NUCL 510
Nuclear Reactor Theory

Fall 2011
Lecture Note 2

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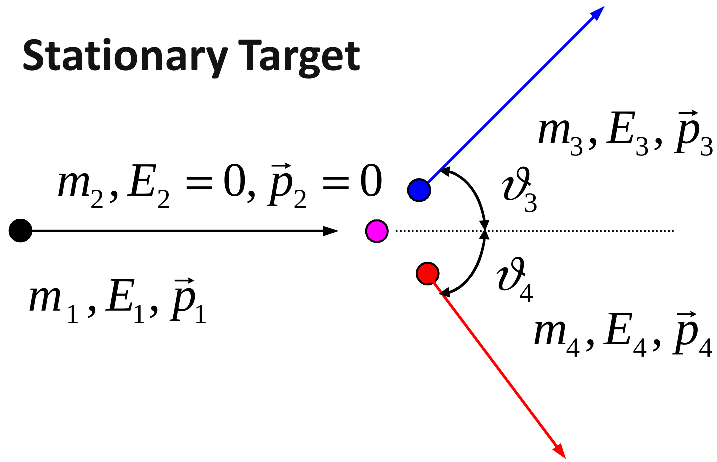
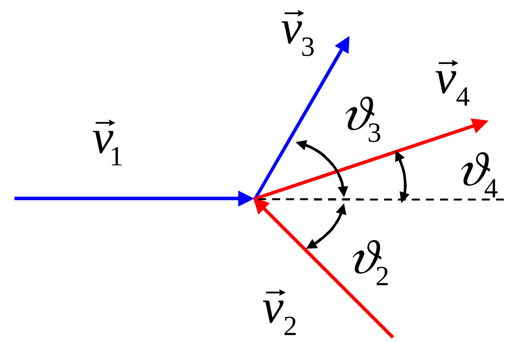
Two-Body Kinematics in Laboratory System (LS)

Stationary Target



Moving Target



- Reaction Q value

$$Q = Q_m - W = (m_1 + m_2 - m_3 - m_4)c^2 - \sum E_{ex}$$

Q_m: mass difference Q value
W: sum of nuclear excitation energies

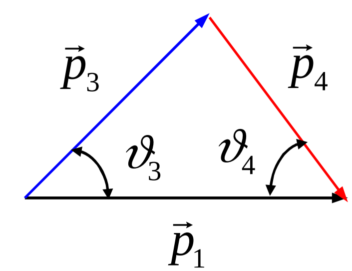
- Energy and momentum conservation equations

$$E_1 + E_2 = E_3 + E_4 - Q$$

$$\vec{p}_1 + \vec{p}_2 = \vec{p}_3 + \vec{p}_4$$

  – If the reaction Q value is very small compared to the rest masses of reactants

$$m_1 + m_2 \cong m_3 + m_4$$



Stationary Target

Center of Mass System (CMS)

- The center of mass (CM) is moving with velocity $\vec{v}_0$ defined as

$$\vec{v}_0 = \frac{m_1\vec{v}_1 + m_2\vec{v}_2}{m_1 + m_2}$$

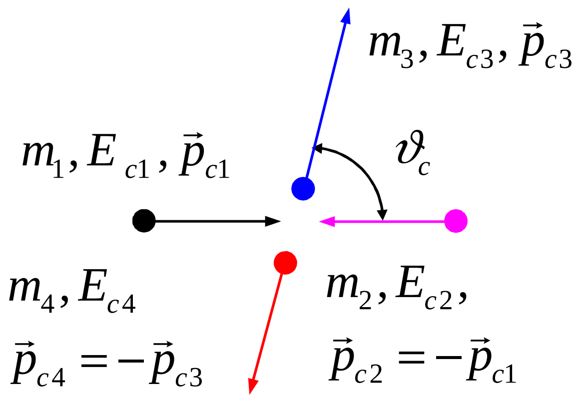
  – In the center-of-mass system, CM is stationary, and hence

$$\vec{v}_{c1} = \vec{v}_1 - \vec{v}_0 = \frac{m_2}{m_1 + m_2}(\vec{v}_1 - \vec{v}_2) = \frac{\mu_m}{m_1}\vec{v}_r$$

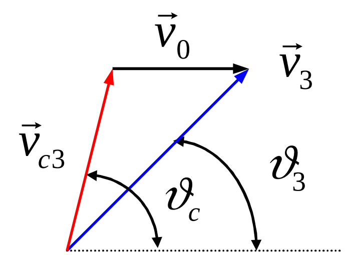
$$\vec{v}_{c2} = \vec{v}_2 - \vec{v}_0 = -\frac{m_1}{m_1 + m_2}(\vec{v}_1 - \vec{v}_2) = -\frac{\mu_m}{m_2}\vec{v}_r$$

$$\mu_m = \frac{m_1 m_2}{m_1 + m_2} \quad \text{(reduced mass)}$$

$$\vec{v}_r = \vec{v}_{c1} - \vec{v}_{c2} = \vec{v}_1 - \vec{v}_2 \quad \text{(relative velocity)}$$



  – The velocity of CM is parallel to the total linear momentum of two reactants and the velocities in the CMS are parallel to the relative velocity between two reactants



Kinetic Energies in CMS before Reaction

- The kinetic energies in CMS before reaction can be written as

$$E_{c1} = \frac{1}{2} m_1 v_{c1}^2 = \frac{1}{2} m_1 \left(\frac{\mu_m}{m_1} \right)^2 v_r^2 \qquad E_{c2} = \frac{1}{2} m_2 v_{c2}^2 = \frac{1}{2} m_2 \left(\frac{\mu_m}{m_2} \right)^2 v_r^2$$

$$E_c^T = E_{c1} + E_{c2} = \frac{1}{2} \mu_m v_r^2 \quad \text{(total kinetic energy in CMS)}$$

$$E_0 = \frac{1}{2}(m_1 + m_2) v_0^2 = \frac{1}{2} \frac{|m_1 \vec{v}_1 + m_2 \vec{v}_2|^2}{m_1 + m_2} \quad \text{(kinetic energy of CM)}$$

  – The total kinetic energy in the laboratory system splits into the total kinetic energy in the center-of-mass system and the kinetic energy of the center-of-mass

$$E_c^T + E_0 = \frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} |\vec{v}_1 - \vec{v}_2|^2 + \frac{1}{2} \frac{|m_1 \vec{v}_1 + m_2 \vec{v}_2|^2}{m_1 + m_2} = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 = E_1 + E_2$$

$$|\vec{a} + \vec{b}|^2 = (\vec{a} + \vec{b}) \cdot (\vec{a} + \vec{b}) = |\vec{a}|^2 + 2\vec{a} \cdot \vec{b} + |\vec{b}|^2$$

