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Challenges beyond Hauser-Feshbach for Nuclear Reaction Modeling

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Introduction

Cross section calculations in the keV to a few tens MeV range with the Hauser-Feshbach codes

- Optical and statistical Hauser-Feshbach models with width fluctuation and pre-equilibrium emission play a central role.
    - width fluctuation models implemented in HF codes give some difference in calculated cross section.
- In general, we may say, the model works pretty well.
    - the Hauser-Feshbach codes, like GNASH, TALYS, Empire, CCONE, CoH_3, etc., have been successfully utilized in nuclear data evaluation for many years.
    - although many phenomenological or empirical treatments of model parameters are involved.

Issues Partially Solved, or Remain

Indeed, we calculate cross sections, but in a proper way?

- Deformed system needs more attention
  - direct inelastic scattering process in HF not so well studied
- Uncertainty in the photon and fission channels could be large
  - photon transmission coefficient from the Giant Dipole Resonance model
  - fission transmission with a simple WKB approximation
- Phenomenological model for pre-equilibrium process still widely used
  - long discussions on quantum mechanical models for PE, which were very active in 1990s, basically disappeared, because
  - The exciton model reasonably works in nuclear data evaluation.
- ... and more

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This talk (or showcase) includes:

- Applicability of the Hauser-Feshbach theory itself
  - width fluctuation correction with direct reaction
- Model parameters for practical calculations
  - incorporating nuclear structure models into the reaction calculations
- Perturbative contributions from the other reaction mechanisms
  - pre-equilibrium, direct/semidirect capture calculation

Width Fluctuation Correction for Spherical Nuclei

The problematic assumption in the Hauser-Feshbach formula

$$\left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_{\mu}} \right\rangle = \frac{\left\langle \Gamma_{\mu a} \right\rangle \left\langle \Gamma_{\mu b} \right\rangle}{\left\langle \Gamma_{\mu} \right\rangle} \tag{1}$$

This leads to the width fluctuation correction (WFC)

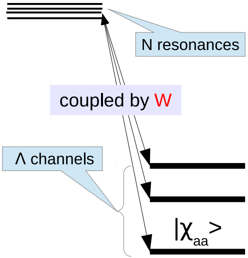
$$\langle \sigma_{ab}^{\mathrm{fl}} \rangle = \frac{T_a T_b}{\sum_c T_c} W_{ab} \tag{2}$$

Rigorously speaking, W_{ab} should be separated into two parts

- the elastic enhancement factor W_a
- the width fluctuation correction factor

Stochastic Scattering Matrix

Generate Resonances with the Random Matrix



$$S_{ab}(E) = \delta_{ab} - 2\pi i \sum_{\mu\nu} W_{a\mu} D^{-1} W_{\nu b} \quad (3)$$

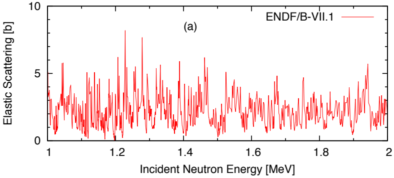
$$D_{\mu\nu} = E\delta_{\mu\nu} - H^{\mathrm{GOE}}_{\mu\nu} + \pi i \sum_{c} W_{\mu c} W_{c\nu} \quad (4)$$

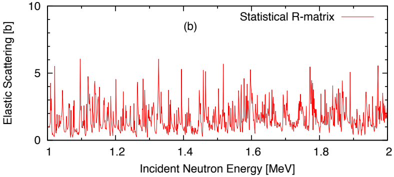
$$\overline{H^{\mathrm{GOE}}_{\mu\nu} H^{\mathrm{GOE}}_{\rho\sigma}} = \frac{1}{N}(\delta_{\mu\rho}\delta_{\nu\sigma} + \delta_{\mu\sigma}\delta_{\nu\rho}) \quad (5)$$

- T_a given by eigenvalues of WW^T
- poles are distributed in $[-2, 2]$
- energy average $\langle |S_{aa}|^2 \rangle$ replaced by ensemble average $\overline{|S_{aa}|^2}$.

