Fundamentals of Nuclear Engineering

Module 5: *Neutron Thermalization*

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Atomic and Nuclear Physics	Basics of Atomic vs. Nuclear structure, definitions of terms used in future modules
Radioactive Decay	Describes radioactive decay processes, half-life vs. decay rate used in future modules
Neutron Induced Reactions	Describes concept of cross sections, neutron induced reaction rates
Nuclear Fuels, Neutron Sources Absorbers, Neutron Poisons	Describes fissionable fuels, neutron sources, absorber materials, and fission product poisons impacting chain reactions
Neutron Thermalization	Describes process of neutron moderation used in thermal reactors, identifies impact of resonance capture which impacts chain reactions
Neutron Diffusion	Describes neutron diffusion model used to analyze chain reactions and other future reactor problems

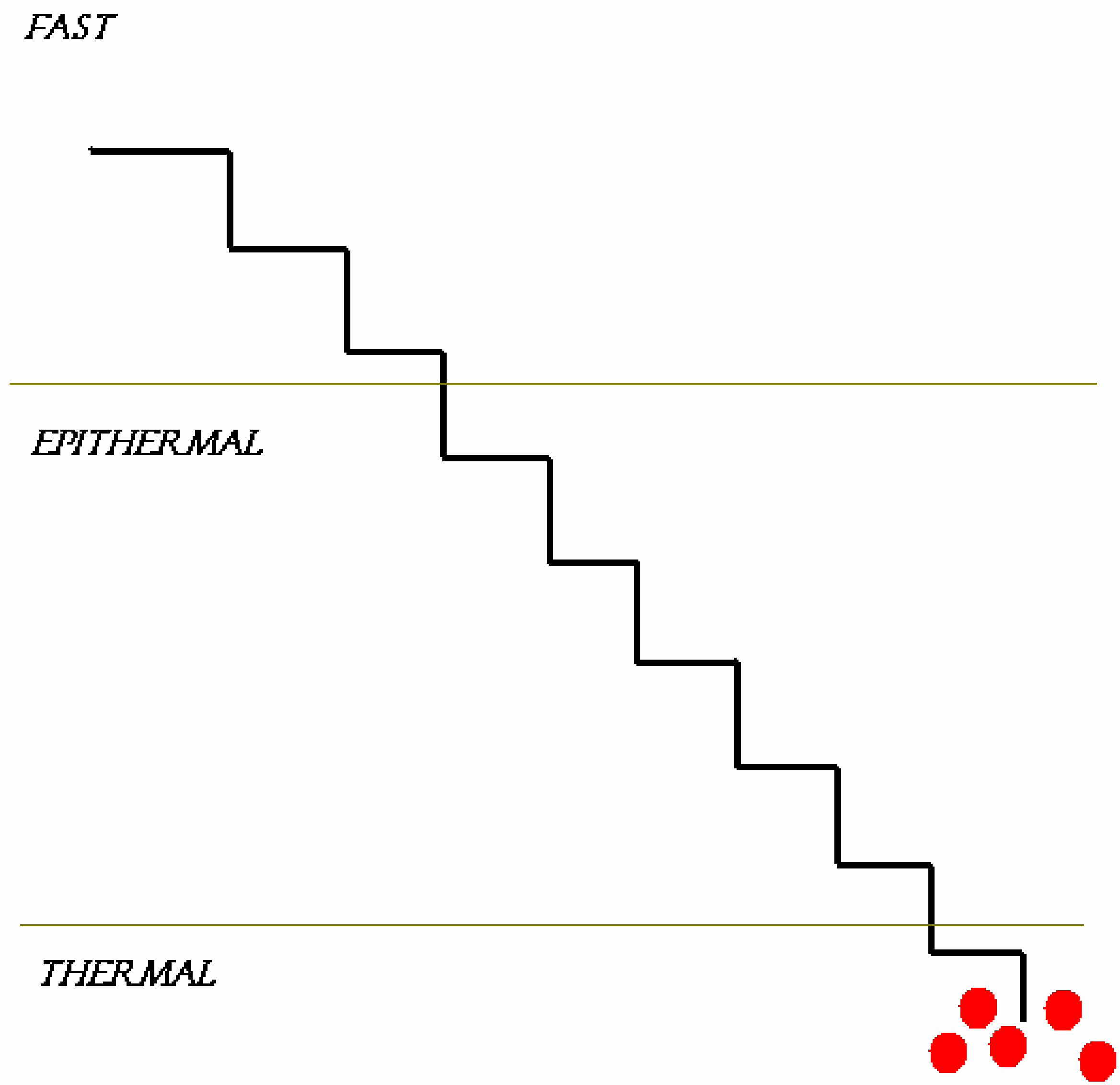
Objectives:

Previous lectures pointed out that fission rate is highest for thermal neutrons (<0.01 eV). This lecture will:

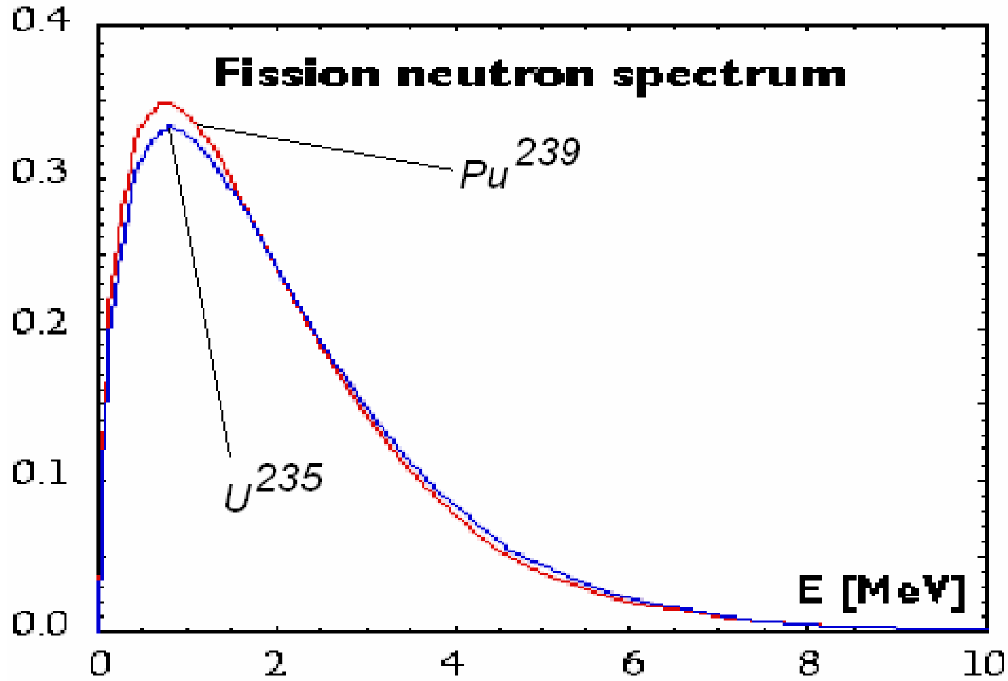
1. Explain process of how 1MeV fission neutrons slow down to <0.01 eV with/without resonance capture
2. Explain *energy transfer* via elastic neutron collisions
3. Explain effect of moderator atomic mass (A) on rate of neutron thermalization
4. Explain effects of neutron capture during slowing down

Neutron Thermalization Can Be Envisioned As Ball Bouncing Down Stairs

- Neutron born at >1 MeV
- First collision occurs
- Neutron enters Epithermal region where resonance capture likely
- Not all neutrons get through
- Neutrons reaching thermal region tend to pile up until absorbed by fissionable material



Fission Neutrons Emitted in >1 MeV Range



- *U^{235}* fission rate higher for thermal neutrons (<<1eV) than for 1MeV fission neutrons
- 1Mev neutron travels at ~*$1.38x10^7$ meters/sec* (or: 0.04c)
- Slowing down fission emitted neutrons to thermal energies increases fission reaction rate
- Principle way to *slow down neutrons* is via *collisions*

