The Interaction of Radiation with Matter: Neutron Interactions

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IEEE Short Course

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Session 3

- Neutron interaction types
  - Scattering
  - Absorption
- Differential scattering cross sections
- Scattering kinematics
- The transport and diffusion equations
- Data resources

Neutron Interaction Types

- Scattering, σ_s
  - Elastic, σ_e
  - Inelastic, σ_{in}
- Absorption , σ_a
  - Capture, σ_γ
  - Fission, σ_f
  - Neutron products, $\sigma_{n,2n}$,…
  - Charged-particle products, $\sigma_{n,p}$, $\sigma_{n,\alpha}$,…

Another View

- Potential scatter (neutron scatters from the nuclear potential) – always elastic scattering
- Compound nucleus formation (tends to occur when neutron energy "matches" a nuclear energy state; thus resonance behavior)
  - Elastic scattering, ${}_Z^AX\left(n,n\right){}_Z^AX$
  - Inelastic scattering, ${}_Z^AX\left(n,n'\right){}_Z^AX^*$
  - Particle emission, ${}_Z^AX\left(n,x\right){}_Z^AX$, where x can be p, d, α, γ, 2n, etc.
  - Fission
- Interference scatter, in between potential and compound nucleus

Neutron Scattering

- Elastic scattering ($Q = 0$)
  - "Potential" scattering from the nuclear potential without entering the nucleus
  - Compound-nucleus scattering in which the neutron enters the nucleus and is expelled with the nucleus still in the ground state
- Inelastic scattering ($Q < 0$)
  - Compound-nucleus scattering in which the neutron enters the nucleus and is expelled with the nucleus in an excited state; neutron KE is given to the nucleus

Neutron Capture

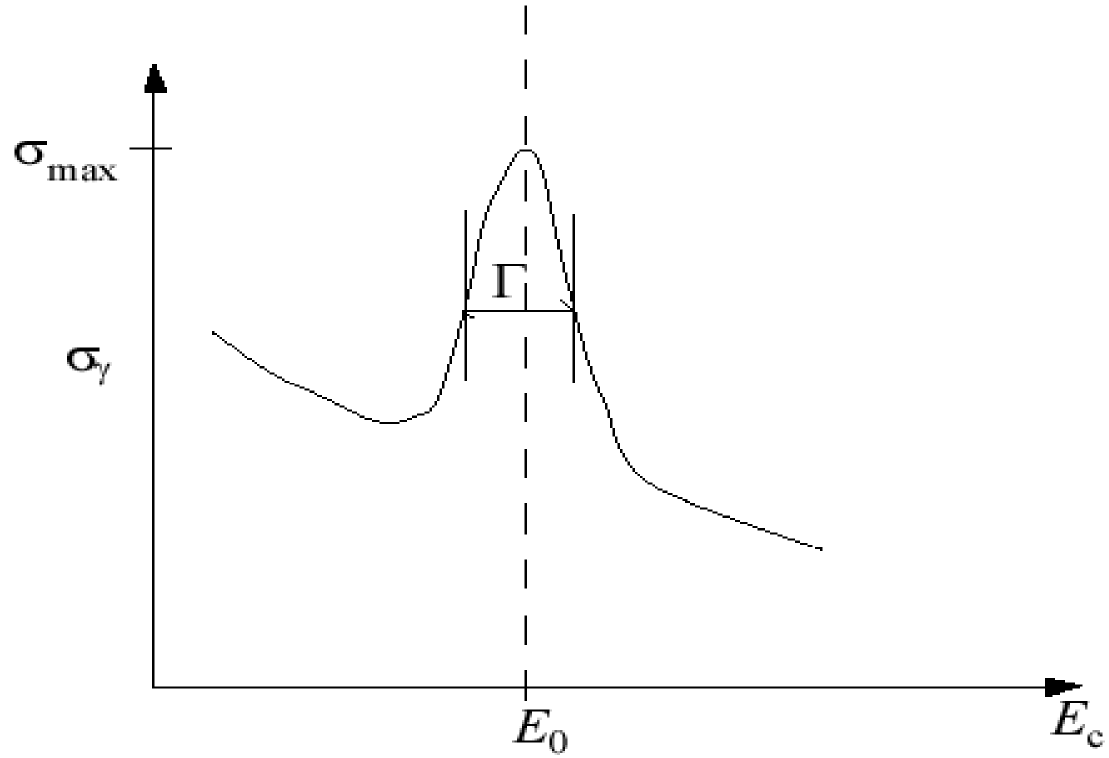
- Compound nucleus is formed and decays to ground state by emission of one or more gammas
- Significant in reactors because resonances create large cross sections for removal of neutrons
- For isolated resonances, Breit-Wigner formula

$$\sigma_\gamma(E_c) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\left(\frac{E_0}{E_c}\right)^{1/2} \frac{1}{1+y^2}, \; y = 2\frac{E_c - E_0}{\Gamma}$$

Isolated Capture Resonance

- E_c is neutron energy
  E_0 is energy of the resonance
  Γ is total line width or FWHM
  Γ_γ is the radiative line width

$$\sigma_0 = \sigma_{\max}\frac{\Gamma}{\Gamma_\gamma}$$

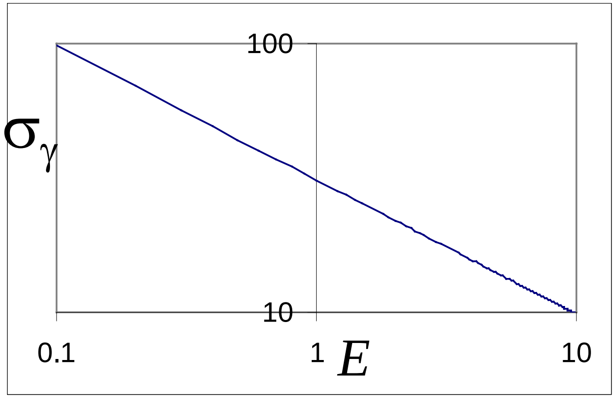


Neutron Cross Sections

- Macroscopic cross section
  - Σ = probability of interaction per unit path length
  - Has units of cm^{-1}
- Microscopic cross section
  - $\sigma = \frac{\Sigma}{N} =$ probability of interaction per unit path length *per atom per unit volume*
  - Unit is cm^2 or b, where 1 b = 10^{-24} cm^2