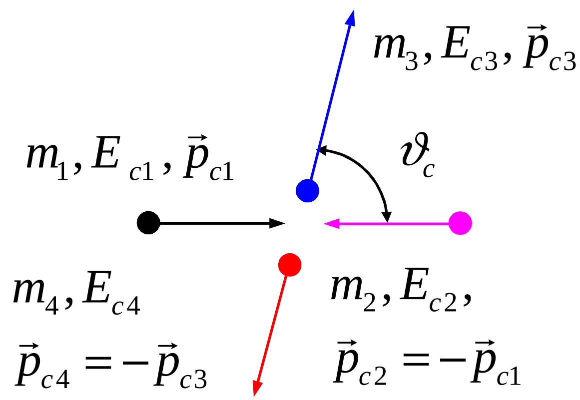
Kinetic Energies in CMS after Reaction

- Velocities in CMS after reaction

$$\vec{v}_0' = \frac{m_3\vec{v}_3 + m_4\vec{v}_4}{m_3 + m_4}$$

$$\vec{v}_{c3} = \vec{v}_3 - \vec{v}_0' = \frac{\mu_m'}{m_3}\vec{v}_r' \qquad \vec{v}_{c4} = \vec{v}_4 - \vec{v}_0' = -\frac{\mu_m'}{m_4}\vec{v}_r'$$

$$\mu_m' = \frac{m_3 m_4}{m_3 + m_4} \qquad \vec{v}_r' = \vec{v}_{c3} - \vec{v}_{c3} = \vec{v}_3 - \vec{v}_4$$



- Kinetic energies in CMS after reaction

$$E_{c3} = \frac{1}{2}m_3 v_{c3}^2 = \frac{1}{2}m_3\left(\frac{\mu_m'}{m_3}\right)^2 (v_r')^2 \qquad E_{c4} = \frac{1}{2}m_4 v_{c4}^2 = \frac{1}{2}m_4\left(\frac{\mu_m'}{m_4}\right)^2 (v_r')^2$$

$$(E_c^T)' = E_{c3} + E_{c4} = \frac{1}{2}\mu_m'(v_r')^2 \qquad E_0' = \frac{1}{2}(m_3 + m_4)(v_0')^2 = \frac{1}{2}\frac{|m_3\vec{v}_3 + m_4\vec{v}_4|^2}{m_3 + m_4}$$

$$(E_c^T)' + E_0' = E_{c3} + E_{c4}$$

Case of Mass Conservation

- If the reaction Q value is very small compared to the rest masses of reactants, then the reactant mass is approximately conserved.
  - If the mass and momentum are conserved, the velocity and kinetic energy of the center-of-mass are not changed as

$$\vec{v}_0' = \frac{m_3\vec{v}_3 + m_4\vec{v}_4}{m_3 + m_4} = \frac{m_1\vec{v}_1 + m_2\vec{v}_2}{m_1 + m_2} = \vec{v}_0$$

$$E_0' = \frac{1}{2}\frac{|m_3\vec{v}_3 + m_4\vec{v}_4|^2}{m_3 + m_4} = \frac{1}{2}\frac{|m_1\vec{v}_1 + m_2\vec{v}_2|^2}{m_1 + m_2} = E_0$$

- For elastic scattering, reactant masses are not changed

$$m_1 = m_3 \qquad m_2 = m_4 \qquad \Rightarrow \mu_m' = \mu_m$$

  - Reaction Q value is exactly zero $Q = 0$
  - Total kinetic energy is conserved $(E_c^T)' = E_c^T$
  - As a result, the relative speed is also invariant $v_r' = v_r$

Non-relativistic Kinematics for Stationary Target (1)

- For a stationary target, $\vec{v}_r = \vec{v}_1 - \vec{v}_2 = \vec{v}_1$
- If the conservation of mass is assumed

$$\mu_m = \frac{m_1 m_2}{m_1 + m_2} = \frac{A}{1+A} m_1 \qquad A = \frac{m_2}{m_1}$$

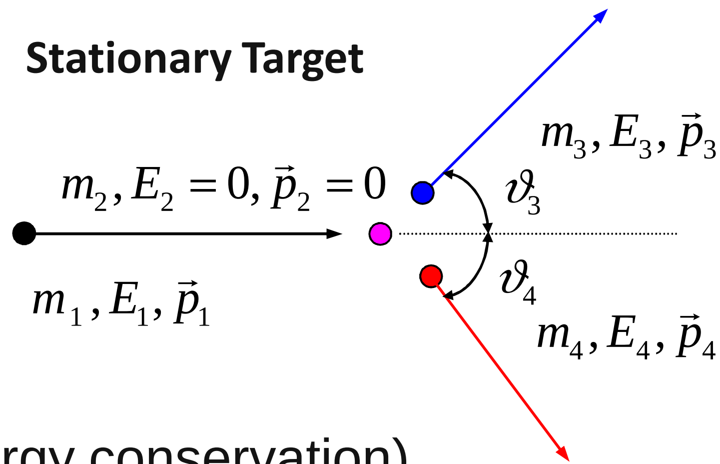
$$\mu_m' = \frac{m_3 m_4}{m_3 + m_4} = \frac{m_3(m_1 + m_2 - m_3)}{m_1 + m_2} = \frac{A'(1+A-A')}{1+A} m_1 \qquad A' = \frac{m_3}{m_1} \quad \left(\begin{array}{l} A' = 1 \text{ for} \\ \text{neutron scattering} \end{array} \right)$$

– Speed and kinetic energy of CM

$$\frac{v_0}{v_1} = \frac{1}{1+A} \qquad \frac{E_0}{E_1} = \frac{(m_1 + m_2) v_0^2}{m_1 v_1^2} = \frac{1}{1+A}$$

– Kinetic energy of incident particle

$$\frac{E_{c1}}{E_1} = \left(\frac{\mu_m}{m_1} \right)^2 = \left(\frac{A}{1+A} \right)^2$$



– Total kinetic energy after reaction (energy conservation)

$$(E_c^T)' = E_3 + E_4 - E_0' \cong E_1 + Q - E_0 = E_c^T + Q = \frac{1}{2} \mu_m v_1^2 + Q = \frac{A}{1+A} E_1 + Q$$

Non-relativistic Kinematics for Stationary Target (2)

- Relative speed of emitted particles

$$\left(\frac{v_r'}{v_0}\right)^2 = \frac{A(1+A)^2}{A'(1+A-A')}\left(1+\frac{1+A}{A}\frac{Q}{E_1}\right)$$

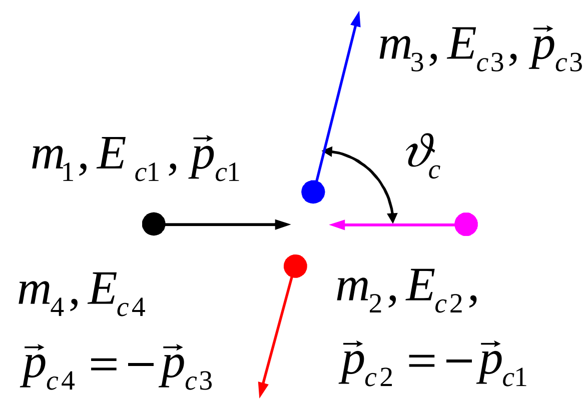
- Speeds of emitted particles relative to CM speed (slide 5)

$$\left(\frac{v_{c3}}{v_0}\right)^2 = \left(\frac{\mu_m'}{m_3}\right)^2\left(\frac{v_r'}{v_0}\right)^2 = \frac{A(1+A-A')}{A'}\left(1+\frac{1+A}{A}\frac{Q}{E_1}\right) \equiv \beta^2$$

$$\left(\frac{v_{c4}}{v_0}\right)^2 = \left(\frac{\mu_m'}{m_4}\right)^2\left(\frac{v_r'}{v_0}\right)^2 = \frac{AA'}{1+A-A'}\left(1+\frac{1+A}{A}\frac{Q}{E_1}\right) \equiv \gamma^2$$

