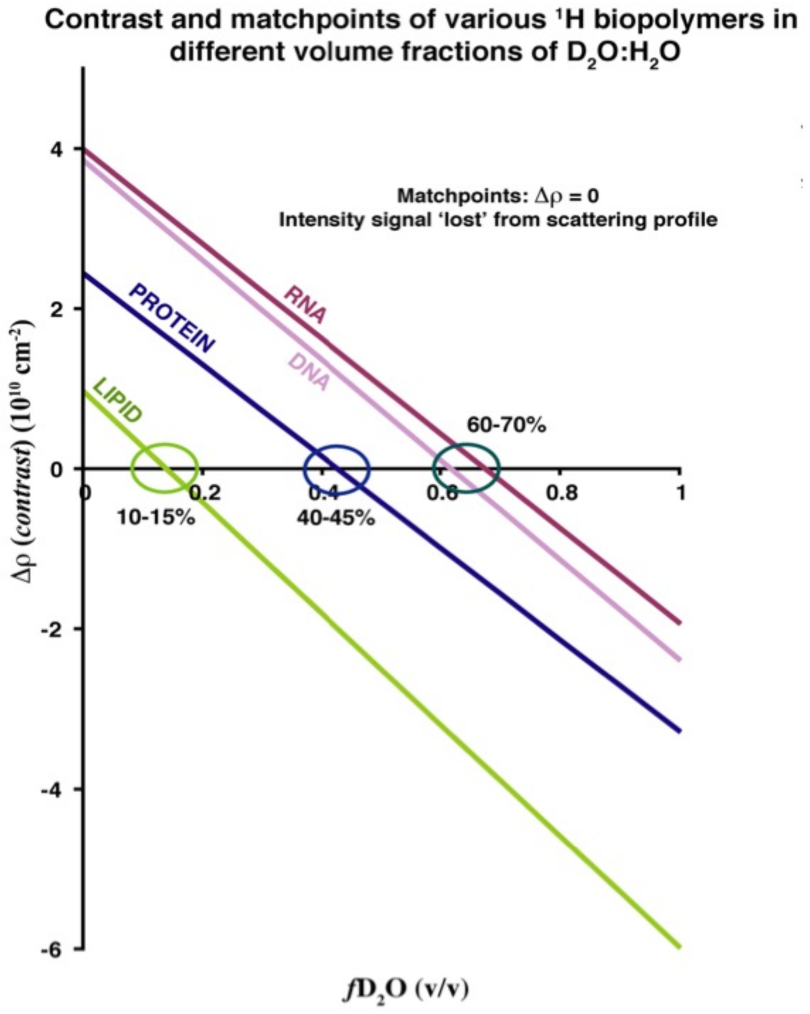


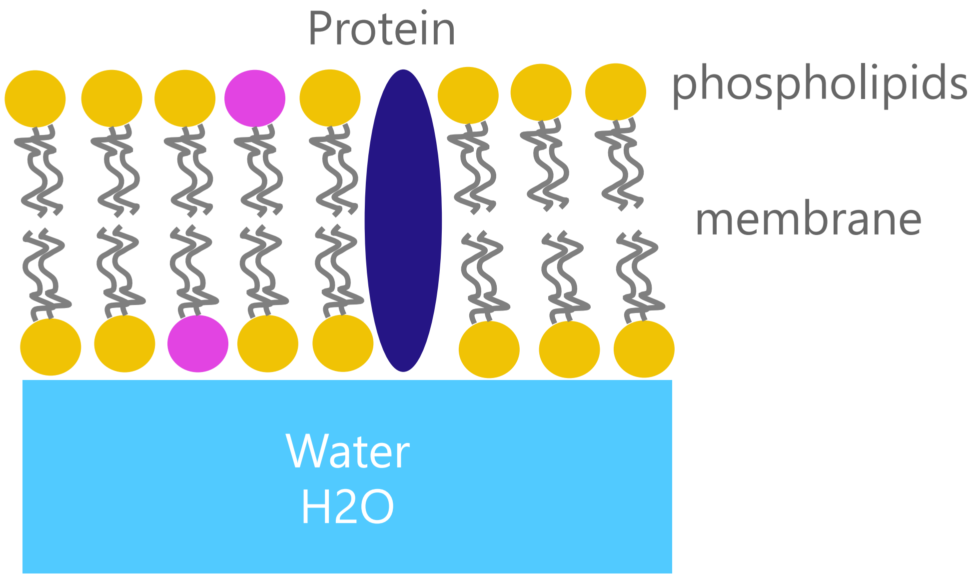
Isotopic substitution – Reflectometry example

