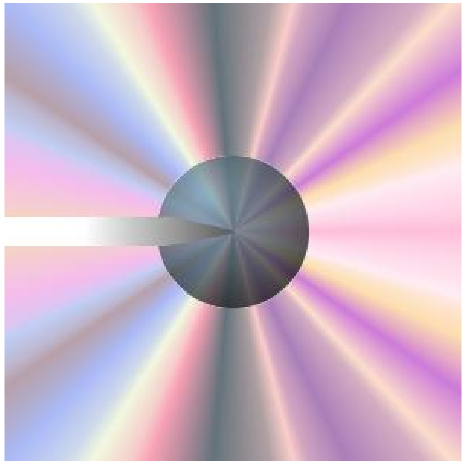
Capture and Preequilibrium Reactions



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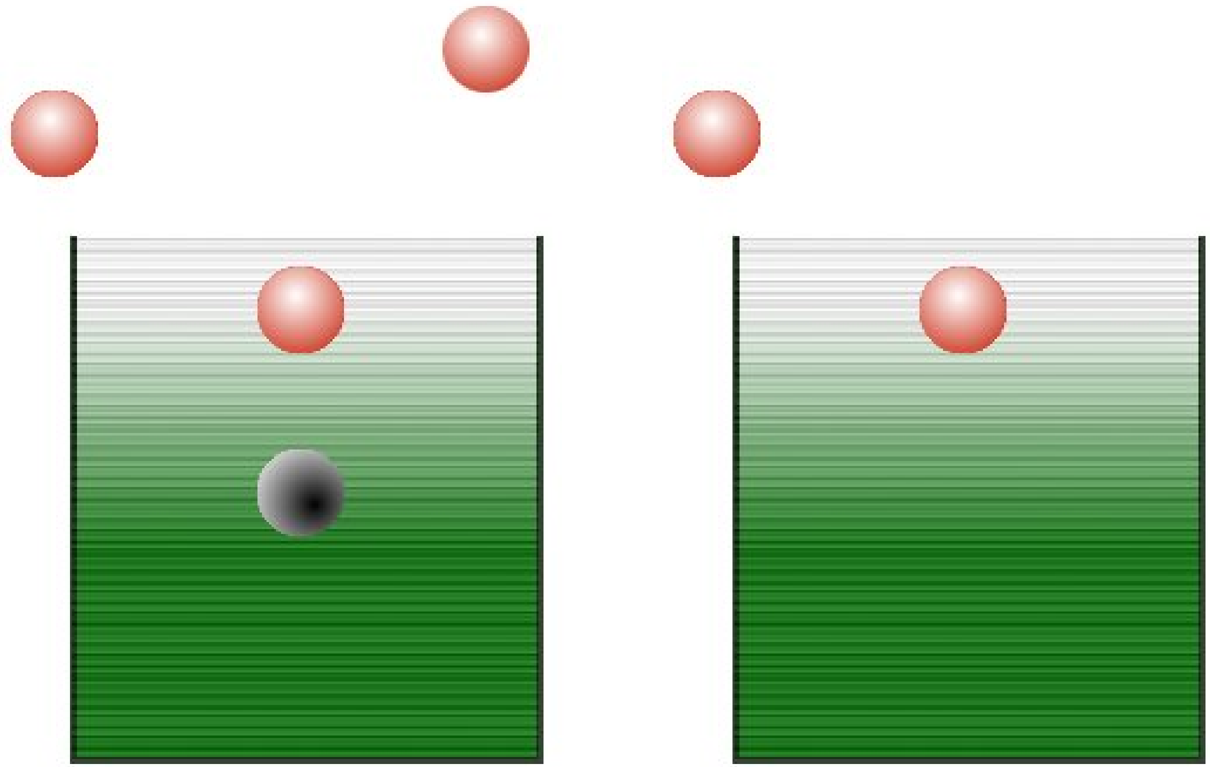
Nuclear Reaction Based on Nuclear Structure Inputs

Nuclear reaction calculation requires many nuclear properties

- discrete level spin and parity — from experimental data
- level density
  - semi-microscopic approach — combinatorial calculation
  - phenomenological approach
    — mass-dependence and shell, pairing energy corrections
- optical potential
- E1 strength function
  - experimental data or Hartree-Fock calculation for GDR
- single-particle wavefunctions and spectroscopic factors for direct/semidirect capture and pre-equilibrium process
- two-body effective interaction

LANL focuses on Capture and Pre-Equilibrium

Single particle states for nuclear reaction calculations



In both cases, the total angular momentum and the excitation energy are determined from the single-particle orbits.

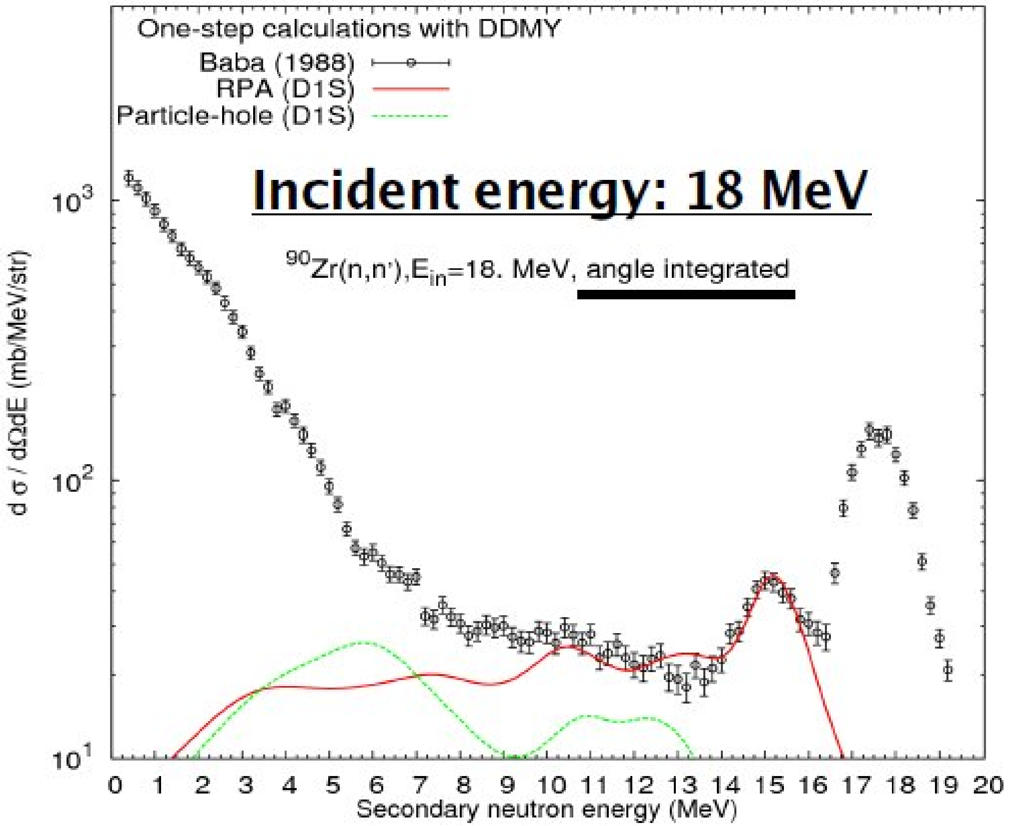
The cross section also depends on the occupation probabilities of each state.