  – Kinetic energies in CMS

$$\frac{E_{c3}}{E_{c1}} = \frac{A'}{A^2}\beta^2 \qquad \frac{E_{c4}}{E_{c1}} = \frac{1+A-A'}{A^2}\gamma^2 = \frac{A'}{1+A-A'}\frac{E_{c3}}{E_{c1}}$$



- Emission angles in CMS

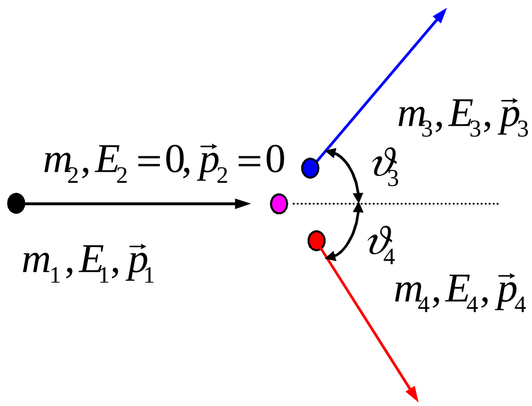
$$\mu_{c3} = \cos\vartheta_{c3} = \cos\vartheta_c = \mu_c \qquad \mu_{c4} = \cos\vartheta_{c4} = \cos(\pi-\vartheta_c) = -\mu_c$$

Non-relativistic Kinematics for Stationary Target (3)

- Kinetic energies in LS after reaction

$$\frac{E_3}{E_1}=\frac{m_3\,|\vec{v}_3|^2}{m_1\,|\vec{v}_1|^2}=\frac{m_3}{m_1}\frac{|\vec{v}_{c3}+\vec{v}_0|^2}{(1+A)^2 v_0^2}=\frac{A'}{(1+A)^2}(\beta^2+2\beta\mu_c+1)$$

$$\frac{E_4}{E_1}=\frac{m_4\,|\vec{v}_4|^2}{m_1\,|\vec{v}_1|^2}=\frac{m_4}{m_1}\frac{|\vec{v}_{c4}+\vec{v}_0|^2}{(1+A)^2 v_0^2}=\frac{1+A-A'}{(1+A)^2}(\gamma^2-2\gamma\mu_c+1)$$



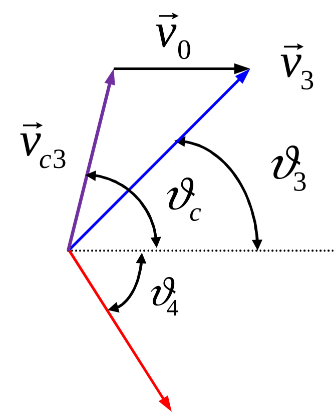
- Emission angles in LS

$$v_3\mu_3=v_{c3}\mu_c+v_0$$

$$\mu_3=\frac{v_1}{v_3}\frac{v_0}{v_1}\left(1+\frac{v_{c3}}{v_0}\mu_c\right)=\sqrt{\frac{E_1}{A'E_3}}\frac{v_0}{v_1}\left(1+\frac{v_{c3}}{v_0}\mu_c\right)=\frac{1+\beta\mu_c}{\sqrt{\beta^2+2\beta\mu_c+1}}$$

$$v_4\mu_4=-v_{c3}\mu_c+v_0$$

$$\mu_4=\frac{v_1}{v_4}\frac{v_0}{v_1}\left(1-\frac{v_{c4}}{v_0}\mu_c\right)=\sqrt{\frac{E_1}{(1+A-A')E_4}}\frac{v_0}{v_1}\left(1-\frac{v_{c4}}{v_0}\mu_c\right)=\frac{1-\gamma\mu_c}{\sqrt{\gamma^2-2\gamma\mu_c+1}}$$

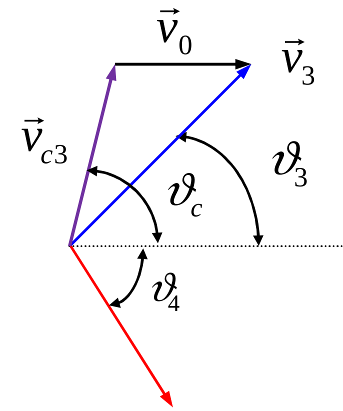


Non-relativistic Kinematics for Stationary Target (4)

- Relation between emitted angles in LS and CMS

$$\mu_c^{\pm} = \frac{-(1-\mu_3^2) \pm \mu_3\sqrt{\mu_3^2-(1-\beta^2)}}{\beta}$$

$$\frac{d\mu_3}{d\mu_c} = \frac{\beta^2(\beta+\mu_c)}{(\beta^2+2\beta\mu_c+1)^{3/2}}$$



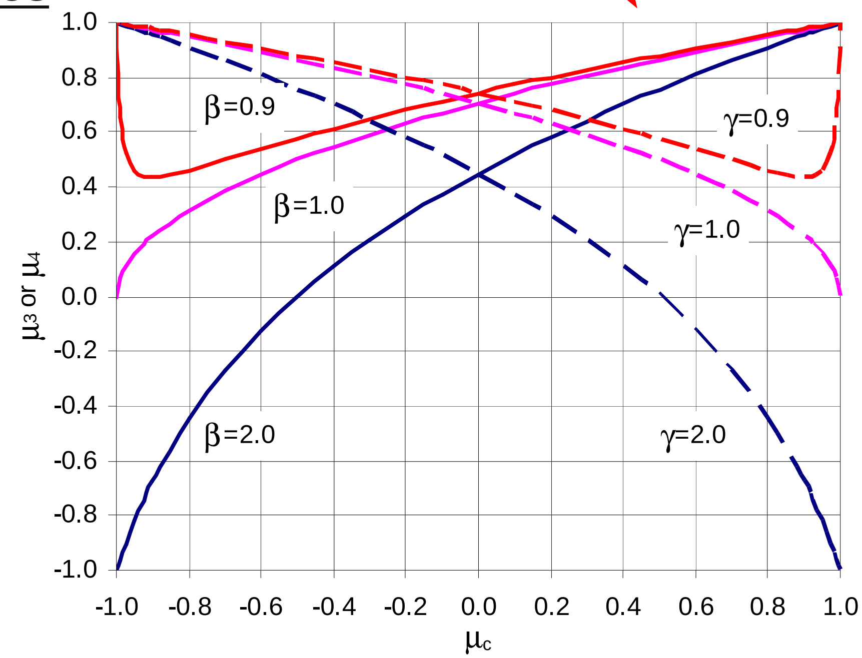
If 0≤β<1, two different angles in CMS correspond to the same direction in LS. Thus <u>two particles with different energies can emerge at the same forward direction in the laboratory system</u>.

$$\mu_{3,\min} = \sqrt{1-\beta^2} \ \text{ at } \mu_c = -\beta \text{ for } 0<\beta<1$$

$$\mu_c^{\pm} = \frac{(1-\mu_4^2) \mp \mu_4\sqrt{\mu_4^2-(1-\gamma^2)}}{\gamma}$$

$$\frac{d\mu_4}{d\mu_c} = -\frac{\gamma^2(\gamma-\mu_c)}{(\gamma^2-2\gamma\mu_c+1)^{3/2}}$$

$$\mu_{4,\min} = \sqrt{1-\gamma^2} \ \text{ at } \mu_c = -\gamma \text{ for } 0<\gamma<1$$



