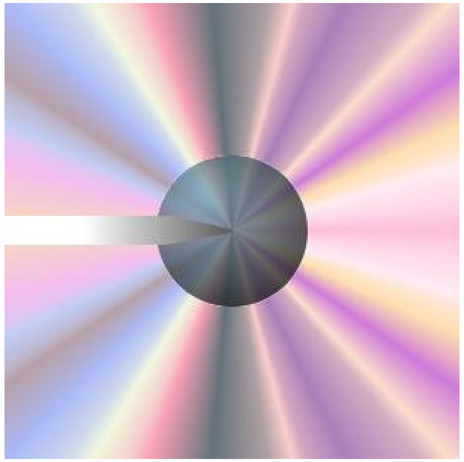
Modeling Scattering Angular Distributions in the Fast Energy Range



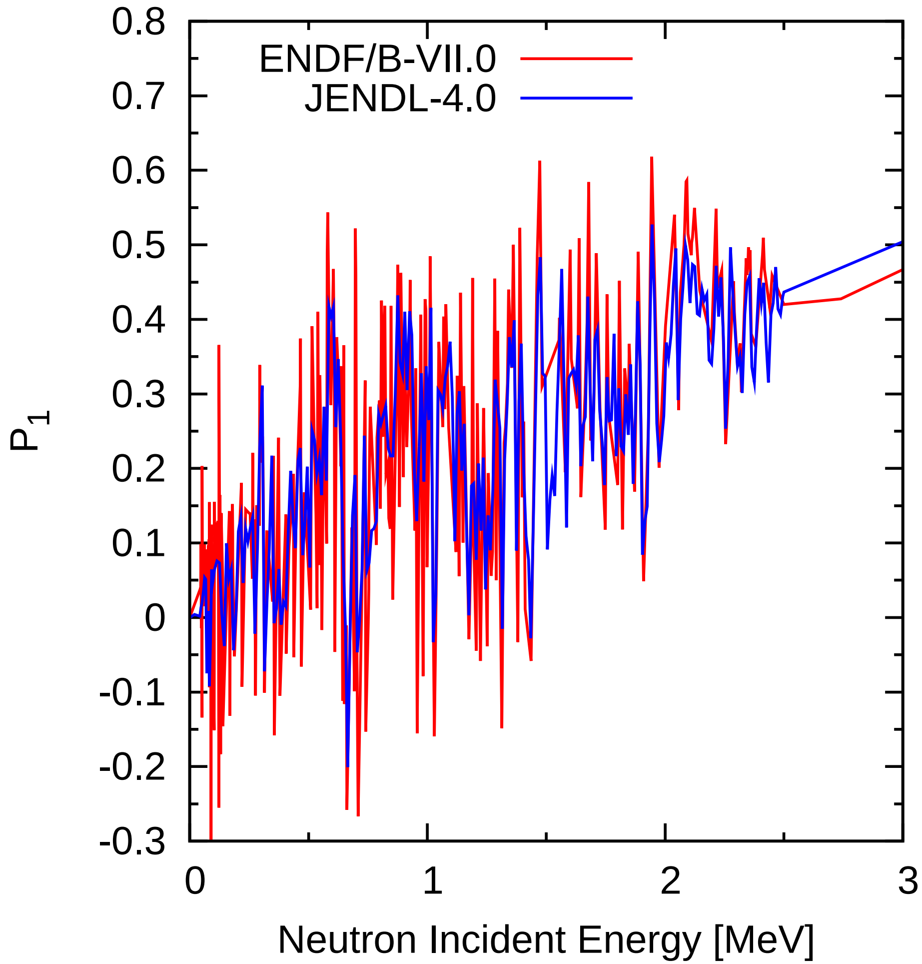
T. Kawano
Theoretical Division
Los Alamos National Laboratory

Los Alamos

Introduction

Importance of Scattering Angular Distribution

- Criticality benchmark calculations imply the significance (high sensitivity to k_{eff}) of elastic scattering angular distributions ($\overline{\mu}$) in the fast energy range.
- These data are generally evaluated with a relatively simple method (optical model).
- When nuclear reaction models cannot predict $\overline{\mu}$ within a desired accuracy, we have to consider new experiments.