Energy Dependence

- Elastic is fairly constant with energy (with exceptions for p-type interactions)
- Inelastic is fairly constant but has resonances close to nuclear excited states
- Capture cross sections often 1/*v* at thermal and epithermal energies
- Some reactions occur only above a threshold energy (see Fig. 2-18 in text)

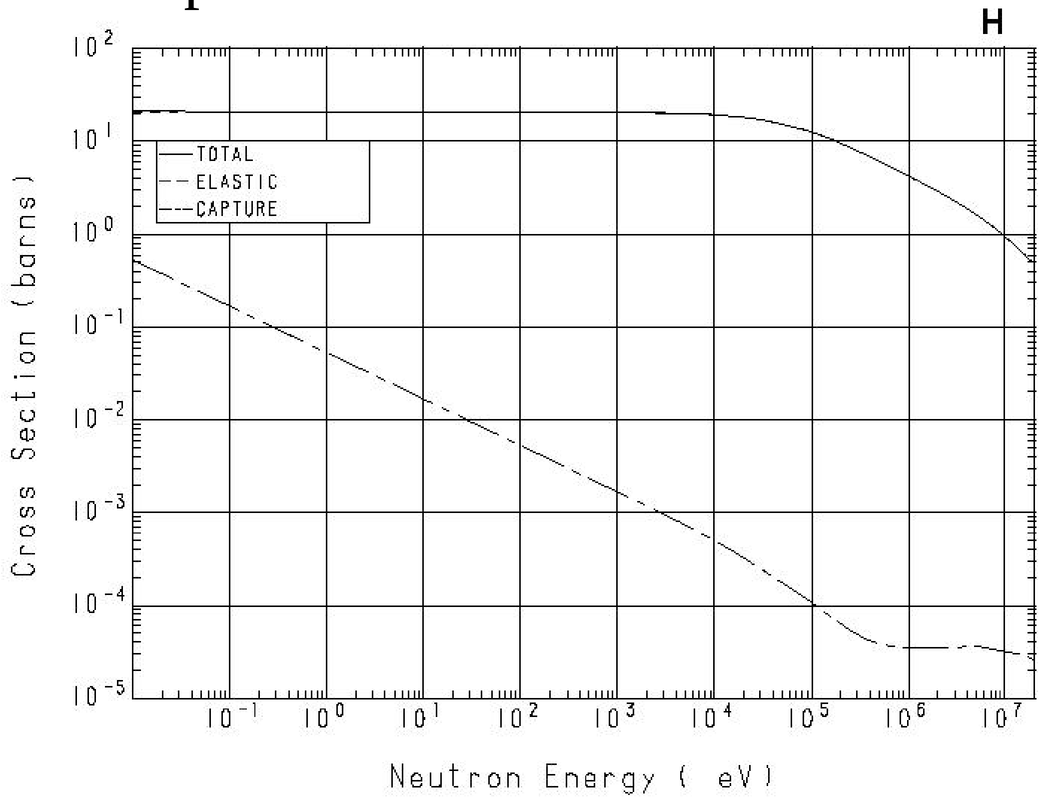


$$1/v \propto 1/\sqrt{E}$$

Hydrogen Cross Sections

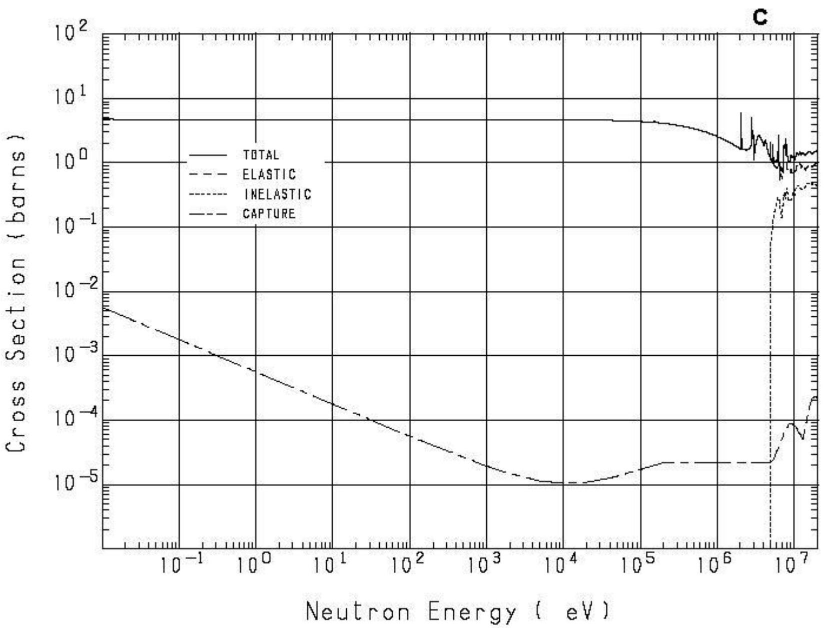
Notes: Elastic and total almost indistinguishable