Kinematics of Knock-on Collision

- Head-on collision: one dimensional collision with neutron and nucleus recoil in opposite directions.
- Glancing collisions are *slightly more complicated* two dimensional events
- Understanding one dimensional events is starting point
- Assuming neutron mass: m traveling at velocity: v
- Relatively stationary nucleus mass: M
- Energy and momentum are conserved

  Energy: $\frac{1}{2}mv^2 + \frac{1}{2}MV^2 = \frac{1}{2}mv^{2\prime} + \frac{1}{2}MV^{2\prime}$

  Momentum: $mv + MV = mv' + MV'$

Kinematics of Knock-on Collision

- Rearranging energy conservation equation:

$$\tfrac{1}{2}mv^2 - \tfrac{1}{2}mv^{2'} = \tfrac{1}{2}MV^{2'} - \tfrac{1}{2}MV^2$$

$$m(v^2 - v^{2'}) = M(V^{2'} - V^2)$$

- Rearranging momentum conservation equation:

$$mv + MV = mv' + MV'$$

$$m(v - v') = M(V' - V)$$

- Dividing energy conservation equation with momentum equation yields:

$$\frac{m(v^2 - v^{2'})}{m(v - v')} = \frac{M(V^{2'} - V^2)}{M(V' - V)}$$

- Or: $v + v' = V' + V$

Kinematics of Knock-on Collision

- Final speed of recoiling nucleus: $V' = (v + v') - V$
- Substitute this in momentum conservation equation:

$$m(v - v') = M(v + v' - 2V)$$

$$-mv' - Mv' = -mv + Mv - 2MV$$

$$(m + M)v' = (m - M)v + 2MV$$

- Solving for v' yields:

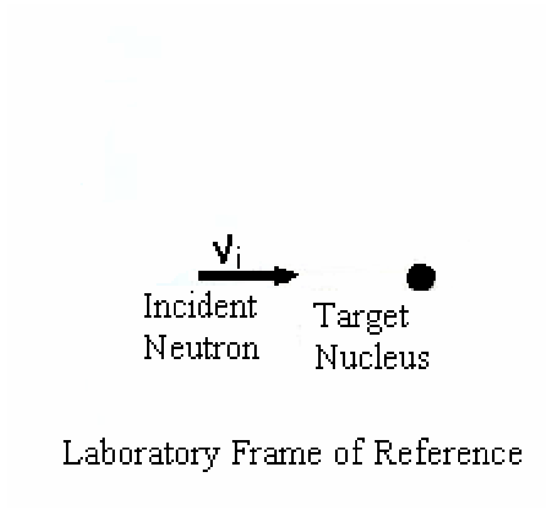
$$v' = (m-M)/(m+M)v + 2m/(m+M)V$$

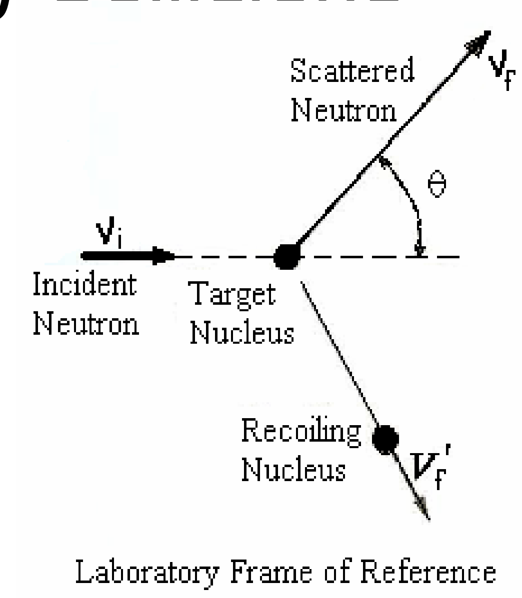
- Kinetic energy of neutron before collision: $E = ½mv^2$
- Kinetic energy of neutron after collision: $E' = ½mv'^2$
- If target nucleus initially at rest: $V \sim 0$, $v' = (m-M)/(m+M)v$
- Kinetic energy after collision is: $E' = ½mv^2 [(m-M)/(m+M)]^2$

Kinematics of Knock-on Collision

- Kinetic energy after collision *E'* is related to initial kinetic energy *E* via factor: $\alpha = [(m\text{-}M)/(m+M)]^2$
- Thus: $E' = \alpha E$
- As further simplification convert to AMU units
- For neutron: $m = 1$,
- For target nucleus: $M = A$,
- Then: $\alpha = [(A\text{-}1)/(A+1)]^2$
- We can now evaluate effectiveness of different nuclei for slowing down neutrons

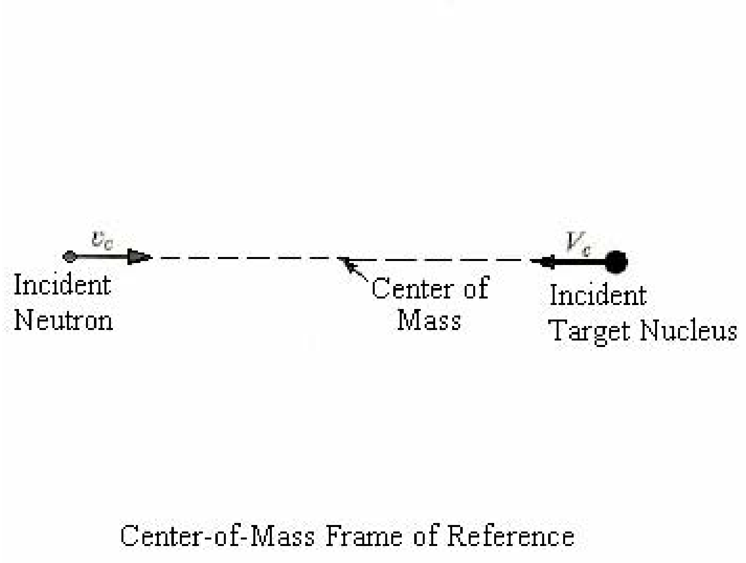
Kinematics of Glancing Collisions

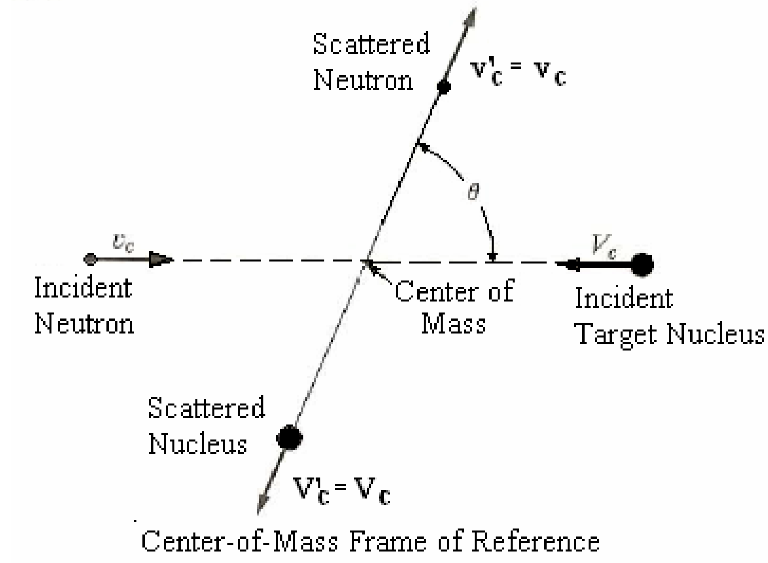




- Viewed from Laboratory Reference Frame – nucleus is stationary, incident neutron has velocity: v_i
- Neutron collides with stationary nucleus at X_0
- Neutron is scattered in new direction, with velocity: v_f'
- Target nucleus recoils, with velocity: V_f'
- Momentum, energy are conserved in elastic collision
- Transformation to *Center of Mass Frame of Reference* simplifies computations of changes in momentum, energy