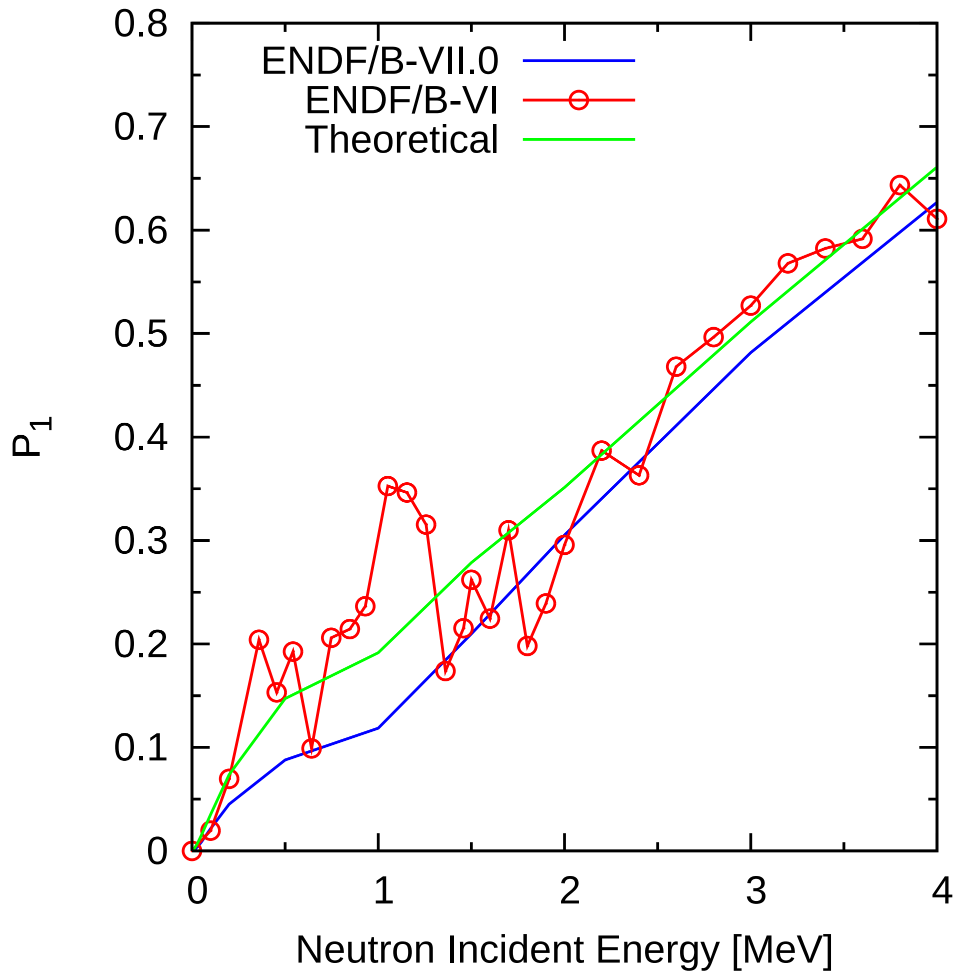


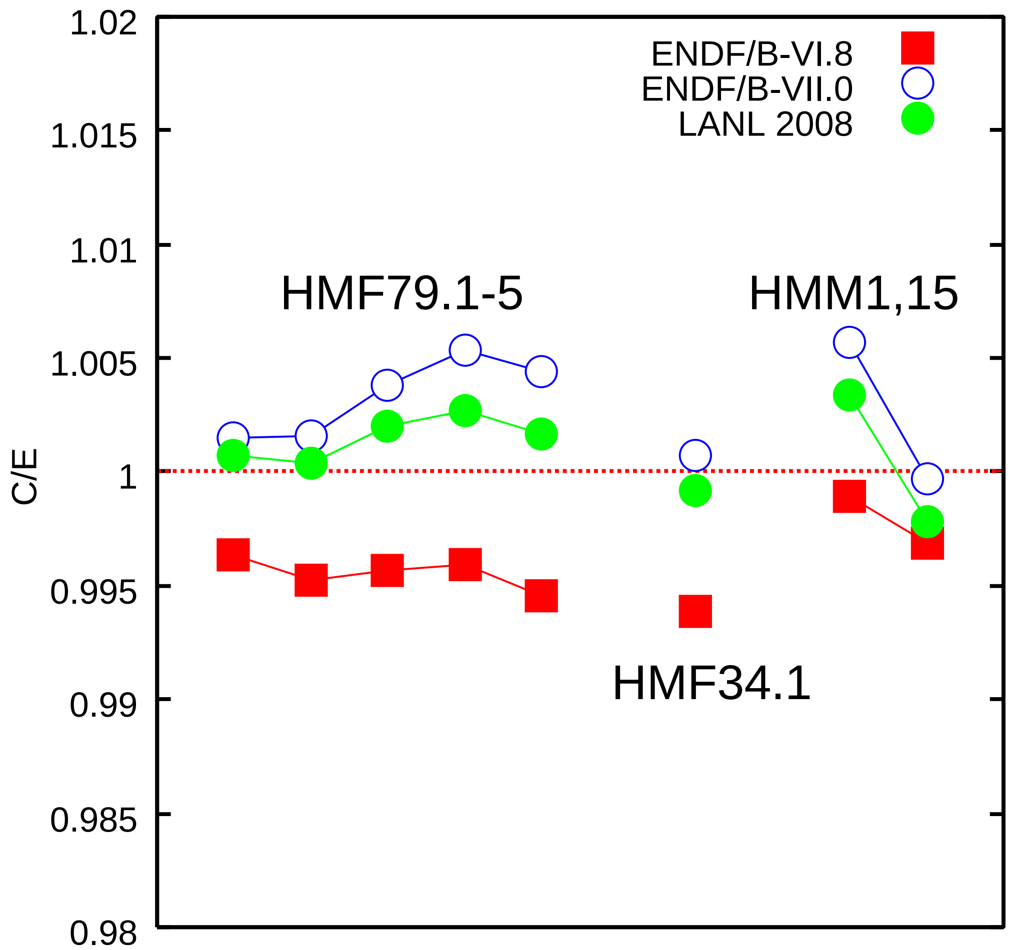
Problems Reported

- Iron shielding benchmark tests are sometimes problematic.
- Criticality safety benchmark test with the Ti-reflector indicated that $\overline{\mu}$ calculated with the optical model does not work so well.
- $\overline{\mu}$ for Na and Fe are by factor 2–3 larger than what we estimate and there is a structure, which cannot be reproduced by a simple optical model calculation.
- Values of $\overline{\mu}$ for ^{238}U in the fast energy range differ considerably among the evaluated data files.

