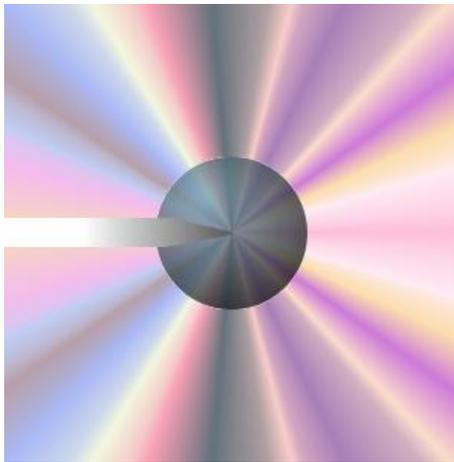


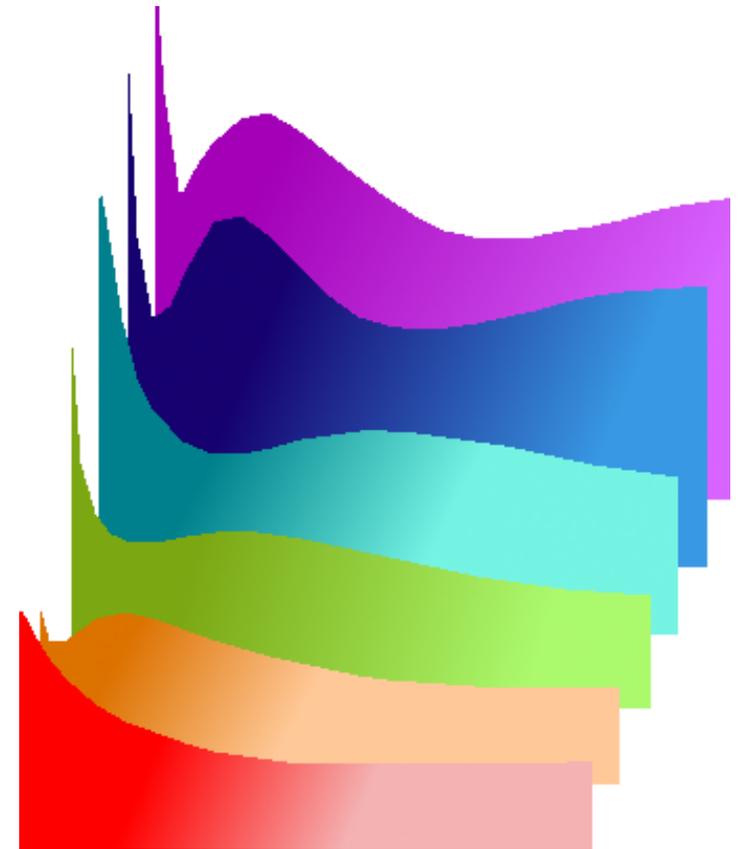
Statistical-Model and Direct-Semidirect-Model Calculations of Neutron Radiative Capture Process



T. Kawano
Theoretical Division
Los Alamos National Laboratory

Nuclear Reactions in the Fast Energy Range

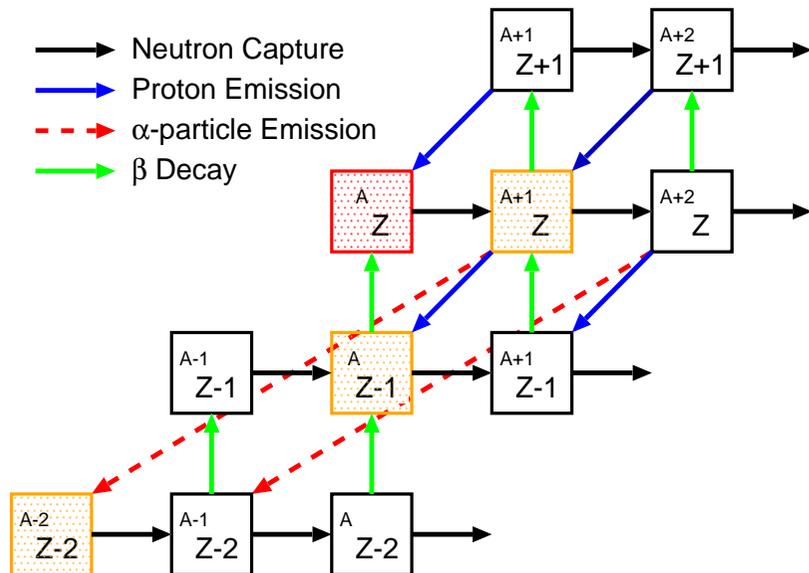
- The **Hauser-Feshbach** statistical theory has been widely used for nuclear reaction data applications,
 - nuclear reaction rates for astrophysics (nucleo-synthesis)
 - nuclear data libraries for energy applications (mainly for neutron)
- however, questions still persist regarding:
 - applicability in the domain of off-stability
 - global inputs
 - level densities, optical potentials,
 - γ -ray strength function
 - nuclear deformation effect
 - width fluctuation correction
$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle \neq \frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\langle \Gamma \rangle}$$
 - inclusive / exclusive observables
 - partial γ -rays, coincidence, etc.
 - Monte Carlo approach to the HF needed
 - interaction on the excited state (isomer)



Nuclear Data for Astrophysical Applications

Nuclear Reaction Rate in Astrophysics

Nuclear Reaction Chain



- Nuclear reactions in astrophysical environments
 - s and r-processes
 - targets are often neutron-rich and unstable
 - neutron capture process is mostly important
 - β -delayed neutron emission and fission
- Model prediction is crucial for
 - reaction cross section
 - Hauser-Feshbach theory
 - nuclear structure, including mass
 - macro/microscopic model, Hartree-Fock

Understanding of the neutron capture process is important to study nucleo-synthesis, which includes models for γ -ray strength function, GDR (Giant Dipole Resonance), nuclear level densities, and spectroscopic factors.

Nucleon Radiative Capture

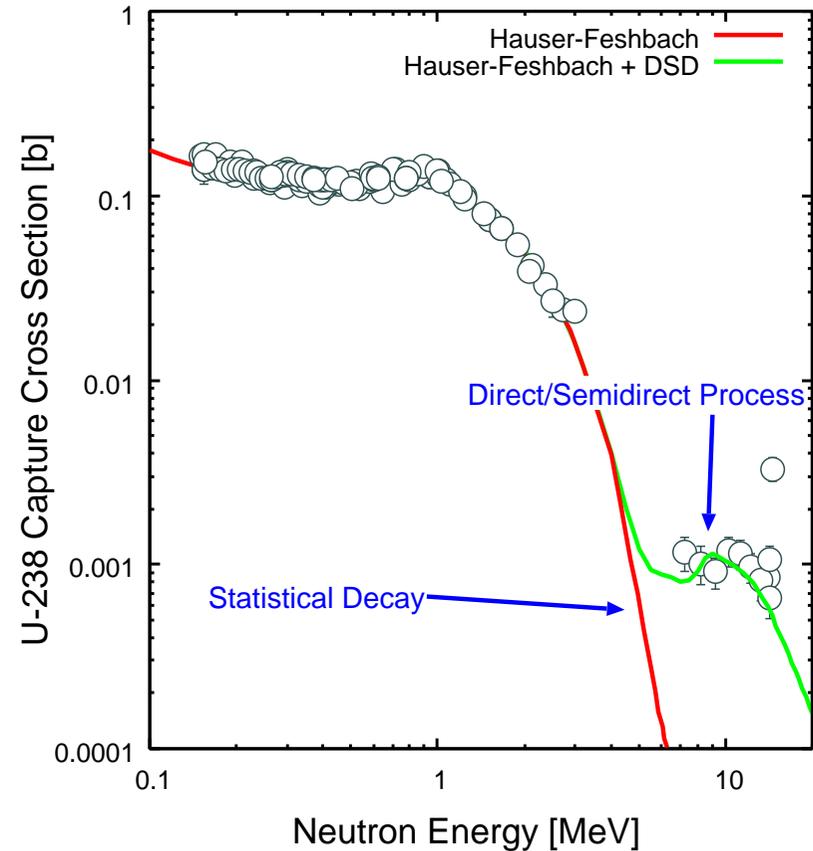
CN and DSD Processes

Compound Reaction

- An incident neutron and a target form a compound nucleus, and it decays.
- Hauser-Feshbach statistical theory, with width fluctuation.
- Cross section decreases rapidly when neutron inelastic channels open.