$$SLD = \frac{\sum_{i=1}^{N} b_{ci}}{V_m}$$

Coherent scattering length of ith atom

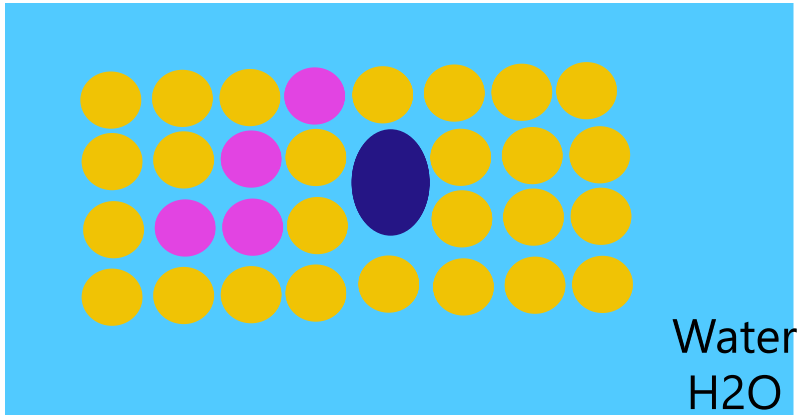
Molecular volume





Side view

Stuff with their SLD, but some heads deuterated



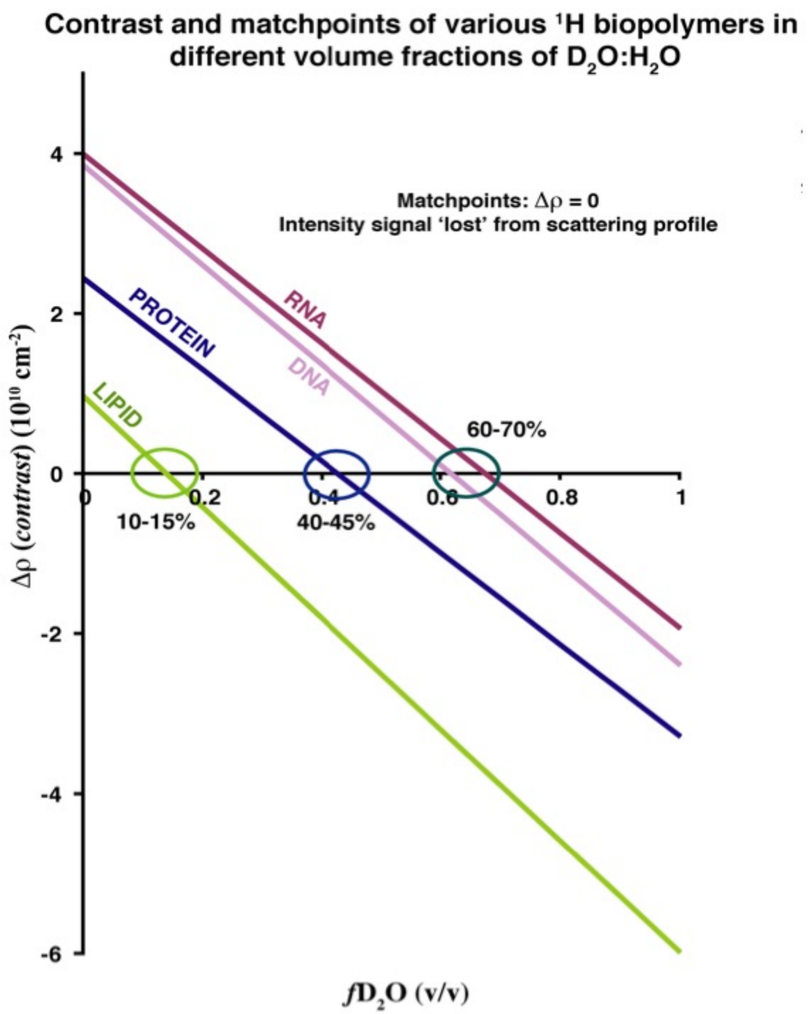
Top view

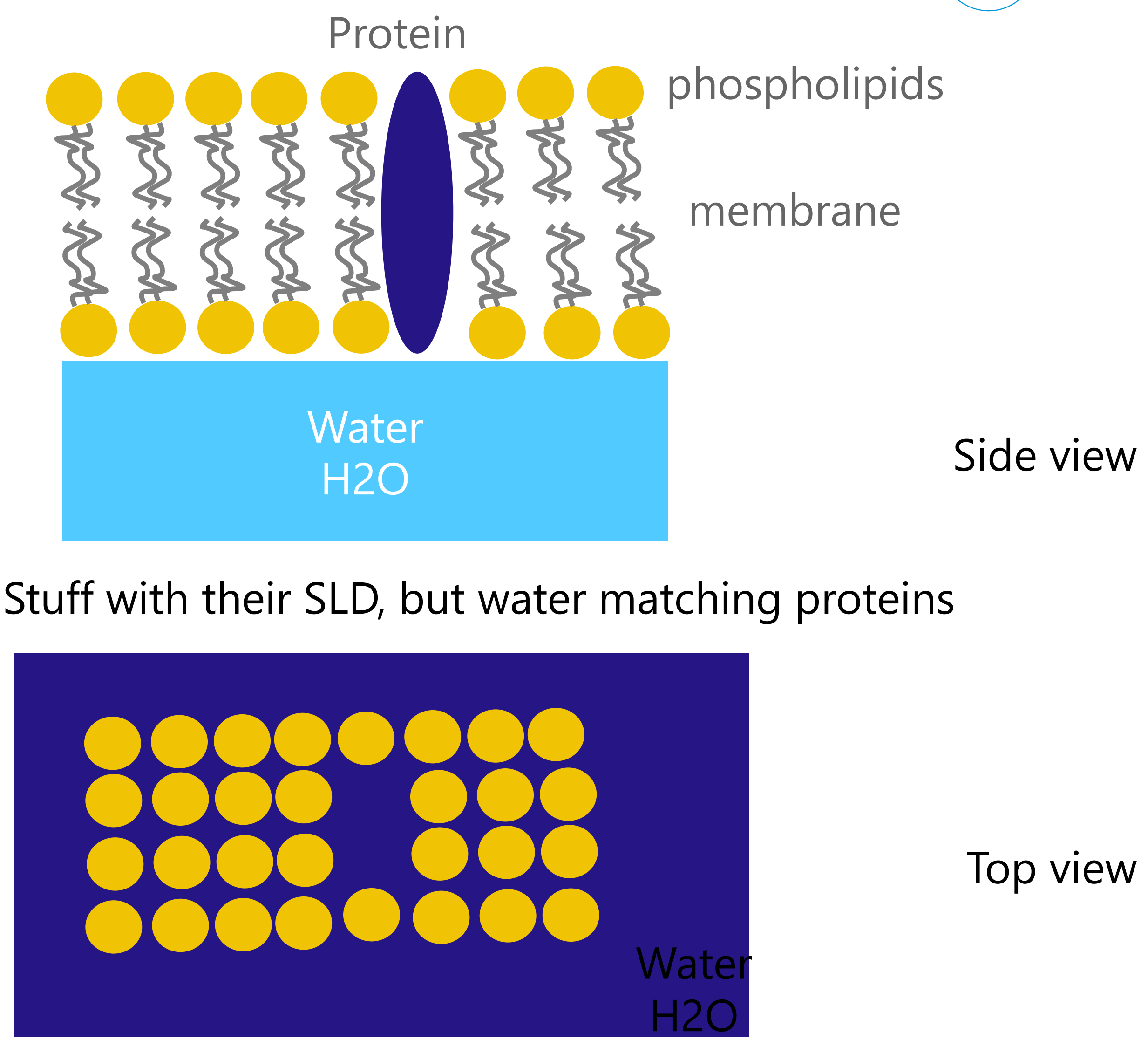
Isotopic substitution – Reflectometry example