Elastic Scattering Angular Distribution and K-eff

P_1 Legendre Coefficient of Ti and k_{eff}



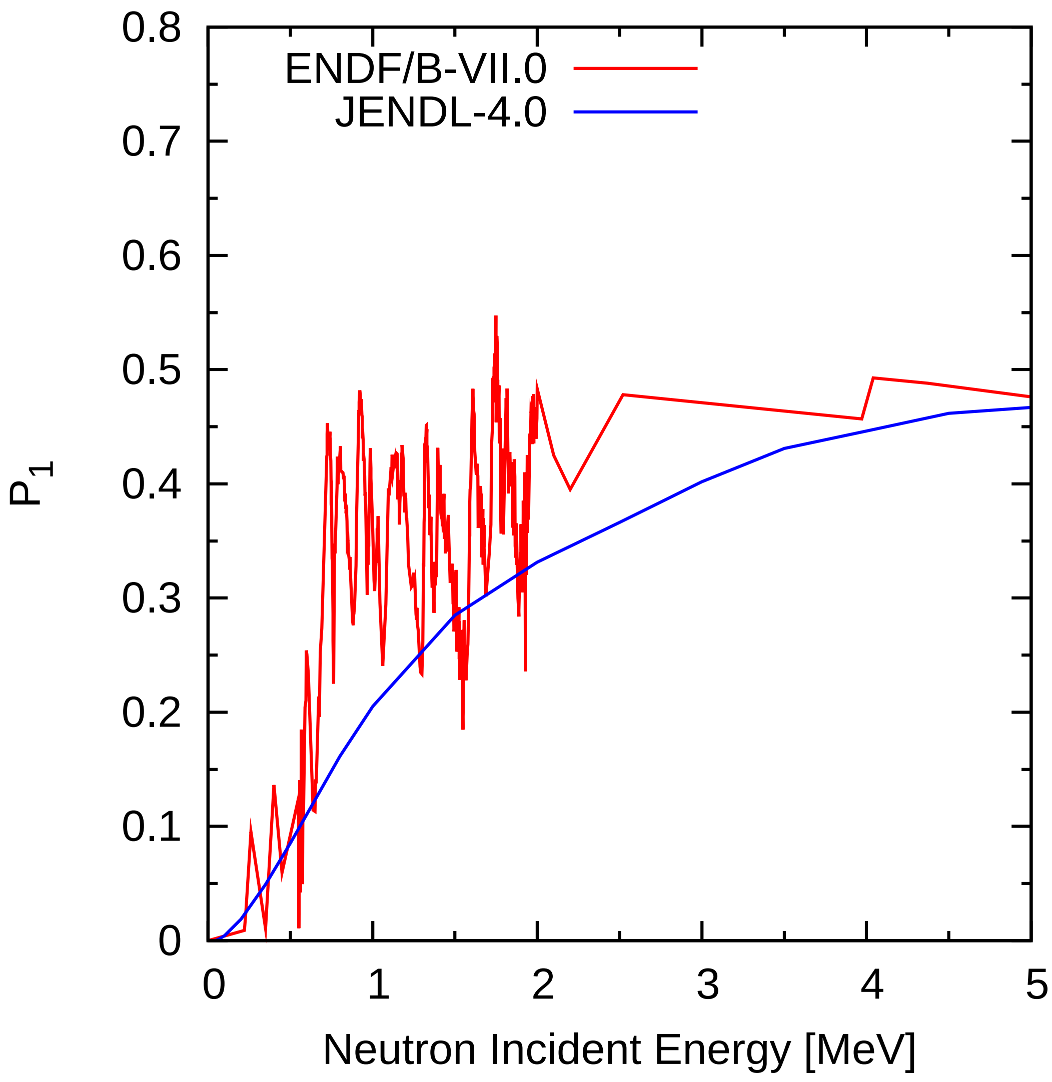


We adopted P_ℓ from ENDF/B-VI up to 4 MeV.

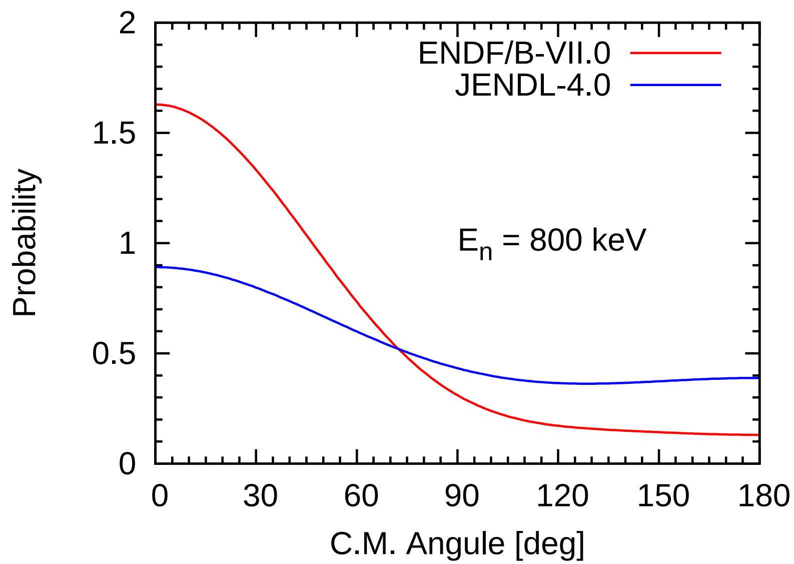
Los Alamos

Na-23 Elastic Scattering Angular Distribution

P_1 Legendre Coefficient for Na23 in ENDF/B-VII and JENDL-4



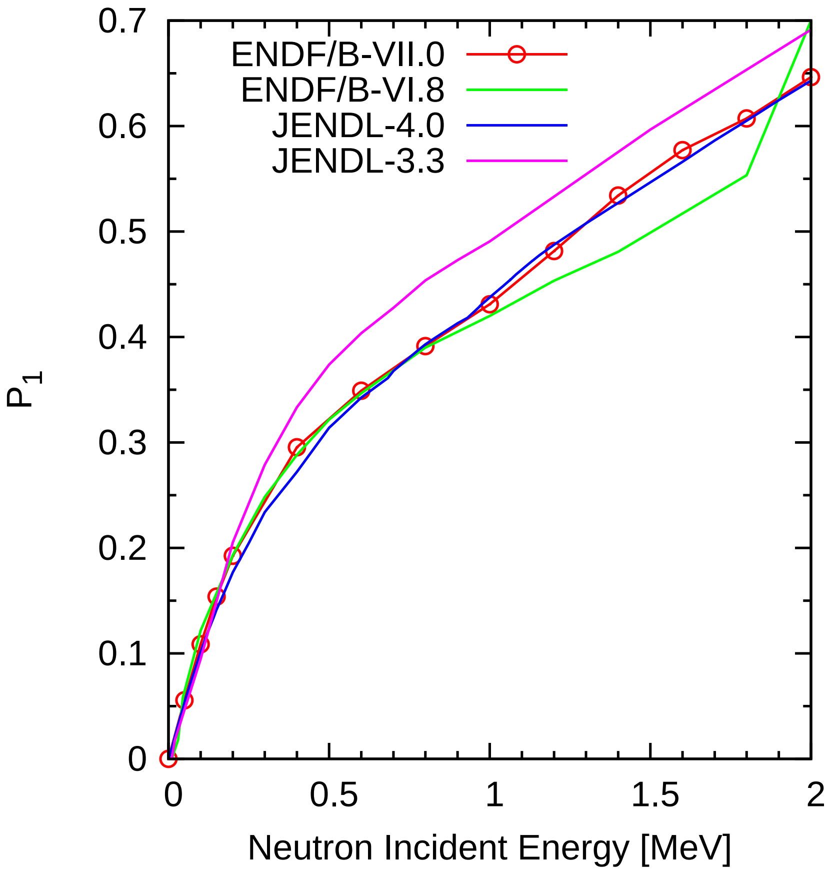
- factor of 2–3 difference in the 500 keV – 1 MeV region
- ENDF/B-VII angular distribution
  - Kinney and Perey data
  - (private communication)
- JENDL-4 angular distribution
  - optical model calculation
  - no structure

