Basic theory I (elastic)

Carl Adams
St. Francis Xavier University

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Outline

1. References
2. Count rates and the differential cross-section.
3. An example of how to calculate differential cross-section from neutron flux and count rate
4. Classical (particle) theory
5. Time dependent perturbation theory and Fermi's Golden Rule
6. Expression for elastic differential cross-section
7. Nuclear scattering
8. Coherent vs. incoherent scattering
9. Reciprocal lattice and nuclear structure factor
10. Magnetic elastic scattering (very brief)

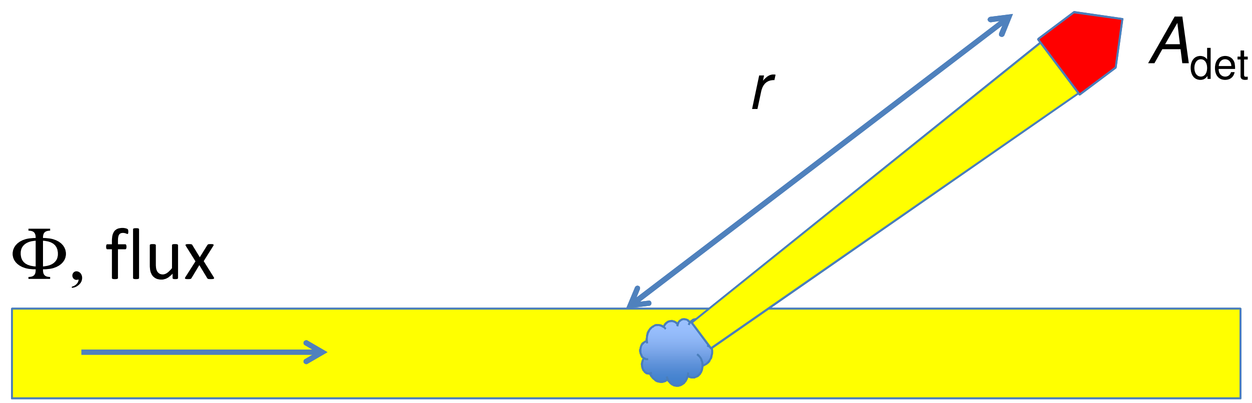
References

- *Theory of Thermal Neutron Scattering* Marshall and Lovesey
- *Neutron Scattering in Condensed Matter Physics* Furrer, Mesot, Strässle
- *Introduction to Quantum Mechanics* Griffiths
- *Introduction to the theory of Thermal Neutron Scattering* Squires
- Another excellent, practical description *Neutron Scattering with a triple-axis spectrometer* Shirane, Shapiro, Tranquada

What determines count rate?

- Sample independent factors
  - Neutron flux (neutrons per cm^2 per second)
  - Geometry/setup of the spectrometer (more neutrons if resolution is “coarse”)
  - Efficiency of detector
- Sample dependent factors
  - If weak scattering: the amount of sample
  - Orientation of sample, scattering angle
  - **Differential cross-section**

Count Rate and Cross-Section

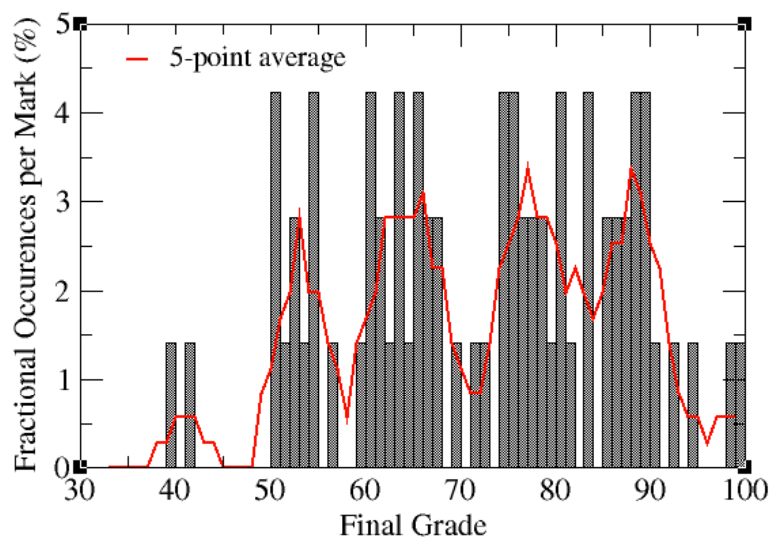


- Would count N particles in Δt seconds e=100%
- N is proportional to Φ, A_{det}, r^{-2}

$$\frac{N}{\Delta t} = D(\text{samp, geo})\,\Phi\,\frac{A_{\text{det}}}{r^2} = D\,\Phi\,\Delta\Omega$$

D(samp, geo) is the **differential cross-section**

Distribution Function-Histogram



- 4% of students with a grade of 80
- Obviously more than 4% with 80 or 81
- There is an implicit “per mark” in the denominator.