$$SLD = \frac{\sum_{i=1}^{N} b_{ci}}{V_m}$$

Coherent scattering length of ith atom

Molecular volume



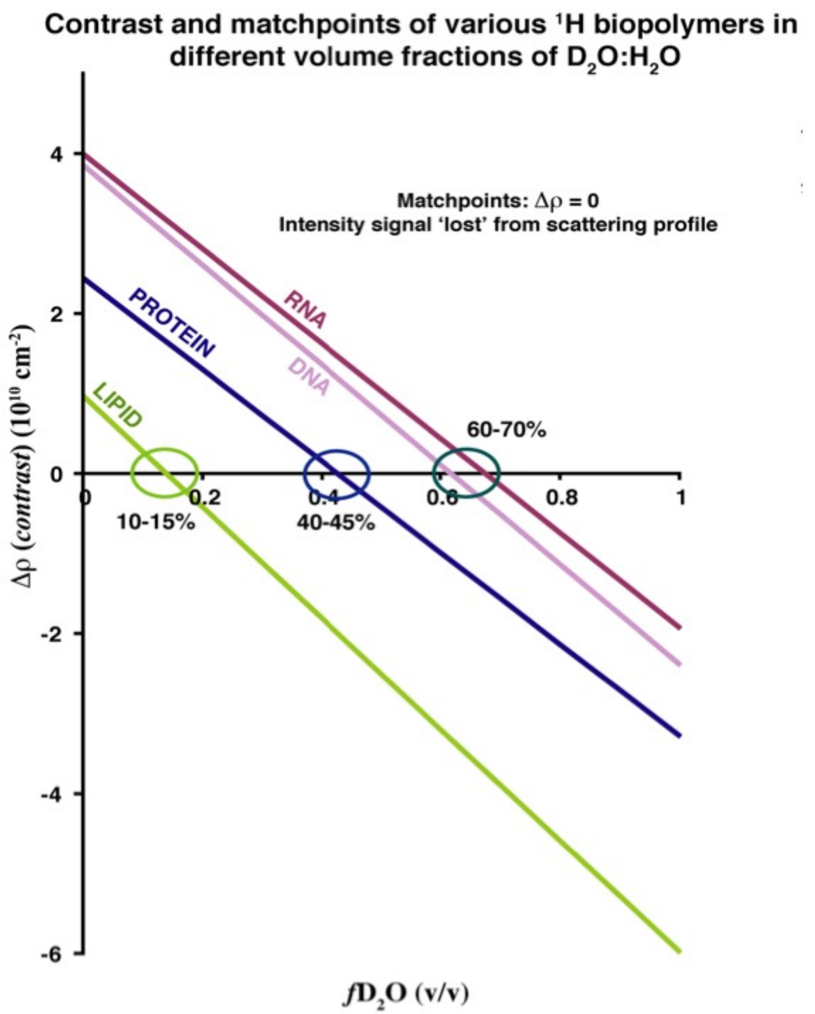


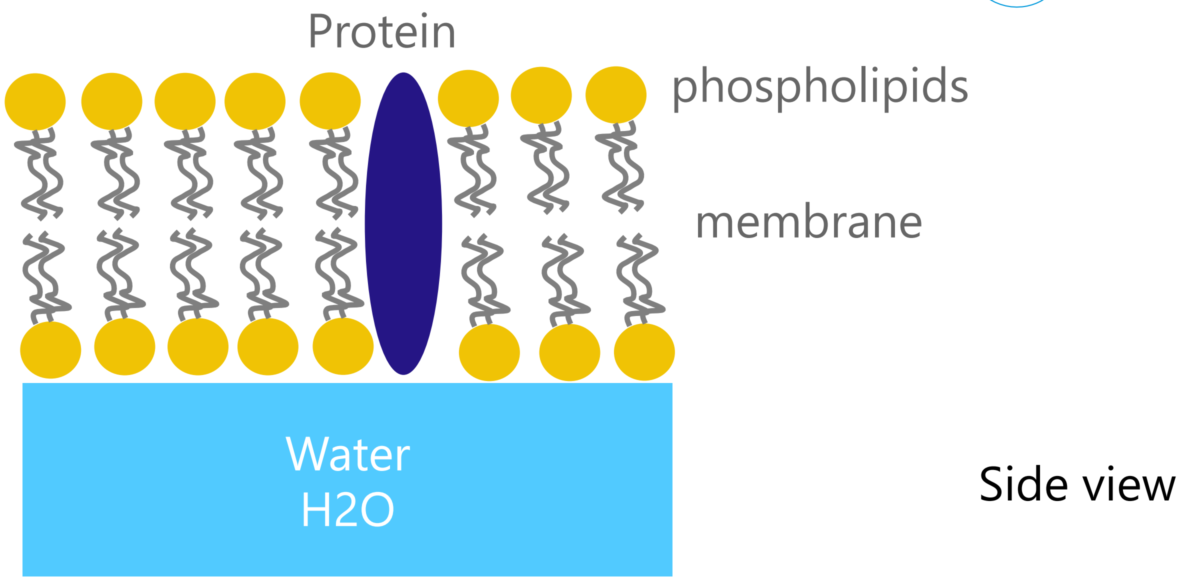
Isotopic substitution – Reflectometry example