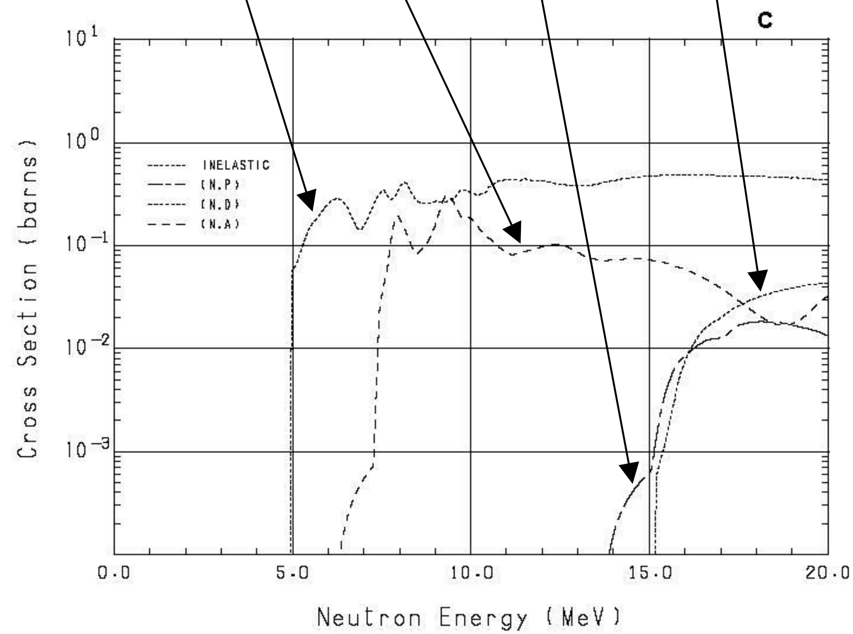
Capture cross section behaves as $1/v$



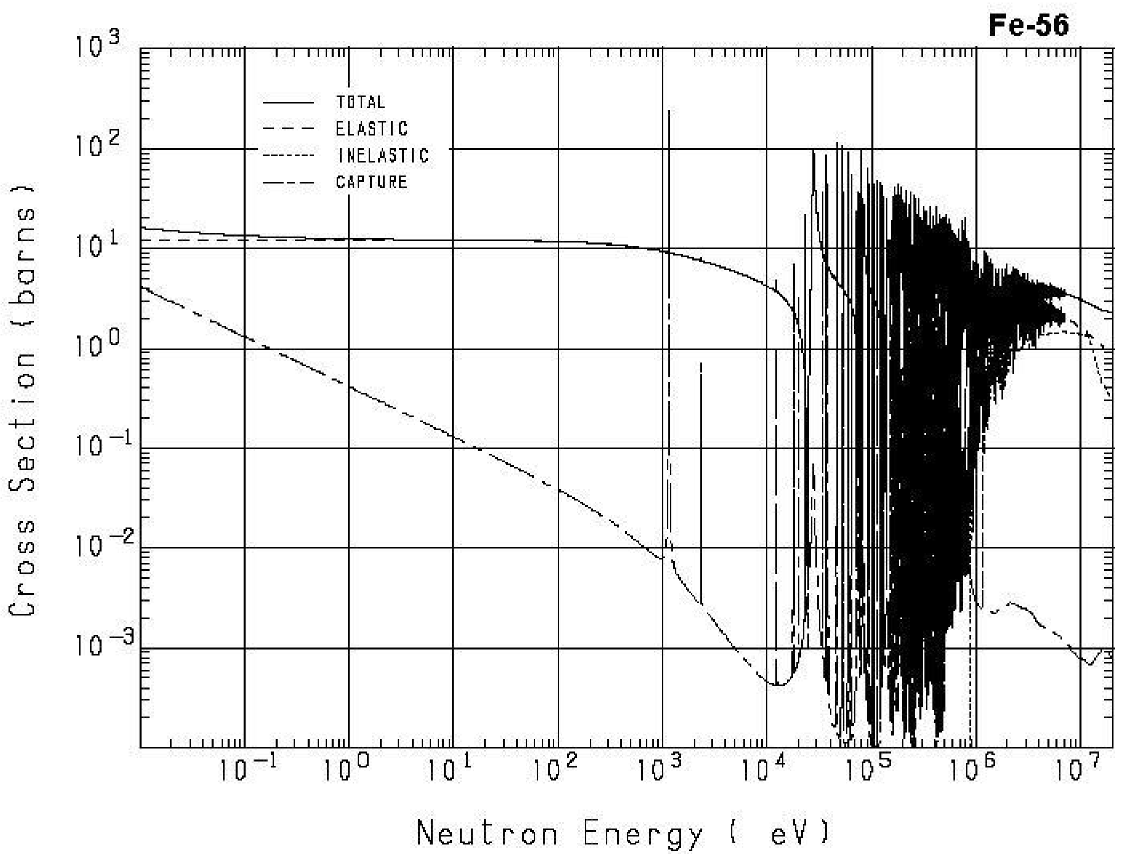
Carbon Cross Sections

Note thresholds: inelastic, (n,α), (n,p), (n,d)