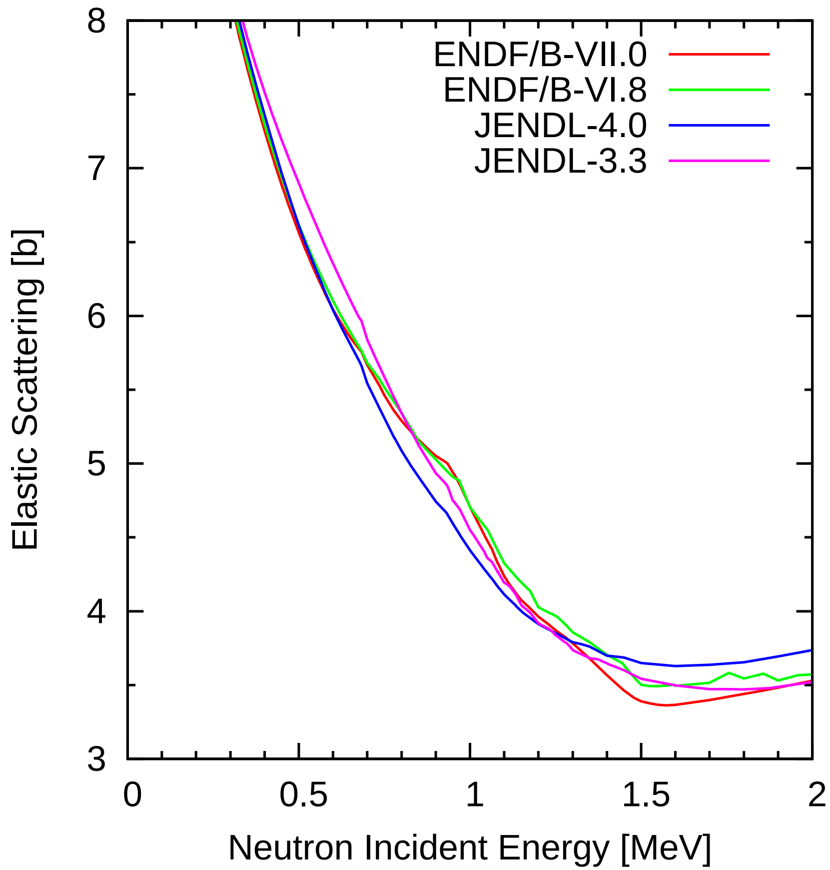


Los Alamos

U-238 Elastic Scattering Cross Sections

P_1 and σ_E for U238 in ENDF and JENDL





- Evaluation performed based on coupled-channels calculations
- Differences come from the optical potential used

Los Alamos

Theory: Scattering Matrices

Reich-Moore R-Matrix Representation

All physical quantities defined by the resonance parameters

$$R_{\alpha\beta}(E) = \sum_i \frac{\sqrt{\Gamma_\alpha^{(i)}\Gamma_\beta^{(i)}}}{E_R^{(i)} - E - i\Gamma_\gamma^{(i)}/2}, \qquad (1)$$

and the scattering matrix is given by

$$S = \frac{I(a)}{O(a)} \frac{1 - R(L^* - B)}{1 - R(L - B)}, \qquad (2)$$

where a the channel radius, $I(r)$ the ingoing and $O(r)$ the outgoing radial wave function, L the logarithmic derivative of the out-going wave function, and B the logarithmic derivative of the radial eigenfunctions.

The averaged total, shape elastic scattering, and reaction cross sections for each entrance channel (s-, p-, ... wave) are given by

$$\sigma_T = \frac{2\pi}{k^2} g\{1 - \mathrm{Re}S\}, \quad \sigma_E = \frac{\pi}{k^2} g|1 - S|^2, \quad \sigma_R = \frac{\pi}{k^2} g\{1 - |S|^2\}. \qquad (3)$$

Elastic Scattering Angular Distribution

Blatt-Biedenharn Formula

$$\frac{d\sigma}{d\Omega} = \sum_L \frac{2L+1}{4\pi} B_L P_L(\cos\theta), \tag{4}$$

where the Legendre coefficient is given by

$$B_L = \frac{\pi}{k^2} \frac{1}{(2i+1)(2I+1)(2L+1)} \sum Z^2(l_1 j_1 l_2 j_2; sL) S_{l_1 j_1} S^*_{l_2 j_2} \tag{5}$$

and Blatt-Biedenharn's Z coefficient is given by

$$Z(l_1 j_1 l_2 j_2; sL) = \hat{l}_1 \hat{l}_2 \hat{j}_1 \hat{j}_2 \langle l_1 l_2 00; sL \rangle W(l_1 j_1 l_2 j_2; sL). \tag{6}$$

- When only the s-wave ($L = 0$) contributes to the scattering matrix element, the angular distribution becomes isotropic.
- Because the S-matrix elements varies rapidly across the resonance range, the scattering angular distribution varies rapidly too.
- Experimental data of scattering angular distributions may have lower energy resolution.

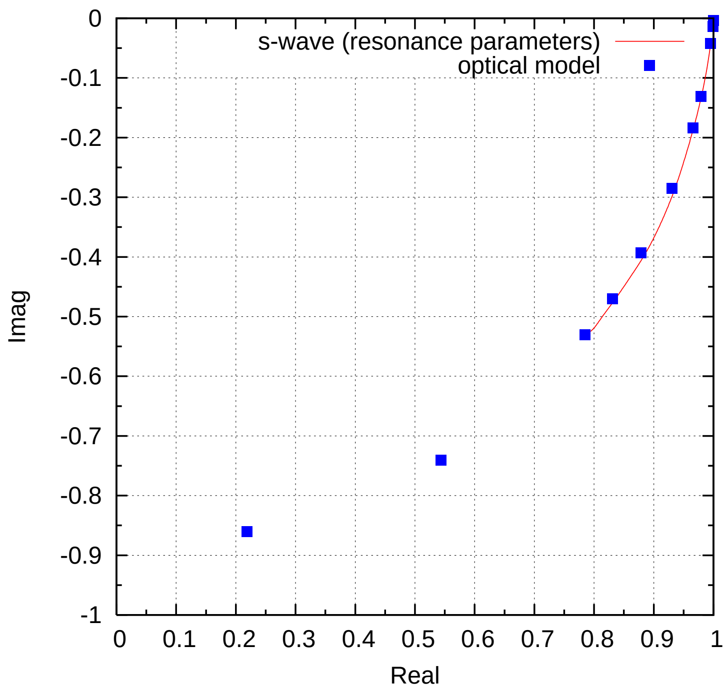
Link Resonances to Optical Model

Lorentzian Energy Averaging

- The optical model gives cross sections averaged over resonances.
- The same average can be obtained in R matrix cross section representation

$$\overline{R} = R(E + iI)$$

- E. Sh. Soukhovitskiĩ, et al., coupled channels potential, adjust the imaginary potential to match the energy averaged S-matrix elements from resonance parameters.



W_s = 2.59 MeV for $E_n < 1.13$ MeV

R' = 9.606 fm (9.6$\pm$ 0.1 in Atlas, Mughabghab)

S_0 = 1.13 $\times 10^{-4}$ ((1.29$\pm$ 0.13) $\times 10^{-4}$, ibid)

S_1 = 2.07 $\times 10^{-4}$ ((2.17$\pm$ 0.19) $\times 10^{-4}$, ibid)