Threshold and Cutoff Energies

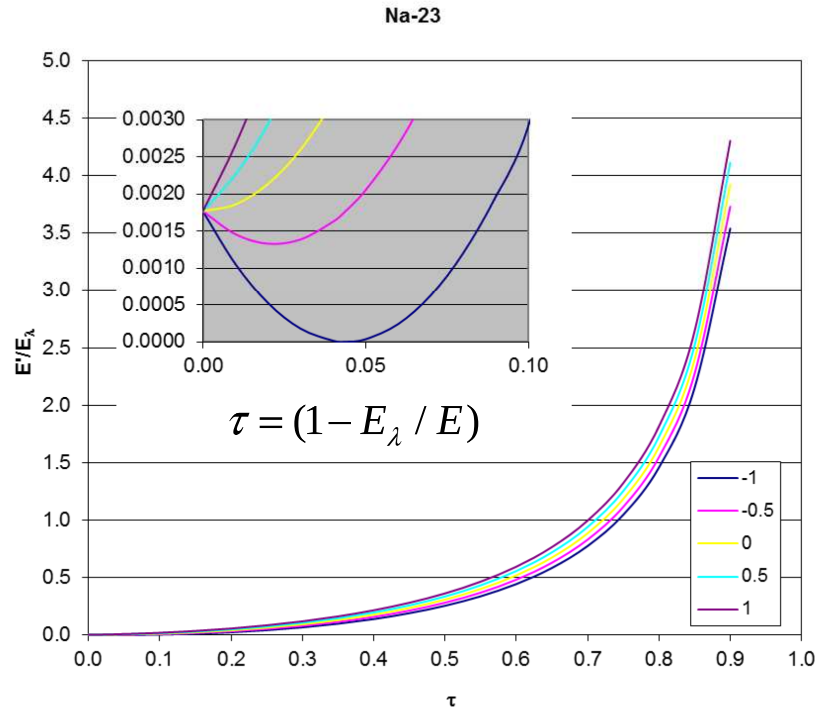
- Threshold energy for endothermic reaction (Q<0)

$$(E_c^T)' = \frac{A}{1+A} E_1 + Q \geq 0 \qquad \Rightarrow E_1 \geq \frac{A+1}{A}(-Q) = E_{th}$$

- Cutoff energy

For Q<0, β increases with increasing incident particle energy E_1. Thus, there exists the largest incident particle energy below which μ_c is dual valued, and hence E_3 is dual valued. This energy is called the cutoff energy for the “double-value” region

$$E_{cut} = \left(1 + \frac{1}{A - A'}\right)(-Q)$$



- For neutron scattering,

$$A' = m_3 / m_1 = 1 \qquad E_{th} = \left(1 + \frac{1}{A}\right)(-Q) \qquad E_{cut} = \left(1 + \frac{1}{A-1}\right)(-Q)$$

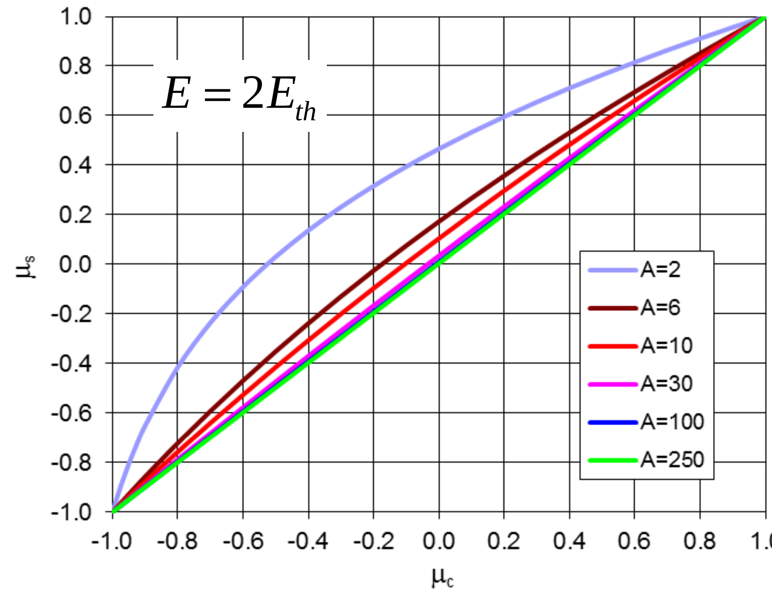
Inelastic Scattering of Neutron

- Effective mass ratio

$$\beta = A\left[1-\frac{1+A}{A}\frac{(-Q)}{E_1}\right]^{1/2} = A\gamma$$

$\beta < 1$ iff

$E_{th} < E < E_{cut}$



- Energies

$$\frac{E_3}{E_1} = \frac{1}{(1+A)^2}(\beta^2 + 2\beta\mu_c + 1)$$

$$\frac{E_4}{E_1} = \frac{A}{(1+A)^2}(\gamma^2 - 2\gamma\mu_c + 1)$$

- Scattering angles

$$\mu_3 = \frac{1+\beta\mu_c}{\sqrt{\beta^2 + 2\beta\mu_c + 1}}$$

$$\Rightarrow \mu_3(E_1,E_3) = \frac{1}{2}\left[(A+1)\sqrt{\frac{E_3}{E_1}} - (A-1)\sqrt{\frac{E_1}{E_3}} + \frac{A(-Q)}{\sqrt{E_1E_3}}\right]$$

$$\mu_4 = \frac{1-\gamma\mu_c}{\sqrt{\gamma^2 - 2\gamma\mu_c + 1}}$$

$$\Rightarrow \mu_4(E_1,E_3) = \frac{1}{2\sqrt{E_1}}\left[\sqrt{A[E_1 - E_3 - (-Q)]} + \frac{E_1 - E_3}{\sqrt{A[E_1 - E_3 - (-Q)]}}\right]$$

Elastic Scattering of Neutron

- For elastic scattering $Q=0$
- Effective mass ratio $\beta = A, \quad \gamma = 1$
- Energies

$$\frac{E_3}{E_1} = \frac{1}{(1+A)^2}(A^2 + 2A\mu_c + 1) \qquad \frac{E_4}{E_1} = \frac{2A}{(1+A)^2}(1-\mu_c)$$

- Scattering angles

$$\mu_3 = \frac{1 + A\mu_c}{\sqrt{A^2 + 2A\mu_c + 1}}$$

$$\mu_c = \frac{1}{A}\left[-(1-\mu_3^2) + \mu_3\sqrt{A^2 - (1-\mu_3^2)}\right]$$

$$\mu_4 = \sqrt{\frac{1-\mu_c}{2}} = \sqrt{\frac{1-\cos\vartheta_c}{2}} = \sin(\vartheta_c / 2)$$