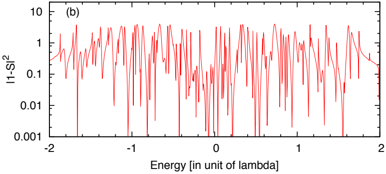
Monte Carlo Generated Cross Sections

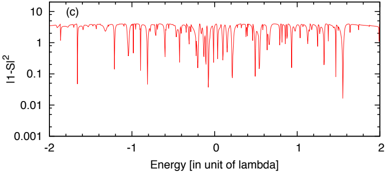
Physical





Mathematical





- Statistical R-matrix includes distributions of d and γ,
- while GOE has a random matrix in the propagator.

Inclusion of Direct Channel

- Approximated Method
  - calculate transmissions from Coupled-Channels S-matrix

$$T_a = 1 - \sum_c |\langle S_{ac} \rangle \langle S^*_{ac} \rangle|^2$$

  - eliminate flux going to the direct reaction channels
  - at least $\sum_a T_a$ gives correct compound formation cross section
  - HF performed in the direct-eliminated cross-section space
- Engelbrecht-Weidenmüller transformation
  - diagonalize S-matrix to eliminate the direct channels
  - HF performed in the channel space
  - transform back to the cross section space
- Kawai-Kerman-McVoy
  - correct at the limit of channel d-o-f $\nu = 2.0$

Implementation of Direct Channel in Stochastic S-Matrix

$$S_{ab} = S_{ab}^{(0)} - i \sum_{\mu} \frac{\gamma_{\mu a}\gamma_{\mu b}}{E - E_\mu - (i/2)\Gamma_\mu} \tag{6}$$

Since $S_{ab}^{(0)}$ is unitary, it can be diagonalized by the orthogonal transformation. However, making a unitary matrix $S_{ab}^{(0)}$ including off-diagonal elements is not so easy.
Instead, we employ a K-matrix method.

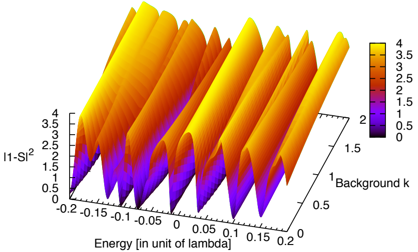
$$K_{ab}(E) = K^{(0)} + \sum_{\mu} \frac{\tilde{W}_{a\mu}\tilde{W}_{\mu b}}{E - E_\mu}. \tag{7}$$

where the background term $K^{(0)}$ is a model parameter. When K is real and symmetric, unitarity of S is automatically fulfilled.

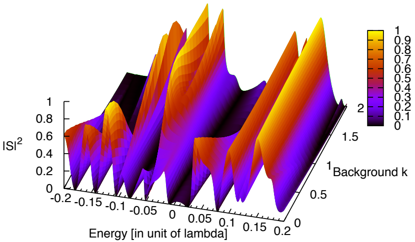
Generated Elastic/Inelastic Cross Sections

Fixed resonances, background component K_{ab} changed from 0 to 2
$N = 100,\ \Lambda = 2$

Elastic



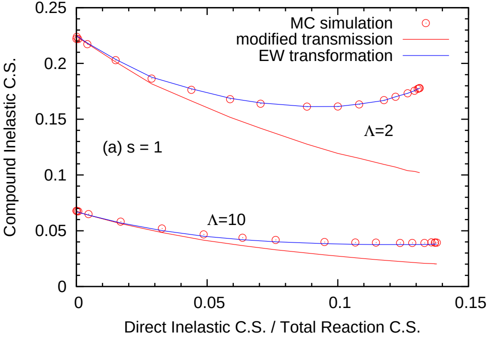
Inelastic



Inelastic scattering cross sections affected by the direct reaction strongly due to the interference between the resonances and the background term.