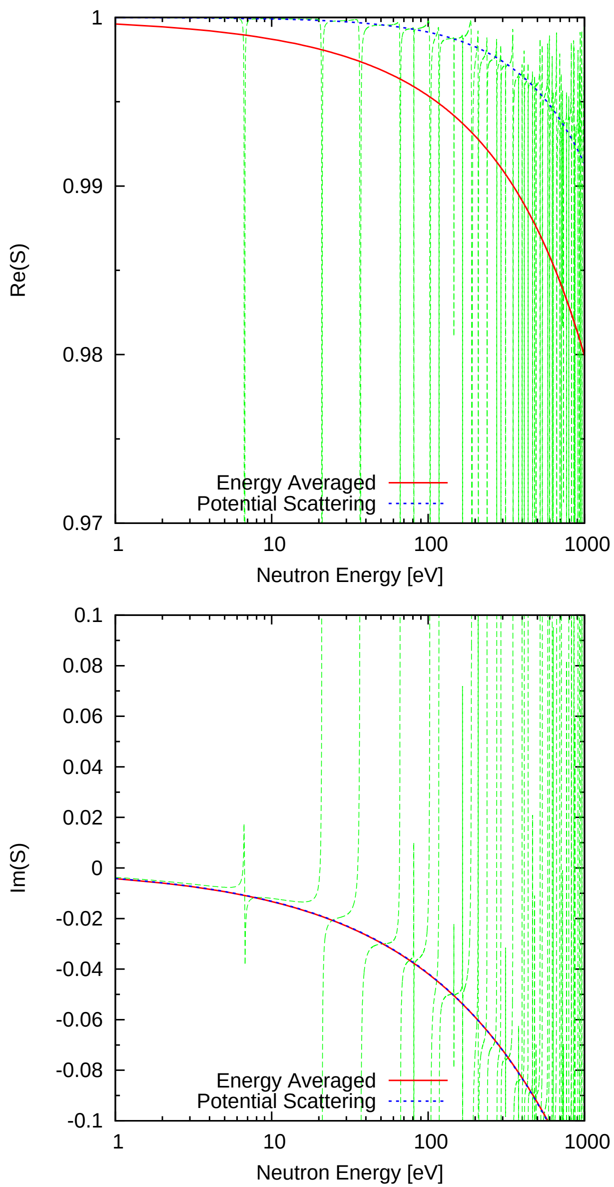
Original SoukhovitskiĩPotential (in the paper)

R' = 9.57 fm

S_0 = 0.95 $\times 10^{-4}$

S_1 = 1.80 $\times 10^{-4}$

S-matrix Background



Common Expression of S-matrix Containing Resonances

$$S_{ab}(E) = S_{ab}^{(0)}(E) - i \sum_{\lambda} \frac{\widehat{g}_{\lambda_a} \widehat{g}_{\lambda_b}}{E - \mathcal{E}_{\lambda}}$$

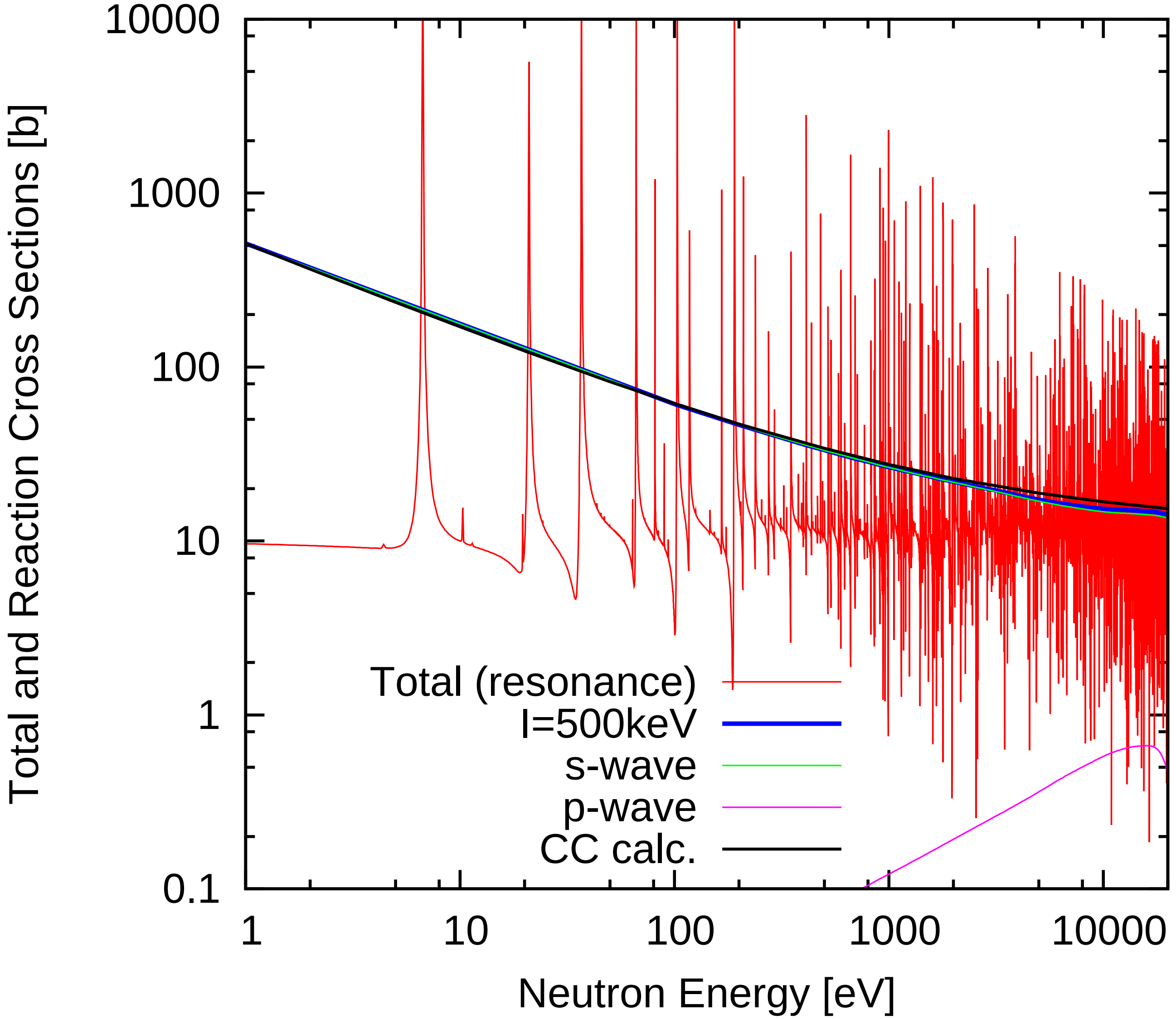
where $S_{ab}^{(0)}(E)$ is the background term, which is nearly energy independent. The phase is not so random.