Diff. Cross-Section: a Ratio as an Area

- $d\Omega$, solid angle in steradians (4π sr in a sphere, the sun 100 μsr, a spectrometer 100-1000 μsr)
- Differential cross-section is the ratio of count rate to flux per unit solid angle

$$D(\text{samp,geo}) = \frac{\left(\dfrac{dN/dt}{\Phi}\right)}{d\Omega} = \frac{"d\sigma"}{d\Omega} = \frac{d\sigma}{d\Omega}$$

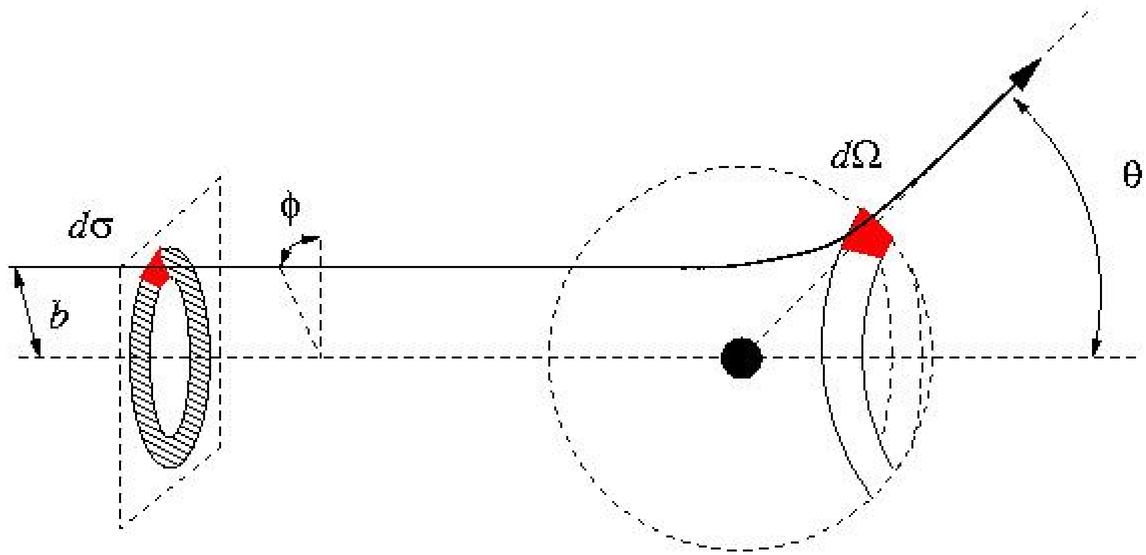
Simple Estimate of Differential Cross Section (an area)

- Incident flux is $\Phi = 1.0 \times 10^7$ neutrons cm^{-2} s^{-1}
- A_{det}=10 cm^2, r=100 cm (0.001 sr), N=3000, Δt=30 s

$$D(\text{samp,geo}) = \frac{Nr^2}{A_{\text{det}}\Phi\,\Delta t} = \frac{(3000)(100)^2}{(10)(10^7)(30)} = 0.01\,\text{cm}^2(\text{sr}^{-1})$$

- If there are 10^{22} atoms, $D=10^{-24}$ cm^2=1 barn (per sr) per atom.