$$SLD = \frac{\sum_{i=1}^{N} b_{ci}}{V_m}$$

Coherent scattering length of ith atom

Molecular volume





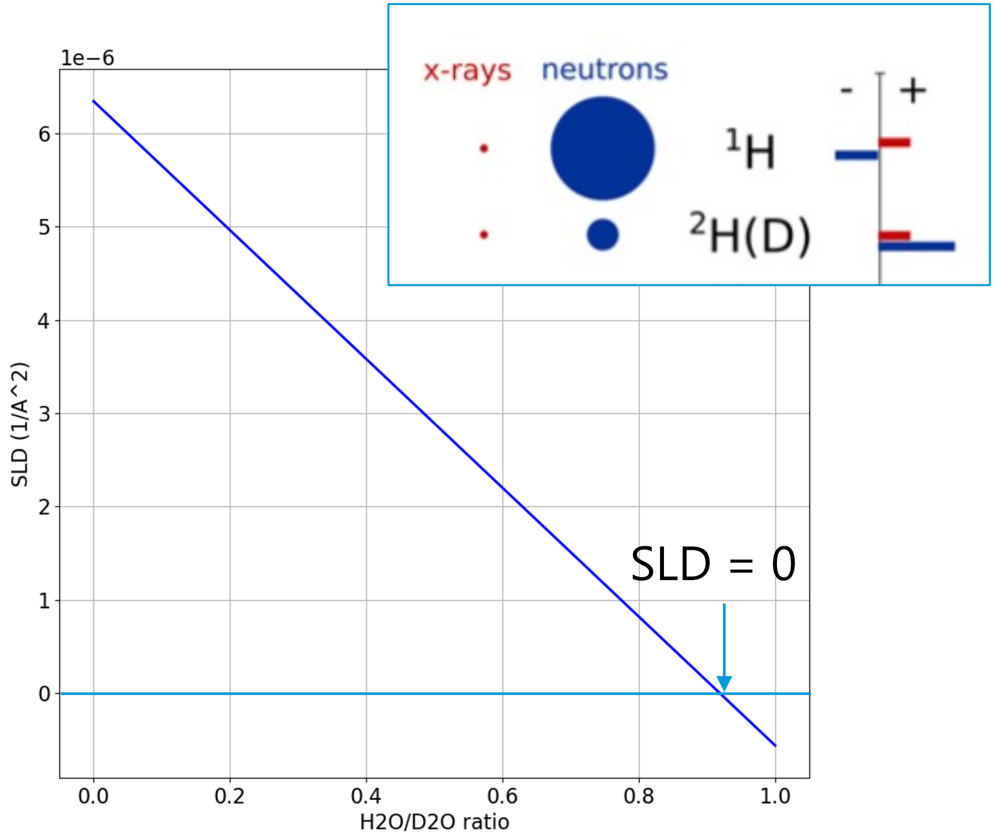
Stuff with their SLD, but water matching heads