Direct/Semidirect Capture

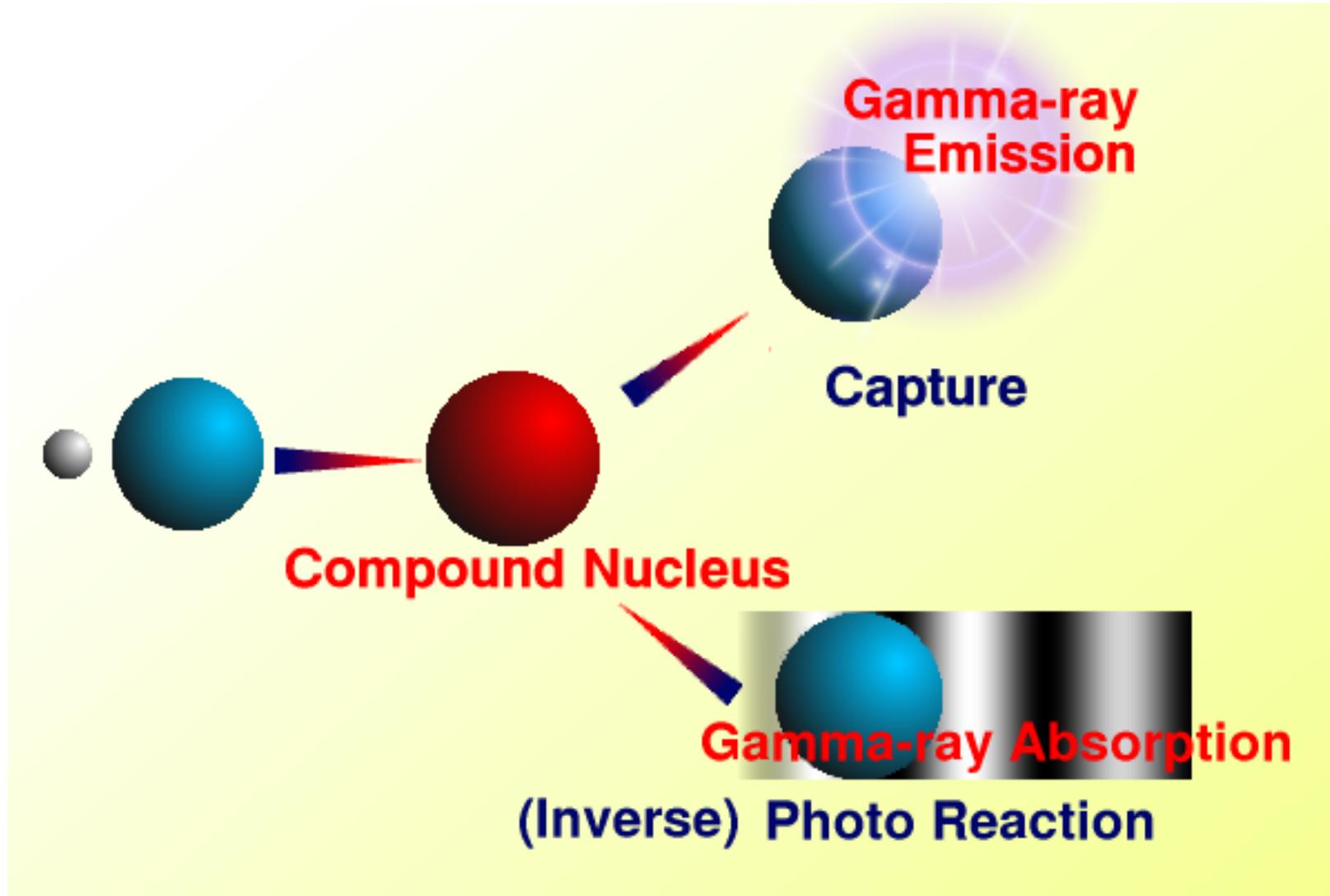
- Direct transition to one of the unoccupied single-particle state.
- Giant Dipole Resonance (GDR)



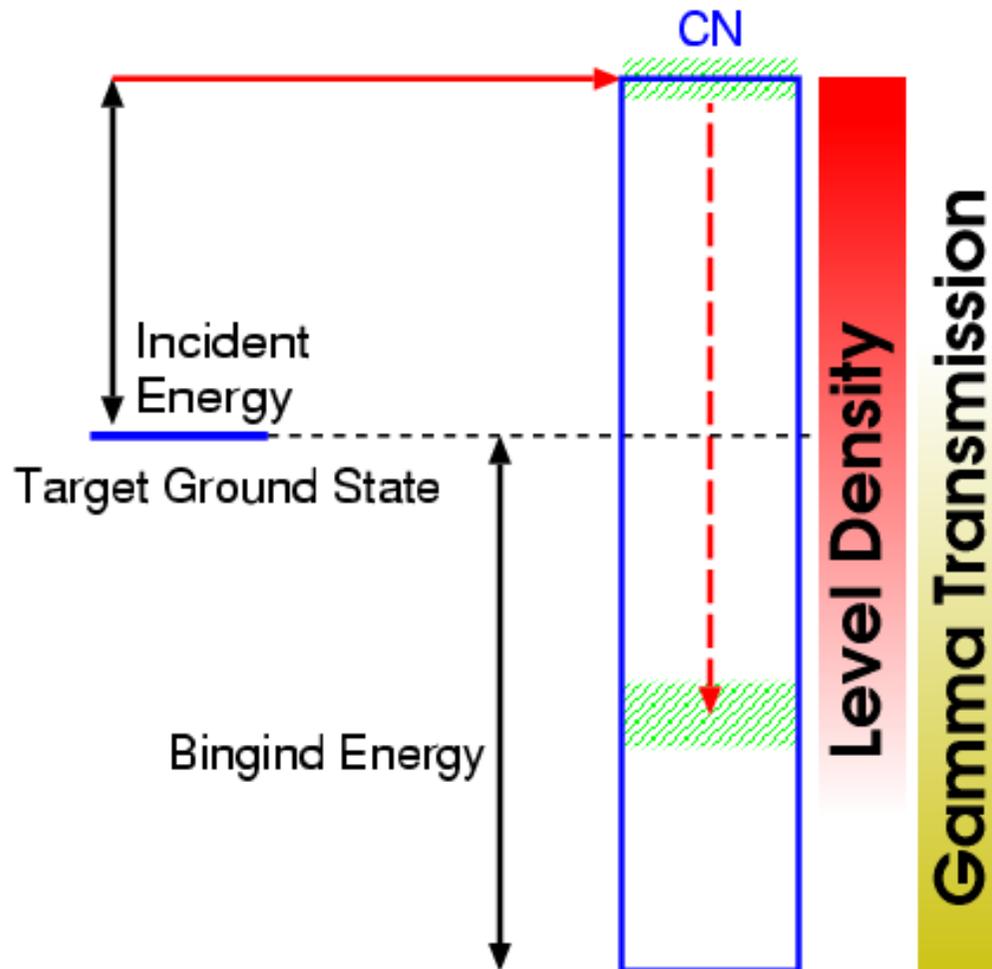
DSD becomes important when (1) incident particle energy is high, or (2) compound capture cross section is small (few resonance, neutron-rich, doubly-closed shell nuclei.)

Photo Emission / Absorption

Inverse process of γ -ray emission



Neutron capture calculations for s and p-process



- Total reaction cross section is determined by the optical model.
- The decay width — the sum of transmission probabilities for all decay processes.
 - The γ -ray radiation width is calculated from the γ -ray absorption probability (the inverse process) and the final state density.
 - Brink's hypothesis is used.
 - Important to understand γ -ray transmission $T_{E1}(E)$, and the level density $\rho(E)$, off-stability.

γ -Ray Strength Function and Transmission

- Standard Lorentzian

$$f_{E1}(E_\gamma) = C\sigma_0\Gamma_0 \frac{E_\gamma\Gamma_0}{(E_\gamma^2 - E_0^2)^2 + E_\gamma^2\Gamma_0^2}$$

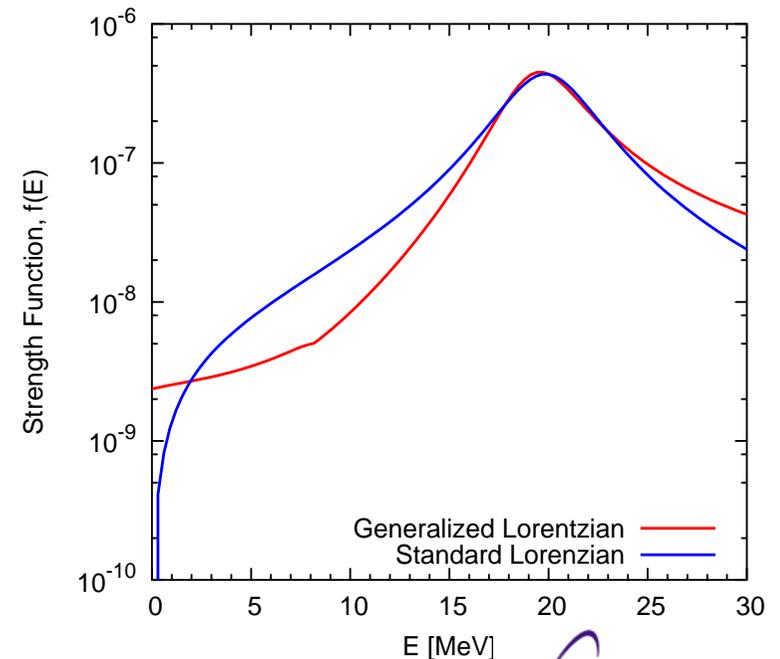
- Generalized Lorentzian, finite value at low energies, energy dependent width

$$f_{E1}(E_\gamma) = C\sigma_0\Gamma_0 \left\{ \frac{E_\gamma\Gamma(E_\gamma, T)}{(E_\gamma^2 - E_0^2)^2 + E_\gamma^2\Gamma^2(E_\gamma, T)} + 0.7 \frac{\Gamma(E_\gamma = 0, T)}{E_0^3} \right\}$$

where $C = 8.68 \times 10^{-8} \text{ mb}^{-1}\text{MeV}^{-2}$, or can be obtained by normalization to an experimental value if available.

The γ -ray transmission coefficient is given by

$$T_{E1}(E_\gamma) = 2\pi E_\gamma^3 f_{E1}(E_\gamma)$$



Normalization of γ -Ray Strength Function

An absolute capture cross section is still hard to predict, however, it can be estimated from average resonance properties.

$$\frac{\langle \Gamma_\gamma \rangle}{D_0} \propto \int_0^{B_n} T_{E1}(E_\gamma) \rho(E_x) dE_x$$