KKM Expression

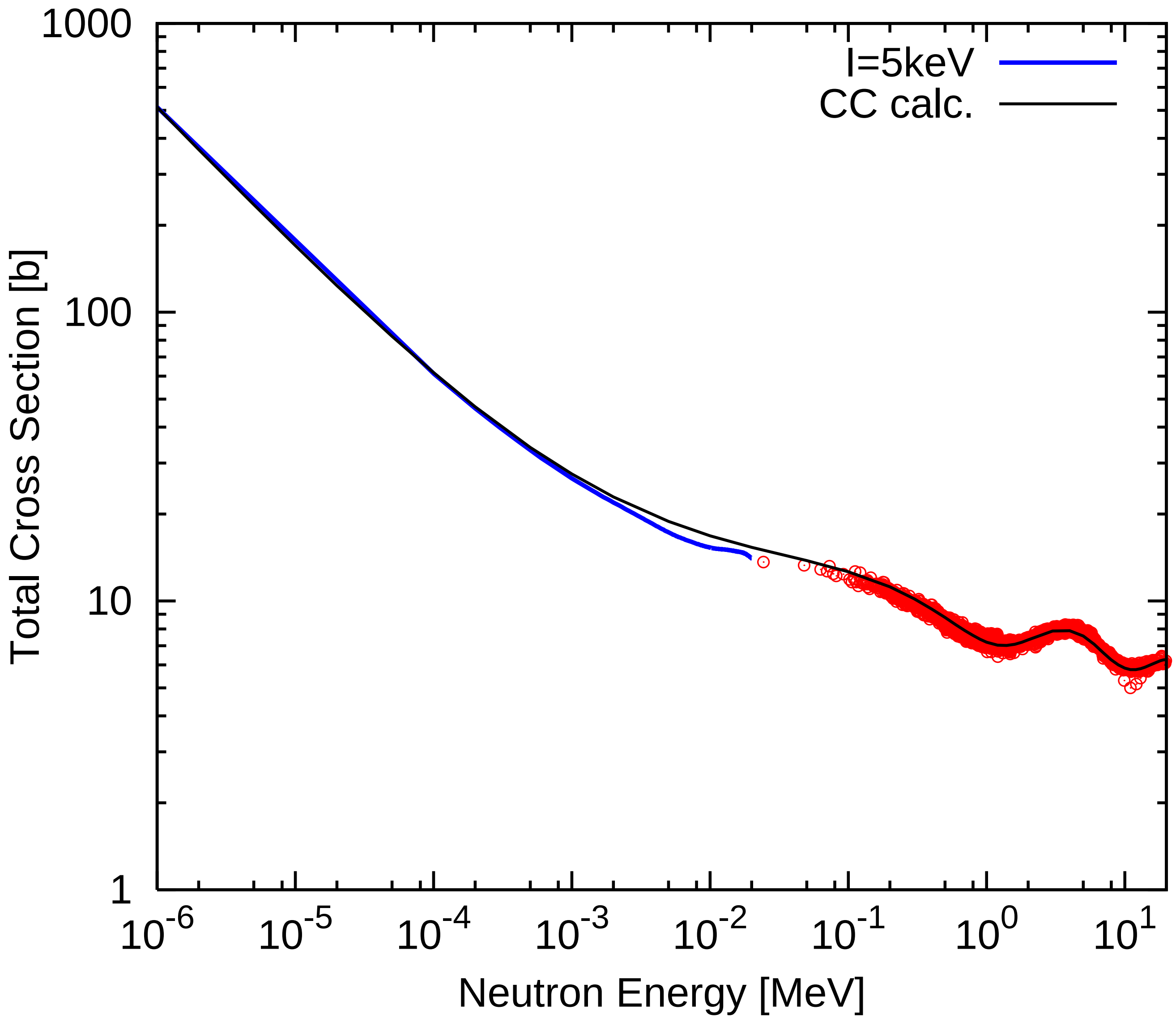
$$S_{ab}(E) = \overline{S}_{ab}(E) - i \sum_{q} \frac{g_{q_a}(E) g_{q_b}(E)}{E - \mathcal{E}_q}$$

where $\overline{S}_{ab}(E)$ is the optical model S-matrix element, and the phase of $g_q(E)$ has a slow q-dependence. The energy average of the resonance sum (second term) becomes zero.

U-238 Total Cross Section in Resonance Range



U-238 Total Cross Section in Higher Energy Region



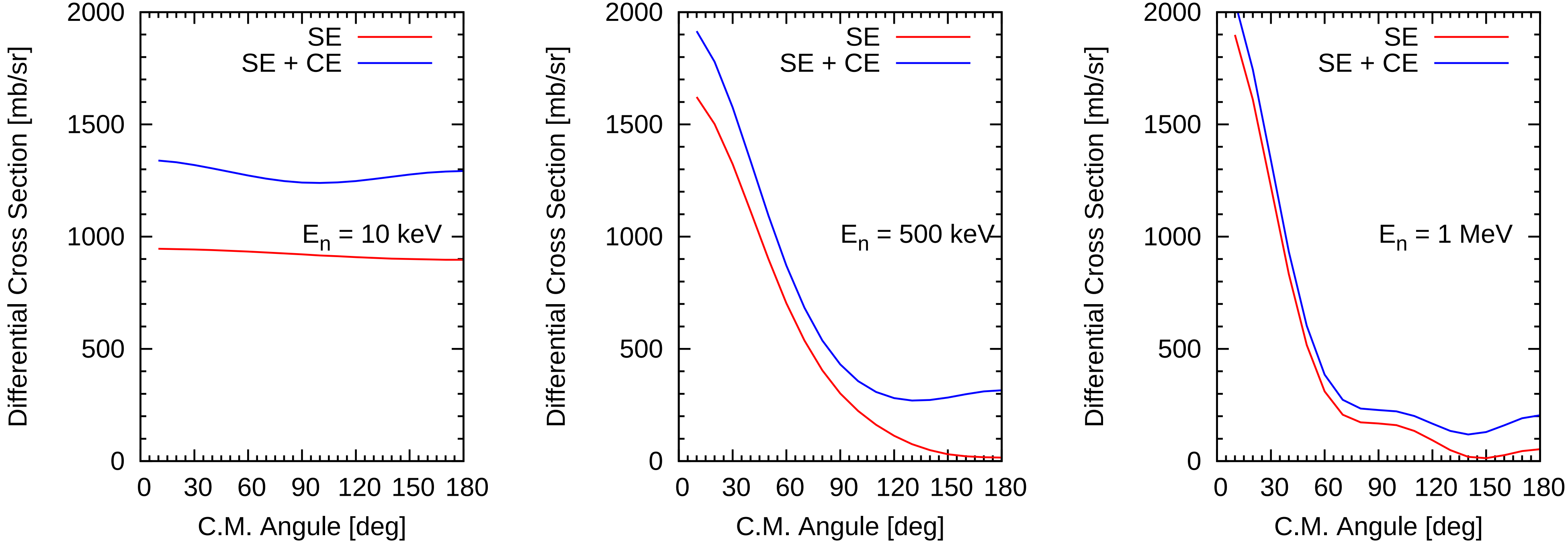
Problems in Extrapolating the Scattering Matrix Elements

- Once energy-averaged scattering matrix elements in the resonance range are well fitted by the optical model, the (shape) scattering angular distribution can be calculated at any energies.
- Anisotropy is seen when the p-wave and higher components start to contribute.
  - At very low energies, the angular distribution is always isotropic (s-wave only)
- The p-wave matrix elements can be fitted by the optical model too. However, there might be missing p-wave resonances.
- In addition to the shape elastic scattering, there is a compound elastic scattering process
  - The compound elastic scattering adds a 90-degree symmetric component to the total scattering angular distribution.
  - The contribution of compound elastic scattering becomes very small, when many inelastic channels open up.