Glancing Collisions in Center of Mass Frame





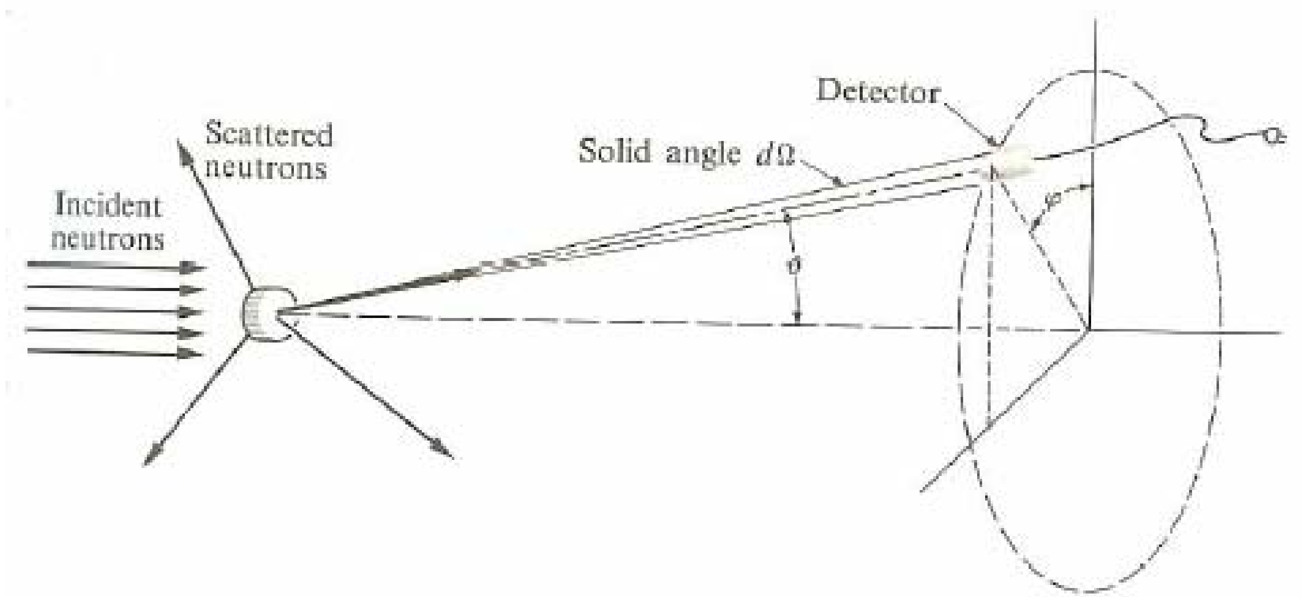
- Center of Mass always remains in fixed location
- Neutron and nucleus move towards each other
- Momentum and energy still conserved

Glancing Collisions in Center of Mass Frame

- Scattering angle in Center of Mass Frame is different
- Note when: $\theta = 180°$, it yields value for Knock-on:
- $E' = E\,[(1+\alpha) + (1-\alpha)\cos(180°)\,]/2 = E\,[(1+\alpha) - (1-\alpha)]/2 = E\,\alpha$
- Note when: $\theta = 0°$, it yields value for missed collision:
- $E' = E\,[(1+\alpha) + (1-\alpha)\cos(0°)\,]/2 = E\,[(1+\alpha) + (1-\alpha)]/2 = E$

Glancing Collisions in Center of Mass Frame

- Maximum kinetic energy loss is for *head-on collision*: $\theta = 180°$
- After <u>*any*</u> collision, neutron energy is between: *E and αE* depending on scattering angle: θ
- Key item is scattering angle distribution, which is described by differential scattering cross section: $d\sigma_S(\theta)/d\Omega(\theta)$
- Solid angle is symmetric about axis: $d\Omega(\theta) = 2\pi \sin(\theta)d\theta$



Glancing Collisions in Laboratory Frame

- *Most likely direction* of scattered neutron *depends on target mass: A*
- Relationship between Laboratory scattering angle *ψ* and Center of Mass scattering angle *θ*:

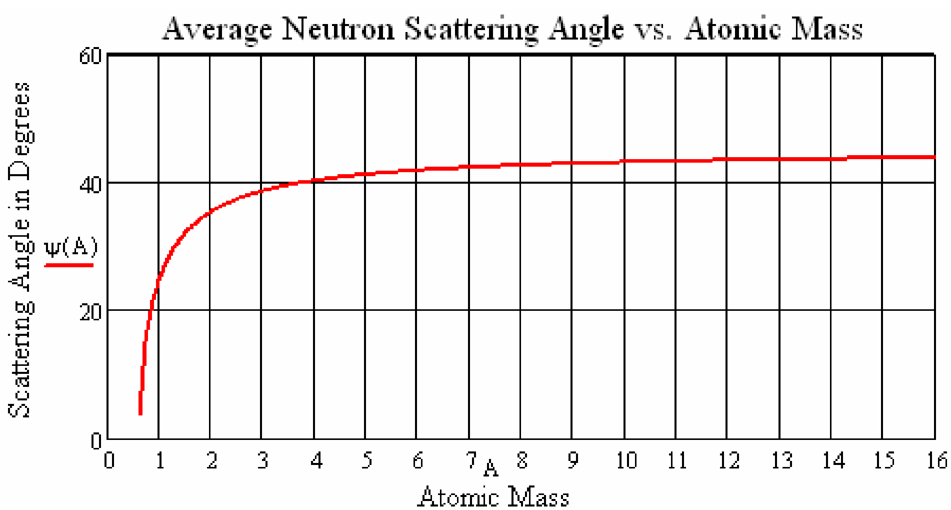
$$\cos(\psi) = \frac{A\cos(\theta)+1}{\sqrt{A^2+2A\cos(\theta)+1}}$$

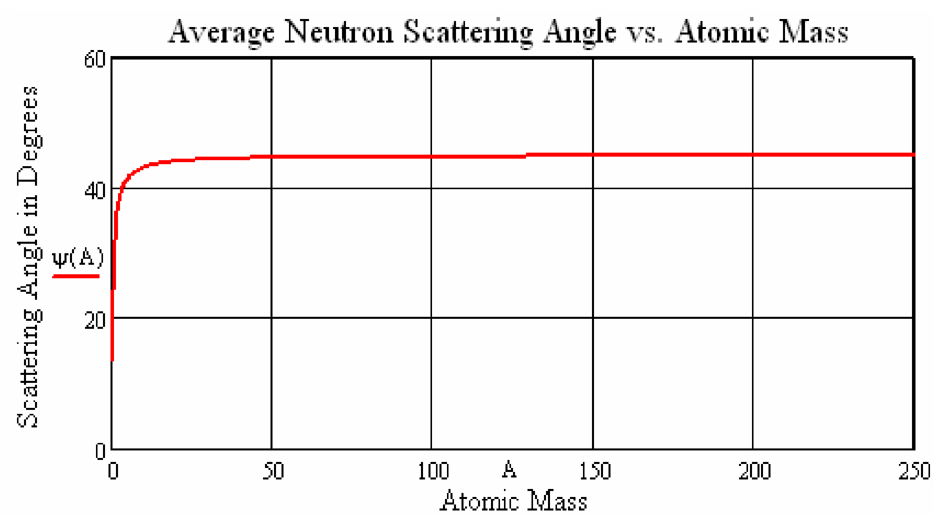
- Computing averaged value of: *cos(ψ)* via change of variables yields:

$$\frac{\int_0^{4\pi}\cos(\psi)d\Omega(\psi)}{\int_0^{4\pi}d\Omega} = \frac{\int_0^{\pi}\frac{A\cos(\theta)+1}{\sqrt{A^2+2A\cos(\theta)+1}}2\pi\sin(\theta)d\theta}{\int_0^{\pi}2\pi\sin(\theta)d\theta} = \frac{2}{3A}$$