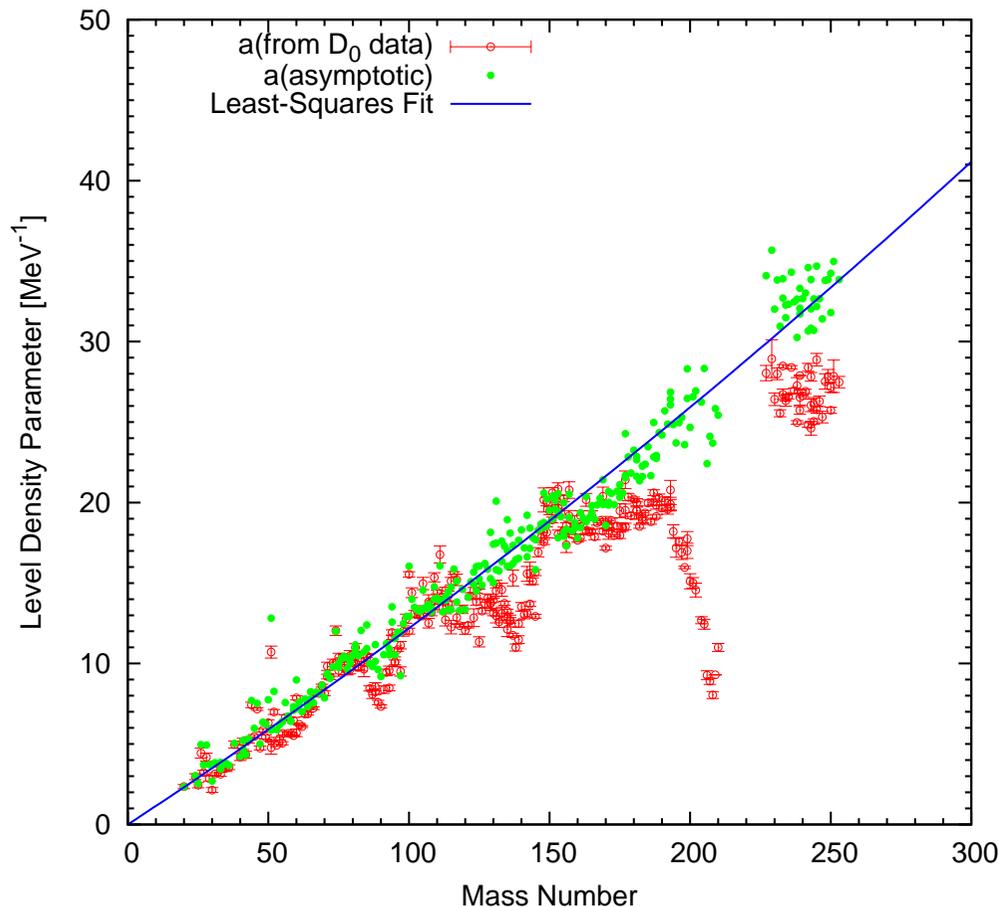
where

- D_0 is the average s-wave resonance spacing near the neutron binding energy:
- $\langle \Gamma_\gamma \rangle$ is the average γ decay width

Compound Nucleus	D_0 keV	$\langle \Gamma_\gamma \rangle$ meV
^{57}Fe	25.4	920
^{91}Zr	6.0	130
^{239}U	0.0208	23.6

or we just re-normalize the calculated capture cross section to experimental data available by adjusting $\langle \Gamma_\gamma \rangle / D_0$.

Level Density Parameter Systematics



Washing-out of Shell Effects

- Shell correction (δW) and pairing energies (Δ) taken from KTUY05 mass formula

$$a = a^* \left\{ 1 + \frac{\delta W}{U} (1 - e^{-\gamma U}) \right\}$$

$$a^* = 0.114A + 7.65 \times 10^{-5} A^2$$

- At low excitation energies, the constant temperature model is used with

$$T = 48.1A^{-0.88} \sqrt{1 - 0.1\delta W}$$

- obtained from discrete level data of more than 1000 nuclei.

TK, S. Chiba, H. Koura, J. Nucl. Sci. Technol., **43**, 1 (2006)

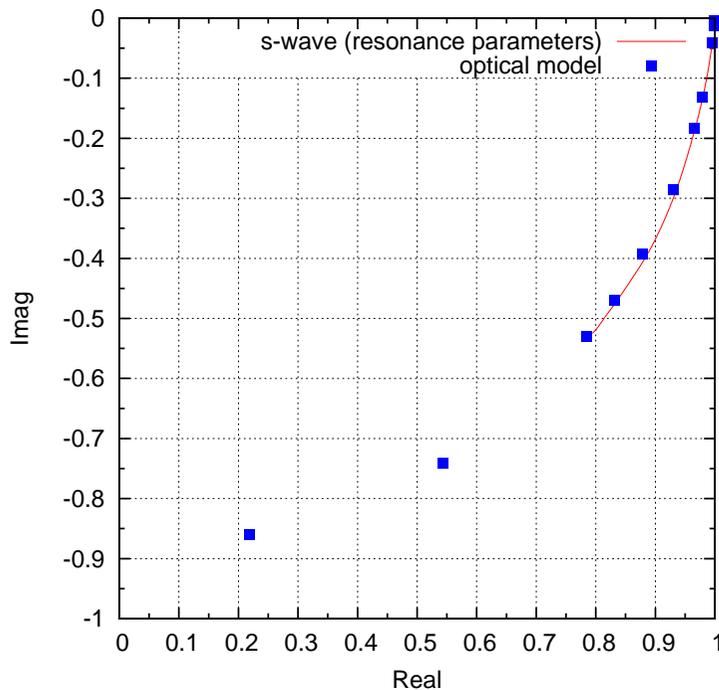
Incorporate Coupled-Channels (CC) method into the HF formula

- Scattering matrix is no longer diagonal.
- Inverse channel problem
 - What is the appropriate transmission coefficient for the excited states ?
 - Replaced by the one for the ground state (historical)
 - Solve the CC equation for the excited state (detailed balance)
- Width fluctuation correction when off-diagonal elements exist
 - Moldauer
 - Engelbrecht-Weidenmüller transformation
 - Kawai-Kerman-McVoy (TK, L.Bonneau, A.Kerman, Nice conf. 2007)
 - Our preliminary results showed that KKM gives almost identical results as Moldauer.
 - Nishioka-Weidenmüller-Yoshida, GOE for coupled-channels

Coupled-Channels Potential Parameters

Modification to the Global CC Potential of Soukhovitskiĭ, et al.

- E. Sh. Soukhovitskiĭ, et al., J. Phys. G: Nucl. Part. Phys. **30**, 905 (2004).
- Adjust the imaginary potential to match the energy averaged S -matrix elements from resonance parameters (TK, F.H. Fröhner, NSE, **127**, 130 (1997)).
- When the S -matrix elements (resonance and optical model) are obtained, total and reaction cross sections are automatically reproduced.



$$W_s = 2.59 \text{ MeV for } E_n < 1.13 \text{ MeV}$$

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

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

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

Original Soukhovitskiĭ Potential (in the paper)

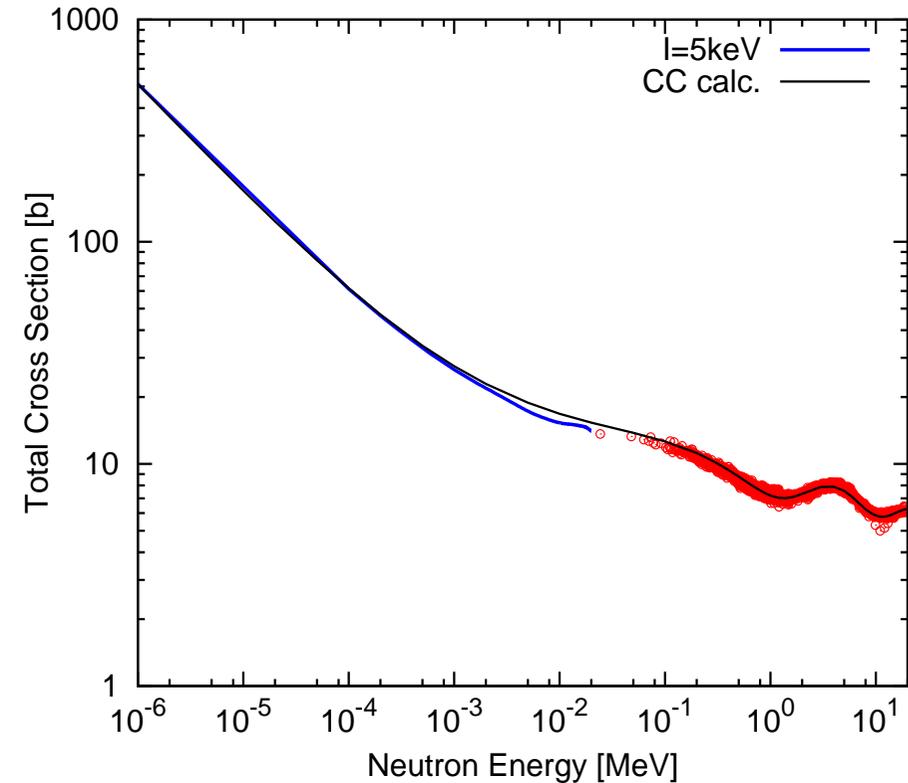
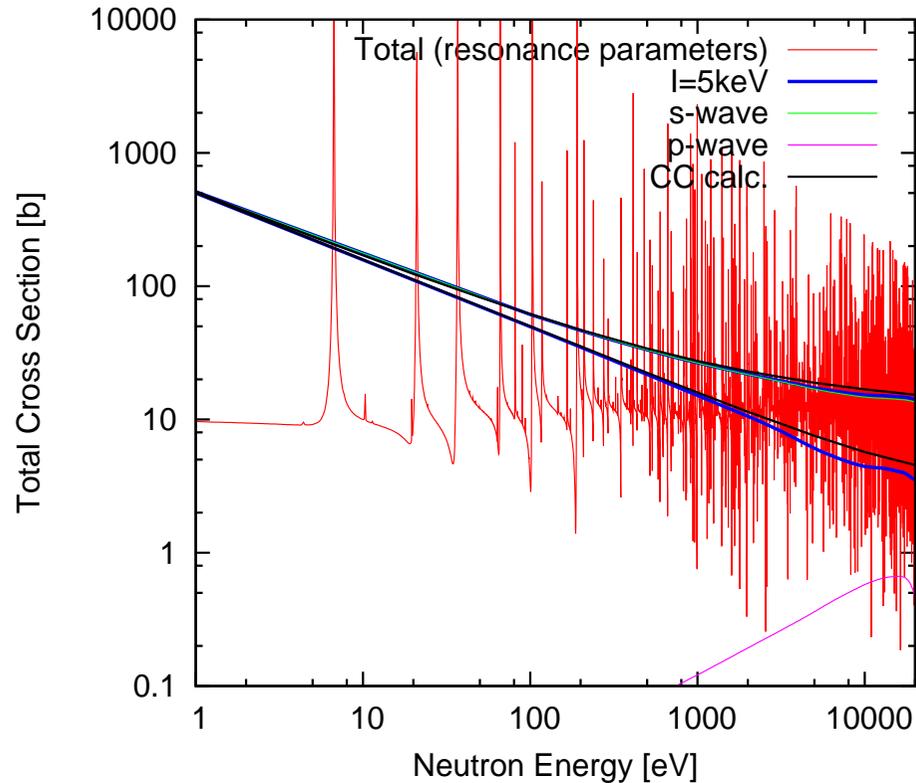
$$R' = 9.57 \text{ fm}$$