Status of Pre-Equilibrium Calculations

Calculations for spherical nuclei

LANL development

- M. Dupuis reported at 2008 Pack Forest meeting
- inelastic scattering on Zr and Pb
- particle-hole excitation from HF-BCS, including u^2, v^2
  - L. Bonneau, TK, et al. Phys. Rev. **C** 75, 054618 (2007)
- collective strength from RPA
- effective interaction (D1S and others)



The pre-equilibrium component in the neutron emission spectra is well-reproduced by the model without any adjustable parameters.

A paper on the spherical calculations in preparation.

Problems in Calculations for Deformed Nuclei

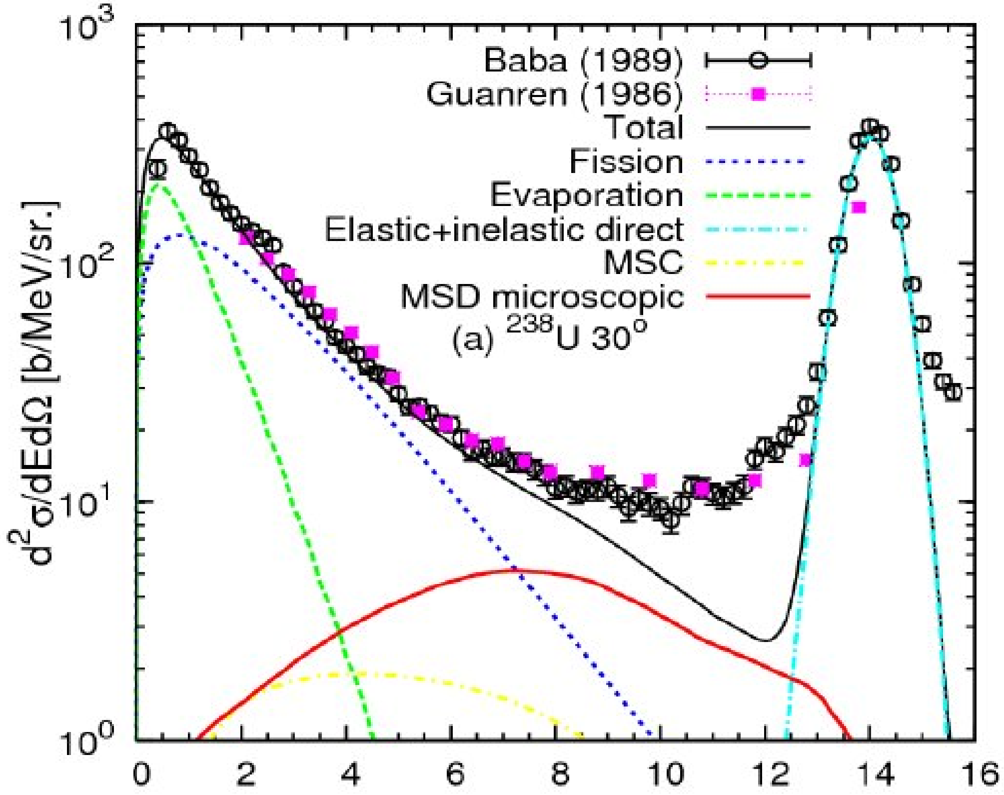
Parallerized DWBA calculation

- significant speed-up for the one-step calculations on deformed nuclei

Missing strength near E_x =3 MeV

- long-standing problem of PE calculations for actinides
- we have been investigating this problem, but have not solved yet.
  - experimental energy resolution
  - back-scattering of neutrons
  - more collectivities