Glancing Collisions in Laboratory Frame

- Solving for average Laboratory Frame scattering angle yields: $\psi = Cos^{-1}(2/3A)$
- For Hydrogen, $A=1$, $\psi = 24.09°$
- For Carbon, $A=12$, $\psi = 43.4°$
- For Uranium, $A=238$, $\psi = 44.9°$





Neutron Slowing Down Density

- Probability of neutron (initial kinetic energy *E)* colliding and resulting in final neutron kinetic energy *E'* is expressed:

$$p(E \rightarrow E')dE' = \frac{-2\pi \sin(\theta) \frac{d\sigma_S(\theta)}{d\theta} d\theta}{\sigma_S}$$

$$E' = \frac{E}{2}\left[(1+\alpha) + (1-\alpha)\cos(\theta)\right]$$

$$dE' = -\frac{E}{2}(1-\alpha)\sin(\theta)d\theta$$

$$p(E \rightarrow E') = \frac{4\pi \frac{d\sigma_S(\theta)}{d\theta}}{\sigma_S E(1-\alpha)}$$

Neutron Slowing Down Density

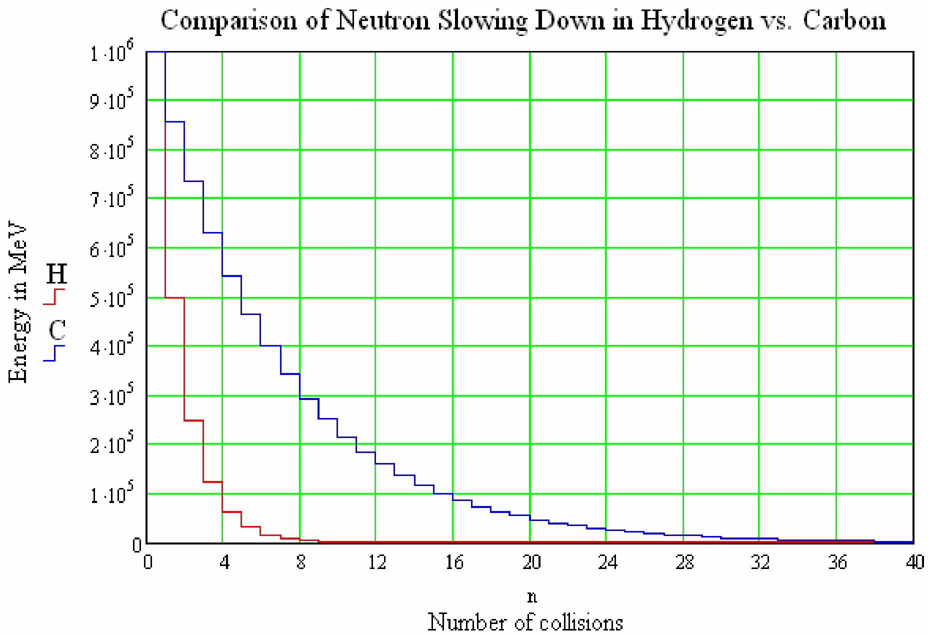
- Common simplification: is to assume *uniform isotropic scattering* throughout solid angle: $d\Omega$
- Then: $d\sigma_s(\theta)/d\Omega(\theta) \sim \sigma_s / 4\pi$
- Probability of kinetic energy dropping from E to E' via collisions:

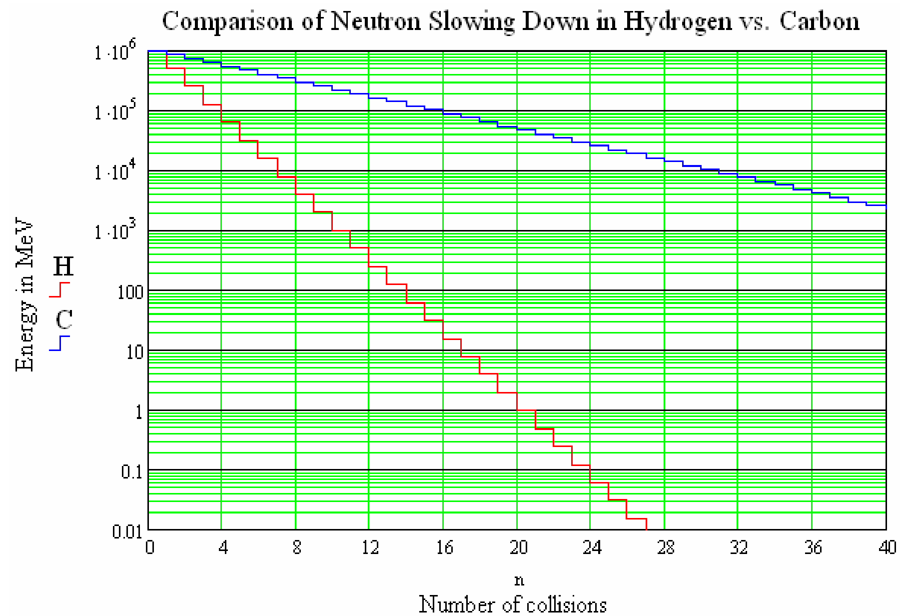
$$p(E \to E') \approx \frac{1}{E(1-\alpha)}$$

- Average energy after one collision is between αE_o and E_o:

$$\langle E' \rangle = \int_{\alpha Eo}^{Eo} E' p(E \to E') dE' = \frac{1}{Eo(1-\alpha)} \int_{\alpha Eo}^{Eo} E' dE' = \frac{(1-\alpha^2)Eo^2}{2Eo(1-\alpha)} = \frac{(1+\alpha)Eo}{2}$$

N Collisions Each Decrease Energy by <E'>





- If each neutron collision decreased energy ***by same*** $<E'>$
- After *n* collisions: $E_n = E_o[(1+\alpha)/2]^n$
- Alternately: $E_n = E_o e^{-n\xi}$ -where: ξ is log energy decrease
- Computing averaged ξ yields:

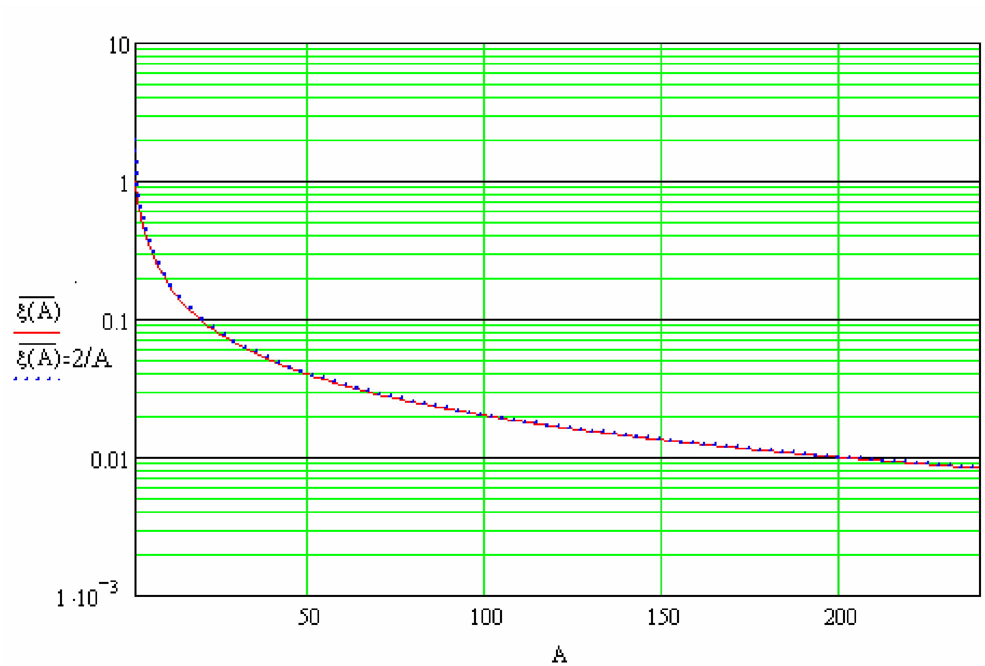
$$\xi = \int_{\alpha Eo}^{Eo} \ln(\frac{Eo}{E'})p(E \rightarrow E')dE' = \frac{1}{Eo(1-\alpha)} \int_{\alpha Eo}^{Eo} \ln(\frac{Eo}{E'})dE' = \frac{\alpha - \alpha\ln(\alpha) - 1}{\alpha - 1}$$