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

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

U-238 Total Cross Section

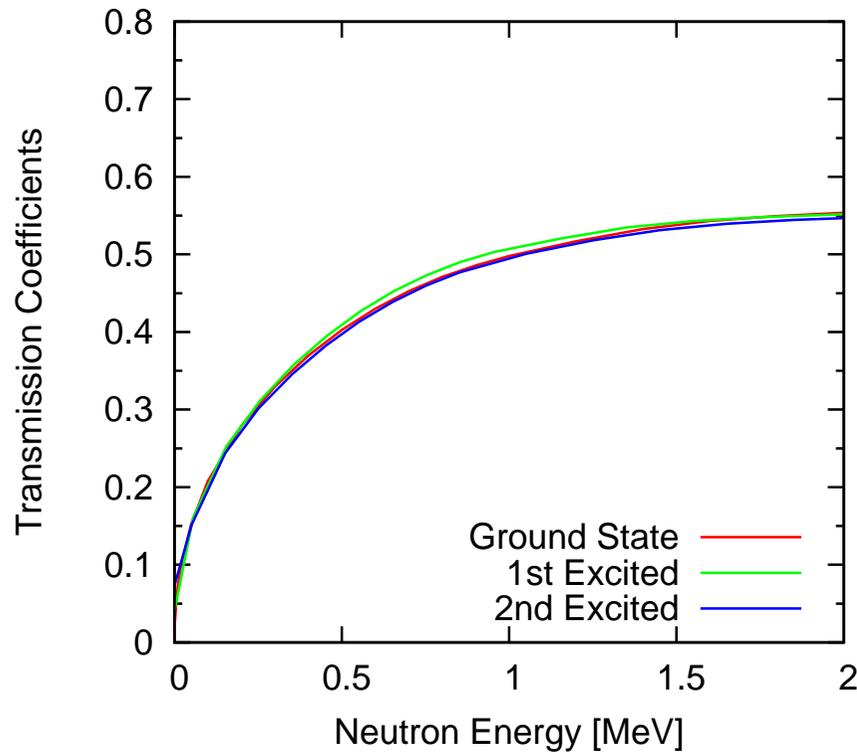
With Modified Soukhovitskiĭ Potential



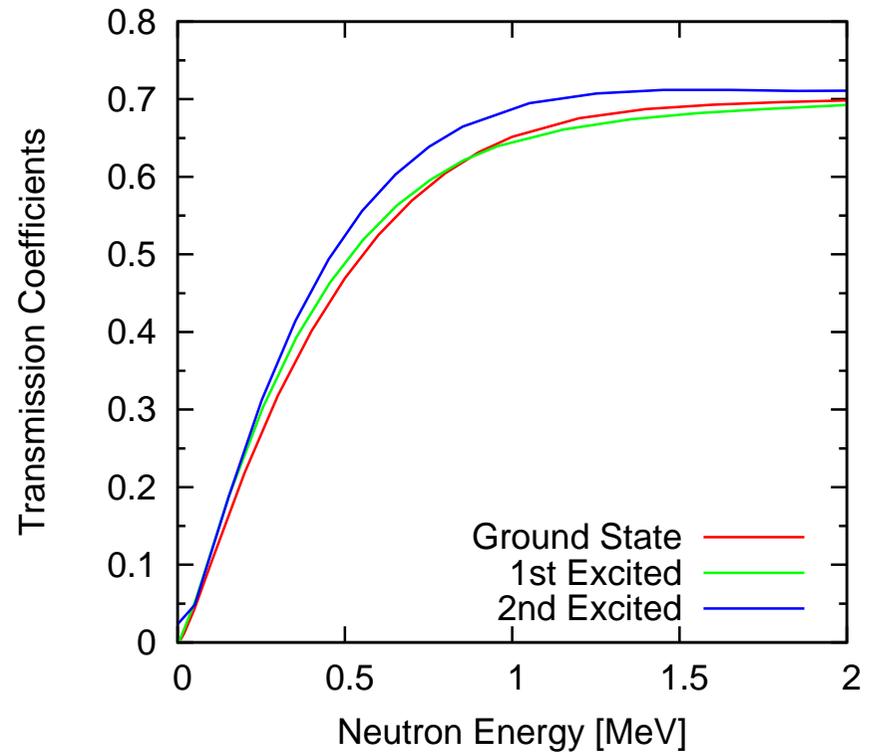
- With the modified Soukhovitskiĭ Potential, the energy averaged total cross section in the resonance range is well-reproduced.
- Above 1.13 MeV, the parameters are the same as the original ones.

Transmission for Inverse Reactions

Transmission Coefficients for the Inverse Channels



s-wave



p-wave

In a usual case, the **ground-state transmission** is used for all the calculation. However, this might underestimate the (n,n') cross-section to the 2^+ and 4^+ states, because the true **transmission to the 2^+ and 4^+** are larger.

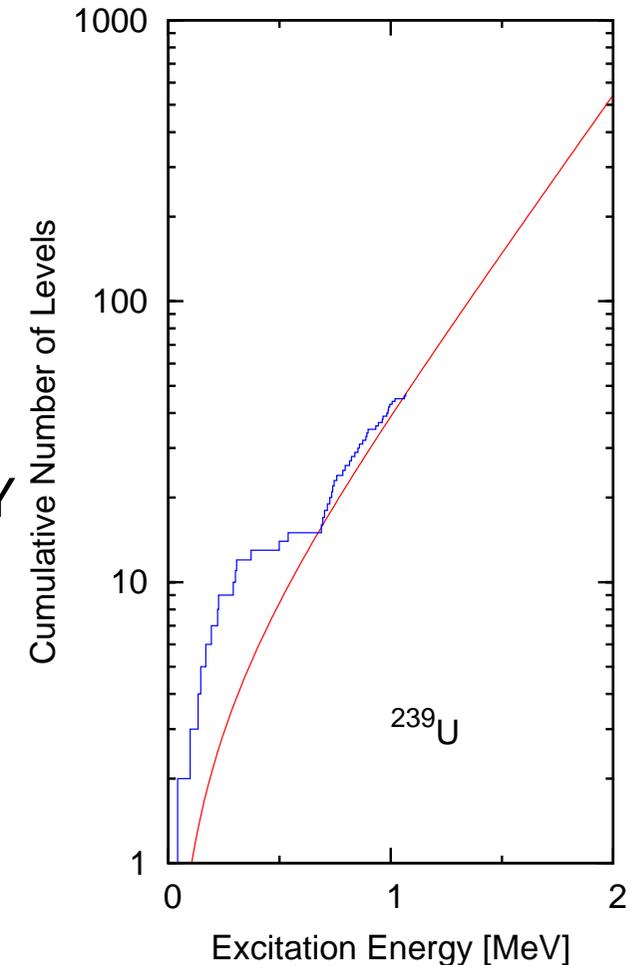
Capture Cross Section Calculations

Model Parameters

- Optical Potential
 - Modified Soukhovitskiĭ
 - CC calculations are made for the G.S. band
 - $0^+ - 2^+ - 4^+ - 6^+ - 8^+$ coupling
 - Spherical potential for the uncoupled states
- Level density
 - Ignatyuk level density formula
 - $a^* = 34.69 \text{ MeV}^{-1}$ for ^{239}U (reproduce $D_0 = 20.3 \text{ eV}$)
 - Shell correction and pairing energies from KTUY mass formula
 - Spin-cut off parameter,

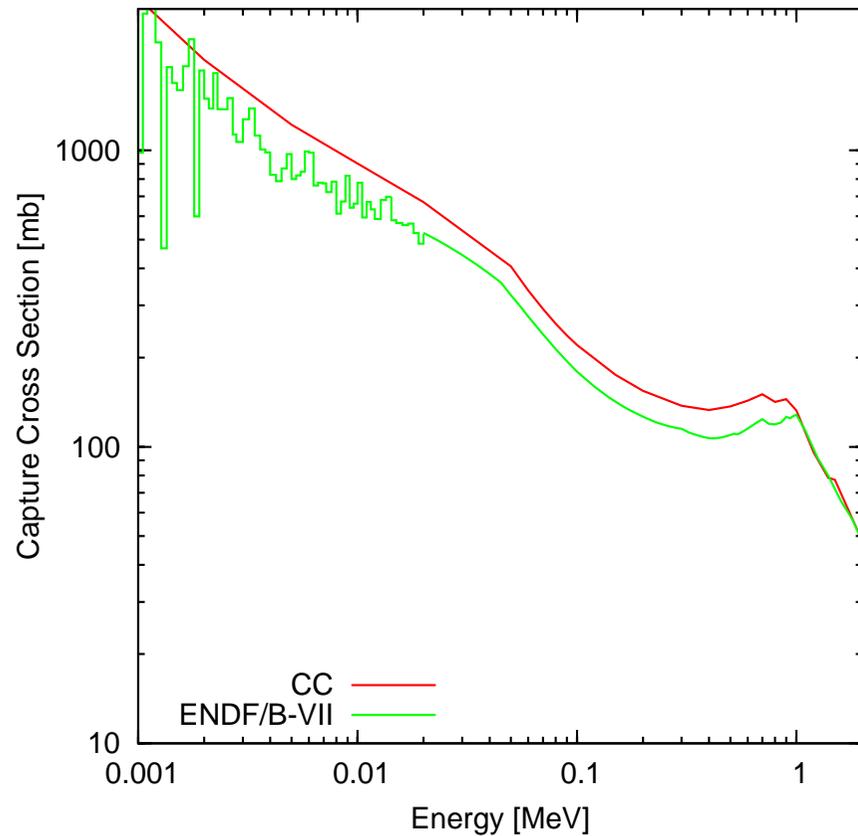
$$\sigma^2 = 3.47 \times 10^{-3} \sqrt{U/aA}^{5/3}$$

- Average γ -ray width
 - $\langle \Gamma_\gamma \rangle = 23.36 \text{ meV}$ from resonance analysis
 - or, to be adjusted if needed