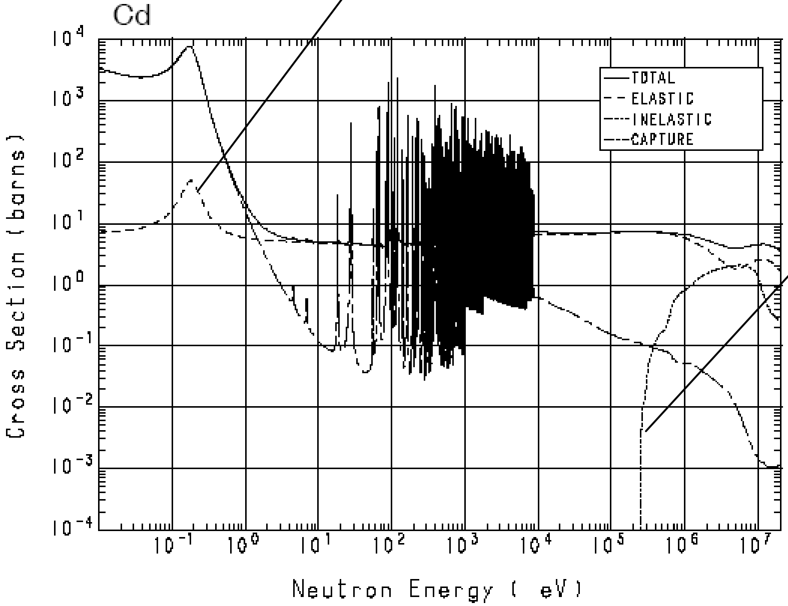
Iron-56 Cross Section



Cadmium Cross Sections

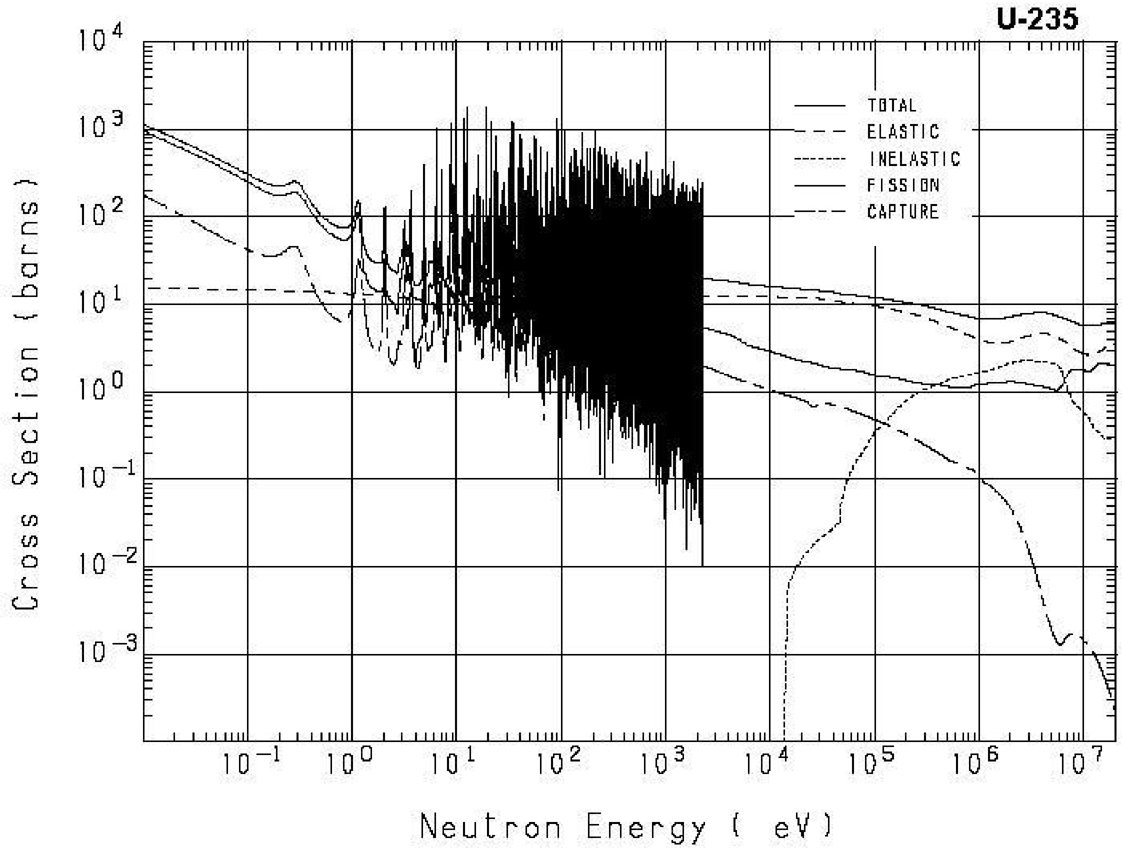
Note: elastic cross section is fairly constant with energy except for one broad resonance

capture cross section is roughly 1/v at low energy and has many resonances from about 10 eV to 10 keV



Inelastic cross section exhibits a threshold at about 250 keV

U-235 Cross Sections



Scattering Cross Sections

- The microscopic scattering cross section can, in principle, be a function of position, energy, and direction
- However, it is almost always true that there is no appreciable dependence on the **incident** neutron direction since nuclei are usually randomly oriented (there often is a dependence on the **change** in direction)
- Thus $\sigma_s(\mathbf{r}, E)$ is the scattering cross section at energy E irrespective of neutron direction
- We rarely have to write $\sigma_s(\mathbf{r}, E, \mathbf{\Omega})$ or $\sigma_s(\mathbf{r}, \mathbf{\Omega})$

Doubly Differential Cross Section

- We interpret $\sigma_s\left(\mathbf{r}, E \to E', \boldsymbol{\Omega} \to \boldsymbol{\Omega}'\right) dE' d\Omega'$ to be the probability per unit differential path length that a neutron of initial energy E and direction $\boldsymbol{\Omega}$ will scatter at $\mathbf{r}$ into a final energy within dE' about E' and a final direction within $d\Omega'$ about $\boldsymbol{\Omega}'$, normalized to one atom per cm^3
- This is called the doubly differential scattering cross section