Predicting the Differential Cross-Section (Classical, Azimuthal Sym)



•Have used classical mechanics to determine the relationship between *b* (impact parameter) and θ

•Assume azimuthal symmetry

•But you can't set *b*; you have uniform flux of particles Φ and a detector at some angle

Classical Diff. Cross-Section

- Solid angle subtended by detector

$$d\Omega = dA/r^2 = \sin\theta \, d\theta \, d\phi$$

- "Area" to scatter to detector at θ

$$d\sigma = b \, d\phi \, db = b(\theta)\left|\frac{db}{d\theta}\right| d\phi \, d\theta$$

- Count rate

$$\frac{N}{\Delta t} = \Phi \, d\sigma = \Phi \, b(\theta)\left|\frac{db}{d\theta}\right| d\phi \, d\theta = \Phi \frac{b(\theta)}{\sin\theta}\left|\frac{db}{d\theta}\right| d\Omega = \Phi \, D(\theta) \, d\Omega$$

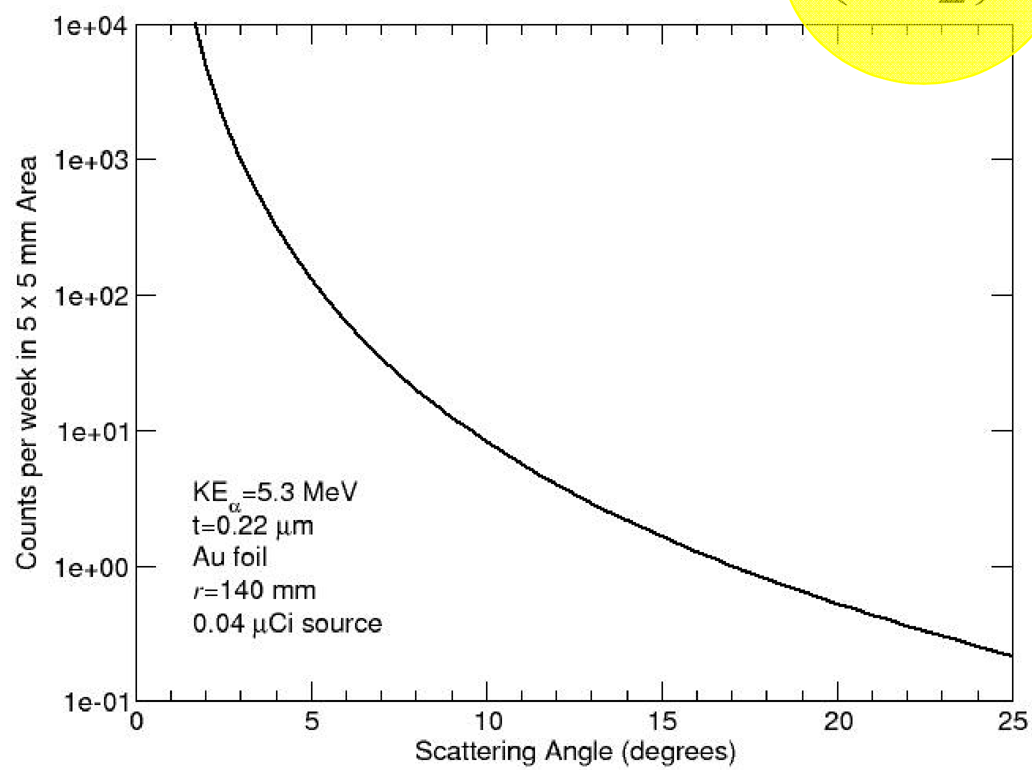
$$D(\theta) = \frac{"d\sigma"}{"d\Omega"} \equiv \frac{d\sigma}{d\Omega} = \frac{b(\theta)}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

Rutherford (Coulomb) Scattering

$$b = \left(\frac{Ze^2}{4\pi\varepsilon_0 E_K}\right)\cot\left(\frac{\theta}{2}\right) \qquad \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \left(\frac{Ze^2}{8\pi\varepsilon_0 E_K}\right)^2 \frac{1}{\left(\sin\frac{\theta}{2}\right)^4}$$

Z=79, E_K=5.3 MeV, θ=25°

$$\frac{d\sigma}{d\Omega} = 1.15\,\text{barns}$$



What determines Φ at the sample?

- Quoting "flux of the reactor" includes all energies and all directions.
- "Front-end" gives a $\Delta\lambda/\lambda$ (or $\Delta k/k$) out of Maxwell distribution

$$k_B T = k_B\,(330\text{ K}) = 28.5\text{ meV} \quad E_i = 36\text{ meV } (\lambda = 1.5\text{ Å})$$

$$\phi(k_i)\,dk_i = \frac{dk_i}{k_i}\left(\frac{E_i}{k_B T}\right)^2 \exp\left(-\frac{E_i}{k_B T}\right)\,\Phi_T = (3\%)\left[\left(\frac{36}{28.5}\right)^2 \exp\left(-\frac{36}{28.5}\right)\right]\left(5\times10^{14}\text{ cm}^{-2}\text{s}^{-1}\right)$$

$$= 6.8\times10^{12}\text{ cm}^{-2}\text{s}^{-1}$$

- Lower case ϕ is a flux "per unit k"