Compound Elastic Scattering Contribution

Shape and Compound Elastic Scattering of U-283

- Compound nuclear reactions calculated with the CoH_3 code.
- All competing channels (capture, inelastic, and fission) included.
- Width fluctuation correction of Moldauer theory.

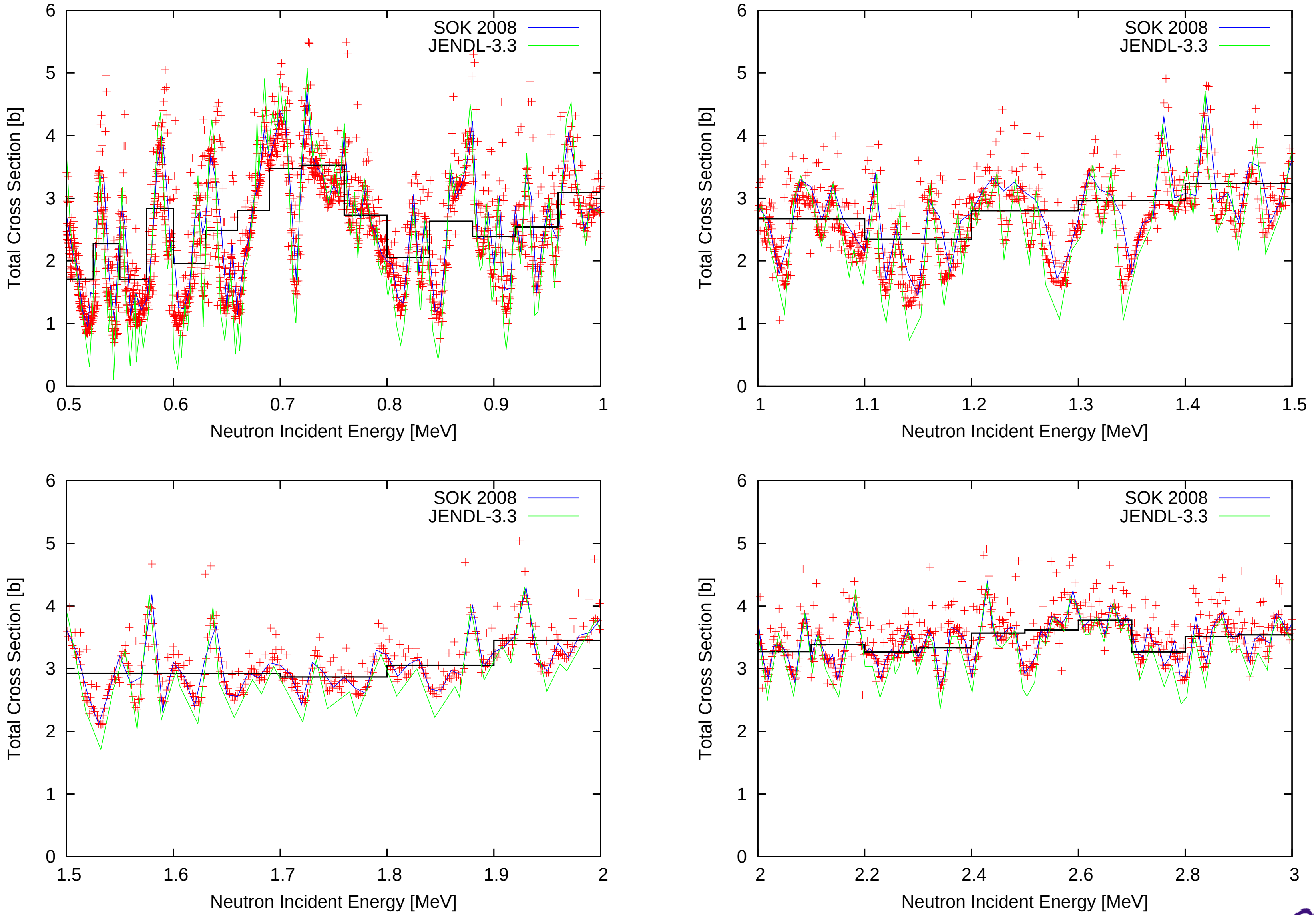


Note: the P_1 values in the modern evaluations (ENDF/B-VII and JENDL-4) agree very well in the U238 case.

Los Alamos

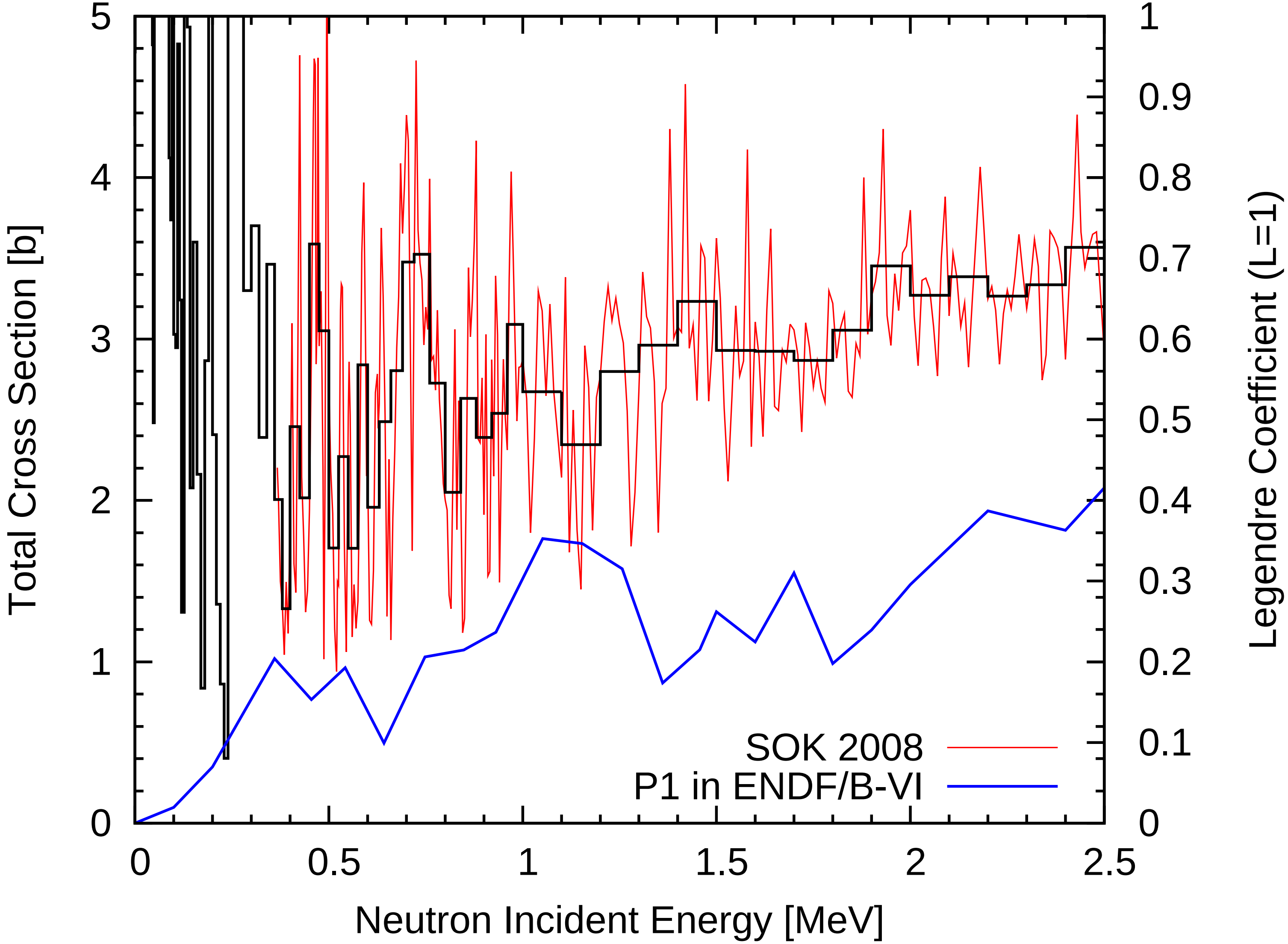
Experimental Data: Intermediate Structure

