Basic theory I (elastic)

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International/Canadian Neutron Scattering Summer School June 4, 2013
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
• Would count \( N \) particles in \( \Delta t \) seconds \( e=100\% \)
• \( N \) is proportional to \( \Phi, A_{\text{det}}, r^{-2} \)

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

\( D(\text{samp, geo}) \) 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 (4\(\pi\) sr in a sphere, the sun 100 \(\mu\)sr, a spectrometer 100-1000 \(\mu\)sr)

- Differential cross-section is the ratio of count rate to flux per unit solid angle

\[
D(\text{samp,geo}) = \left( \frac{dN/\text{dt}}{\Phi} \right) \frac{d\sigma}{d\Omega} = \text{"d}\sigma\text{"} \frac{d\sigma}{d\Omega}
\]
Simple Estimate of Differential Cross Section (an area)

- Incident flux is $\Phi = 1.0 \times 10^7$ neutrons cm$^{-2}$ s$^{-1}$
- $A_{\text{det}} = 10$ cm$^2$, $r = 100$ cm (0.001 sr), $N = 3000$, $\Delta t = 30$ 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 $\theta$
- Assume azimuthal symmetry
- But you can’t set $b$; you have uniform flux of particles $\Phi$ 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 \( \theta \)

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

• 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

\[
b = \left( \frac{Ze^2}{4\pi\varepsilon_0 E_K} \right) \cot \left( \frac{\theta}{2} \right)
\]

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

\( Z=79, \ E_K=5.3 \text{ MeV}, \ \theta=25^\circ \)

\[
\frac{d\sigma}{d\Omega} = 1.15 \text{ barns}
\]
What determines $\Phi$ 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

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

  \[
  \phi(k_i) dk_i = \frac{dk_i}{k_i} \left( \frac{E_i}{k_B T} \right)^2 \exp \left( - \frac{E_i}{k_B T} \right) \Phi_T = (3\%) \left[ \left( \frac{36}{28.5} \right)^2 \exp \left( - \frac{36}{28.5} \right) \right] \left( 5 \times 10^{14} \text{ cm}^{-2} \text{s}^{-1} \right)
  \]

  \[
  = 6.8 \times 10^{12} \text{ cm}^{-2} \text{s}^{-1}
  \]

- Lower case $\phi$ is a flux “per unit $k$”
Φ Estimate: Discriminate direction

• A solid angle of acceptance (approx)
  Horizontal 0.5° and vertical 2°

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

\[
\Phi_{\text{samp}} = \frac{\phi(k_i) \, dk_i \, d\Omega}{4\pi} = 1.6 \times 10^8 \, \text{cm}^{-2}\text{s}^{-1}
\]

• (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 \( k = \frac{2\pi}{\lambda} \)
- \( f(\theta) \) is the **scattering amplitude** and is a complex number with dimensions of length

\[ \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \]

- \( f(\theta) \) 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 $\propto |c_f(t)|^2 / t$

(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

\[(H + V(t))\Psi(t) = i\hbar \frac{\partial \Psi}{\partial t}\]

- Evolution of “final state” for weak perturbation

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

- 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

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

- The 2nd term $\rightarrow$ a delta-function $\times 2\pi\hbar t$ 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 $d\Omega$)

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

- Transition rate from Squires’ Eqn. 2.2
- $\rho_{\vec{k}_f}$ is the # of final states per unit energy
- $\lambda$ are the labels describing the sample state
- Can also include spin degrees of freedom for the neutron $\sigma$
Cross-section from Transition Rate

\[
\left( \frac{d\sigma}{d\Omega} \right)_{\lambda_i \rightarrow \lambda_f} = \frac{\sum_{\overline{k}_f \text{ in } d\Omega} W_{\overline{k}_i, \lambda_i \rightarrow \overline{k}_f, \lambda_f}}{\Phi} = \frac{1}{\Phi} \frac{1}{d\Omega} \sum_{\overline{k}_f \text{ in } d\Omega} W_{\overline{k}_i, \lambda_i \rightarrow \overline{k}_f, \lambda_f}
\]

• 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” × “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 $d^3k$ and a $dE_f$: how many states are available (box with ‘$L$’)?
Cross-section Result

\[ \# = \rho_k'(E_f) \frac{d^3k_f}{dE_f} dE_f = \left( \frac{L}{2\pi} \right)^3 \frac{k_f^2 dk_f d\Omega}{\hbar^2 k_f} \frac{dE_f}{m} = \left( \frac{L}{2\pi} \right)^3 \frac{mk_f}{\hbar^2} d\Omega dE_f \]

\[ \rho_k'(E_f) = \left( \frac{L}{2\pi} \right)^3 \frac{mk_f}{\hbar^2} d\Omega \]

- Incident flux involves \( L^3 \) as well

\[ \Phi = \frac{\nu_i}{L^3} = \frac{\hbar k_i}{mL^3} \]
Differential Cross-Section

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

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

(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.