Isotopic substitution – Reflectometry example

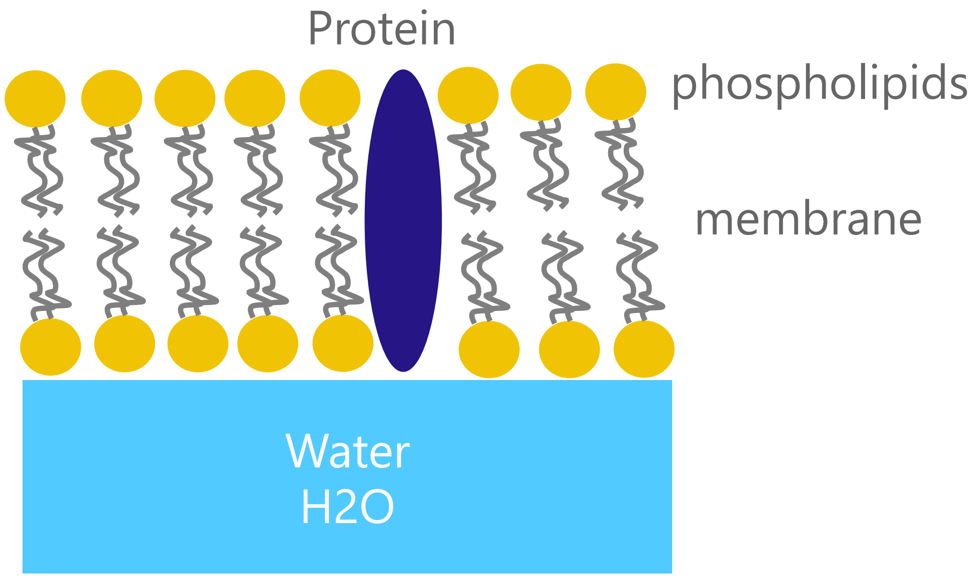
$$SLD = \frac{\sum_{i=1}^{N} b_{ci}}{V_m}$$