Computations of Average log Energy Decrease

- Using definition of α in terms of A: α = *[(A-1)/(A+1)]²*

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

- An approximation that works for large *A: ξ ~ 2/A*



Neutron Slowing Down Efficiency

Nucleus:	A:	α:	ξ:
Hydrogen ($_1H^1$)	1	0	1.000
Deuterium ($_1H^2$)	2	0.0123	0.725
Graphite ($_6C^{12}$)	12	0.7160	0.158
Oxygen ($_8C^{16}$)	16	0.8789	0.120
Iron ($_{26}Fe^{56}$)	56	0.9311	0.035
Lead ($_{82}Pb^{208}$)	208	0.9810	0.009585
Uranium ($_{92}U^{238}$)	238	0.9833	0.00838

Neutron Slowing Down Efficiency

- One "*head-on*" neutron collision with H nucleus can effectively stop fission neutron with $E_f \sim 1\text{-}3\ MeV$
- Considering "*average collisions*" with H, $E_T = E_f e^{-n\xi}$ and solving for "n" number of collisions to reach thermal energy $E_T = 0.025eV$, yields:

$$n = ln(E_f / E_T)/\xi = ln(10^6 eV/ 0.025eV)/1.0 = 17.5 \text{ collisions}$$

- Performing same calculation for C graphite, $\xi = 0.158$, yields:

$$n = 110.8 \ collisions$$

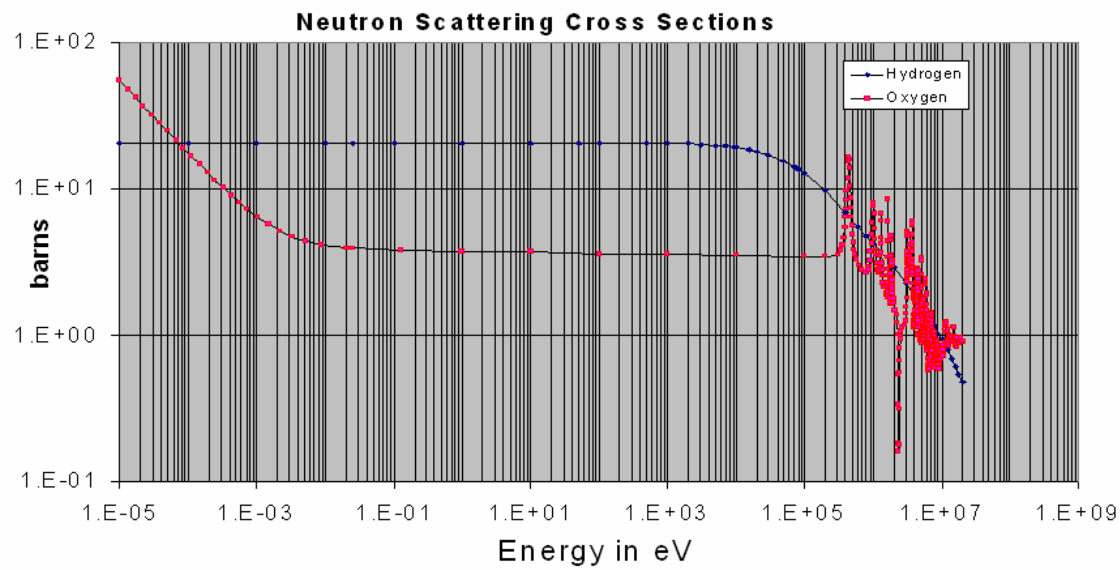
- Heavy metal elements such as Iron, Lead, Uranium are even *less effective* in slowing down fission neutrons

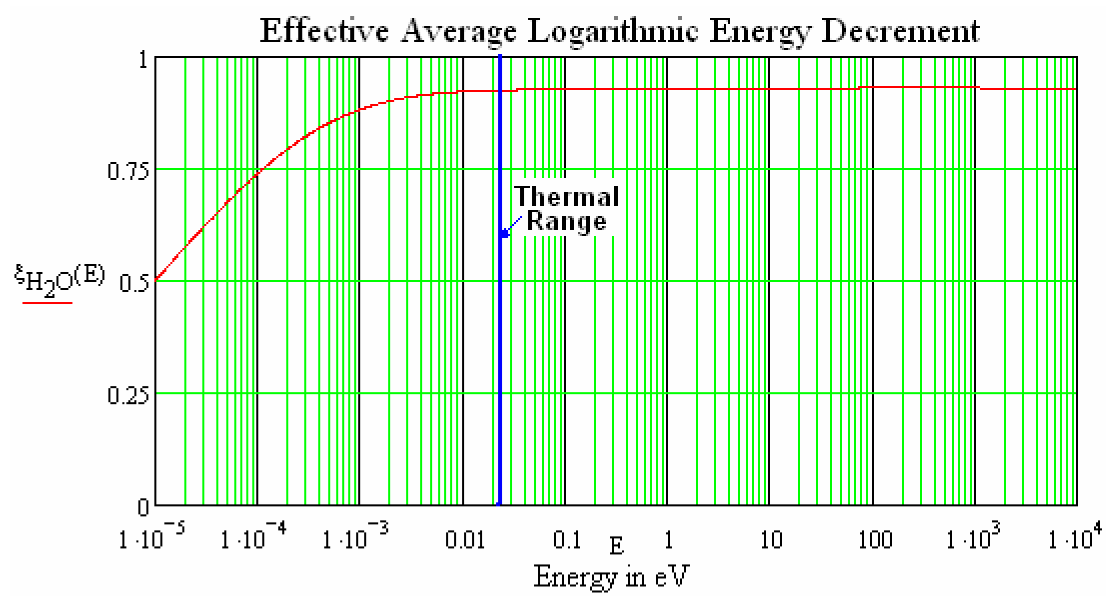
ξ for Composite Moderators

- In most cases neutron slowing down occurs in moderator with more than one type of target (e.g.: H_2O)
- Effective value of ξ is computed based on cross-section weighted average:

$$\bar{\zeta}_{H_20}(E) = \frac{2\sigma_s(E)_H \zeta_H(E) + \sigma_s(E)_O \zeta_O(E)}{2\sigma_s(E)_H + \sigma_s(E)_H}$$