Differential Cross Sections

- The total scattering cross section is just

$$\sigma_s(\mathbf{r}, E) = \int_{4\pi} \int_0^\infty \sigma_s(\mathbf{r}, E \to E', \boldsymbol{\Omega} \to \boldsymbol{\Omega}') \, dE' d\Omega'$$

- Similarly,

$$\sigma_s(\mathbf{r}, E, \boldsymbol{\Omega} \to \boldsymbol{\Omega}') = \int_0^\infty \sigma_s(\mathbf{r}, E \to E', \boldsymbol{\Omega} \to \boldsymbol{\Omega}') \, dE'$$

$$\sigma_s(\mathbf{r}, E \to E') = \int_{4\pi} \sigma_s(\mathbf{r}, E \to E', \boldsymbol{\Omega} \to \boldsymbol{\Omega}') \, d\Omega'$$

are the (singly) differential scattering cross sections

Probability Density Function

- A function $f(x)$ is a probability density function (PDF) if
  - It is defined on an interval $[a,b]$
  - It is non-negative on the interval
  - It is normalized such that $\int_a^b f(x)\,dx = 1$
- $f(x)dx$ = probability that a random sample from f will be within dx about x

Alternative Formulation

- We can express the singly differential cross sections

$$\sigma_s(r,E,\mathbf{\Omega}\to\mathbf{\Omega}') = \sigma_s(r,E)\, f_{\Omega}(\mathbf{\Omega}\to\mathbf{\Omega}')$$

$$\sigma_s(r,E\to E') = \sigma_s(r,E)\, f_E(E\to E')$$

where $f_E(E\to E')$ and $f_{\Omega}(\mathbf{\Omega}\to\mathbf{\Omega}')$ are PDFs

- This notation separates the cross section (with units of area) from the probability density
- f_E has units of MeV^{-1}, f_{Ω} has units of sr^{-1}
- Thus $\sigma_s(r,E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')$ has units cm^2 MeV^{-1} sr^{-1}

Rotational Invariance

- It is almost always true that
  - Scattering and azimuthal angles are independent
  - The probability of scattering from one direction to another is dependent only on the cosine of the scattering angle

$$f\left(\mathbf{\Omega} \to \mathbf{\Omega}'\right) = f\left(\mathbf{\Omega} \bullet \mathbf{\Omega}'\right) f_{\psi}\left(\psi\right) = \frac{1}{2\pi} f_{\omega}\left(\omega_s\right)$$