Coherent scattering length of ith atom

Molecular volume

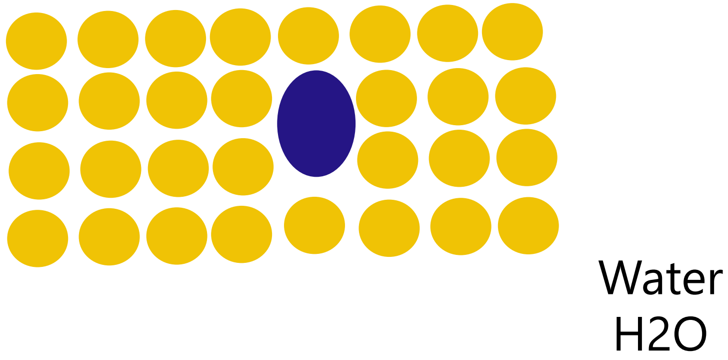


H2O / H2O



Side view

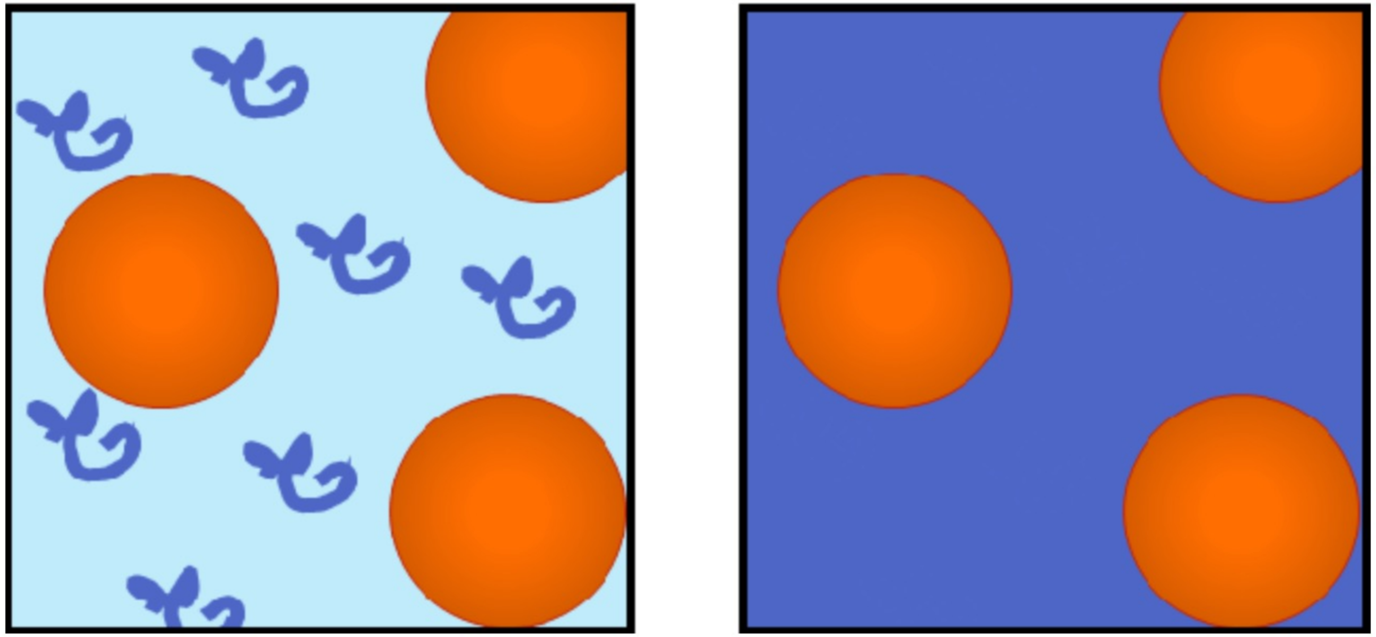
8% di D2O in H2O = non refletive water

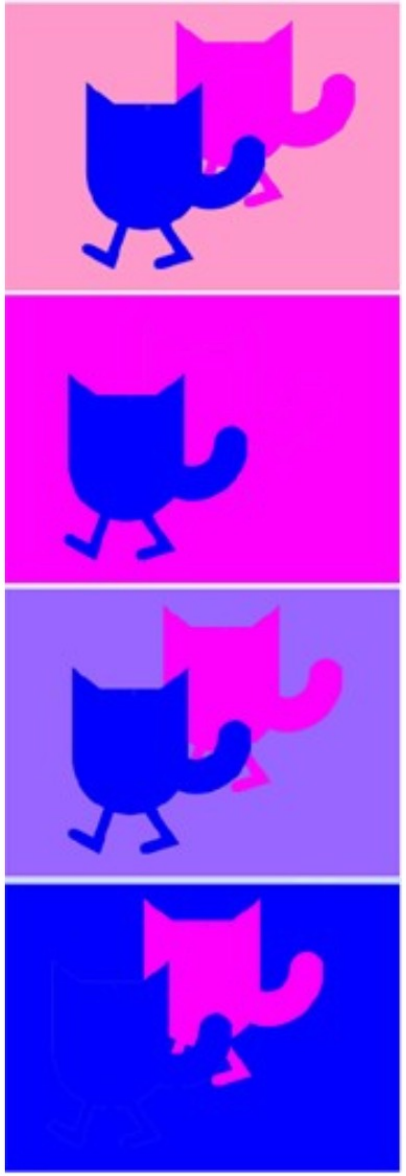


Top view

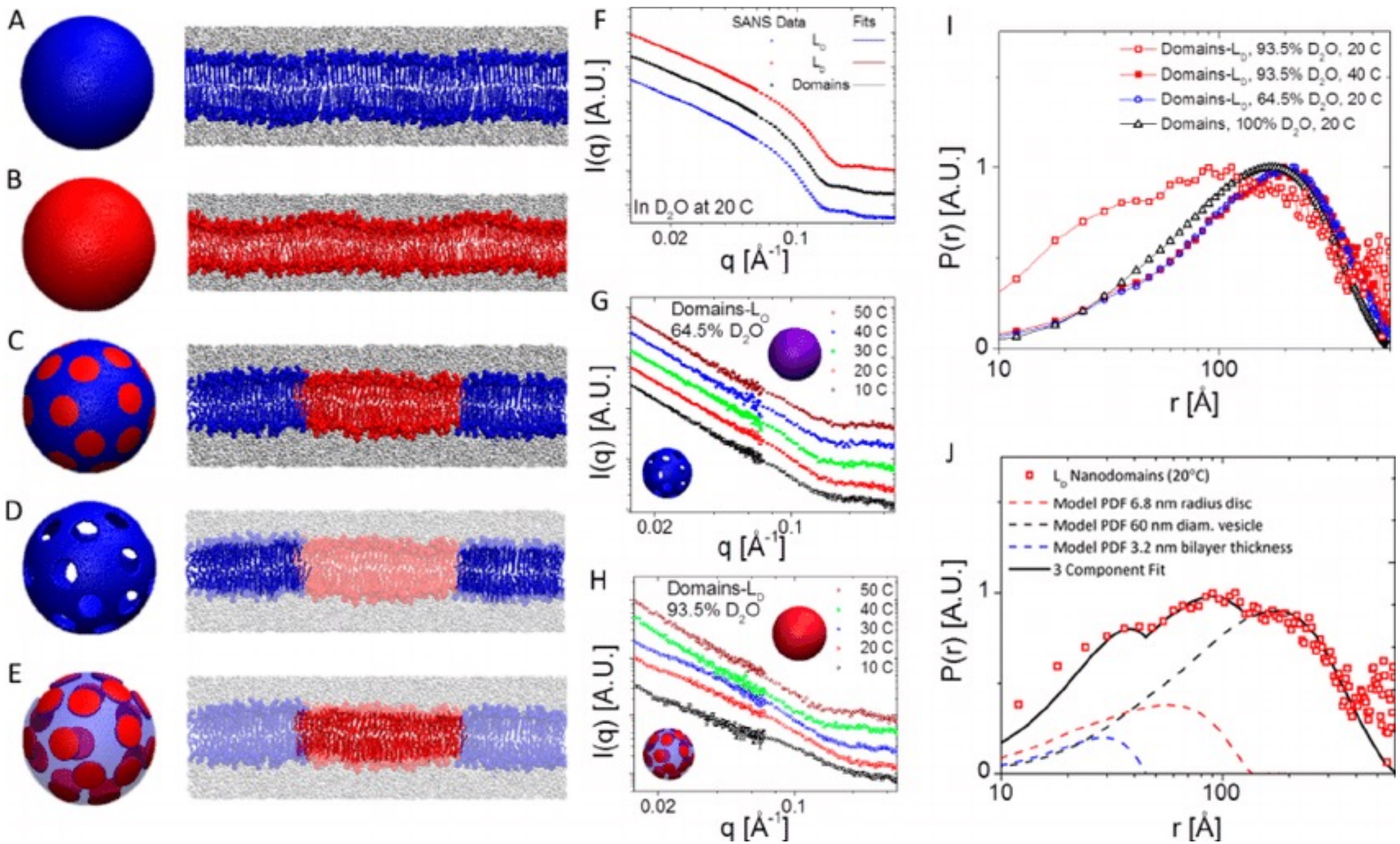
full contrast
silica + PEG in D_2O

PEG match point
silica + PEG in 15% D_2O





SANS data



A
B
C
D
E
F
SANS Data
Fits
Domains
In D2O at 20 C
I(q) [A.U.]
q [Å-1]
G
Domains-Lo
64.5% D2O
50 C
40 C
30 C
20 C
10 C
H
Domains-LD
93.5% D2O
I
Domains-LD, 93.5% D2O, 20 C
Domains-LD, 93.5% D2O, 40 C
Domains-Lo, 64.5% D2O, 20 C
Domains, 100% D2O, 20 C
P(r) [A.U.]
r [Å]
J
LD Nanodomains (20°C)
Model PDF 6.8 nm radius disc
Model PDF 60 nm diam. vesicle
Model PDF 3.2 nm bilayer thickness
3 Component Fit