Φ Estimate: Discriminate direction

- A solid angle of acceptance (approx)

Horizontal 0.5° and vertical 2°

$$d\Omega = \frac{dA}{r^2} = \frac{dx\,dy}{r^2} = \left(\frac{0.5^\circ}{57.3^\circ}\right)\left(\frac{2^\circ}{57.3^\circ}\right) = 304\ \mu\text{srad}$$

$$\Phi_{\text{samp}} = \frac{\phi(k_i)\,dk_i\,d\Omega}{4\pi} = 1.6\times10^{8}\ \text{cm}^{-2}\text{s}^{-1}$$

- (High? Monochromator? Resolution?)
- Nuclear reactors aren't lasers! Or synchrotrons! Closer to a high vacuum!

Modifications to Cross-Section for **Quantum** Neutron Scat.

- The incoming and scattered particles are replaced by an incoming plane wave and an outgoing wave (Born approx, weak scattering)
- The quantum state of the system (sample plus beam) changes as a result of the interaction between the incoming wave and the sample
- In every case the interaction potential *V* is included in some fashion and you want to find the likelihood of a transition.

Interpretations and Methods of Quantum Scattering

$$\psi(r,\theta) \approx A\left(e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right), \text{ for large } r$$

- Incoming plane wave and outgoing wave $k=2\pi/\lambda$
- $f(\theta)$ is the **scattering amplitude** and is a complex number with dimensions of length

$$\frac{d\sigma}{d\Omega} = \left|f(\theta)\right|^2$$

- $f(\theta)$ depends on the sample, geometry, and k. Usually not stated as simple function.
- Will **use Fermi's Golden Rule to calculate a transition rate**

Time-dependent Perturbation Theory

(some of the quantum details)

- The sample and neutron wave have a Hamiltonian *H* (can be used to find total energy and also "evolves" the quantum system)
- How likely is a transition between an incoming neutron wave and initial sample state to a final sample state with a scattered neutron wave of a possibly different energy?

$$\Psi(t) = c_i(t)\,\psi_i \exp\left(-\frac{iE_i t}{\hbar}\right) + c_f(t)\,\psi_f \exp\left(-\frac{iE_f t}{\hbar}\right)$$

- Transition probability per unit time $\propto \left|c_f(t)\right|^2 / t$

(Note: the sample is not in a specific state but instead is in some kind of spread of states because of finite temperature. Let's investigate a single state and do the averaging over the "ensemble" of states later.)

Details: T-dep. Perturbation Theory

- Time-dep Schrödinger equation

$$\left(H + V(t)\right)\Psi(t) = i\hbar \frac{\partial \Psi}{\partial t}$$

- Evolution of "final state" for weak perturbation

$$c_f(t) \approx \frac{1}{i\hbar}\int_0^t \left\langle \psi_f \left| V(t') \right| \psi_i \right\rangle \exp\left(\frac{i}{\hbar}(E_f - E_i)t'\right) dt'$$

- If *V*(*t*) is sinusoidal (i.e. a wave)

$$V(t) = V\exp\left(\frac{-iEt}{\hbar}\right) + V^{+}\exp\left(\frac{iEt}{\hbar}\right)$$

Transition Probability at large *t*

- Use energy absorption as an illustration

$$P_f(t) = \left|c_f(t)\right|^2 = \frac{1}{\hbar^2}\left|\langle \psi_f | V | \psi_i \rangle\right|^2 \left[\frac{\sin\left\{\frac{1}{2}\frac{\left(E-(E_f-E_i)\right)t}{\hbar}\right\}}{\frac{1}{2}\frac{\left(E-(E_f-E_i)\right)}{\hbar}}\right]^2$$

- The 2nd term -> a delta-function x $2\pi\hbar$ *t* for long times. Sensitive to final density of states
- For a transition rate, the *t* term cancels out.