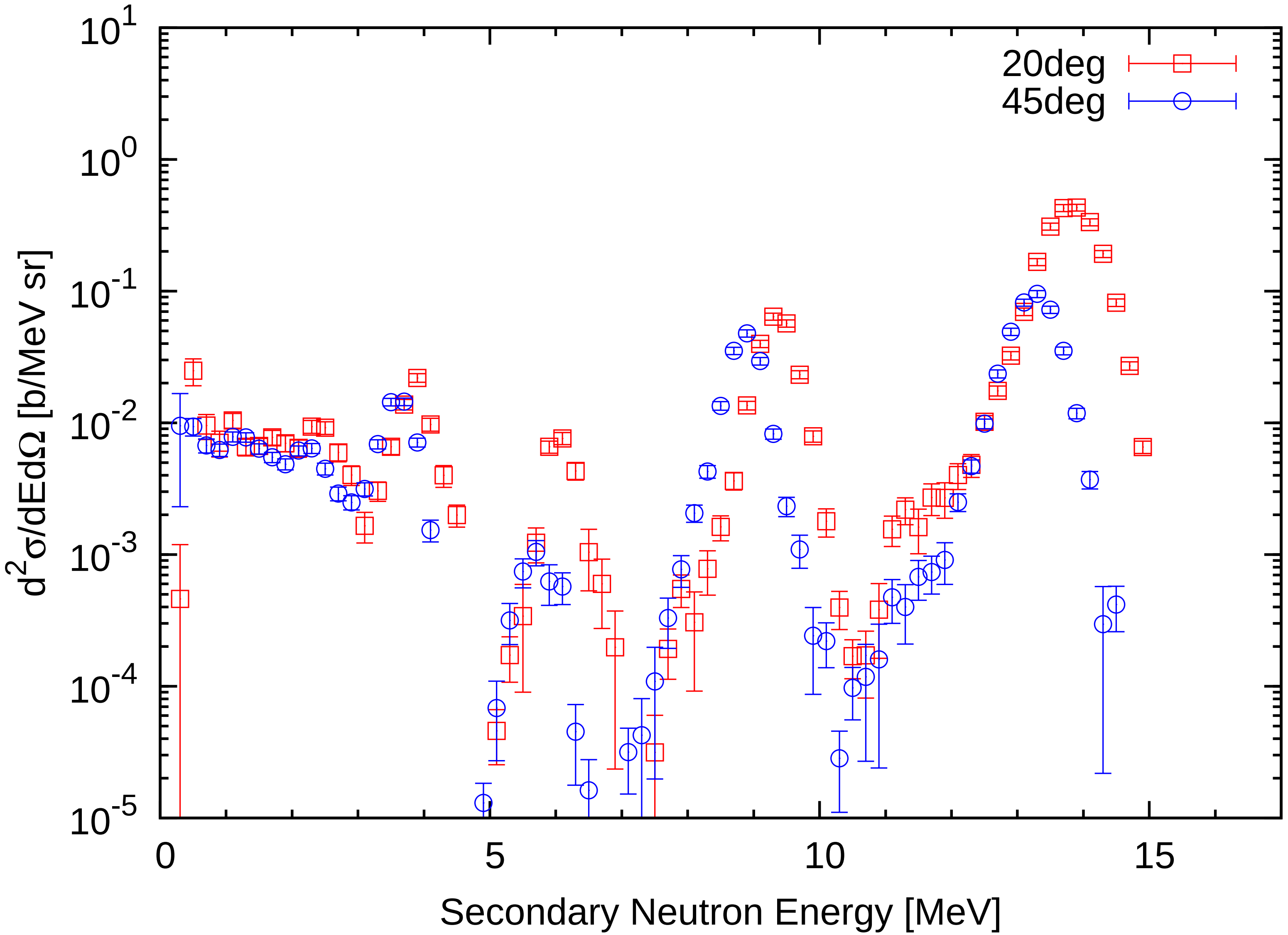
    — deformed RPA needed
  - BCS calculation too simple ?



In Year 3, calculations with the deformed RPA model (development at LLNL) planned, but have not been completed yet.

Non-Symmetric Energy Resolution

Double differential cross section data on C at 14 MeV



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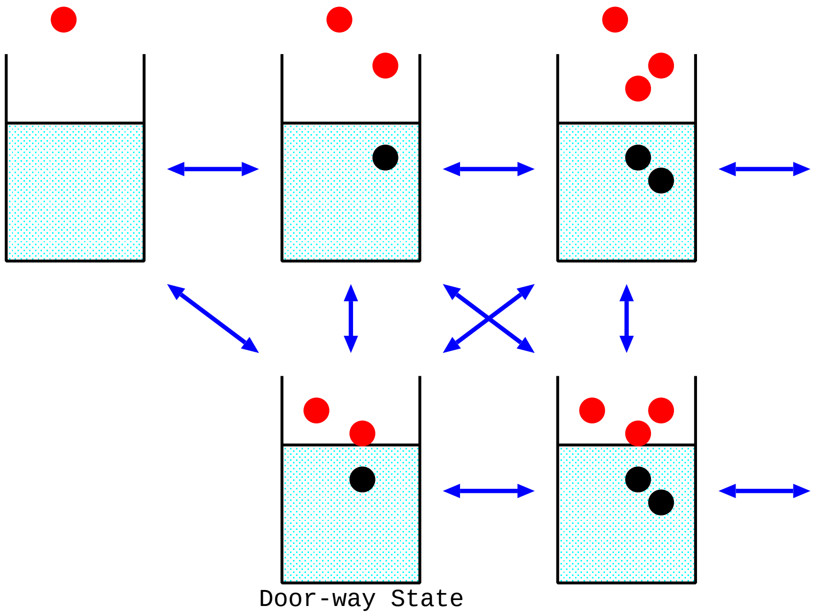
QM Pre-Equilibrium Theory : Future Direction

Possible further development

- deformed QRPA for collective enhancement
- rigorous coupling with the Hauser-Feshbach compound theory
  - spin / parity conservation
  - $P \rightarrow Q$ damping
- higher steps
  - two-step formalism and interference effect
  - sudden approximation
  - T.Kawano, S.Yoshida, Phys. Rev. C, **64**, 0246031 (2001)
  - only important for nucleon incident energies above 40 MeV or so
- realistic energy broadening to compare with experimental data



Nucleon Capture Process

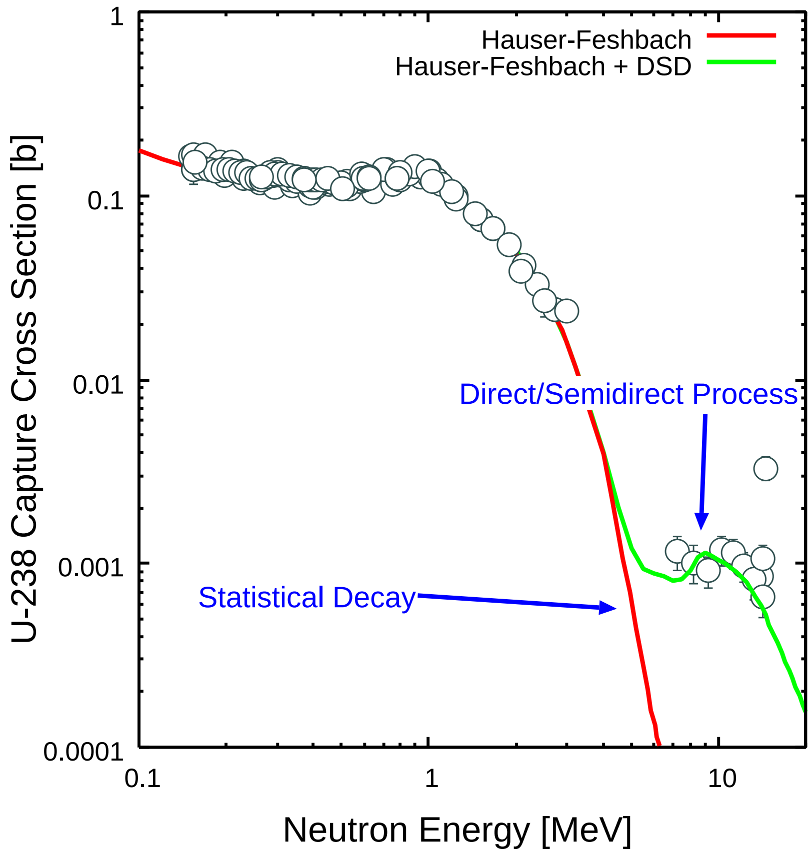
Compound Nucleus and Direct/Semidirect Processes

Compound Reaction

- Incident neutron and 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.)