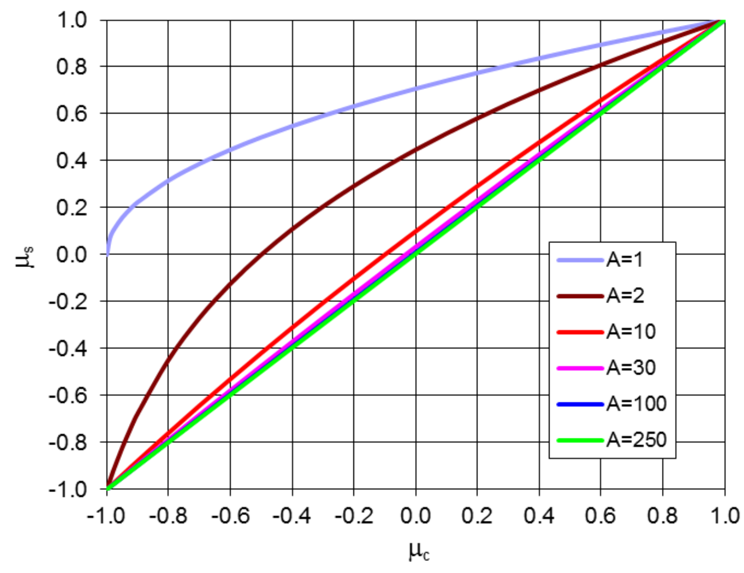
$$\mu_c = 1 - 2\mu_4^2$$

$A = 1 \quad \mu_3 = \sqrt{\dfrac{1+\mu_c}{2}} \geq 0$

$$\cos^2\vartheta_3 = \frac{1+\cos\vartheta_c}{2} = \cos^2\frac{\theta_c}{2}$$

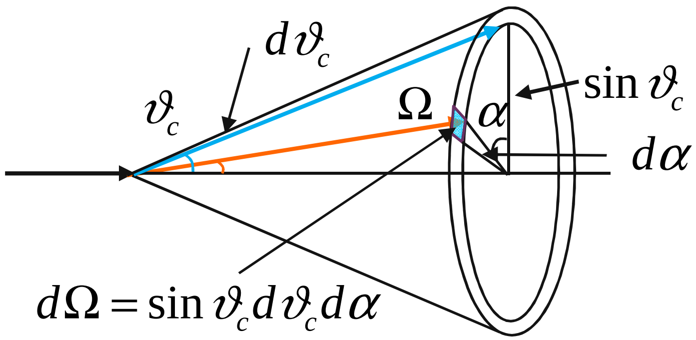
$$\Rightarrow \vartheta_3 = \frac{\theta_c}{2}$$

$\Rightarrow$ No backward scattering



Cross Sections for Neutron Scattering

- In CMS, scattering of low- and intermediate-energy neutrons is nearly isotropic. In fact, for hydrogen, it is isotropic up to about 30 MeV.



$$\sigma_s(E,\mu_c) \cong \frac{\sigma_s(E)}{4\pi}$$

- Generally, the heavier the nuclide, the lower the energy above which elastic scattering becomes anisotropic. Thus the differential scattering cross section is well represented by a low-order Legendre polynomial expansion in the form

$$\sigma_s(E,\mu_c) \cong \frac{\sigma_s(E)}{4\pi}\sum_{n=0}^{N}(2n+1)\, f_n(E)P_n(\mu_c)$$

$$f_0 = 1 \text{ in ENDF}$$

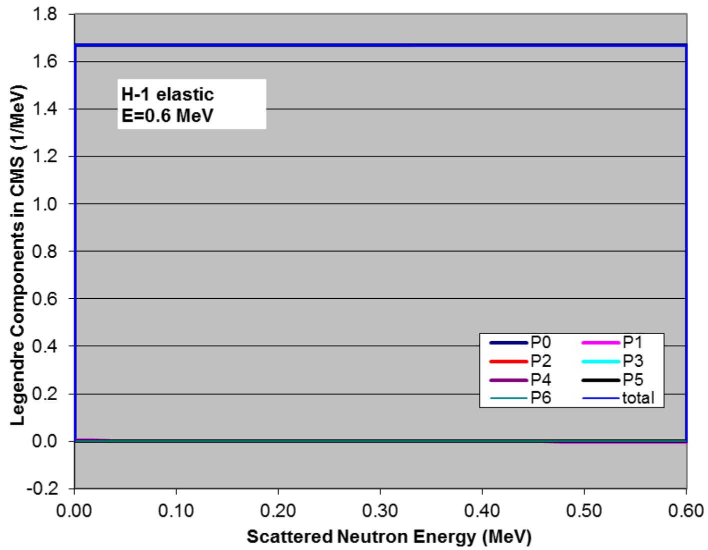
- The relation between the laboratory and center-of-mass scattering angular distributions may be obtained from a formal change of independent variable

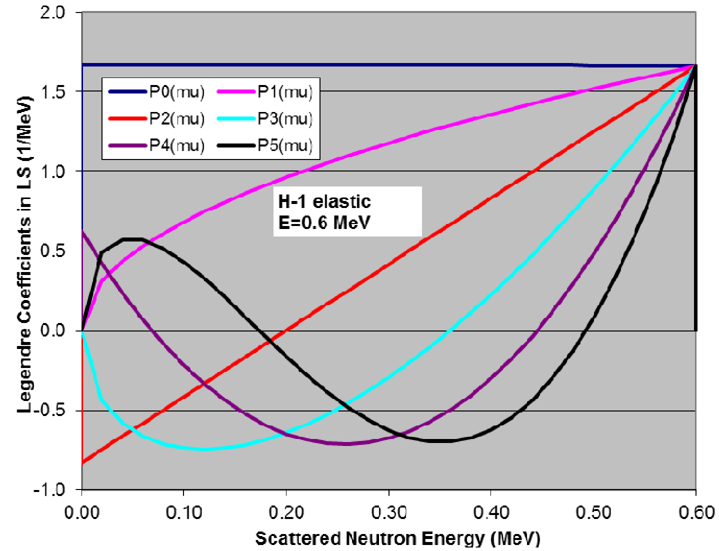
$$\sigma_s(E,\mu_s)d\mu_s = \sigma_s(E,\mu_c)d\mu_c$$

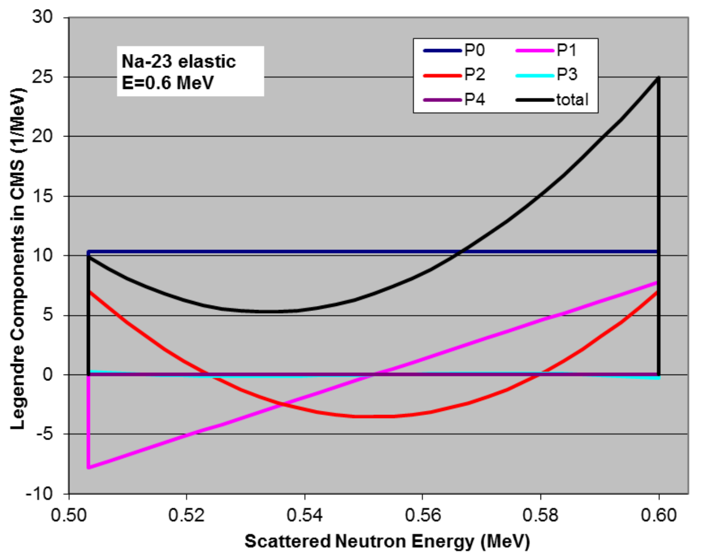
$$\frac{d\mu_c^{\pm}}{d\mu_3} = \pm\frac{(\beta^2+2\beta\mu_c^{\pm}+1)^{3/2}}{\beta^2(\beta+\mu_c^{\pm})}$$