Fermi (Dirac)'s Golden Rule

- Fermi's Golden Rule (for scattering into $d\Omega$)

$$\sum_{\vec{k}_f \text{ in } d\Omega} W_{\vec{k}_i,\lambda_i \to \vec{k}_f,\lambda_f} = \frac{2\pi}{\hbar} \rho_{\vec{k}_f}(E_f) \left| \left\langle \vec{k}_f \, \lambda_f \middle| V \middle| \vec{k}_i \lambda_i \right\rangle \right|^2$$

- Transition rate from Squires' Eqn. 2.2
- $\rho_{\mathbf{kf}}$ is the # of final states per unit energy
- λ are the labels describing the sample state
- Can also include spin degrees of freedom for the neutron σ

Cross-section from Transition Rate

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda_i \to \lambda_f} = \frac{\left(\dfrac{\sum\limits_{\vec{k}_f \text{ in } d\Omega} W_{\vec{k}_i,\lambda_i \to \vec{k}_f,\lambda_f}}{\Phi}\right)}{d\Omega} = \frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\vec{k}_f \text{ in } d\Omega} W_{\vec{k}_i,\lambda_i \to \vec{k}_f,\lambda_f}$$

- Squires' Eqn. 2.1
- Will we get the correct cancellation?
- Yes, use a "box" for normalisation.

Density of States

- Generalised definition “# of states”= “density of states” x “volume”
- Counting/standing wave argument then use the chain rule to get the correct units for “volume” (an energy volume in this case)
- Neutron waves scattered into a $d^3\mathbf{k}$ and a dE_f : how many states are available (box with ‘L’)?

Cross-section Result

$$\# = \rho_{\vec{k}'}(E_f)\frac{d^3\mathbf{k}_f}{dE_f}dE_f = \left(\frac{L}{2\pi}\right)^3 \frac{k_f^2\,dk_f\,d\Omega}{\frac{\hbar^2 k_f}{m}dk_f}dE_f = \left(\frac{L}{2\pi}\right)^3 \frac{mk_f}{\hbar^2}d\Omega dE_f$$

$$\rho_{\vec{k}'}(E_f) = \left(\frac{L}{2\pi}\right)^3 \frac{mk_f}{\hbar^2}d\Omega$$

- Incident flux involves L^3 as well

$$\Phi = \frac{\upsilon_i}{L^3} = \frac{\hbar k_i}{mL^3}$$

Differential Cross-Section

The L^6 term is removed by considering the normalisation factors of the neutron wavefunction.

$$\left|\left\langle f\middle|V\middle|i\right\rangle\right|^2 = \left|\iiint_{L^3\,\text{box}} dx\,dy\,dz\;\psi^*_{\vec{k}_f}(\vec{r})V(\vec{r};\vec{R}_j)\;\psi_{\vec{k}_i}(\vec{r})\right|^2 = \frac{1}{L^6}\left|\int d\mathbf{r}\,e^{-i\vec{k}_f\cdot\vec{r}}V(\vec{r};\vec{R}_j)\,e^{i\vec{k}_i\cdot\vec{r}}\right|^2$$

(Have assumed that the state of the sample is unchanged. Need to relax this for inelastic scattering/partial differential cross-section. Also contains the Born approximation for weak scattering.)

Combine previous terms to obtain **differential cross-section.** Now just exponentials in matrix element.

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\left\langle\vec{k}_f\middle|V(\vec{R}_j)\middle|\vec{k}_i\right\rangle\right|^2$$

How can we sum over 10^{22} atoms?

- Maybe each one sends a wave that is independent of the others and incoherent (random phase over atoms would do it)

$$\left| \left\langle f \left| \sum_j V_j(\vec{r}-\vec{R}_j) \right| i \right\rangle \right|^2 = \sum_j \left| \left\langle f \left| V_j(\vec{r}-\vec{R}_j) \right| i \right\rangle \right|^2$$

- Or else we need to keep the "cross terms" **interference**

Fourier Transform of *V*

- Take advantage of the periodicity of the lattice?

$$V(\vec{r}) = \sum_j V_j(\vec{r} - \vec{R}_j) \qquad \vec{x}_j = \vec{r} - \vec{R}_j$$

$$\left\langle \vec{k}_f \middle| V \middle| \vec{k}_i \right\rangle = \sum_j \int d\,\vec{r}\, \exp\left(i\left(\vec{k}_i - \vec{k}_f \right) \bullet \vec{r} \right) V(\vec{r} - \vec{R}_j)$$

$$\left\langle \vec{k}_f \middle| V \middle| \vec{k}_i \right\rangle = \sum_j \int d\,\vec{x}_j\, \exp\left(i\,\vec{Q} \bullet \left(\vec{x}_j + \vec{R}_j \right) \right) V(\vec{x}_j)$$

$$\left\langle \vec{k}_f \middle| V \middle| \vec{k}_i \right\rangle = \sum_j \exp(i\vec{Q} \bullet \vec{R}_j) \int d\,\vec{x}_j\, \exp\left(i\,\vec{Q} \bullet \vec{x}_j \right) V(\vec{x}_j)$$

Interaction?