DSD Theory for Deformed Nuclei

DSD Amplitudes

$$T_d \propto \sqrt{S_{ljK}} \langle R_{ljK}(r) | r | R_{LJ}(r) \rangle$$

$$T_s \propto \sqrt{S_{ljK}} \langle R_{ljK}(r) | h(r) | R_{LJ}(r) \rangle$$

DSD with Hartree-Fock BCS Theory

spectroscopic factor S_{ljK}

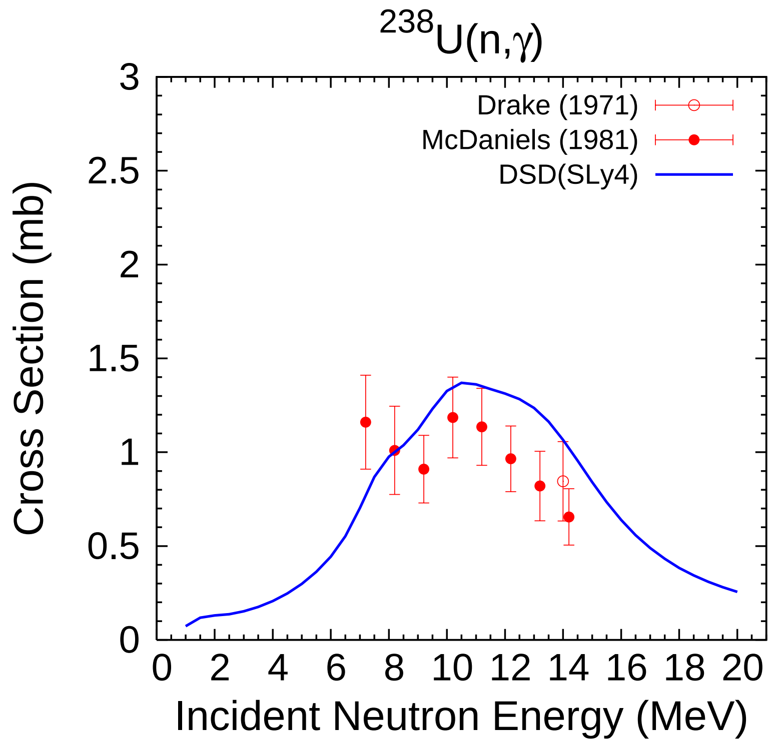
- single-particle occupation probabilities, $v^2 = 1 - u^2$
- no experimental data needed

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

- HF-BCS calculation and decomposition into spherical HO basis
- consistent treatment for all nuclei from spherical to deformed nuclei

U-238 Calculated Result

We have validated our model against the existing experimental data.



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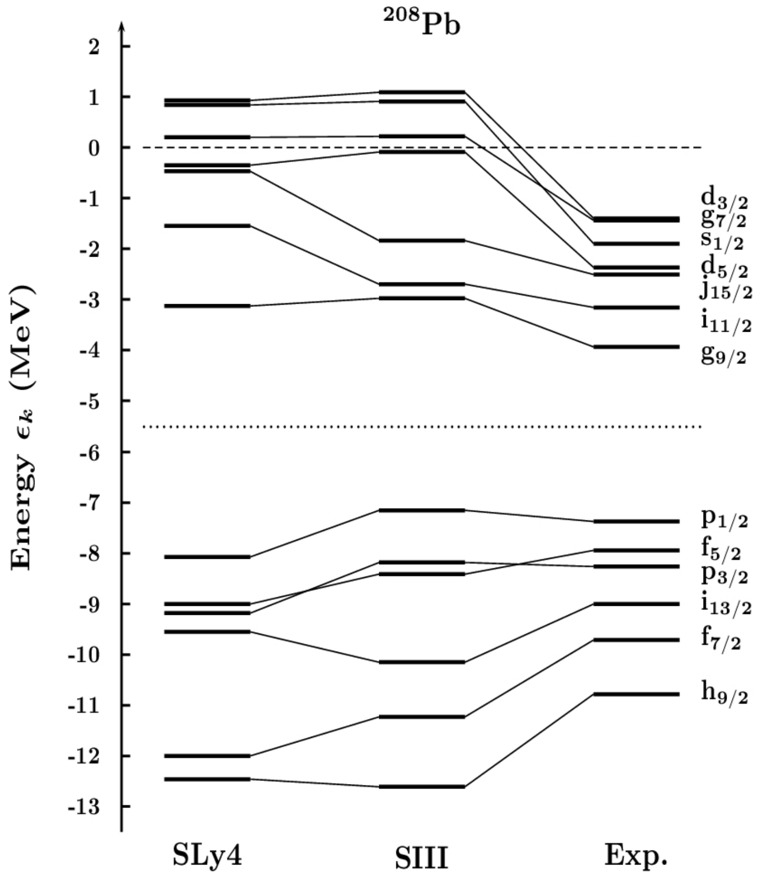
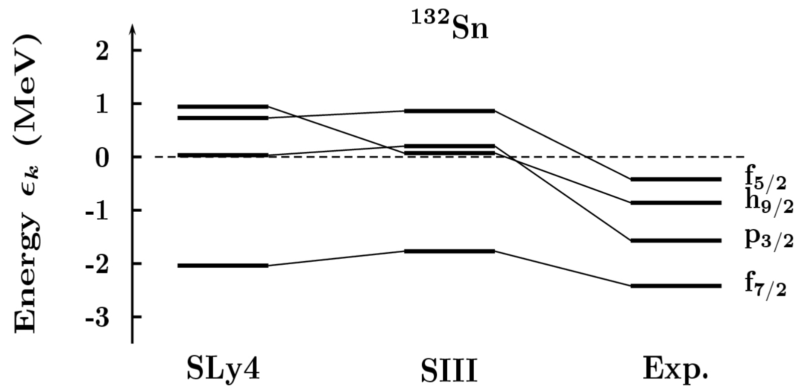
Single-Particle Energies Crucial

Bound or Unbound





Weakly bound levels $\longrightarrow$ very sensitive to the effective force

Prediction of single-particle energies is crucial

Odd Target

Occupation Probabilities

The BCS model gives occupation probabilities $v^2 = 1 - u^2$ of each single-particle state. They can be related to spectroscopic factors for a captured neutron.