  - where

$$\omega_s = \cos\theta_s$$

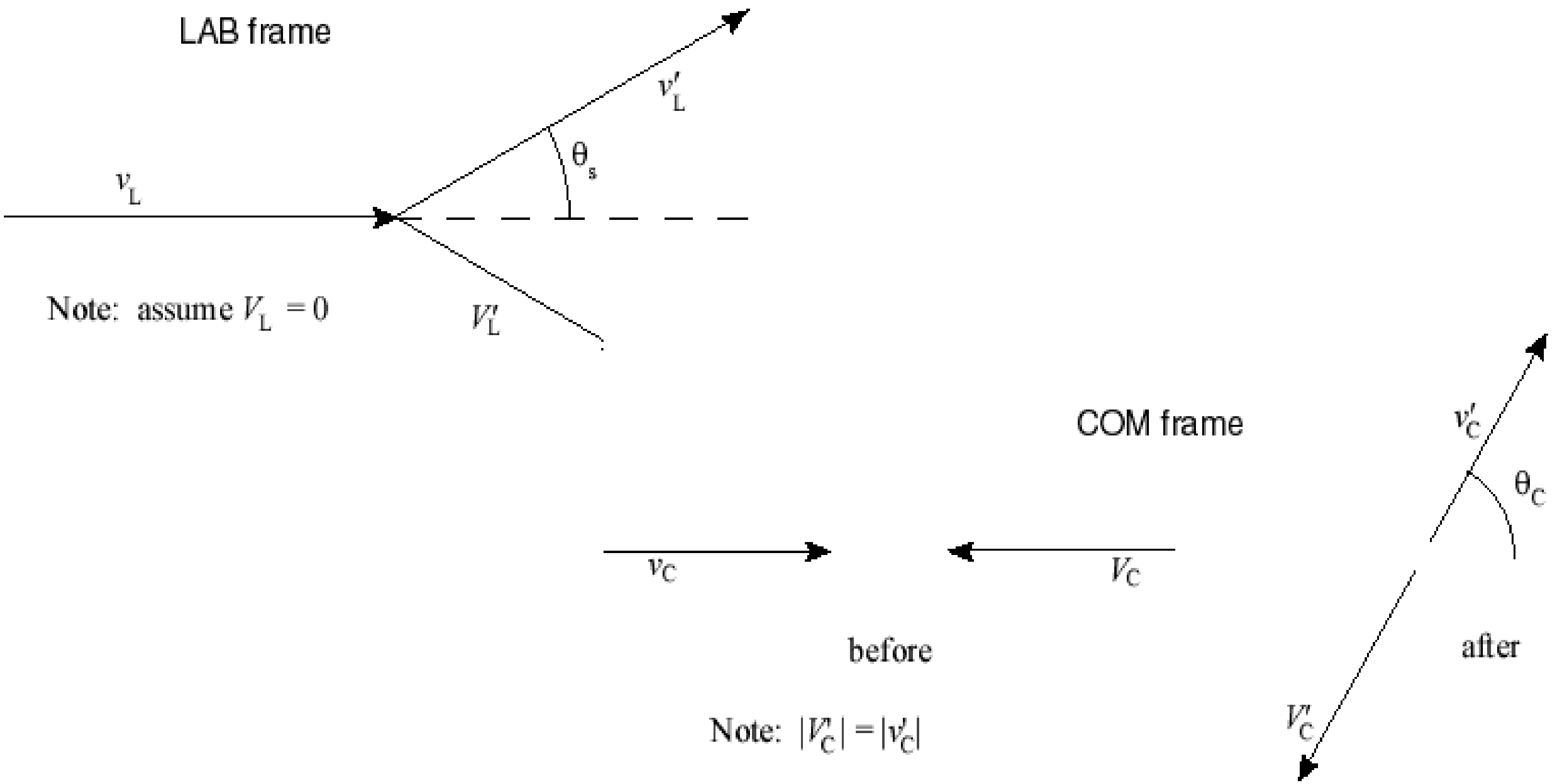
Simplification

- Because of rotational invariance, we often write

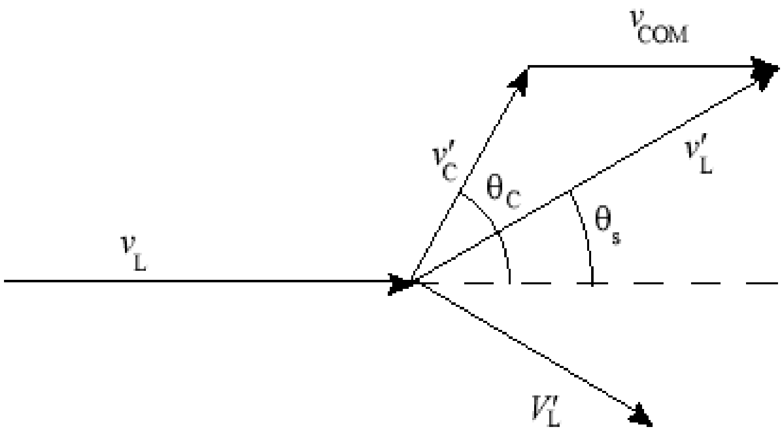
$$\sigma_s\left(\mathbf{r}, E \to E', \mathbf{\Omega} \to \mathbf{\Omega}'\right) = \sigma_s\left(\mathbf{r}, E\right)\frac{1}{2\pi} f\left(E \to E', \omega_s\right)$$

- Note θ_s is the scattering angle in the LAB system
- Neutron scattering is generally not isotropic in the LAB system but generally is isotropic in the COM system

LAB and COM Systems



Relationship between Systems



The velocities in the LAB and COM systems are related through the velocity of the center of mass v_{COM}

Elastic Scattering

- For elastic scattering, we can apply
  - Conservation of energy
  - Conservation of momentum
- Then it can be shown that

$$\tan\theta_s = \frac{\sin\theta_c}{\frac{1}{A} + \cos\theta_c}$$

- θ_s is scatter angle in LAB system, θ_c is scatter angle in COM system, and *A* is atomic mass of the nucleus

Elastic Scattering in COM System

- This can be rewritten as

$$\boxed{\omega_s = \frac{1 + A\omega_c}{\sqrt{A^2 + 2A\omega_c + 1}}}$$

- Elastic scattering usually is isotropic in the COM frame; thus

$$f(\omega_c) = \frac{1}{2}, \ -1 \le w_c \le 1$$

and we use the relation above to obtain ω_s

Inelastic Scatter in COM Frame

- For inelastic scattering,

$$\omega_s = \frac{\gamma + \omega_C}{\sqrt{\gamma^2 + 2\gamma\omega_C + 1}}$$

where

$$\gamma = \frac{v_{COM}}{v'_C} = \left[A^2 + \frac{A\left(A+1\right)Q}{E} \right]^{-1/2}$$

with Q the Q-value of the interaction

- Note $\gamma \rightarrow 1/A$ as $Q \rightarrow 0$ and the above reduces to the previous formula for elastic scattering

Scatter-angle/Energy Relationship

- There is a one-to-one relationship between scattering angle and energy loss
- A neutron that scatters through a small angle loses little energy compared to one that scatters through a large angle
- Let E be the energy before the scatter, E' be the energy after the scatter, and define

$$\alpha = \left(\frac{A-1}{A+1} \right)^2$$

Elastic Scatter

- For elastic scattering, we find

$$E' = \frac{A^2 + 2A\cos\theta_c + 1}{(A+1)^2} E$$

- Also, for isotropic scatter in the COM frame (s-wave scattering)

$$f(E \rightarrow E') = \frac{1}{(1+\alpha)E}, \ \alpha E \le E' < E$$

$$= 0, \text{ otherwize}$$

Alternative Formulation

- The doubly differential scattering cross section alternatively can be written

$$\sigma_s\left(\mathbf{r}, E \to E', \Omega' \to \Omega\right) = \frac{1}{2\pi}\sigma_s\left(\mathbf{r}\right) f\left(E \to E'\right)\delta\left(\omega_s - S\left(E, E'\right)\right)$$

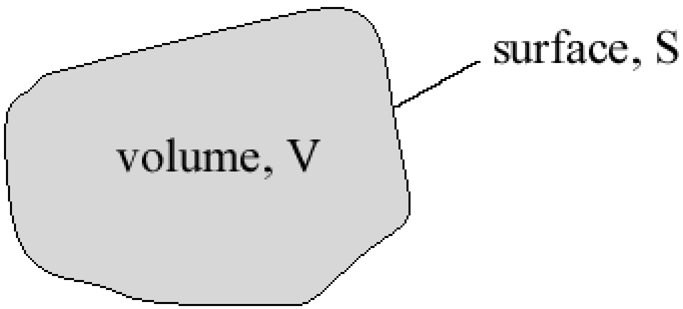
where

$$S\left(E, E'\right) = \frac{1}{2}\left[\left(A+1\right)\sqrt{\frac{E}{E'}} - \left(A-1\right)\sqrt{\frac{E'}{E}}\right]$$