Fluctuation in the Measured Total Cross Section



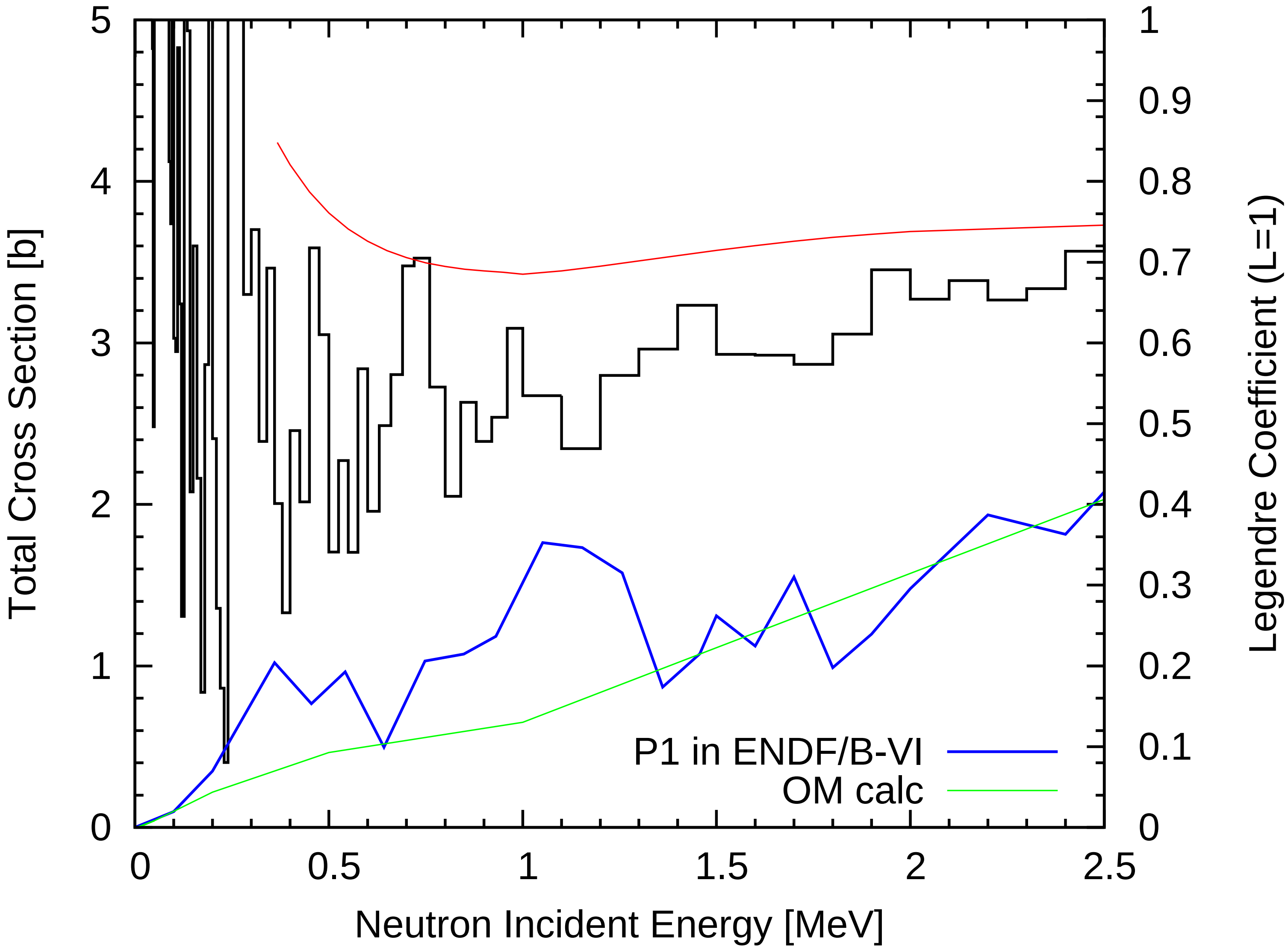
Measured Total Cross Section and P1

Are They Correlated ?



Group-Averaged Total Cross Section and P1

Difference Between OM calc. and Group Cross Sections



Key Issues In The Intermediate Structure Region

- The intermediate structure (or door-way states) observed in the experimental total cross sections cannot be predicted by any model.
  - The experimental data are essential.
- Direct measurement of scattering angular distributions at narrow incident energy step.
  - There are some experimental data available for Ti, Na, and so on, although the origin of the data are often not tractable.
  - Recovery of experimental activities — see T. Hill
- Indirect estimation method from the experimental total cross sections and the optical model calculation
  - We need more careful modeling, theoretical development.

Conclusion

Understanding Scattering Angular Distributions in the Fast Energy Range

- The scattering angular distributions can be calculated by the R and S matrices in the resonance range.
- An extrapolation from the resolved resonance region into the unresolved resonance range is possible, but uncertainties may inflate.
- In the higher energy region, experimental total cross sections show strong fluctuations, which cannot be reproduced with the theoretical models.
- However, there is an indication that one can relate the experimental total cross section to the optical model calculation.
  - More theoretical investigations needed.
  - Check other isotopes to which scattering angular distribution measurements were made.
- International cooperative project under OECD/NEA, WPEC subgroup 35 initiated in 2010.