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

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

• Or else we need to keep the “cross terms” interference
Fourier Transform of $V$

• Take advantage of the periodicity of the lattice?

\[
V(\vec{r}) = \sum_j V_j(\vec{r} - \vec{R}_j) \quad \vec{x}_j = \vec{r} - \vec{R}_j
\]

\[
\langle \vec{k}_f | V | \vec{k}_i \rangle = \sum_j \int d\vec{r} \exp\left(i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}\right) V(\vec{r} - \vec{R}_j)
\]

\[
\langle \vec{k}_f | V | \vec{k}_i \rangle = \sum_j \int d\vec{x}_j \exp\left(i\vec{Q} \cdot (\vec{x}_j + \vec{R}_j)\right) V(\vec{x}_j)
\]

\[
\langle \vec{k}_f | V | \vec{k}_i \rangle = \sum_j \exp(i\vec{Q} \cdot \vec{R}_j) \int d\vec{x}_j \exp\left(i\vec{Q} \cdot \vec{x}_j\right) V(\vec{x}_j)
\]
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)

\[ \psi_{sc}(\vec{r}) \propto -\frac{b_j}{r} \exp(ik_f r) \]

• This matches earlier formalism with complex scattering length “b” playing the role of \( f(\theta) \).

\[ \frac{d\sigma}{d\Omega} = |b|^2 \]
What potential would give \( b \)?

- Delta-function potential with parameter \( a \)
  
  \[
  V(\vec{r}) = a\delta^3(\vec{r})
  \]

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

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

- 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

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

- Can write the mod-squared as double sum

\[ \left| \langle \vec{k}_f \middle| V \middle| \vec{k}_i \rangle \right|^2 = \left( \frac{2\pi\hbar^2}{m} \right)^2 \sum_{j,j'} b_j^* b_{j'} \exp\{i\vec{Q} \cdot (\vec{R}_j - \vec{R}_{j'})\} \]
Better expression: possible states of sample/neutron

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

\[
\frac{d\sigma}{d\Omega} = \sum_{\lambda,\sigma} p_{\lambda} p_{\sigma} \sum_{j'j} \exp\{i\vec{Q} \cdot (\vec{R}_j - \vec{R}_{j'})\} \langle \sigma\lambda | b_{j'}^* b_j | \sigma\lambda \rangle
\]

- Marshall and Lovesey (1.16a)

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

- The dependence on neutron spin averages out
Coherent and Incoherent Parts

• If different atoms there is no correlation between the ‘$b$’ values; otherwise perfect

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

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

Average of $b$
Strict geometry

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

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
- $x\ 4\pi$ for $\sigma_{\text{coh}}$ etc.

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

$$|b|^2 = \sum_{\xi} c_{\xi} \frac{1}{2I_{\xi} + 1} \left\{ (I_{\xi} + 1)|b_{\xi}^+|^2 + I_{\xi}|b_{\xi}^-|^2 \right\}$$
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 \( \vec{Q} \cdot \vec{R}_j = 2\pi n \) 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

\[
\begin{align*}
\vec{A} &= 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \\
\vec{B} &= 2\pi \frac{\vec{c} \times \vec{a}}{\vec{a} \cdot (\vec{b} \times \vec{c})} \\
\vec{C} &= 2\pi \frac{\vec{a} \times \vec{b}}{\vec{a} \cdot (\vec{b} \times \vec{c})}
\end{align*}
\]

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

\( \vec{Q} = \vec{G}(hkl) \) is Bragg's Law
Non-Bravais: Structure Factor

- Still require $\mathbf{Q} = \mathbf{G}$ but some reflections may be reduced or systematically absent

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

$$F_N\left(\mathbf{G}(hkl)\right) = \sum_j b_j \exp\left(i\mathbf{G} \cdot \mathbf{d}\right)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh}} = N \left(\frac{2\pi}{\nu_0}\right)^3 \sum_{\mathbf{G}(hkl)} \left|F_N(hkl)\right|^2 \delta^3(\mathbf{Q} - \mathbf{G}(hkl))$$

- $\nu_0$ 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

\[
\frac{d\sigma}{d\Omega} = (\gamma_0)^2 \left( \frac{1}{2} g F(\bar{Q}) \right)^2 \sum_{\alpha\beta} \left( \delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2} \right) \times \sum_j \exp (i \bar{Q} \cdot \bar{R}_j) \langle \hat{S}_0^\alpha \rangle \langle \hat{S}_j^\beta \rangle
\]

\[
F_d (\bar{Q}) = \int \rho_{\text{unpaired} \, e, d} (\bar{r}) \exp (i \bar{Q} \cdot \bar{r}) \, d\bar{r}
\]

- Also need to include a magnetic form vector
- \( \gamma = 1.913, \ r_0 = 2.82 \) 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.