- The delta function sifts the appropriate value of ω_s given the final energy

The Neutron Transport Equation

- Consider an arbitrary volume *V* bounded by surface *S*



- Assume the volume *V* does not change with time

Further Assumptions

- Neutron decay can be ignored (~10 minute half life)
- The neutron can be treated as a point particle (thermal neutron wavelength is ~4.5×10^{-9} cm, small with respect to inter-atomic distances and very small respect to macroscopic distances)
- Interactions with electrons are negligible
- Neutron-neutron interactions can be ignored
- Neutron-nuclei interactions are point interactions
- Can ignore effects of spin, magnetic moment, gravity

NTE Derivation

- From the previous definition of neutron density

$$\frac{\partial}{\partial t}[dEd\Omega\int_V n(\mathbf{r},E,\Omega,t)d^3r] =$$

The time rate of change of the density of neutrons within volume *V* that have energies within *dE* about *E* and direction within $d\Omega$ about $\mathbf{\Omega}$ at time *t*

Gains and Losses

- This rate of change is related to the rate of gains and losses
- Replace n by $\dfrac{\varphi}{v}$
- Since V is constant, we can interchange the order of differentiation and integration and obtain

$$\boxed{\frac{dEd\Omega}{v}\int_V \frac{\partial}{\partial t}\varphi(\mathbf{r},E,\Omega,t)d^3r = \text{rate of gain in } V \text{ - rate of loss in } V}$$

Gain Mechanisms

- Neutron sources within V that emit neutrons into dE about E and $d\Omega$ about $\mathbf{\Omega}$,
- neutrons having energies within dE about E and directions within $d\Omega$ about $\mathbf{\Omega}$ that stream into V through S
- neutrons within V having energy E' and direction $\mathbf{\Omega}'$ that scatter into energy within dE about E and direction within $d\Omega$ about $\mathbf{\Omega}$.

Loss Mechanisms

- neutrons having energies within dE about E and directions within $d\Omega$ about $\mathbf{\Omega}$ that stream out of V through S
- neutrons having energies within dE about E and directions within $d\Omega$ about $\mathbf{\Omega}$ that interact within V
  - absorption removes neutrons but scattering also removes them from the specific energy and direction intervals they occupied

Sources

- Define the source rate s such that

$s(\mathbf{r}, E, \Omega, t)d^3 r dE d\Omega =$ rate at which neutrons are introduced into d^3r about $\mathbf{r}$ with energies within dE about E and moving in directions within $d\Omega$ about Ω at time t

- Thus

$\int_V s(\mathbf{r}, E, \Omega, t)d^3 r dE d\Omega =$ rate at which neutrons are introduced into V with energies within dE about E and moving in directions within $d\Omega$ about $\mathbf{\Omega}$ at time t

Intermediate Result

- We have established

$$\frac{dE\,d\Omega}{v}\int_V \frac{\partial}{\partial t}\varphi(\mathbf{r},E,\Omega,t)\,d^3r = \text{(source rate + streaming-in rate}$$

+ in-scatter rate – streaming-out rate - interaction rate) of neutrons within dΩ about and *dE* about *E* in *V* at time *t*

- Substitute appropriate forms and use Gauss' theorem relating volume and surface integrals of vector quantities

The Neutron Transport Equation

- Eventually, we obtain the integro-differential form of the neutron transport equation (NTE)

$$\frac{1}{v}\frac{\partial \varphi\left(\mathbf{r},E,\mathbf{\Omega},t\right)}{\partial t}+\mathbf{\Omega}\bullet\vec{\nabla}\varphi\left(\mathbf{r},E,\mathbf{\Omega},t\right)+\Sigma_t\varphi\left(\mathbf{r},E,\mathbf{\Omega},t\right)=$$

$$\int_{4\pi}\int_0^\infty \Sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega})\varphi(\mathbf{r},E',\mathbf{\Omega}',t)dE'd\Omega'+s\left(\mathbf{r},E,\mathbf{\Omega},t\right)$$

- This can be expressed simply as 1/*v* times the time rate of change of φ = source rate + in-scattering rate
  - net leakage rate – removal rate

Integral Form of the NTE

- A general case of the integtral form can be written

$$\varphi\left(\mathbf{r},E,\hat{\mathbf{\Omega}}\right)=\int_V\int_0^\infty\int_{4\pi}L\left(\mathbf{r},\mathbf{r}',E,\mathbf{\Omega}\right)\Sigma_s\left(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega}'\right)\varphi\left(\mathbf{r}',E',\mathbf{\Omega}'\right)d\Omega'dE'd^3r'+$$
$$\int_V L\left(\mathbf{r},\mathbf{r}',E,\mathbf{\Omega}\right)s\left(\mathbf{r}',E,\mathbf{\Omega}\right)d^3r'$$

where

$$L\left(\mathbf{r},\mathbf{r}',E,\mathbf{\Omega}\right)=\frac{e^{-\Sigma_t(E)|\mathbf{r}-\mathbf{r}'|}}{\left|\mathbf{r}-\mathbf{r}'\right|^2}\delta\left[\mathbf{\Omega}-\frac{\mathbf{r}-\mathbf{r}'}{\left|\mathbf{r}-\mathbf{r}'\right|}\right]$$

and the two-dimensional delta function is defined such that

$$\int_{4\pi}\delta\left(\mathbf{\Omega}-\mathbf{\Omega}_0\right)f\left(\mathbf{\Omega}\right)d\Omega=f\left(\mathbf{\Omega}_0\right)$$