Spectroscopic factors for even and odd targets

The probability of nucleon capture into the orbit j is proportional to the probability of the orbit j being empty [Yoshida, PR15, 2122 (1961)].

$$S_{ljK} = (2j+1)u_j^2 \times \frac{2}{2j+1} \qquad \text{for even target}$$

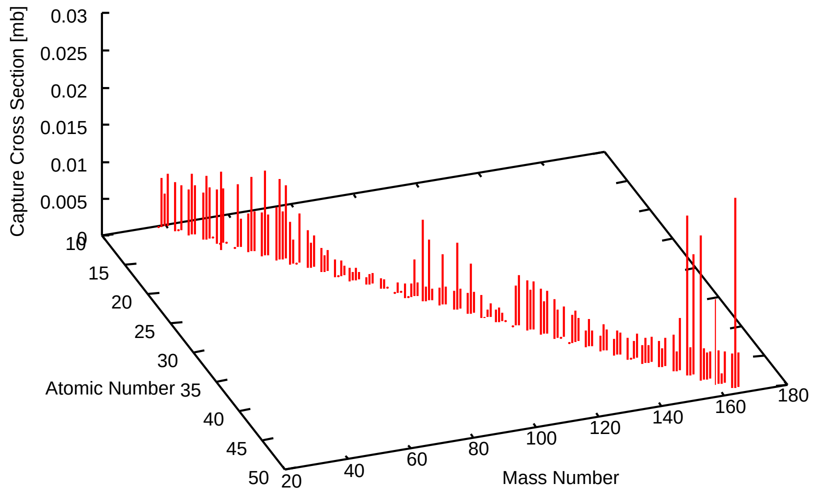
$$S_{ljK} = v_j^2 \times \frac{2}{2j+1} \qquad \text{for odd target}$$

This simplified formalism tested for the proton incident case. In general, experimental data for the odd target are scarce, and the validation might be difficult.

Capture Reaction Rate Calculations

Astrophysical reaction rates for r-process

- We have performed the neutron capture reaction calculations for more than 130, as a part of the augmented astrophysical rate database
- Capture reactions near the neutron drip-line ⇒ DSD dominant



"Neutron reactions in accreting neutron stars: A new pathway to efficient crust heating," S. Gupta, T. Kawano, P. Möller, Phys. Rev. Lett. **101**, 231101 (2008).

- Large scale calculations impact on nuclear astrophysics communities and energy applications, if we are able to provide the rate database.
- We are planning to perform the global calculation for all unstable isotopes.
- More microscopic inputs (E1 strength function, s.p. spectra) needed

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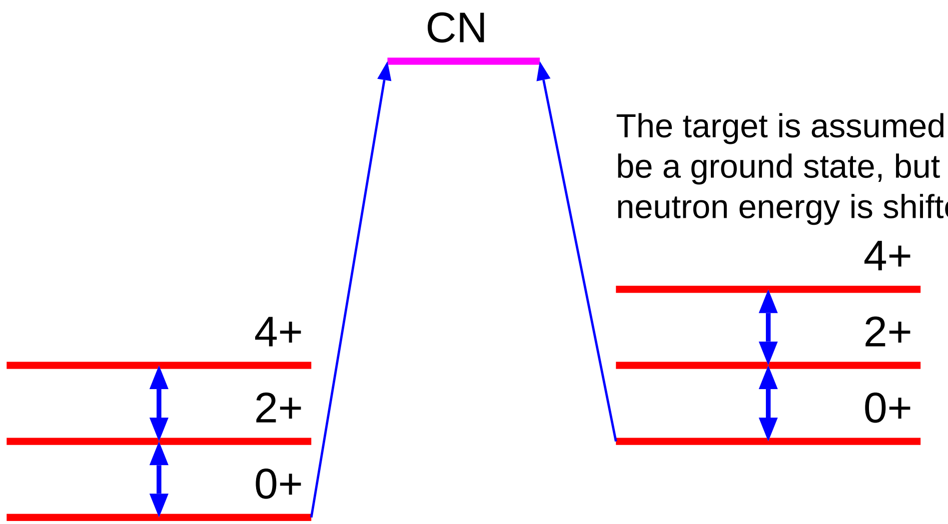
Neutron Reaction on Deformed Nuclei

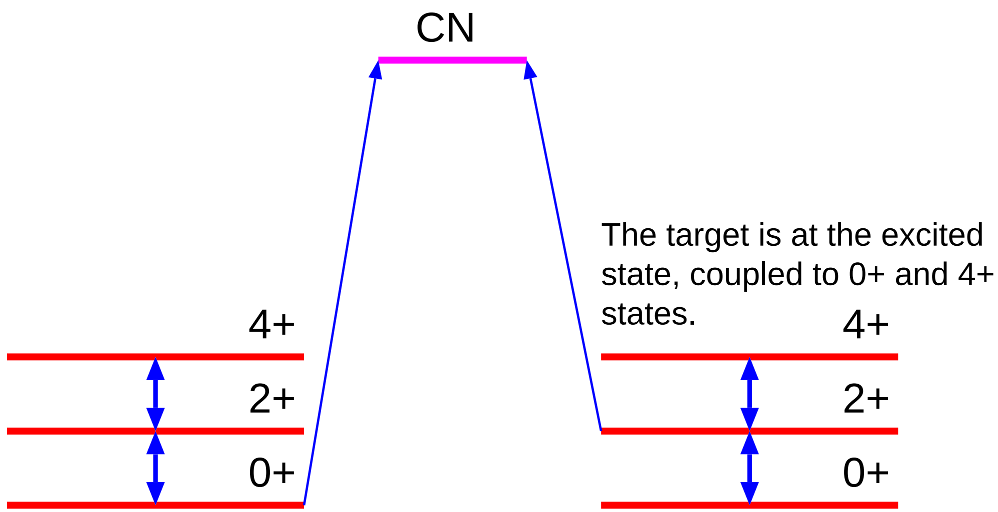
Modification to Hauser-Feshbach Theory at Low Energies

- Incorporate Coupled-Channels (CC) method into Hauser-Feshbach formula
  - 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)