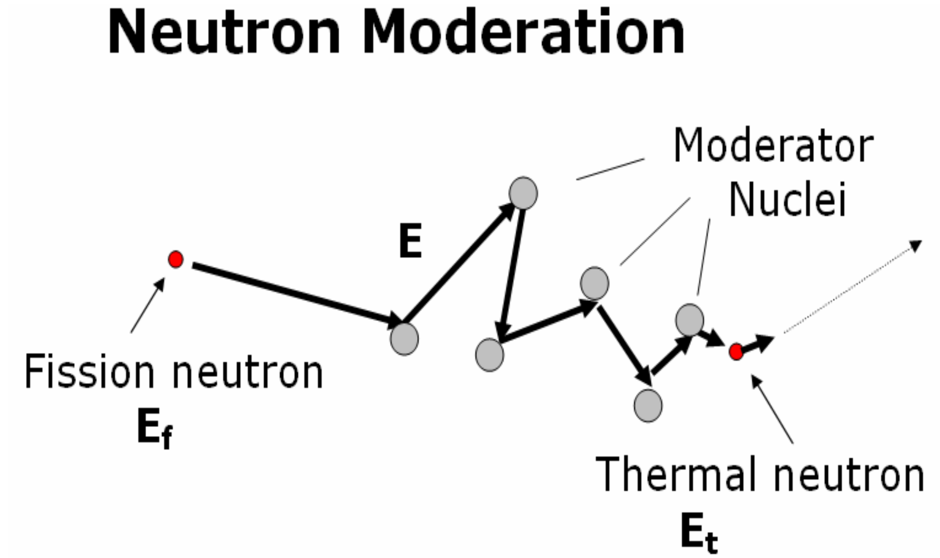
- $\xi_{H2O}(E) \approx 0.93$ in region $0.025eV < E < 10^5 eV$

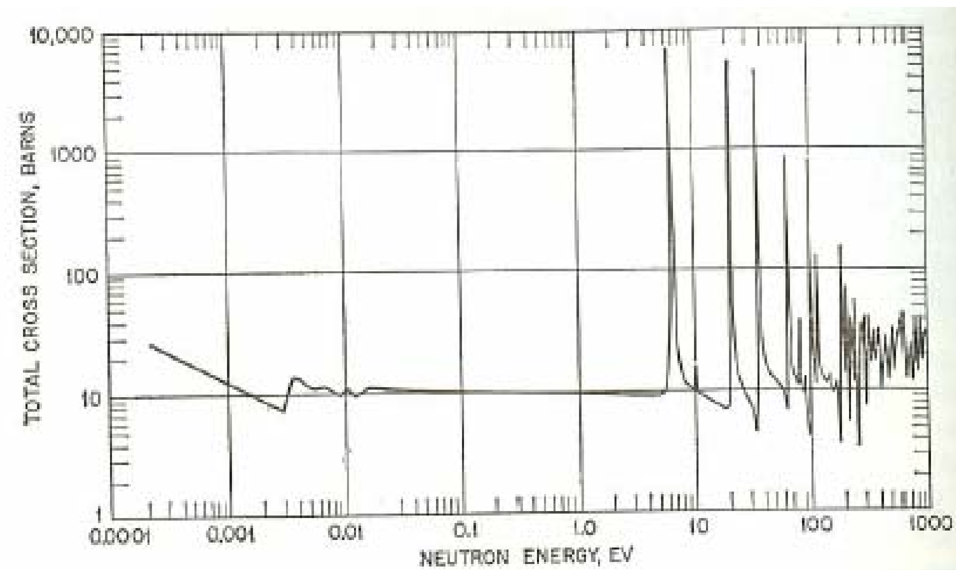




What Happens During Neutron Moderation

- Fission neutrons emitted with distributed energies: $E_f \geq 1\ MeV$
- Based upon $\Sigma_{tot}(E)$ probability of interaction, interactions occur
- Neutron reduces speed (energy) as neutron undergoes *repeated collisions* while *moving away from fission source*
- Mean free path between collisions decreases as speed decreases
- *Possibility of resonance capture* in *< 1keV* region increases as speed decreases,





Total cross section of uranium-238 as function of neutron energy

Neutron Thermalization Without Capture

Neutron Thermalization Without Capture

- This is "idealistic case" – misses impact of resonance capture removing neutrons
- Assume: "*near infinite*" medium → no loss at boundaries
- Assume: Fast neutrons produced by fission, thermal neutrons consumed by fission – *in thermal region*
- On average: rate which neutron with energy: *E* collides into energy: E' , is: $P(E \rightarrow E')dE' = dE' / E$

Neutron Thermalization Without Capture

- "*Slowing down density*": $q(E)$ (neutrons <E /cm^2-sec)

- Overall rate of neutrons arriving at this energy is given by: $q(E)\, dE / E\, \xi(E)$

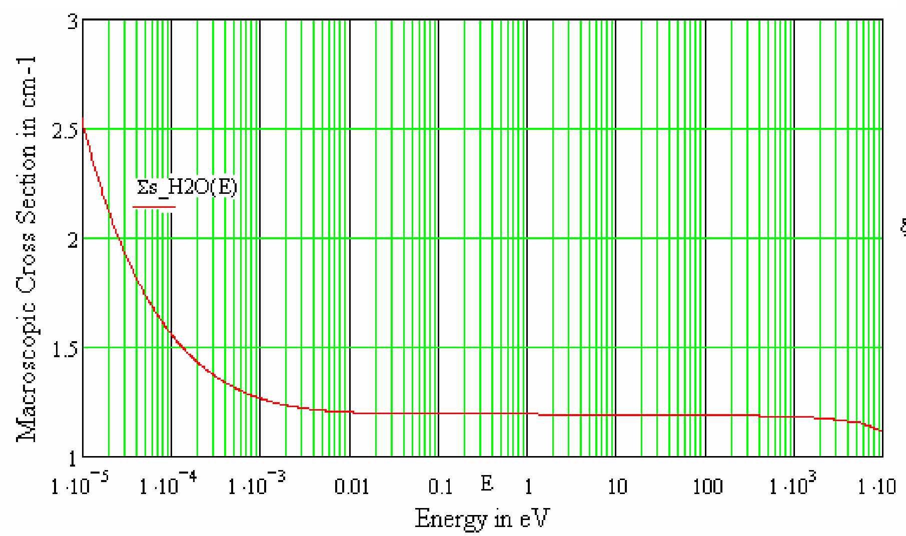
- This must match rate neutrons loose energy within small energy window *dE, and* is proportional to collision rate