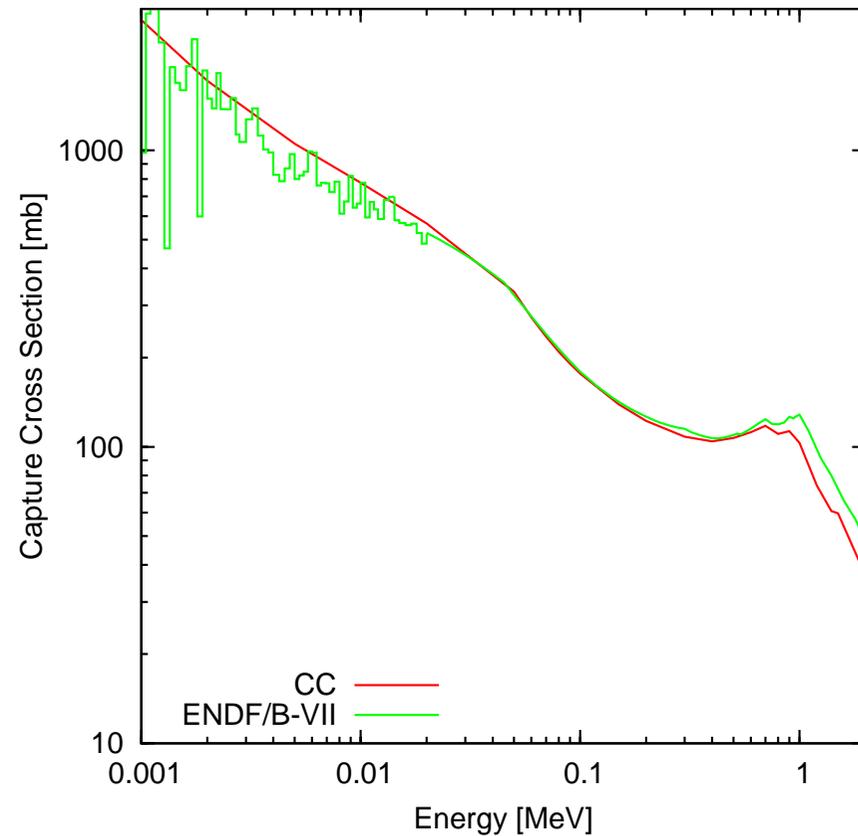


U-238 Results

Comparison with ENDF/B-VII (a part of standards evaluation)



$$\langle \Gamma_\gamma \rangle = 23.36 \text{ meV}$$

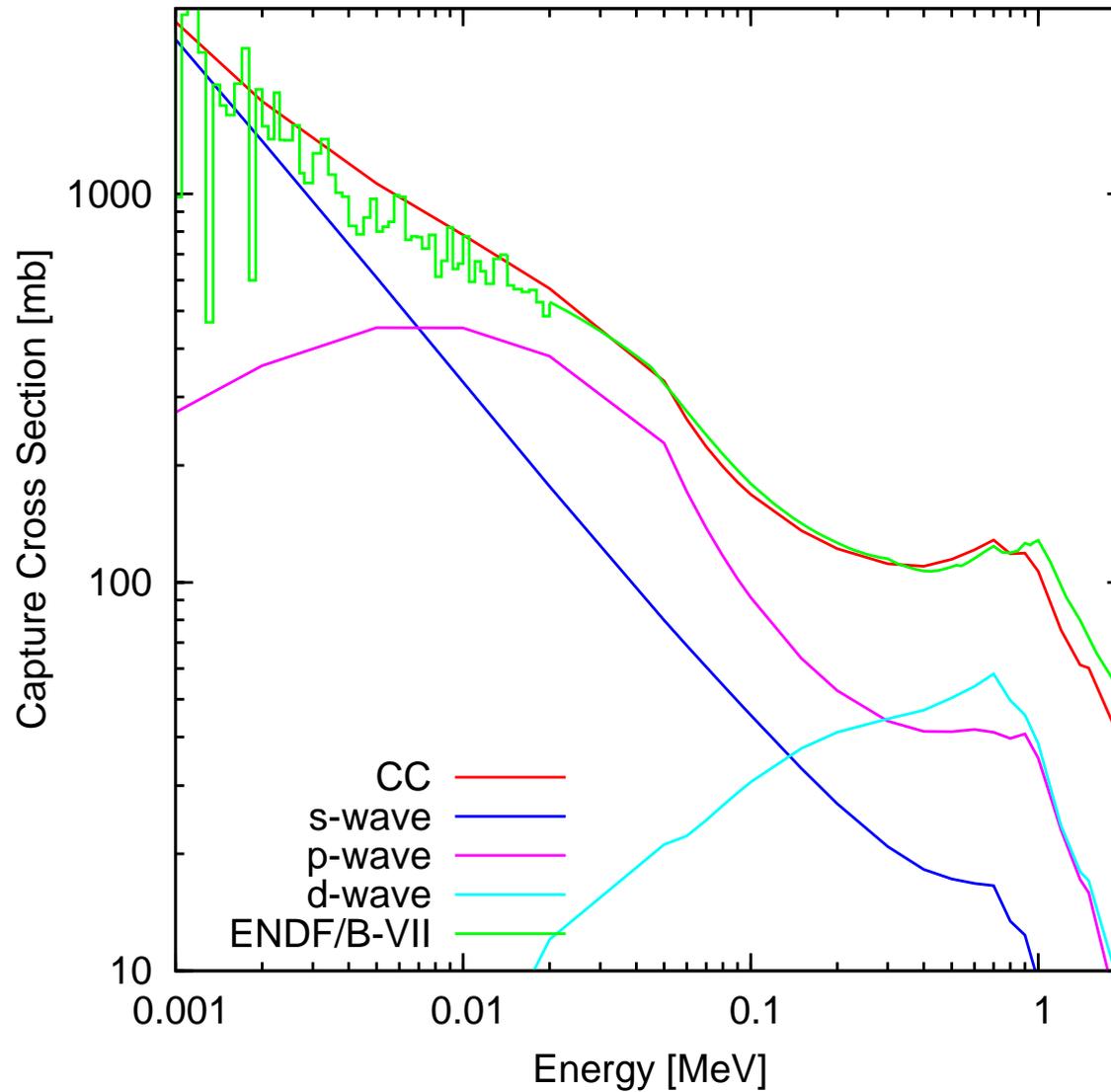


$$\langle \Gamma_\gamma \rangle = 17.83 \text{ meV}$$

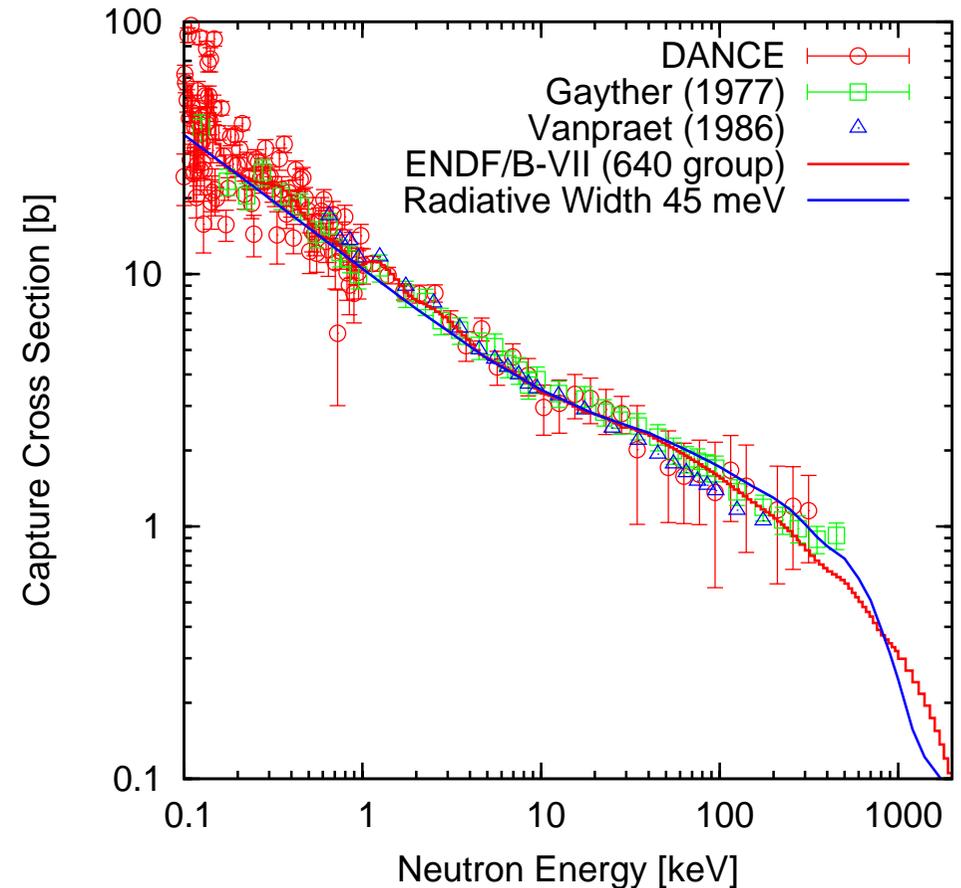
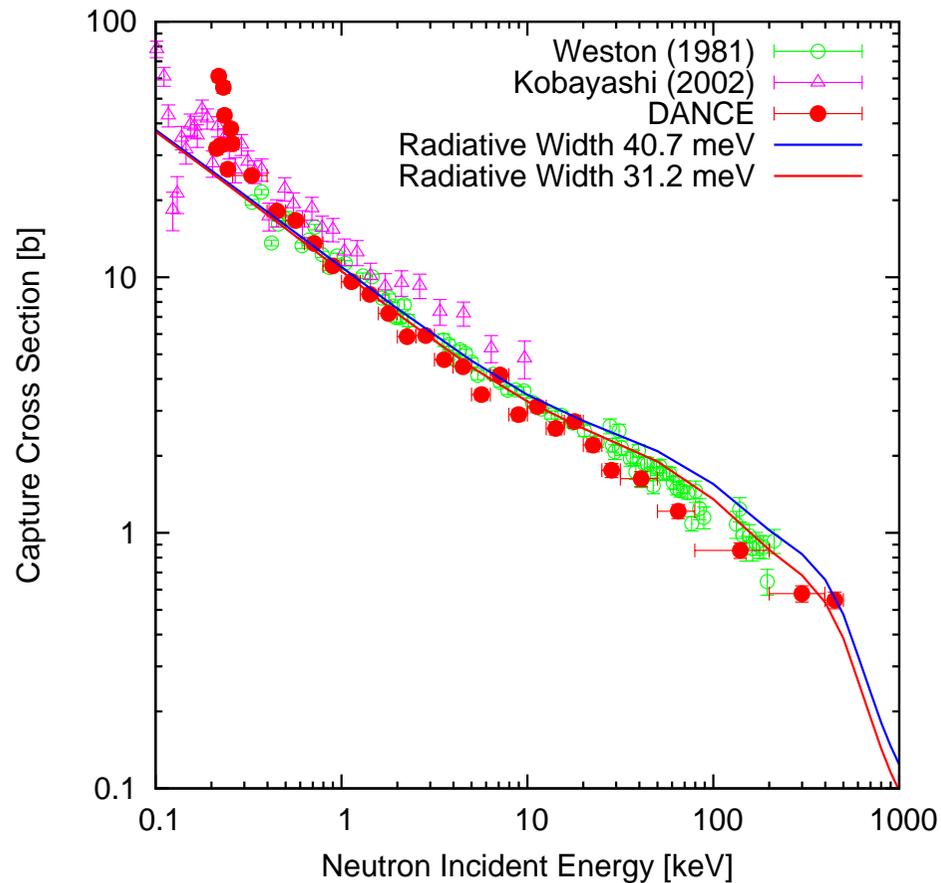