Neutron Emission Probabilities $\propto$ Transmission



Usual HF calculation



Detailed balance

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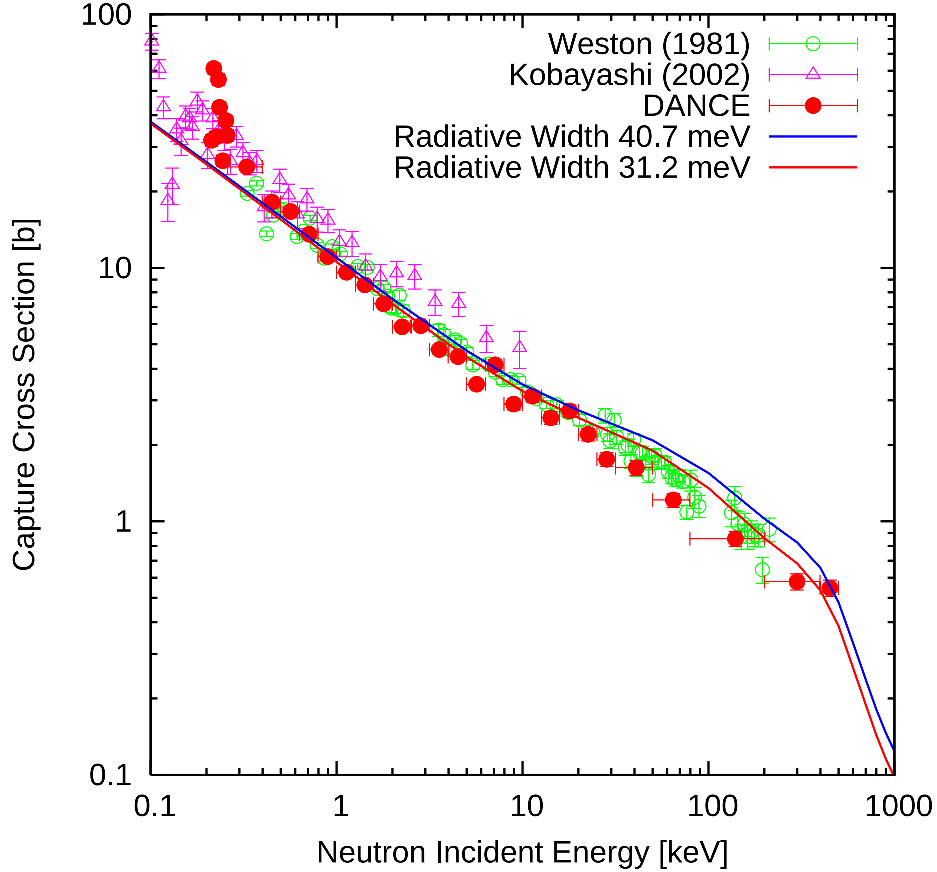
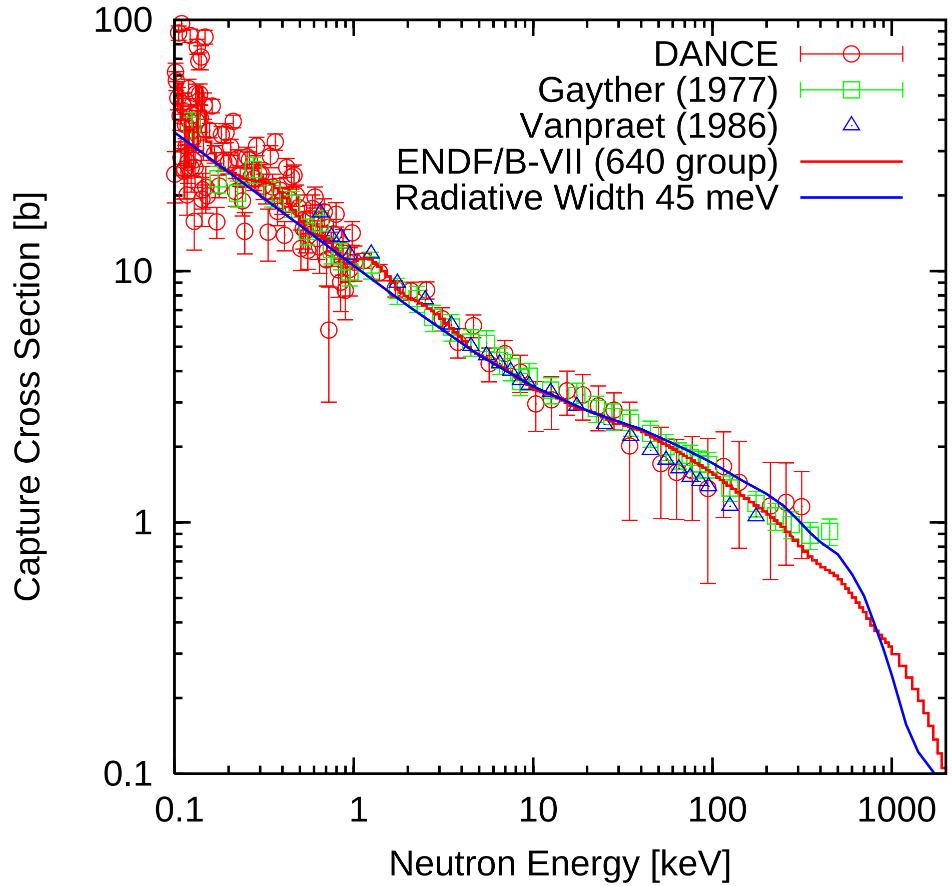
Comparisons with LANSCE / DANCE Data

Np237



Am241



E.-I. Esch, et al. Phys. Rev. C **77**, 034309 (2008)

M. Jandel, et al. Phys. Rev. C **78**, 034609 (2008)

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A New Hauser-Feshbach Model Code

Essential Tool to calculate cross sections

- All model developments, including the Hatree-Fock structure calculations, optical potential, DSD capture, pre-equilibrium process, and compound nuclear reactions, need to be validated against observable quantities — experimental data.
- An enterprise model code is essential for practical purposes (applications)
- A new proto-type Hauser-Feshbach model code written at LANL
  - C++
  - GPL
- We plan to release this code as a part of SciDAC collaboration

Modules Included, To Be Included

Current developing version

- Cross section calculation for $A \geq 10$ and $E \geq 1$ keV
- Spherical optical model and coupled-channels model for the entrance channel
- Direct/semidirect capture, for a simple spherical Nilson diagram
- Classical exciton model for pre-equilibrium reaction
- Width fluctuation by Moldauer's heuristic method
- Phenomenological inputs — level density, E1 strength function, PE strength