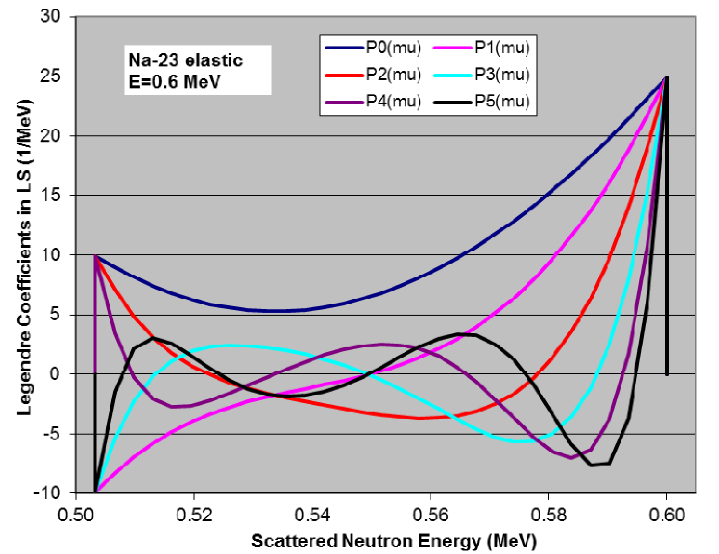
For elastic scattering and for inelastic scattering with single value of μ_c, only the positive sign applies, and there is single value of E_3. However, for inelastic scattering with dual values of E_3, there are two values of μ_c.

Sample Legendre Coefficients

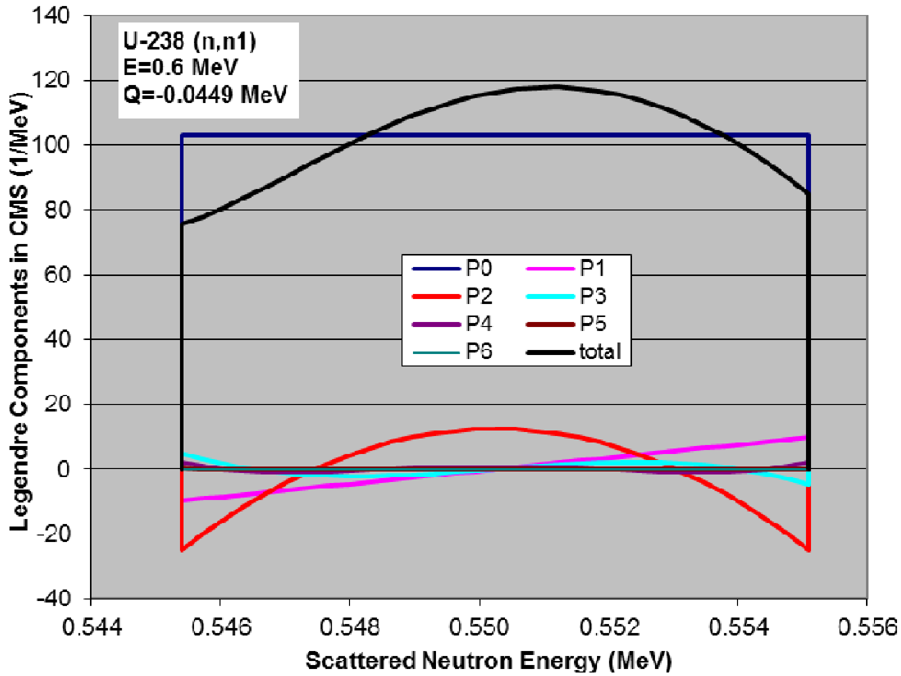


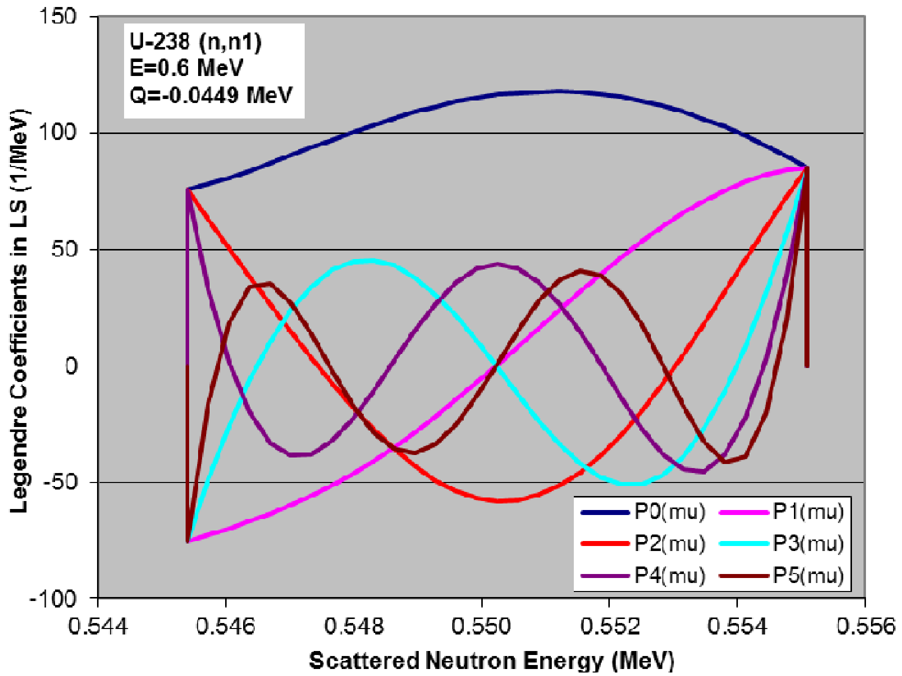






Sample Legendre Coefficients



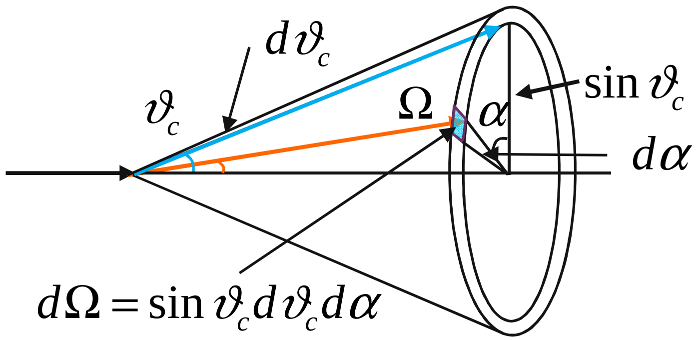


Average Energy Transfer in Neutron Scattering

- Scattering into a particular range of energies requires scattering within an associated range of directions, that is