- Nucleus-neutron… inverse square? (joke!) Actually don’t know but take advantage of it being really short range.
- Electron-neutron… electron creates a magnetic field which interacts with the magnetic dipole moment of the neutron and there a lot of electrons in a lot of places with lots of different magnetic fields…

Bound Scattering Length

- If we consider a fixed, single nucleus then the scattering of thermal neutrons (wavelength much greater than the interaction distance) the scattering will be pure *S*-wave (result of diffraction theory)

$$\psi_{sc}(\vec{r}) \propto -\frac{b_j}{r}\exp\left(ik_f r\right)$$

- This matches earlier formalism with complex scattering length "*b*" playing the role of *f*(θ).

$$\frac{d\sigma}{d\Omega} = \left|b\right|^2$$

What potential would give *b*?

- Delta-function potential with parameter *a*

$$V(\vec{r}) = a\delta^3(\vec{r})$$

$$\left|\left\langle f\left|V\right|i\right\rangle\right|^2 = \left|\int_{\text{all space}} d\vec{r}\,\exp\left(i\left(\vec{k}_i - \vec{k}_f\right)\bullet\vec{r}\right) a\delta^3(\vec{r})\right|^2 = \left|a\right|^2$$

$$a = \frac{2\pi\hbar^2}{m} b \qquad V(\vec{r} - \vec{R}_j) = \frac{2\pi\hbar^2}{m} b_j \delta^3(\vec{r} - \vec{R}_j)$$

- Fermi pseudo potential
- *b* is determined by experiment

A System of Many Nuclei

$$V(\vec{r}) = \sum_j V_j(\vec{r} - \vec{R}_j) = \left(\frac{2\pi\hbar^2}{m}\right)\sum_j b_j\,\delta^3(\vec{r} - \vec{R}_j)$$

- Now doing the Fourier Transform is easy

$$\left\langle \vec{k}_f \middle| V \middle| \vec{k}_i \right\rangle = \frac{2\pi\hbar^2}{m}\sum_j b_j \exp(i\vec{Q}\bullet\vec{R}_j)$$

- Can write the mod-squared as double sum

$$\left|\left\langle \vec{k}_f \middle| V \middle| \vec{k}_i \right\rangle\right|^2 = \left(\frac{2\pi\hbar^2}{m}\right)^2 \sum_{j'j} b^*_{j'}\, b_j \exp\left\{i\vec{Q}\bullet\left(\vec{R}_j - \vec{R}_{j'}\right)\right\}$$

Better expression: possible states of sample/neutron

- You don't know the exact spin states of all of the nuclei or the neutrons

$$\frac{d\sigma}{d\Omega} = \sum_{\lambda,\sigma} p_\lambda p_\sigma \sum_{j'j} \exp\left\{i\vec{Q}\bullet\left(\vec{R}_j - \vec{R}_{j'}\right)\right\}\left\langle \sigma\lambda \middle| b_{j'}^{*} b_j \middle| \sigma\lambda \right\rangle$$

- Marshall and Lovesey (1.16a)

$$\overline{b_{j'}^{*} b_j} = \sum_{\lambda} p_\lambda \left\langle \lambda \middle| b_{j'}^{*} b_j \middle| \lambda \right\rangle \quad \frac{d\sigma}{d\Omega} = \sum_{j'j} \exp\left\{i\vec{Q}\bullet\left(\vec{R}_j - \vec{R}_{j'}\right)\right\} \overline{b_{j'}^{*} b_j}$$

- The dependence on neutron spin averages out

Coherent and Incoherent Parts

- If different atoms there is no correlation between the *'b'* values; otherwise perfect

$$\overline{b_{j'}^{*} b_{j}} = \left|\overline{b}\right|^{2} + \delta_{j,j'}\left(\overline{\left|b\right|^{2}} - \left|\overline{b}\right|^{2}\right)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh}} = \left|\overline{b}\right|^{2}\left|\sum_{j}\exp\left\{i\vec{Q}\bullet\vec{R}_{j}\right\}\right|^{2}$$