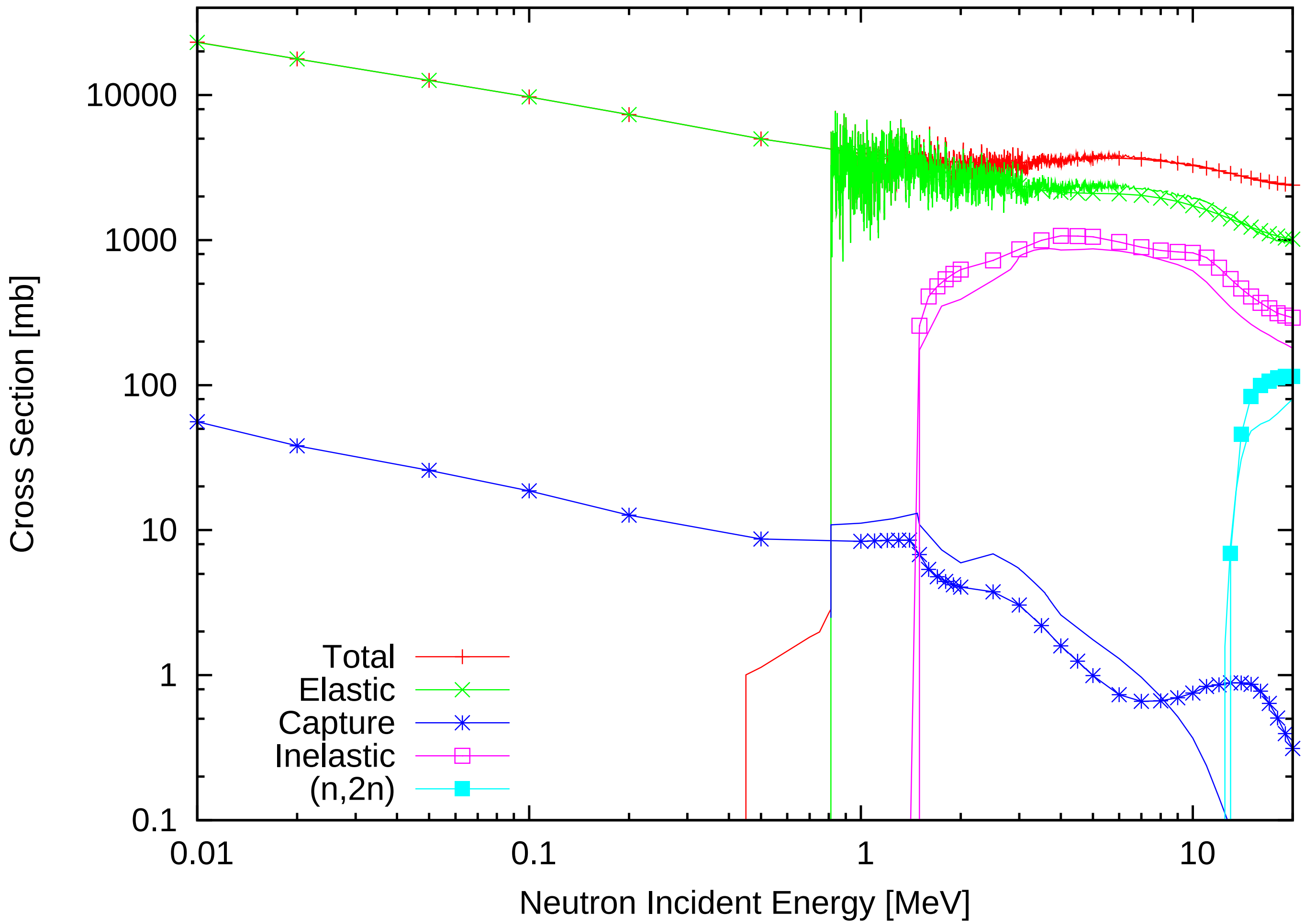
UNEDF Achievements can be included

- Single-particle states for the DSD capture
- Semi-microscopic level densities
- E1 strength function by the Hartree-Fock calculations
- KKM, width fluctuation when strongly coupled channels exist
- FKK, microscopic description of the one-step reaction

and more ...