Partial Wave Contribution

Decomposition into Each Partial-Wave Contribution



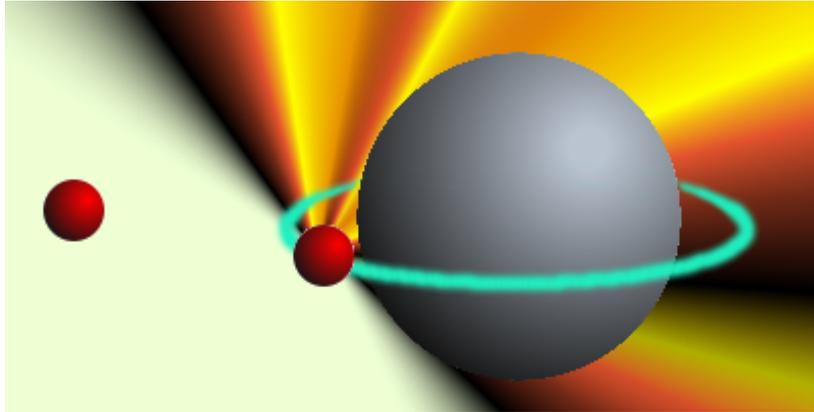
Comparisons with DANCE Data



When the calculated capture cross section for ^{241}Am is averaged over the Jezebel spectrum, it gives a 5% higher value than that for ENDF/B-VII.

Direct/Semidirect Nucleon Capture Model

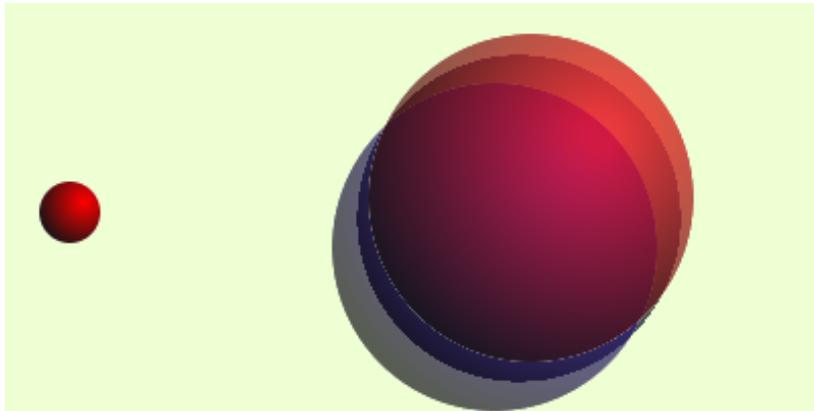
Direct Capture



- Electric dipole radiation transition from optical potential to single-particle state
- Amplitude

$$T_d = C_d \langle R_{nlj} | r | R_{LJ} \rangle$$

Semidirect (Collective) Capture



- Excite GDR, and decay into single-particle state
- Vibration-particle coupling, $V_1 h(r)$
- Amplitude

$$T_s = C_s \langle R_{nlj} | V_1 h(r) | R_{LJ} \rangle \\ \times \frac{|M_{GDR}|^2}{E_\gamma - E_{GDR} + i\Gamma_{GDR}/2}$$

Model Improvements

spectroscopic factor S_{ljK}

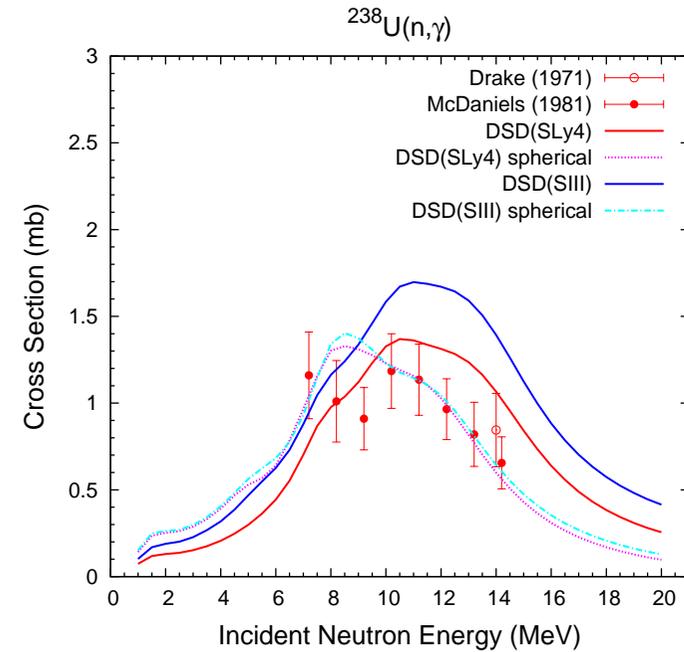
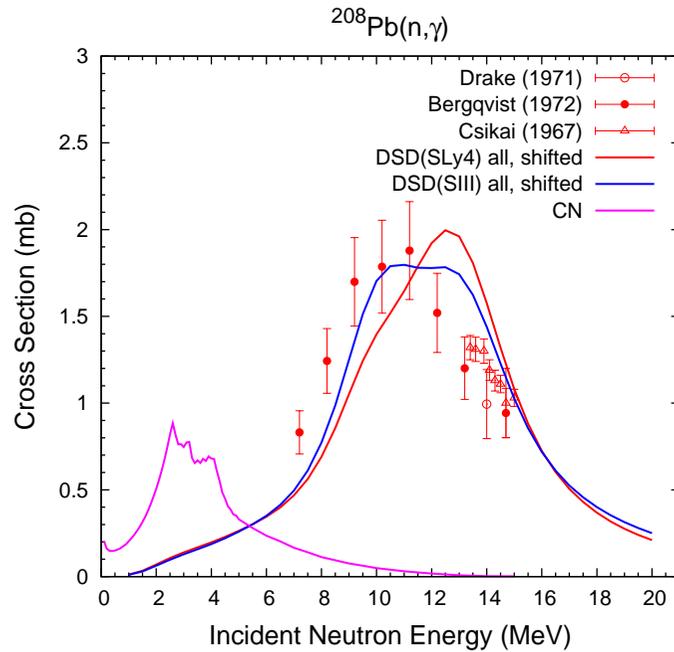
- previous studies
 - experimental data (often not available for astrophysical calculations)
- DSD/HF-BCS
 - single-particle occupation probabilities
 - no experimental data needed

single-particle wave-function, $R_{ljK}(r)$

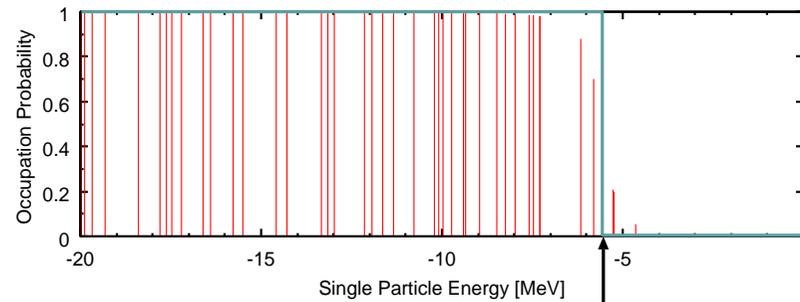
- previous studies
 - spherical Woods-Saxon, Nilsson model, coupled-channels model to bound states
- DSD/HF-BCS
 - HF-BCS calculation and decomposition into spherical HO basis
 - consistent treatment for all nuclei from spherical to deformed nuclei