Neutron Diffusion Equation

- Under the diffusion approximation (that the angular flux density can be expressed as a two-term expansion in spherical harmonics) and a few other assumptions, the NTE can be reduced to the neutron diffusion equation

$$\frac{1}{v}\frac{\partial\varphi\left(\mathbf{r},Et\right)}{\partial t}+\vec{\nabla}\bullet D\left(\mathbf{r},E\right)\vec{\nabla}\varphi\left(\mathbf{r},E,t\right)+\Sigma_a(\mathbf{r},E)\varphi\left(\mathbf{r},Et\right)=s_0\left(\mathbf{r},Et\right)$$

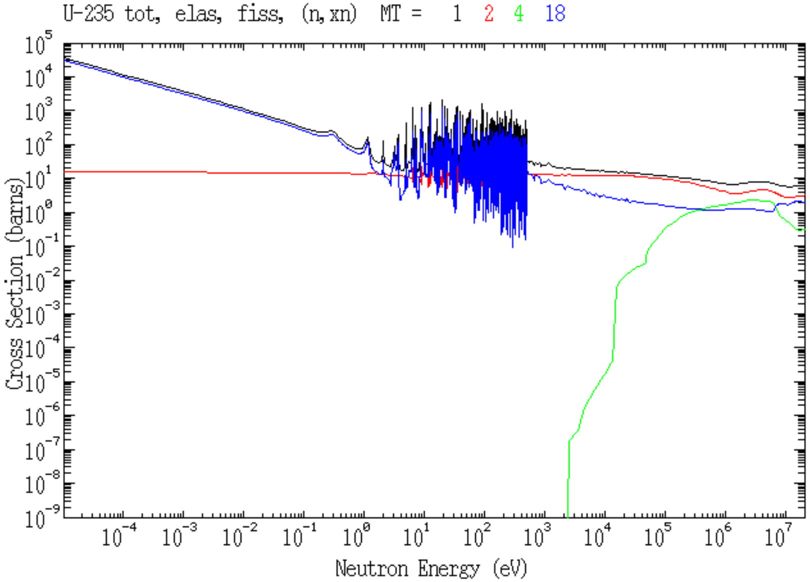
where D is known as the diffusion coefficient

Neutron Cross Section Data

- It is very important to have detailed cross section data files, because of the resonances and thresholds in neutron cross sections
- A well-known data set is called the ENDF (Evaluated Nuclear Data File) cross section file
- It is available at the National Nuclear Data Center at Brookhaven National Laboratory at **http://www.nndc.bnl.gov/**

Alternative Neutron Data Files

- Another excellent evaluated neutron data file is available from the Japan Atomic Energy Research Institute
- It is called the JENDL file, which is available on the world wide web



http://wwwndc.tokai-sc.jaea.go.jp/jendl/jendl.html

Review of Transport Calculations

- Various forms of transport equations exist for the various types of radiation
- They cannot all be solved by the same techniques
- Thus, we have a suite of methods for calculating quantities such as detector response, dose, etc.
- Note that most quantities of interest depend on interaction rates and thus we often seek flux density or fluence

General Approaches

- For photons and sometimes for neutrons, we can use approximate buildup and albedo schemes
- These involve calculating the uncollided flux at a point or in a region (at a distance *d* from a point source in a uniform medium, the uncollided flux is simply $\varphi^{(0)}(d) = S_0 \frac{e^{-\Sigma d}}{4\pi d^2}$
- Then the total flux can be estimated as

$$\varphi(d) = B(d)\varphi^{(0)}(d)$$

Numerical Schemes

- There are several numerical schemes for solving transport and diffusion equations, such as
  - Discrete ordinates (consider the flux at discrete positions, use a quadrature to estimate the in-scattering integral, and numerically solve a system of algebraic equations in terms of the finite unknown flux values
  - Function expansion methods, such as S_n, which reduce to finding a finite number of expansion coefficients
  - Order-of-scatter approaches (find uncollided flux, then use as a source to find once-collided flux, etc.)

Monte Carlo Methods

- Since flux densities can be considered to be expected values, we can use Monte Carlo simulation techniques
- Monte Carlo is based on the law of large numbers (Bernoulli, 1713, in *Ars Conjectandi* or "The Art of Conjecturing") and the central limit theorem
- The power of MC is that the standard deviation in the estimate varies at worst as $1/N^{1/2}$

What is Monte Carlo?

- MC is a powerful form of ***quadrature***
  - Estimates expected value integrals
  - Applies to problems of arbitrary dimensionality
  - Highly flexible and adaptable
- MC is also a means of ***simulation***
  - Conduct numerical “experiments” to estimate outcomes of complex processes
  - Experiments run on a computer, dart board, etc.
  - Highly intuitive

Law of Large Numbers

- It can be shown that, almost surely,

$$\bar{x} = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} x_i = \int_a^b x f(x)\,dx = \langle x \rangle$$

  i.e., the sample mean eventually approaches the population mean

- The central limit theorem can be used to estimate how large must *N* be to achieve a desired precision

Some General-Purpose MC Codes

- MCNP (comes in various flavors) – coupled neutron, photon, electron transport
  - **http://www-rsicc.ornl.gov/**
- EGSnrc or EGS4 – coupled photon, electron transport
  - **http://www.irs.inms.nrc.ca/EGSnrc.html**
- GEANT – object-oriented code for treating various radiation types over broad energy ranges
  - **http://geant4.web.cern.ch/geant4/**

Other General-purpose MC Codes

- PENELOPE – coupled photon, electron transport
  - **http://www.nea.fr/html/dbprog/peneloperef.html**
- MCSHAPE – photon transport accounting for polarization
  - **http://shape.ing.unibo.it/**
- SRIM – the Stopping and Range of Ions in matter; performs heavy charged particle transport and contains extensive stopping power data
  - **http://www.srim.org/**