Example I: n + Ni58 Reactions

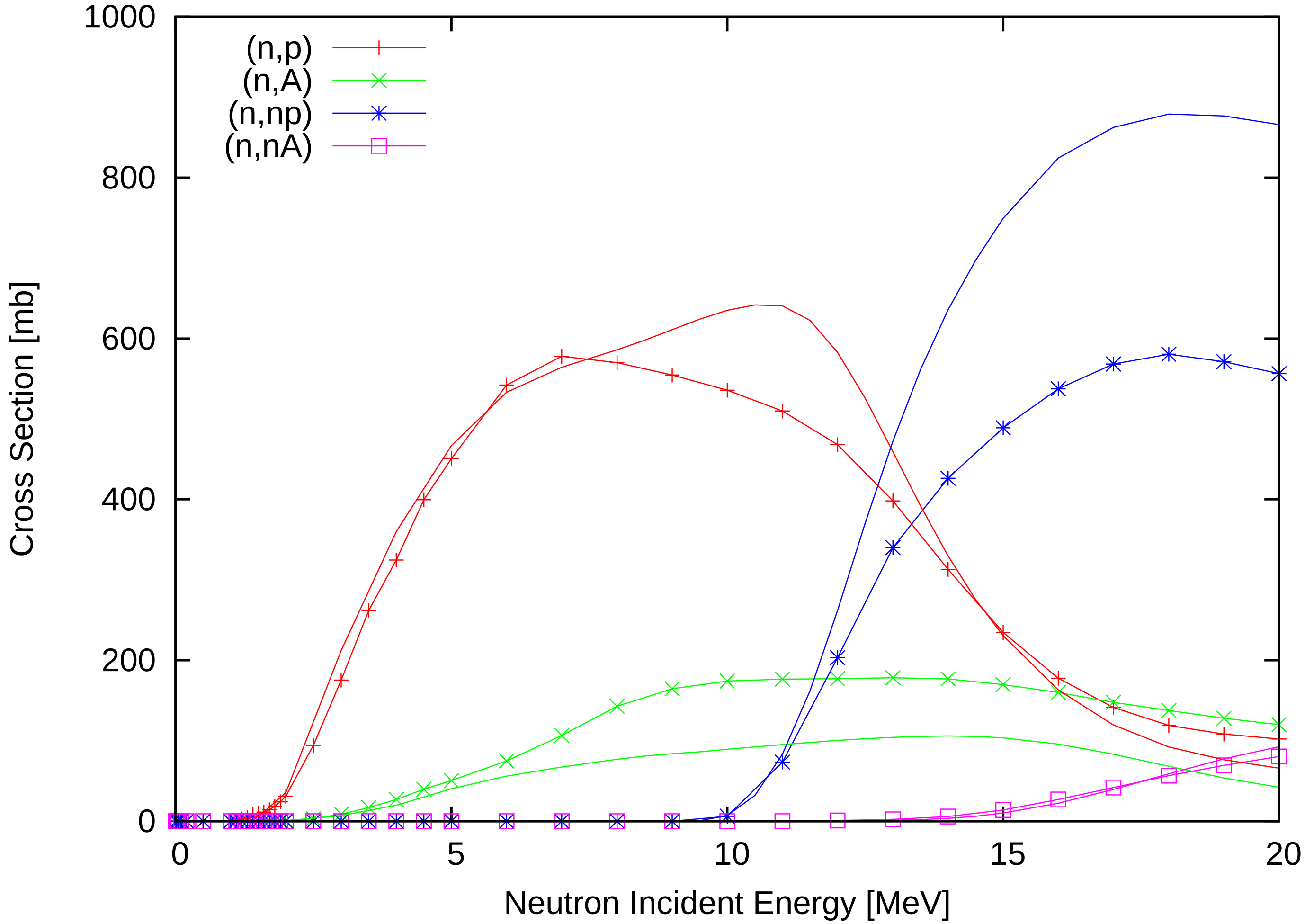
Comparison with evaluated data



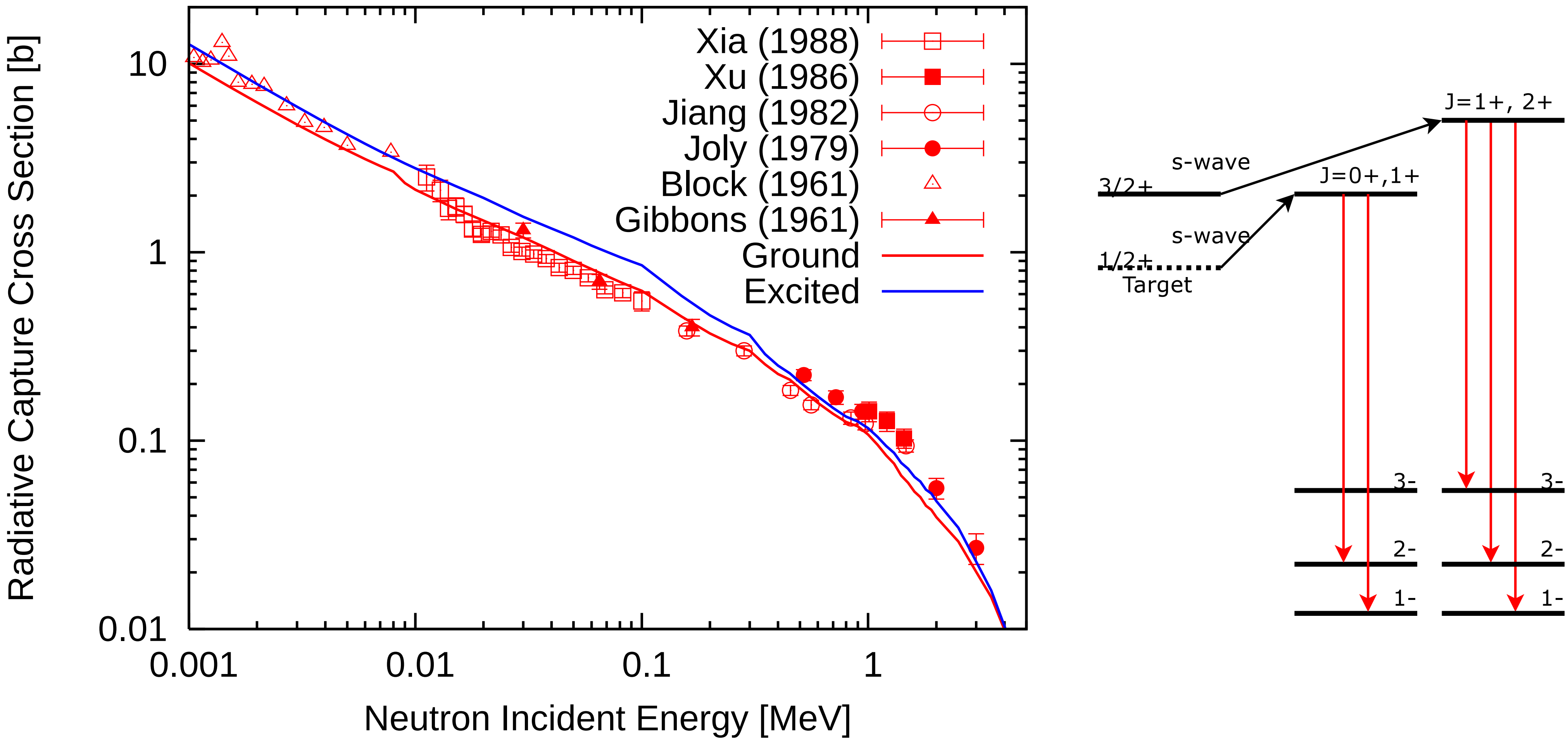
can be used for astrophysical reaction rate calculations

Example I: n + Ni58 Reactions, cont'd

Comparison with evaluated data



Example II: Reaction on the Excited State, Tm169



20% to 50% enhancement observed for the excited state case, due to the total compound formation, the spin of CN, and the spin phase space accessible by E1 transition.

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Concluding Remarks

Nuclear Reaction based on Hartree-Fock-BCS states

Pre-Equilibrium

- Spherical calculation looks reasonable
- Problems found for the deformed case
- We have investigated the possible reasons, but still need more work to understand.

Nucleon Capture

- Direct/semidirect capture model
- Even target cases well established
- Odd cases underway
- To compare the calculated results with experimental data, full Hauser-Feshbach model calculations needed.
- We plan to utilize microscopic inputs for the Hauser-Feshbach calculation
  - level densities from single-particle states
  - E1 strength function for neutron capture reaction on nuclei off-stability