Inelastic Scattering Enhancement

Compound inelastic scattering cross section as a function of $\sigma_{\mathrm{DI}}/\sigma_{\mathrm{R}}$



- The approximation method using the modified transmission coefficients does not work when the direct channels are strong,
- since the compound inelastic scattering cross sections will be largely underestimated.
- This happens when
  - direct cross section is strong
  - the number of open channels small

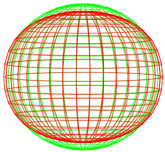
Limited Nuclear Structure Information

Nuclear structure information is involved in the Hauser-Feshbach calculation

- low-lying discrete state E_x, J^π, and γ-ray branching ration
    - can be tabulated in a supplemental file
    - IAEA maintains RIPL
- quantities calculated with nuclear mean-field theories
    - ground state deformation β_2, β_4 (also in RIPL)
    - single-particle levels and occupation probabilities
    - fission barriers

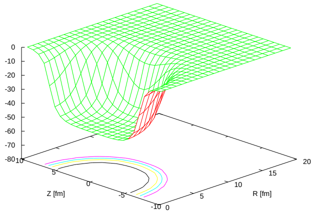
A natural extension of our Hauser-Feshbach codes is to include some simple nuclear mean-field models.

Mean-Field Models Added to CoH_3

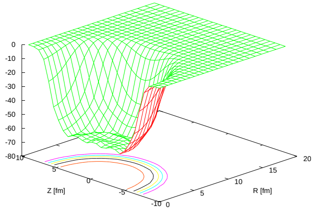


^{197}Au

- FRDM Finite-Range Droplet Model
- HF-BCS Skyrme Hartree-Fock BCS Model
  clone of Bonneau's code, rewritten in C++



FRDM

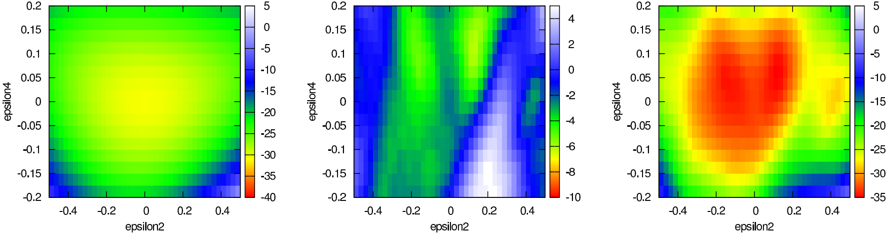


HF-BCS

Combining FRDM and HF-BCS

Use FRDM potential as an initial potential in the Hartree-Fock iteration

Pt-194



macro energy micro energy total

- iteration converges quickly
- can avoid being trapped by local minima
- if spherical WS is used, HF iteration can go either prolate / oblate shape depending on the initial condition

Direct/SemiDirect (DSD) Capture with HF-BCS

DSD Amplitudes

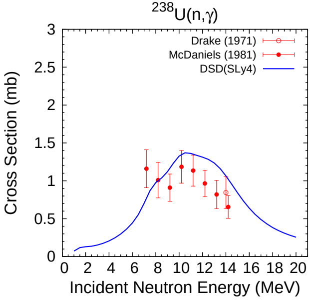
$$T_d \propto \sqrt{S_{ljK}} \langle R_{ljK}(r) | r | R_{LJ}(r) \rangle \qquad T_s \propto \sqrt{S_{ljK}} \langle R_{ljK}(r) | h(r) | R_{LJ}(r) \rangle \quad (8)$$

DSD with Hartree-Fock BCS Theory
spectroscopic factor S_{ljK}

- single-particle occupation probabilities, $v^2 = 1 - u^2$

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



Bonneau, TK, et al. PRC **75**, 054618 (2007)