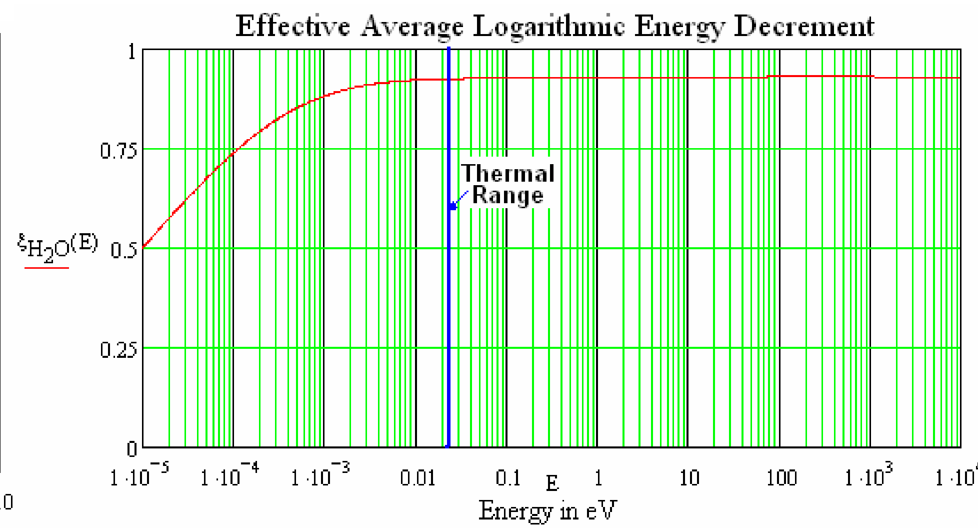
$$\Phi(E)\, \Sigma_s(E)\, dE$$

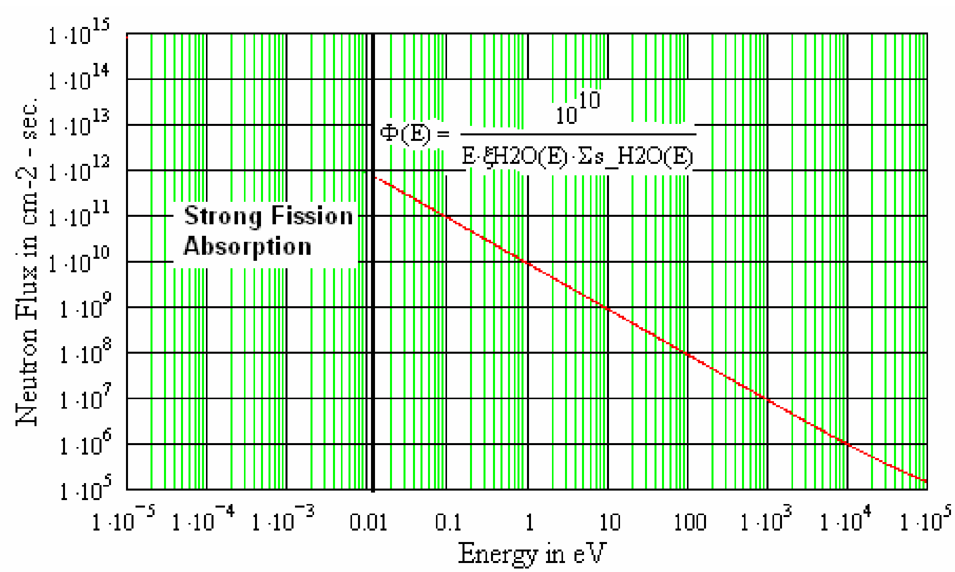
- $q(E)\, dE / E\, \xi(E) = \Phi(E)\, \Sigma_s(E)\, dE$ and from this:

$$\Phi(E) = q(E) / \Sigma_s(E)\, E\, \xi(E)$$

Simplified Plot of: $\Phi(E) = q(E) / \Sigma_s(E)\, E\, \xi(E)$







- Relatively smooth $\Sigma_s(E)$, $\xi(E)$, in ***epithermal energy range,*** and no strong absorbers gives relatively smooth $1/E$ flux

Neutron Thermalization With Capture

Neutron Thermalization With Capture

- With presence of strong absorber materials, $\Sigma_c(E)$ will impact simple $1/E$ shape of $\Phi(E)$
- Standard approach is to compute:

$$\frac{\partial q(E)}{\partial E} dE = \Sigma c(E)\Phi(E)dE$$

- Expression for unperturbed flux becomes:

$$(\Sigma s(E) + \Sigma c(E))\Phi(E) = \frac{q(E)}{E\xi(E)}$$

$$\Phi(E) = \frac{q(E)}{E\xi(E)(\Sigma s(E) + \Sigma c(E))}$$

Neutron Thermalization With Capture

- Substituting $\Phi(E)$ expression into *differential slowing down density equation* yields:

$$\frac{\partial q(E)}{\partial E} = \Sigma c(E)\Phi(E) = \frac{\Sigma c(E) q(E)}{E\xi(E)(\Sigma s(E) + \Sigma c(E))}$$

- Integrating this expression from *E* down to *E'* yields:

$$\int_{q(E')}^{q(E)} \frac{\partial q(E)}{q(E)} dq(E) = \ln\left(\frac{q(E)}{q(E')}\right) = \int_{E'}^{E} \frac{\Sigma c(E) dE}{\xi(E)(\Sigma c(E) + \Sigma s(E))E}$$

$$\frac{q(E)}{q(E')} = \exp\left[\int_{E'}^{E} \frac{\Sigma c(E) dE}{\xi(E)(\Sigma c(E) + \Sigma s(E))E}\right]$$

$$\frac{q(E')}{q(E)} = \exp\left[-\int_{E'}^{E} \frac{\Sigma c(E) dE}{\xi(E)(\Sigma c(E) + \Sigma s(E))E}\right]$$

Neutron Thermalization With Capture

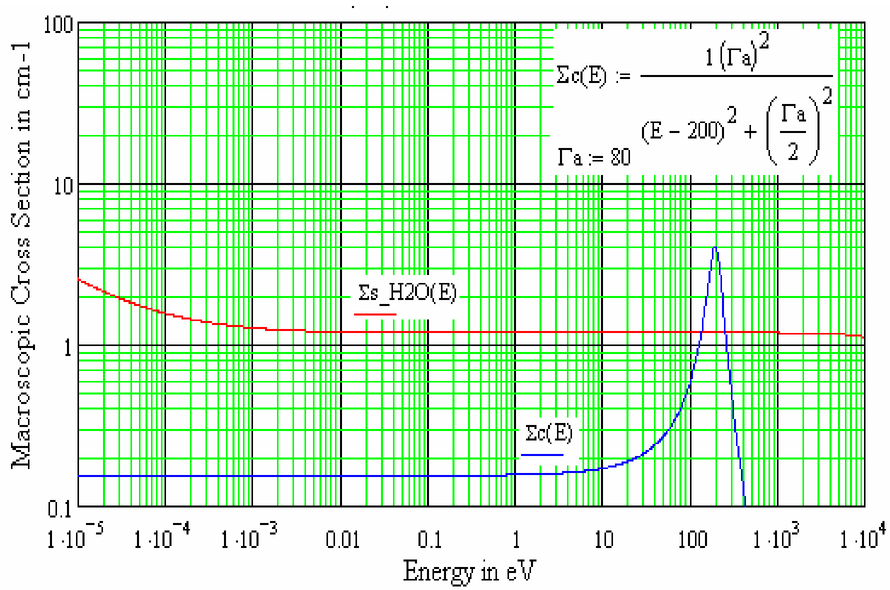
$$\frac{q(E')}{q(E)} = \exp\left[-\int_{E'}^{E} \frac{\Sigma c(E)dE}{\xi(E)(\Sigma c(E) + \Sigma s(E))E} \right]$$

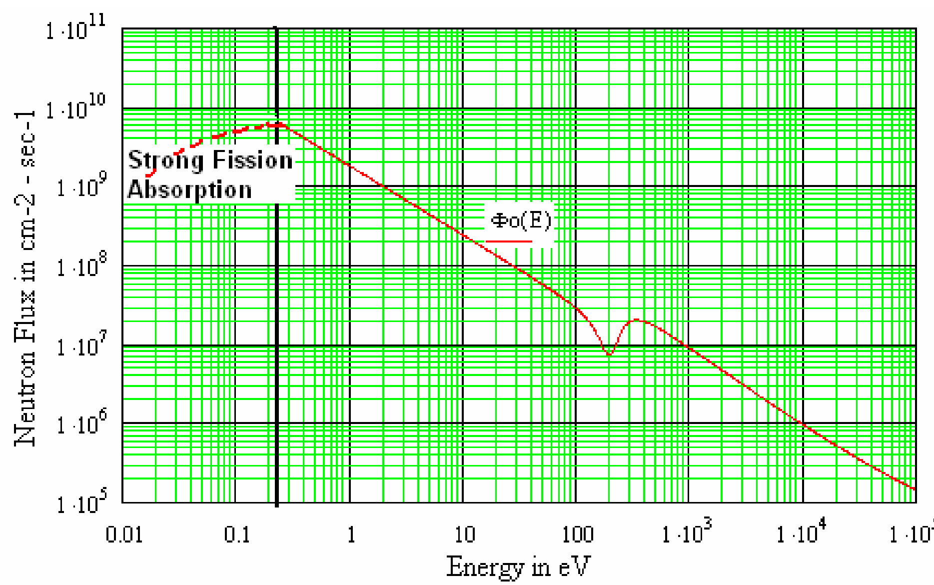
- This is fraction of neutron slowing down density *after downscattering* from E to E'.