Average of *b*
Strict geometry

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{incoh}} = N\left\{\overline{\left|b\right|^{2}} - \left|\overline{b}\right|^{2}\right\} = N\,\overline{\left|b - \overline{b}\right|^{2}}$$

Deviation from
average of *b*

Calculating Coherent and Incoherent Scattering Lengths

- b^+ and b^- are the scattering lengths for total spin equal to I+1/2 and I-1/2 if I is the spin of the nucleus
- the multiplicity of the I+1/2 state is larger than the I-1/2 state
- Multiple isotopes
- x 4π for σ_{coh} etc.

$$\bar{b} = \sum_{\xi} c_{\xi} \frac{1}{2I_{\xi}+1}\left\{(I_{\xi}+1)b_{\xi}^{+} + I_{\xi}b_{\xi}^{-}\right\}$$

$$\overline{|b|^2} = \sum_{\xi} c_{\xi} \frac{1}{2I_{\xi}+1}\left\{(I_{\xi}+1)\left|b_{\xi}^{+}\right|^2 + I_{\xi}\left|b_{\xi}^{-}\right|^2\right\}$$

Practical Examples

- Hydrogen (proton) is a very strong incoherent scatterer (80 b incoh, 1.8 b coh); deuterium much less so (6.0 b, 2.1 b)
- Vanadium-51 has very little coherent scattering (0.03 b) because of a match between b^+ and b^-
- Natural boron, cadmium, gadolinium are strong absorbers

Reciprocal Lattice

- Want $\vec{Q} \bullet \vec{R}_j = 2\pi n$ for coherent scattering.
- This means that $\vec{Q}$ will be a **reciprocal lattice vector.**

$\vec{a}, \vec{b}, \vec{c}$ are lattice vectors $\vec{R}_j = n\vec{a} + m\vec{b} + l\vec{c}$ for a Bravais lattice

$$\vec{A} = 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \bullet \left(\vec{b} \times \vec{c}\right)} \qquad \vec{B} = 2\pi \frac{\vec{c} \times \vec{a}}{\vec{a} \bullet \left(\vec{b} \times \vec{c}\right)} \qquad \vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{a} \bullet \left(\vec{b} \times \vec{c}\right)}$$

$\vec{G}(hkl) = h\vec{A} + k\vec{B} + l\vec{C}$ is the reciprocal lattice

$\vec{Q} = \vec{G}(hkl)$ is Bragg's Law

Non-Bravais: Structure Factor

- Still require **Q=G** but some reflections may be reduced or systematically absent

$$j \text{ atoms in unit cell at positions } \vec{d}_j = d_{j1}\vec{a} + d_{j2}\vec{b} + d_{j3}\vec{c}$$

$$F_N\left(\vec{G}(hkl)\right) = \sum_j \overline{b_j} \exp\left(i\vec{G} \bullet \vec{d}\right)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh}} = N\frac{(2\pi)^3}{v_0} \sum_{\vec{G}(hkl)} \left|F_N(hkl)\right|^2 \delta^3\left(\vec{Q} - \vec{G}(hkl)\right)$$

- V_0 is the volume of the unit cell
- Nuclear structure factor F_N is very useful

Elastic Magnetic Scattering

- Use a similar analysis for magnetism with a different "vector style" interaction

αβ are Cartesian components

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{el}} = (\gamma r_0)^2 \left(\frac{1}{2} g F(\vec{Q})\right)^2 \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2}\right) \times \sum_j \exp\left(i\vec{Q} \bullet \vec{R}_j\right) \left\langle \hat{S}_0^\alpha \right\rangle \left\langle \hat{S}_j^\beta \right\rangle$$

$$F_d(\vec{Q}) = \int \rho_{\text{unpaired } e, d}(\vec{r}) \exp\left(i\vec{Q} \bullet \vec{r}\right) \, d\vec{r}$$

- Also need to include a magnetic form vector
- γ=1.913, r_0=2.82 fm (classical r of electron)

Elastic Scattering: Going Forward

- Although underlying theory can be fairly complex. Most of the time the experimentalist uses “rules of thumb”.
- Although it “looks” hard a lot of key simplifications that make neutron scattering easier to interpret.
- Bragg peaks from coherent scattering
- Nuclear scattering is from “point” objects and neutron spin averages out. Not so for magnetic scattering.