Calculated Results

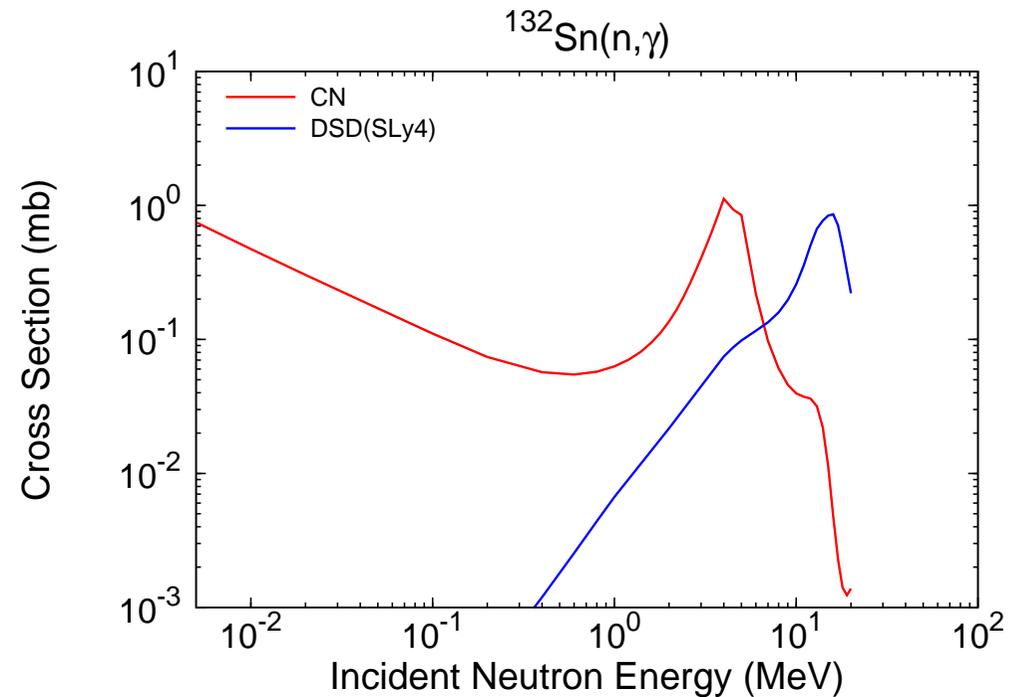
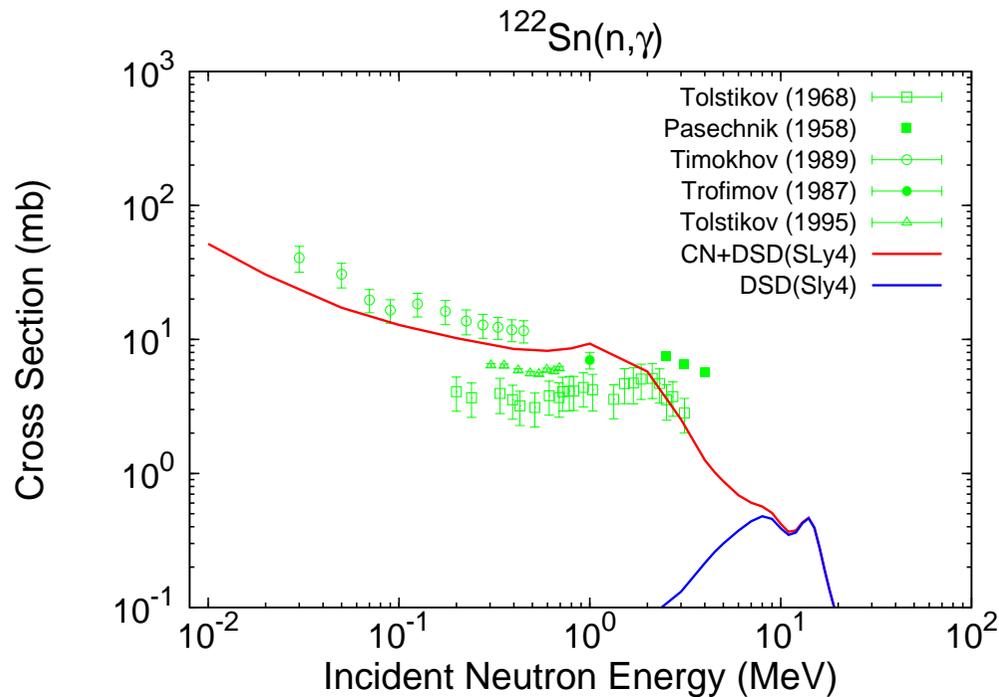
DSD Cross Sections for Spherical and Deformed Cases



Occupation Probabilities for U-238



Neutron Capture Off-Stability — Sn-122, 132



- Since global Hartree-Fock-BCS calculations for all nuclides are feasible, this technique will be a powerful tool to estimate the neutron capture rates in the r-process.
- HF calculation problems for the odd nuclei still exist.
- Proton capture calculations underway.

Applications of the Hauser-Feshbach Model to Different Areas

Combining with nuclear structure calculations

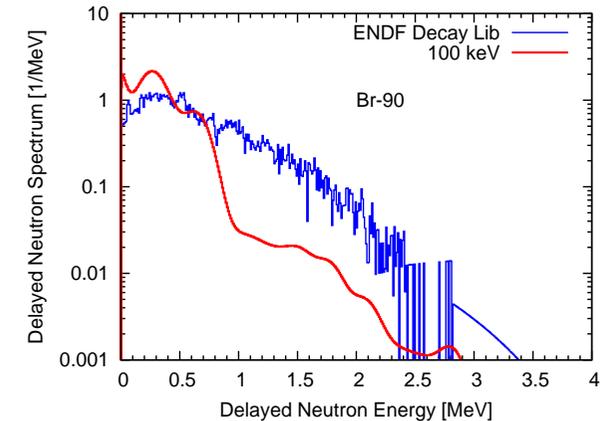
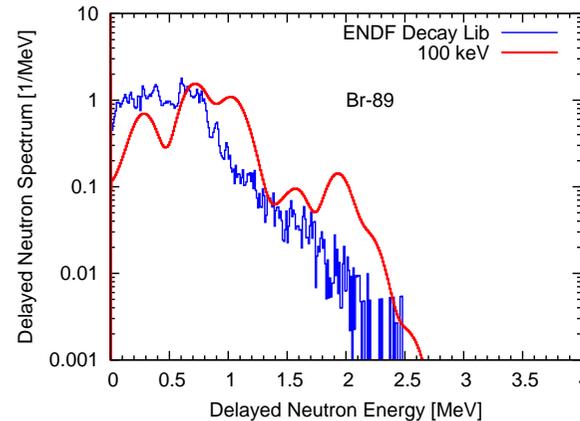
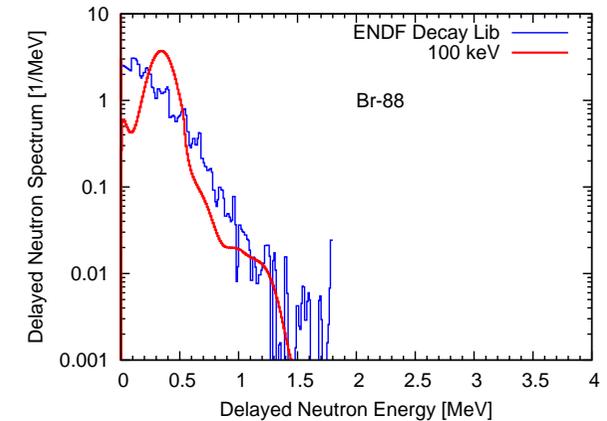
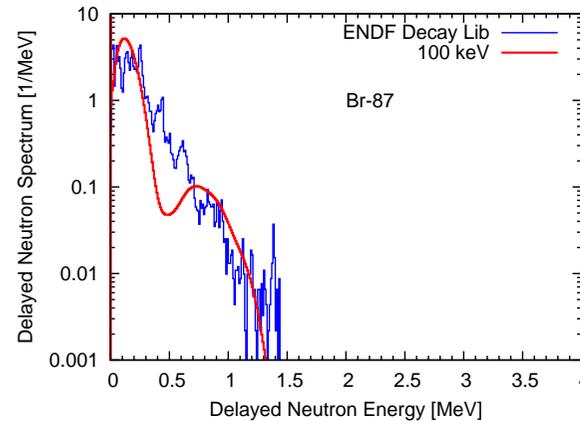
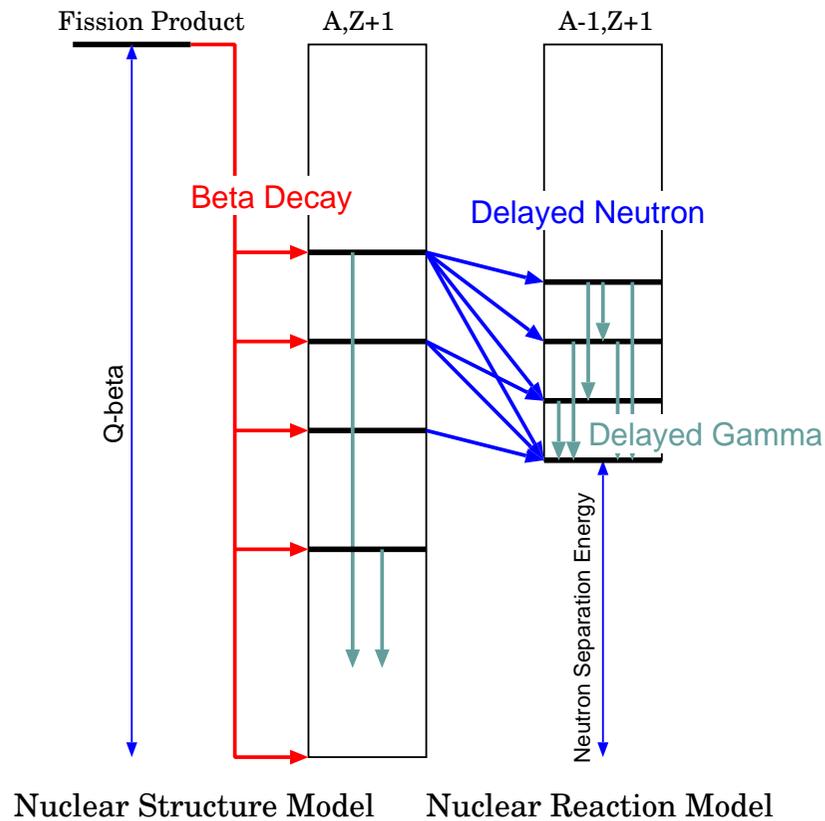
- β -decay and electron capture produce highly excited states of nuclei, and the excitation energies can be larger than the neutron separation energy.
- Nuclear structure models, such as QRPA, predict final states of β -decay and EC.
- Compound decay from a daughter nucleus at given E_x, J^π .

Monte Carlo approach to the Hauser-Feshbach

- HF gives an integrated cross-section for all possible intermediate transitions.
- However, recent experiments are sometimes conducted by measuring partial γ -rays, coincidence with a particular γ -ray transition, selected events such as a fixed γ -ray multiplicity.
- Correlation information is needed.