- Expression is used in calculating fraction of neutron loss during thermalization (due to *resonance capture*)

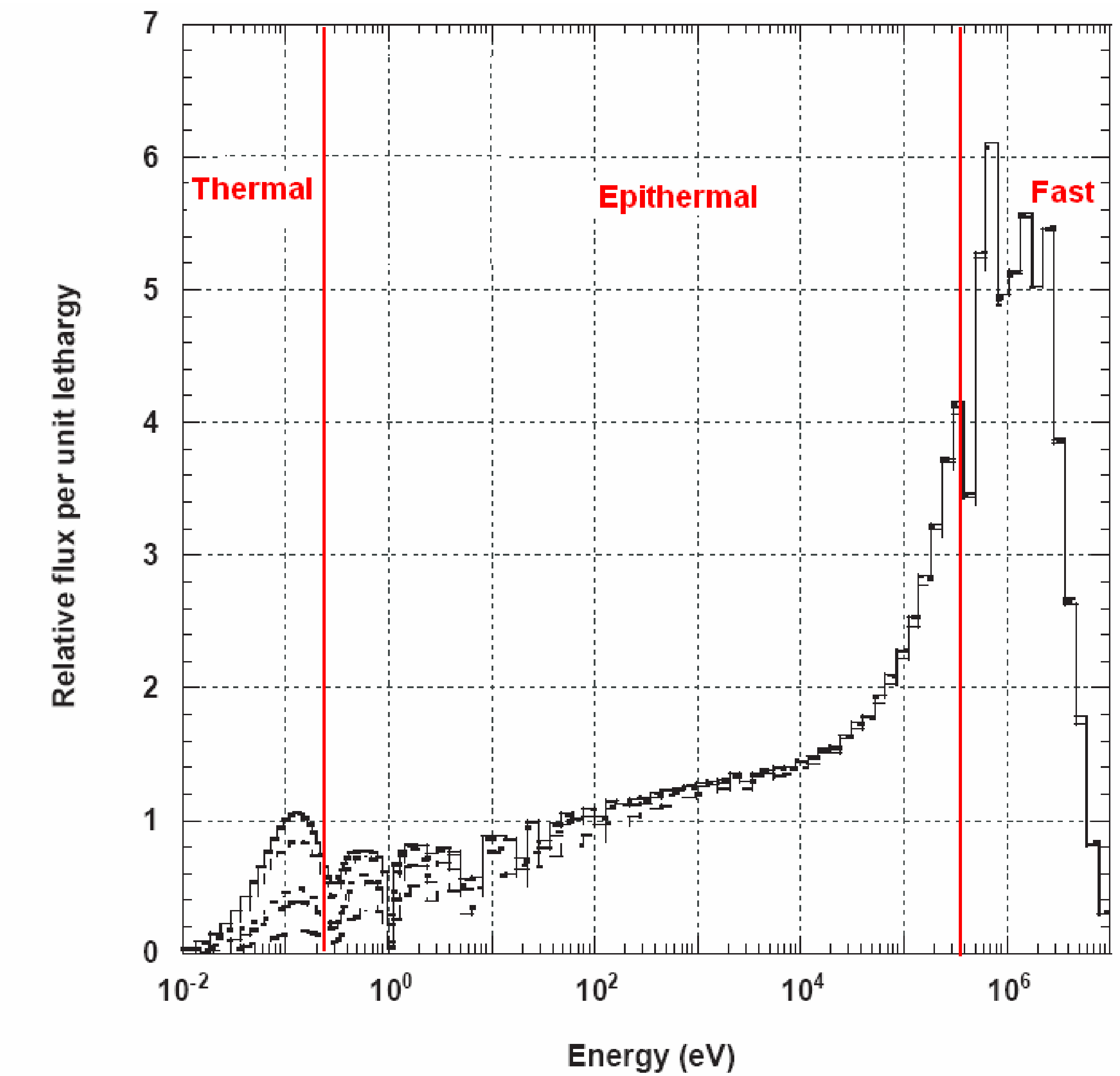
Example: $\Phi(E) = q(E) / E\, \xi(E)\, (\Sigma_s(E) + \Sigma_c(E))$

- *For illustrative purposes*: assume presence of: "*Coloradium*"
- "*Coloradium"* has 200eV resonance absorption $\Sigma_c(E)$, $\Gamma=80eV$
- Using derived expression for $q(E)$, insert into $\Phi(E)$ expression
- This yields following for $\Phi(E)$ *with just one resonance*
- Overall $\Phi(E)$ is lower, as would be expected, and has drop in region of resonance.
- Consider: *effect of hundreds of resonances!*





Calculated $\Phi(E)$ for 3000Mw$_t$ PWR Core



Taken from:

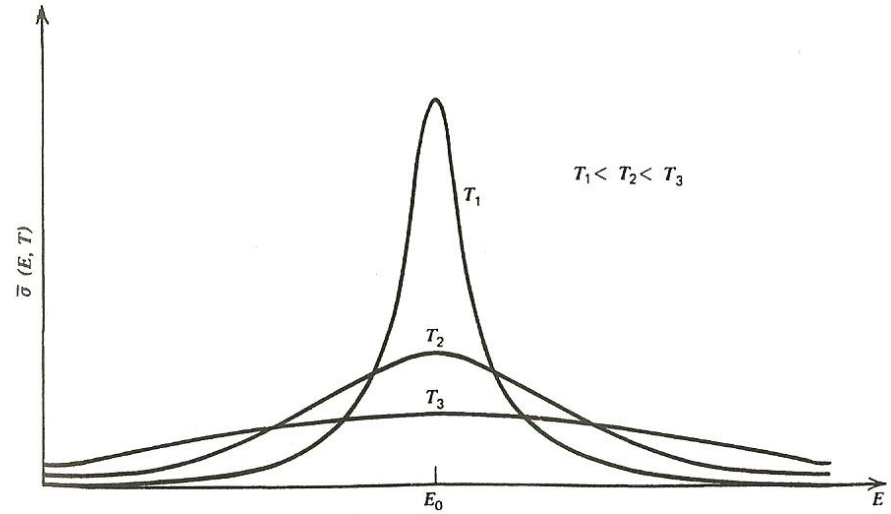
A. Waris, H. Sekimoto, "Characteristics of Several Equilibrium Fuel Cycles of PWR", *Journal of Nuclear Science and Technology*, Vol.38, No.7 p.517-526, July 2001.

Effect of increased temperature

- Doppler effect on broadening of cross sections noted previously
- Expression for slowing down density depends on cross sections

$$\frac{q(E')}{q(E)} = \exp\left[-\int_{E'}^{E} \frac{\Sigma c(E)dE}{\xi(E)(\Sigma c(E) + \Sigma s(E))E}\right]$$

- Increasing temperature increases capture rate during thermalization
- Thus: fewer neutrons reach thermal energies



Doppler-broadening of a resonance with increasing temperature.

Resonance Integral Plays Important Role in Criticality Evaluations

- Fraction of neutron density which survive slowing down from energy E to below E' is called "*Resonance Integral*"

$$\frac{q(E')}{q(E)} = \exp\left[-\int_{E'}^{E} \frac{\Sigma c(E) dE}{\xi(E)(\Sigma c(E) + \Sigma s(E))E} \right]$$

- It *appears again* in discussing reactor criticality
- Given that $\Sigma_c(E)$, $\Sigma_s(E)$ *are* actually *hundreds of resonances*, direct computation of *Resonance Integral* requires clever numerical computation
- Fortunately: simplifications exist which show trends of things such as *temperature dependence on resonance widths*

Summary on Slowing Down Neutrons

- 1-3 Mev neutrons slow can slow down to 0.01-0.025 eV in *one Head-on collision* with Hydrogen in water molecule
- 'Head-on' collisions are *not average*: thermalizing could take 17-18 glancing like collisions with H_2O molecules
- Heavier materials are *less efficient* in slowing neutrons
- Overall neutron population undergoes thermalizing but fraction is lost due to *resonance captures*
- Resonance capture fraction $q(E')/q(E)$ if computed with all proper $\Sigma(E)$, $\xi(E)$ can estimate resonance losses