Coupled-Channels Calculation with FRDM

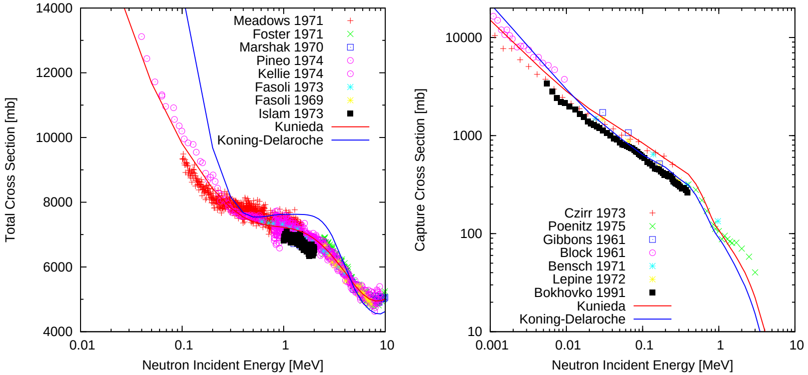
Expansion of FRDM shape by Spherical Harmonics

$$r(\theta,\phi) = R_0 + R_0 \sum_{l=1} \sum_{m=-l}^{l} \beta_{lm} Y_l^m(\theta,\phi) \tag{9}$$

$$\begin{aligned} {}^{165}\mathrm{Ho} \quad & (\epsilon_2 = 0.267, \epsilon_4 = 0.02, \epsilon_6 = 0.017) \\ \simeq \quad & (\beta_2 = 0.291, \beta_4 = 0.009, \beta_6 = -0.0197, \beta_8 = -0.006, \ldots) \end{aligned} \tag{10}$$

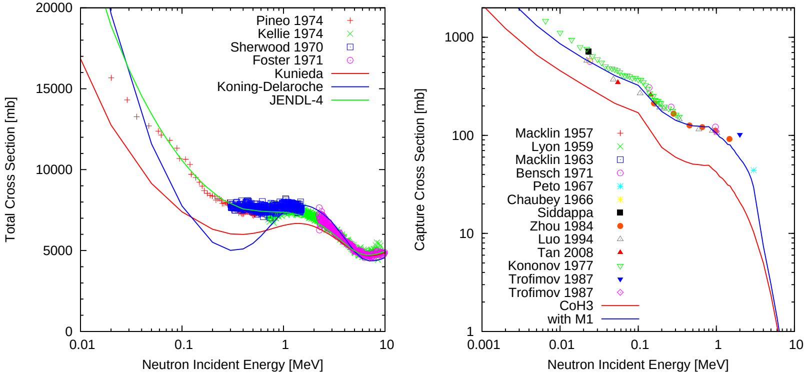
- We cannot use FRDM potential directly as a real part of optical potential (R_0 tends to be smaller)
- Use the deformation for the global CC potential by Kunieda et al.

FRDM + Kunieda Potential Calculation, Ho-165



The calculated capture cross section also depends on other quantities, such as level density, photon-strength function. This is just an example!

FRDM + Kunieda Potential Calculation, Sm-152



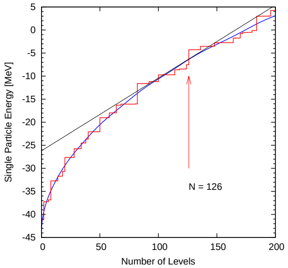
It turned out that capture is sensitive to a small M1 photon strength at low energy — scissors/twist mode
($E = 3$ MeV, $\Gamma = 3$ MeV, and $\sigma_0 = 0.5$ mb).

J. L. Ullmann et al. PRC **89**, 034603 (2014); M. Guttormsen et al. PRC **89**, 014302 (2014)

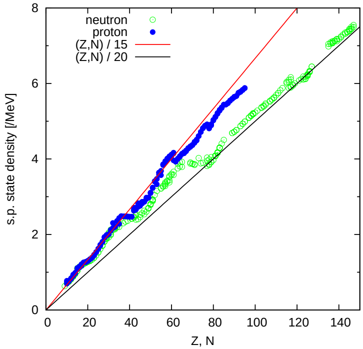
Strutinsky Method for Single-Particle State Density

Level (state) densities in the pre-equilibrium process

$$\omega = \frac{g^n (E - A_{ph})^{n-1}}{p!h!(n-1)!}$$



^{208}Pb single-particle levels



g is given by the tangent at E_F in the FRDM strutinsky method

Mean-Field Single-Particle States for MSC/MSD

The quantum mechanical pre-equilibrium calculations benefit from the mean-field models — a smooth transition of DWBA from discrete final states to a continuum.