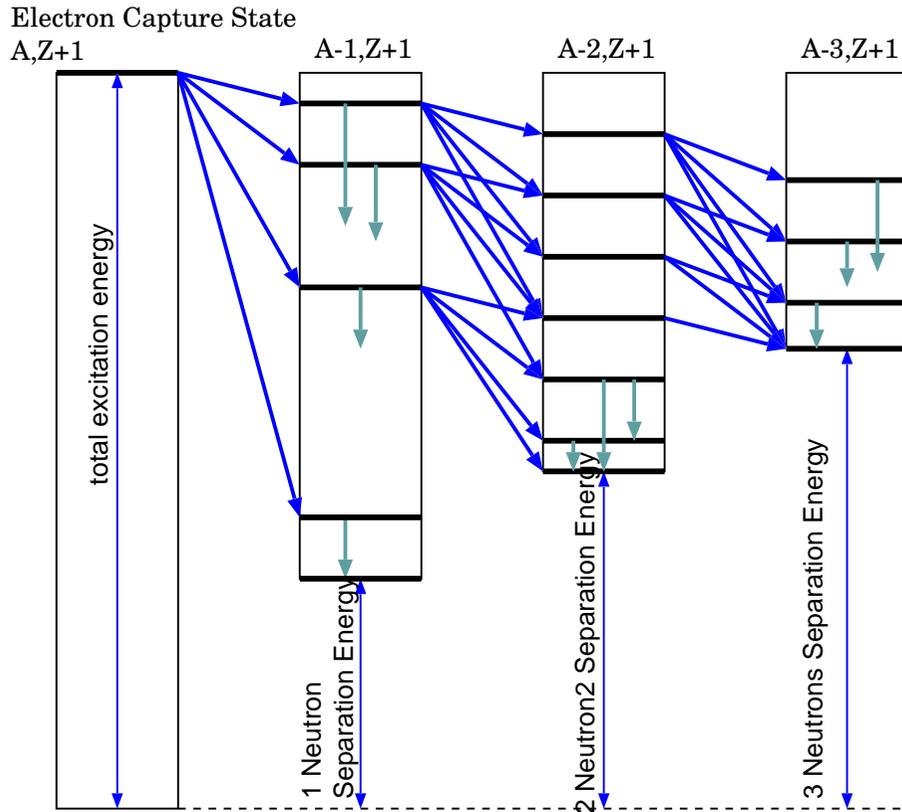
Application of HF to Delayed Neutron Emission

QRPA and Hauser-Feshbach model for Beta-Delayed Neutron



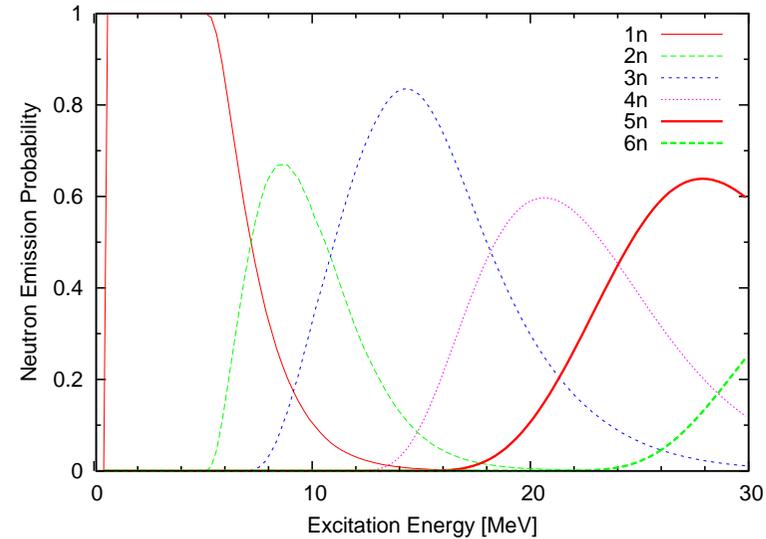
We assume that the excited state after β -decay is a compound state, having a fixed J value, $|I - 1| \leq J \leq I + 1$, where I is the spin of precursor.

Sequential Neutron Emissions

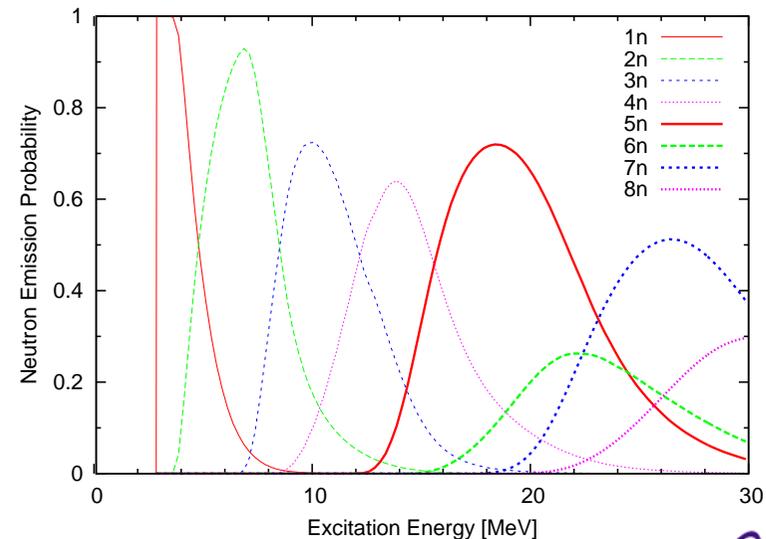


Electron capture produces a highly excited state, which subsequently decays by emitting several neutrons (very fast process).

Si-43



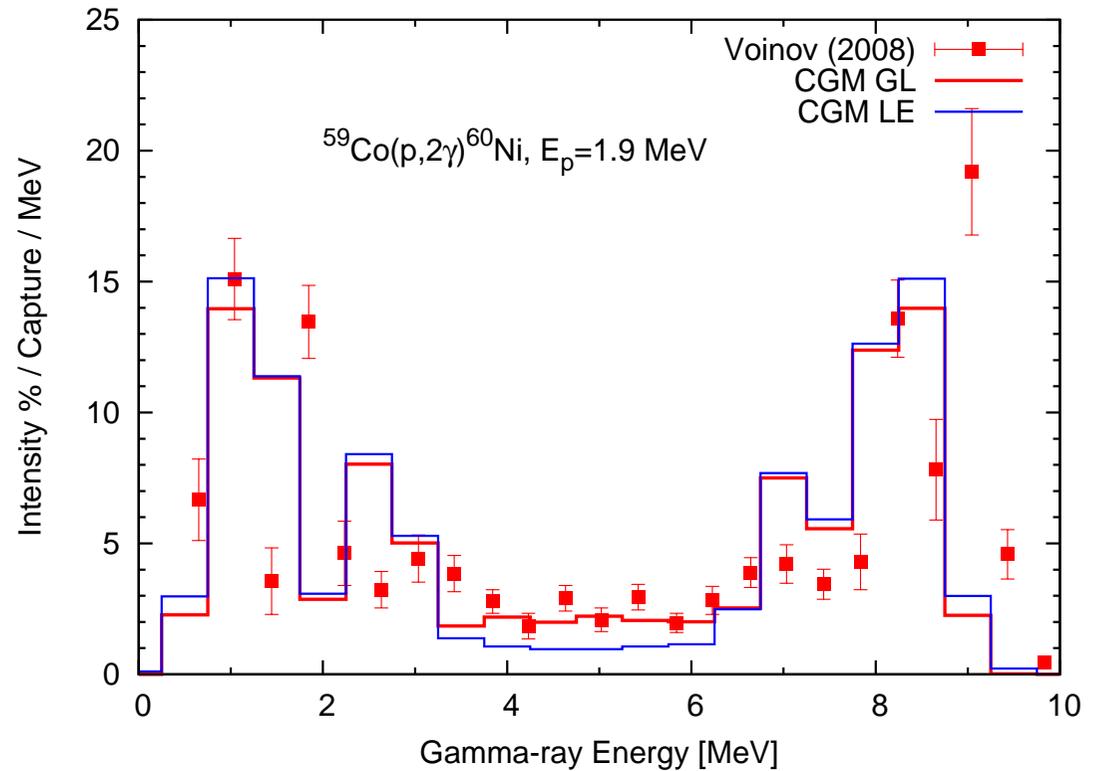
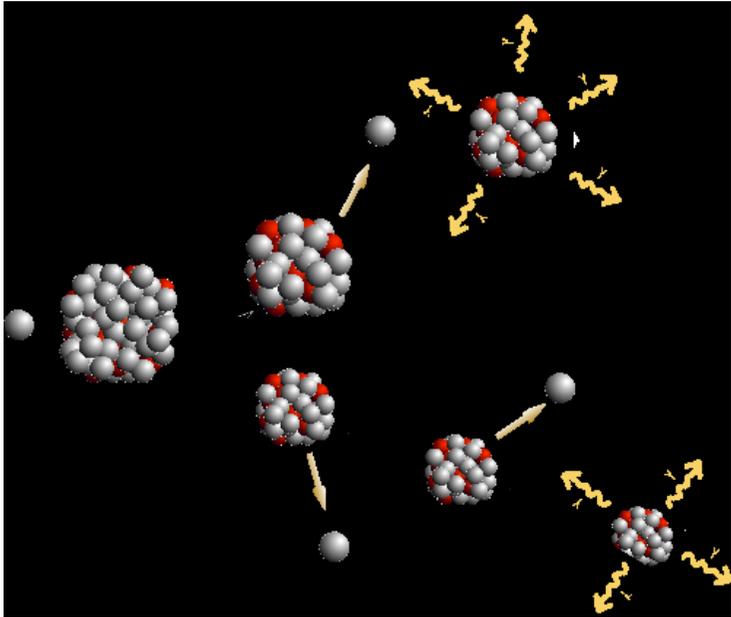
Sr-118



Monte Carlo Simulation for Particle Emission

Application of Monte Carlo to Hauser-Feshbach Model at LANL

- β -delayed γ
- prompt fission neutron spectrum
 - n- γ correlation
 - γ -ray competition
- γ -ray cascading
 - γ -ray multiplicity dist.



A preliminary result of the γ -ray spectra from proton capture for the multiplicity 3 case (2 γ -rays and the $2^+ \rightarrow 0^+$ transition). Data taken from the proc. of Yosemite conference, 2008

Nuclear Reaction Modeling: Recent Development for Astrophysics

Compound Nuclear Reaction

- Improved Hauser-Feshbach model for capture reaction, including nuclear deformation effect, which supports experimental data at LANSCE with DANCE.

Direct/Semidirect Nucleon Capture

- The Hartree-Fock BCS theory for the DSD process has a potential to predict neutron capture cross-sections near the neutron drip-line.

Extension of the Hauser-Feshbach Model Applications

- Beta-delayed and EC neutron emission
- Prompt fission neutron spectra
- Monte Carlo approach : correlations of particle emissions