$$\sigma_s(E_1,E_3)dE_3 = 2\pi\sigma_s(E_1,\mu_c)d\mu_c$$

$$\sigma_s(E_1,E_3) = \frac{4\pi(1+A)^2}{2\beta E_1}\sigma_s(E,\mu_c)$$



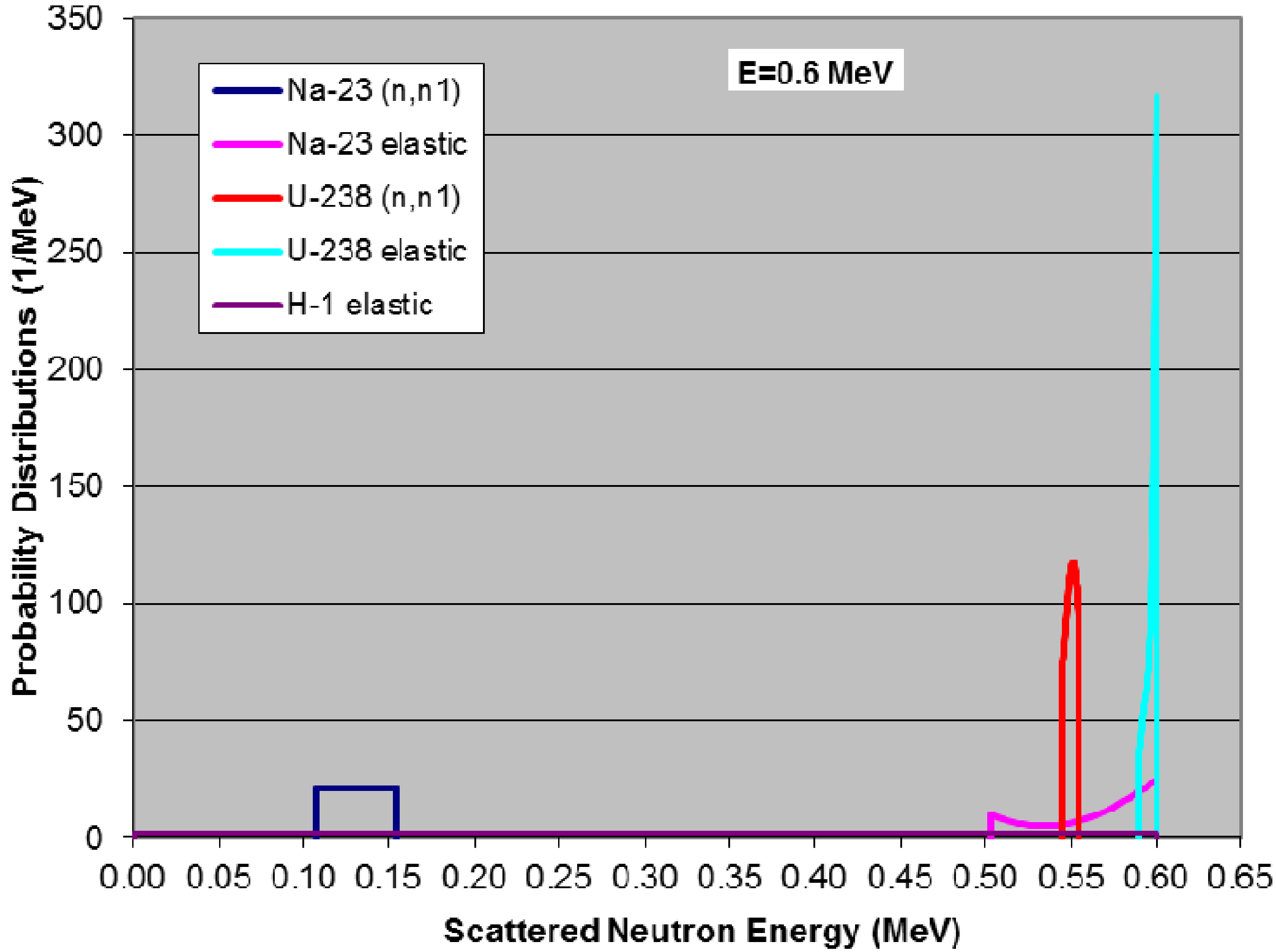
- Thus, the average energy of scattered neutron can be obtained as

$$\frac{<E_3>}{E_1} = \frac{1}{\sigma_s(E_1)}\int_{E'_{\min}}^{E'_{\max}} dE_3 \frac{E_3}{E_1}\sigma_s(E_1,E_3) = \frac{2\pi}{\sigma_s(E_1)}\int_{-1}^{1} d\mu_c \frac{E_3}{E_1}\sigma_s(E_1,\mu_c)$$

- The average recoil energy of target can be obtained as

$$\frac{<E_4>}{E_1} = 1 - \frac{<E_3>}{E_1} + \frac{Q}{E_1}$$

Scattered Neutron Energy Distribution



Doppler Broadening (1)

- The laboratory cross section should be defined to agree with the observed reaction rate.
  - The cross section is determined by the relative speed, as opposed to the laboratory speed of neutron
  - The Doppler broadened cross section will not generally be the same as the cold cross section
- If $P(\vec{V})d\vec{V}$ is the probability at temperature T that a nucleus (or atom) has velocity $\vec{V}$ within $d\vec{V}$ about $\vec{V}$, the observed reaction rate that a neutron with velocity $\vec{v}$ will collide with a nucleus is

$$R(v,T) = v\sigma(v,T) = \int [v_r \sigma(v_r,0)] P(\vec{V}) d\vec{V}$$

- If the velocity distribution of the target nuclei is isotropic, we have

$$P(\vec{V})d\vec{V} = \frac{1}{4\pi} P(V)dVd\mu d\varphi$$

$$\sigma(v,T) = \frac{1}{2v}\int_{-1}^{1} d\mu \int_{0}^{\infty} dV [v_r \sigma(v_r,0)] P(V)$$

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Doppler Broadening (2)

- The relative speed can be written as

$$v_r = |\vec{v} - \vec{V}| = (v^2 + V^2 - 2vV\mu)^{1/2}$$

- The Jacobian transformation from the cosine of scattering angle to the relative speed is given by

$$d\mu = v_r dv_r / vV$$

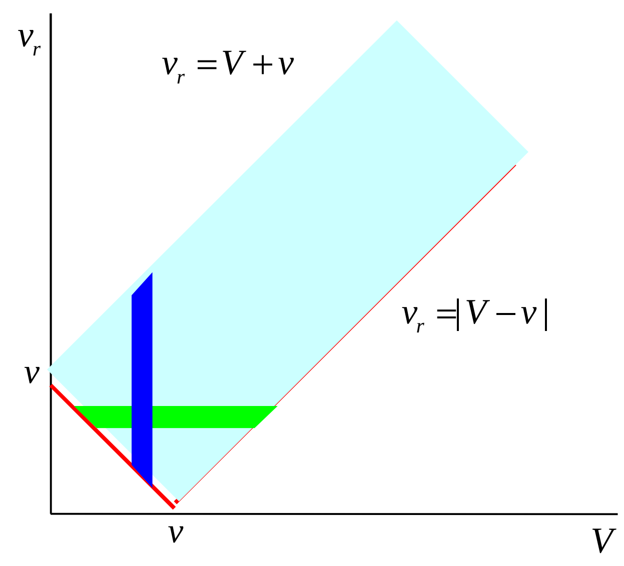
- If the velocity distribution of the target nuclei is isotropic, we have

$$\sigma(v,T) = \frac{1}{2v^2}\int_{|v-V|}^{v+V}[v_r\sigma(v_r,0)]v_r dv_r \int_0^\infty P(V)\frac{dV}{V}$$

$$= \frac{1}{2v^2}\int_0^\infty [v_r\sigma(v_r,0)]v_r dv_r \int_{|v-v_r|}^{v+v_r} P(V)\frac{dV}{V}$$

- For the Maxwellian monatomic (or free) gas model, the distribution of nuclei speed is given by

$$P(V)dV = 4\pi\left(\frac{\beta}{\pi}\right)^{3/2} V^2 e^{-\beta V^2} dV; \quad \beta = \frac{M}{2kT}$$



Doppler Broadening (3)

- The Doppler broadened cross section is obtained as

$$\sigma(v,T)=\frac{2\beta^{3/2}}{\sqrt{\pi}v^2}\int_0^\infty [v_r\sigma(v_r,0)]v_r dv_r \int_{|v-v_r|}^{v+v_r} Ve^{-\beta V^2}dV$$

$$=\frac{\beta^{1/2}}{\sqrt{\pi}v^2}\int_0^\infty [v_r\sigma(v_r,0)]v_r\left[e^{-\beta(v-v_r)^2}-e^{-\beta(v+v_r)^2}\right]dv_r$$