- They tend to be lengthy calculations, and not so practical in the nuclear data evaluation.
- Simplification applied
  - TUL in Empire, or Koning and Akkermans [PRC **47**, 724 (1993)]
  - random sample of particle-hole pairs by Kawano and Yoshida (2001).
- There is very little progress in this area nowadays, except for at CEA.
- Dupuis first time implemented QRPA in MSD.

P-H Excitation for One-Step MSD Reaction

$$\frac{d^2\sigma_{ba}}{dEd\Omega} = \frac{(2\pi)^4}{k_a^2} \sum_{\mu} |\langle \chi_b^{(-)} u_{m\mu} | \mathcal{V} | \chi_a^{(+)} u_0 \rangle|^2 \rho_{m\mu}(E_x) \tag{11}$$

Unperturbed State Density from FRDM / HF

$$\rho_m^{(0)}(E) = \sum_{\mu} \delta(E - \epsilon_{m\mu}) \tag{12}$$

Exciton State Density for fixed $J\pi$

$$\rho_m(E) = -\sum_{\mu} \frac{1}{\pi} \mathrm{Im} \frac{1}{E - \epsilon_{m\mu} - \sigma_m(E)} \tag{13}$$

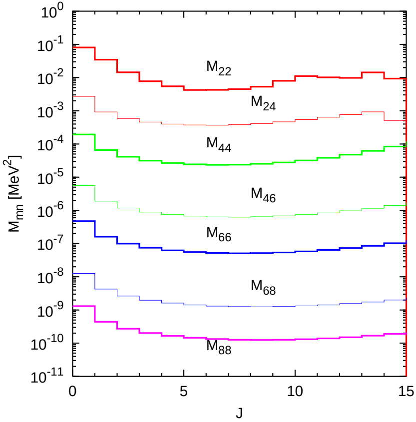
Saddle Point Equation with Second Moment $\mathcal{M}$ of M.E.

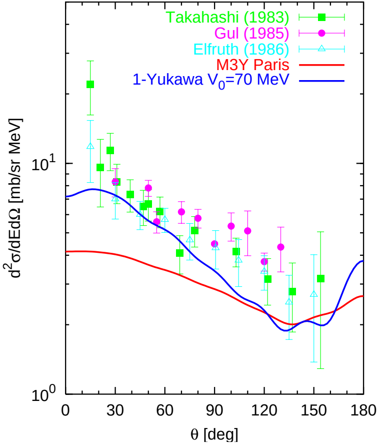
$$\sigma_m(E) = \sum_{n} \mathcal{M}_{mn} \int \rho_n^{(0)}(\epsilon) \frac{1}{E - \epsilon - \sigma_n(E)} d\epsilon \tag{14}$$

TK, S. Yoshida, PRC, **64**, 024603 (2001)

Calculated One-Step MSD DDX

^{208}Pb(n,n') reaction at $E_{in} = 14.5$, $E_{out} = 7.5$ MeV





TK, S.Yoshida, unpublished.

Concluding Remarks

- Direct reaction channels should be properly included in the Hauser-Feshbach codes.
  - Engelbrecht-Weidenmüller transformation, or KKM
- Nuclear structure (mean-field calculation) input
  - will reduce the number of phenomenological adjustable parameters
  - The M1 photon strength will be a key to handle spiky capture channel
- Quantum mechanical pre-equilibrium process
  - we should shed light on this again for better understanding of neutron inelastic scattering from actinides
  - maybe need more practical models for nuclear data evaluations