- This can be rewritten in terms of energy as

$$\sigma(E,T)=\frac{\alpha^{1/2}}{2\sqrt{\pi E}}\int_0^\infty [\sqrt{E_r}\sigma(E_r,0)]\left[e^{-\alpha(\sqrt{E}-\sqrt{E_r})^2}-e^{-\alpha(\sqrt{E}+\sqrt{E_r})^2}\right]dE_r$$

$$E=\frac{1}{2}mv^2;\quad E_r=\frac{1}{2}mv_r^2;\quad \alpha=\frac{2\beta}{m}=\frac{M}{mkT}=\frac{A}{kT}$$

- For large $\alpha\sqrt{EE_r}$ $(\sim AE/kT)$, the second exponential can be ignored, compared to the first

$$\sigma(E,T)=\frac{\alpha^{1/2}}{2\sqrt{\pi E}}\int_0^\infty [\sqrt{E_r}\sigma(E_r,0)]e^{-\alpha(\sqrt{E}-\sqrt{E_r})^2}dE_r$$

Psi-Chi Method for Doppler Broadening (1)

- The major contribution to this remaining integral comes from a narrow range of E_r, either close to E or close to some other energy E_0 (usually the peak of a resonance). This assumption allows a Taylor expansion of E_r, which in turn yields the approximation

$$\alpha(\sqrt{E}-\sqrt{E_r})^2 \approx \left(\frac{E_r - E}{\Delta}\right)^2$$

$$\Delta = 2\left(\frac{E}{\alpha}\right)^{1/2} = \left(\frac{4kTE}{A}\right)^{1/2} \quad \text{(Doppler width)}$$

- In the psi-chi (ψ-χ) method, a third approximation is introduced by extending the lower limit of integration to -∞

$$\sigma(E,T) = \frac{1}{\Delta\sqrt{\pi E}} \int_{-\infty}^{\infty} [\sqrt{E_r}\,\sigma(E_r,0)] e^{-[(E_r-E)/\Delta]^2} dE_r$$

- Single-level Breit-Wigner formula for an isolated s-wave resonance

$$\sigma_a(E) \approx \sigma_0 \frac{\Gamma_a}{\Gamma_r} \frac{1}{1+x^2} \quad (a=\gamma, f)$$

$$\sigma_0 = \frac{4\pi}{k^2} g_J \frac{\Gamma_n}{\Gamma} \quad \text{(peak value of the resonance)}$$

$$\sigma_n(E) \approx 4\pi a^2 + \sigma_0 \frac{\Gamma_n}{\Gamma} \frac{1}{1+x^2} + \sigma_0 ka \frac{2x}{1+x^2}$$

$$x = \frac{E - E_0}{\Gamma/2}$$

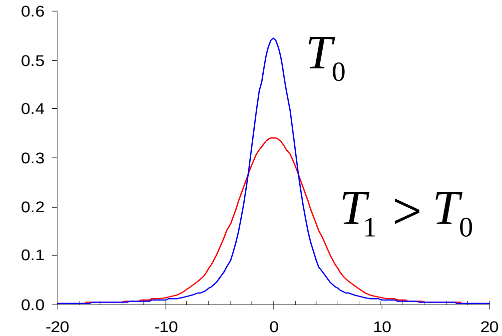
Psi-Chi Method for Doppler Broadening (2)

- The symmetric and anti-symmetric Doppler broadened line shape functions can be approximated as

$$\psi(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{1}{1+w^2}\exp\left[-\frac{\xi^2}{4}(x-w)^2\right]dw$$

$$\chi(x,\xi)=\frac{\xi}{\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{w}{1+w^2}\exp\left[-\frac{\xi^2}{4}(x-w)^2\right]dw$$

$$\xi=\frac{\Gamma}{\Delta}$$



- The Doppler broadened line shapes ψ and χ can be represented as convolution integrals of Lorentzian L and Gaussian kernel G as

$$\psi(x,\xi)=\int_{-\infty}^{\infty}L(w)G(x-w;\xi)dw=L(x)*G(x,\xi)$$

$$\chi(x,\xi)=\int_{-\infty}^{\infty}2wL(w)G(x-w,\xi)dw=[2xL(x)]*G(x,\xi)$$

$$L(x)=\frac{1}{1+x^2}$$

$$G(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\exp\left(-\frac{\xi^2}{4}x^2\right)$$

- ✓ Lorentzian L and 2xL represent the natural line shapes of ψ and χ at 0K, respectively
- ✓ Gaussian kernel G represents the pure Doppler shape

Scattering Function for Monatomic Gas (1)

- For an energy-independent s-wave scattering, which is isotropic in the center of mass system, the scattering function can be obtained as

$$\sigma_s(E) f_s(E \to E', \mu_0) = \frac{\sigma_{s0}(1+A^{-1})^2}{2} \frac{A}{2E'} \delta\left\{\mu_0 - \frac{1}{2}\left[(A+1)\sqrt{\frac{E'}{E}} - (A-1)\sqrt{\frac{E}{E'}}\right]\right\}$$

- The energy transfer function is the integral of the scattering function over all scattering angles

$$\sigma_s(E) f_s(E \to E') = 2\pi \int_{-1}^{1} \sigma_s(E) f_s(E \to E', \mu_0) d\mu_0$$

$$\sigma_s(v) f_s(E \to E') = \frac{\sigma_{s0}\eta^2}{2E}\left\{\operatorname{erf}\left(\eta\sqrt{\frac{E'}{kT}} - \rho\sqrt{\frac{E}{kT}}\right) \mp \operatorname{erf}\left(\eta\sqrt{\frac{E'}{kT}} + \rho\sqrt{\frac{E}{kT}}\right)\right.$$
$$\left. + e^{(E-E')/kT}\left[\operatorname{erf}\left(\eta\sqrt{\frac{E}{kT}} - \rho\sqrt{\frac{E'}{kT}}\right) \pm \operatorname{erf}\left(\eta\sqrt{\frac{E}{kT}} + \rho\sqrt{\frac{E'}{kT}}\right)\right]\right\}$$

$$\eta = \frac{A+1}{2\sqrt{A}} \qquad \rho = \frac{A-1}{2\sqrt{A}}$$

✓ Here the upper signs are to be used for $E' > E$ and the lower signs for $E' < E$

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Scattering Function for Monatomic Gas (2)

- When the temperature approaches zero or the thermal motion of target nuclides is negligible relative to the neutron energy, the energy transfer function is reduces to that for stationary target

$$\sigma_s(v) f_s(E \to E') = \begin{cases} \dfrac{\eta^2}{E} = \dfrac{\sigma_{s0}}{(1-\alpha)E}, & \alpha E \le E' \le E \\ 0, & E' > E \ \text{ or } \ E' < \alpha E \end{cases}$$

- For a proton gas (A=1), η=1 and ρ=0, and the energy transfer function becomes

$$\sigma_s(v) f_s(E \to E') = \frac{\sigma_{s0}}{E} \begin{cases} e^{(E-E')/kT} \operatorname{erf}\sqrt{E/kT}, & E' > E \\ \operatorname{erf}\sqrt{E'/kT}, & E' < E \end{cases}$$