Theoretical Issues on 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 utilized in nuclear data evaluation successfully.
  - 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 WKF 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
  - Exciton model reasonably works in nuclear data evaluation
- ... and more

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I will focus on neutron inelastic scattering issues in the modelling.
This talk includes:

- Width fluctuation correction with direct reaction
- Quantum mechanical pre-equilibrium models

Statistical Model — Hauser-Feshbach

Energy average cross section over many resonances

$$
\begin{aligned}
\left\langle \sigma_{ab}^{\mathrm{fl}} \right\rangle &= \sum_{\mu} \left\langle \left| \frac{g_{\mu a} g_{\mu b}}{E - W_\mu} \right|^2 \right\rangle \\
&= \frac{1}{\Delta E} \int_{E' - \Delta E/2}^{E' + \Delta E/2} \frac{\Gamma_{\mu a} \Gamma_{\mu b}}{(E' - E_\mu)^2 + \Gamma_\mu / 4} dE' \\
&= \left\langle \frac{2\pi}{D} \frac{\Gamma_{\mu a} \Gamma_{\mu b}}{\Gamma_\mu} \right\rangle \\
&\simeq \frac{2\pi}{D} \frac{\langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle}{\langle \Gamma_\mu \rangle} = \frac{T_a T_b}{\sum_c T_c} \qquad (1)
\end{aligned}
$$

where

$$
T_c = 2\pi \frac{\langle \Gamma_c \rangle}{D} \qquad (2)
$$

Width Fluctuation Correction

The problematic assumption in the Hauser-Feshbach formula

$$\left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle = \frac{\langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle}{\langle \Gamma_\mu \rangle} \tag{3}$$

This leads to the width fluctuation correction (WFC)

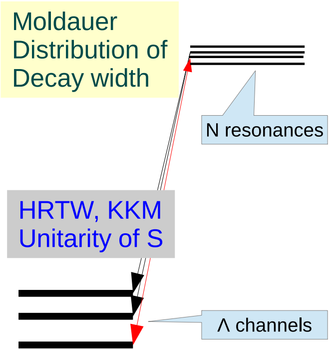
$$\langle \sigma_{ab}^{\mathrm{fl}} \rangle = \frac{T_a T_b}{\sum_c T_c} W_{ab} \tag{4}$$

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

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

Methods to Derive Width Fluctuation Correction

- Heuristic Method
  - generate resonances using Monte Carlo technique, and average them numerically
  - Moldauer (1980)
  - HRTW Hofmann, et al. (1975, 1980)
- Projection Operator Method
  - KKM, Kawai-Kerman-McVoy (1973)
  - using randomness of decay amplitude phase
- Maximum Entropy Method
  - Mello and Seligman (1980)
  - Fröhner (1986)



All models have some approximations, phenomenological parameters, or require numerical calculations.

GOE Triple Integral - Exact Solution for $N \to \infty$

Generalized Scattering Matrix

$$S_{ab} = S_{ab}^0 - 2i \sum_{\lambda\mu} \gamma_{\lambda a}^t (D^{-1}) \gamma_{\mu b} \quad (5)$$

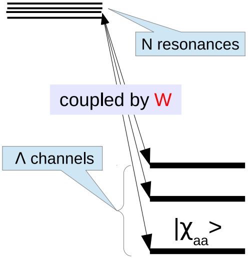
$$D_{\lambda\mu} = \delta_{\lambda\mu} E - (H_{QQ})_{\lambda\mu} - (W_Q)_{\lambda\mu} \quad (6)$$

where the matrix H_{QQ} is replace by GOE. Verbaarschot, Weidenmüller, Zirnbauer obtained the $\langle S_{ab}^{\mathrm{fl}}(E_1) S_{cd}^{\mathrm{fl}}(E_2) \rangle$ in a triple integral, which is believed to be the correct answer.

$$\begin{aligned} \langle |S_{ab}|^2 \rangle &= |\langle S_{ab} \rangle|^2 + \frac{T_a T_b}{8} \int_0^\infty d\lambda_1 \int_0^\infty d\lambda_2 \int_0^1 d\lambda \mu(\lambda, \lambda_1, \lambda_2) \\ &\times \Pi_c \frac{1 - T_c \lambda}{\sqrt{(1 + T_c \lambda_1)(1 + T_c \lambda_2)}} J_{ab}(\lambda, \lambda_1, \lambda_2) \end{aligned} \quad (7)$$

Stochastic Scattering Matrix

Generate Resonances with the Random Matrix



$$S_{ab}(E) = \delta_{ab} - 2\pi i \sum_{\mu\nu} W_{a\mu} D^{-1} W_{\nu b} \tag{8}$$

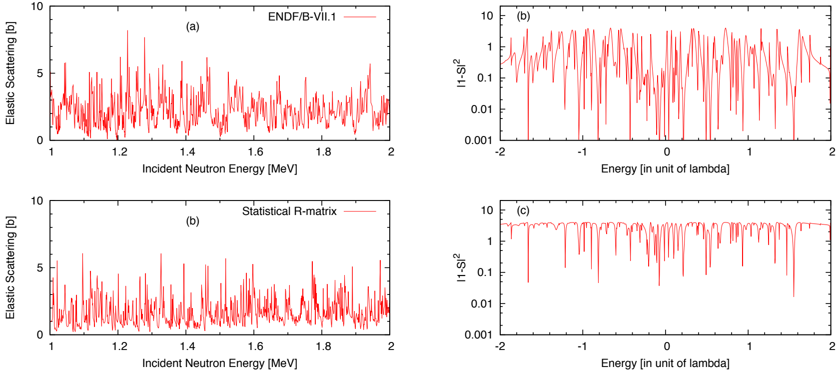
$$D_{\mu\nu} = E\delta_{\mu\nu} - H^{\mathrm{GOE}}_{\mu\nu} + \pi i \sum_{c} W_{\mu c} W_{c\nu} \tag{9}$$

$$\overline{H^{\mathrm{GOE}}_{\mu\nu} H^{\mathrm{GOE}}_{\rho\sigma}} = \frac{\lambda^2}{N} (\delta_{\mu\rho}\delta_{\nu\sigma} + \delta_{\mu\sigma}\delta_{\nu\rho}) \tag{10}$$

- λ is a scale parameter $(= 1.0)$
- T_a given by eigenvalues of WW^T
- average spacing $d = \pi\lambda/N$, and strength $s = \langle\gamma^2\rangle/d$
- poles are distributed in $[-2\lambda, 2\lambda]$
- We assume that the energy average $\langle|S_{aa}|^2\rangle$ can be replaced by the ensemble average $\overline{|S_{aa}|^2}$.

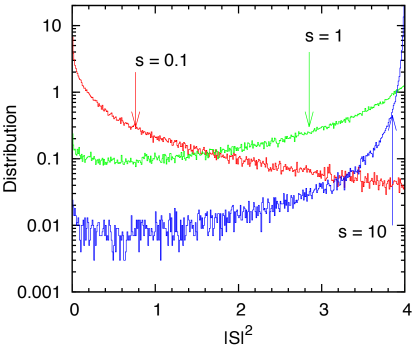
Monte Carlo Generated Cross Sections

Physical | Mathematical



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

Ensemble Average at the Center of GOE



$$s = \frac{\langle \gamma^2 \rangle}{d}$$

Input

- $N = 100,\ \Lambda = 2,\ s = 1$
- $T_a = 0.708,\ T_b = 0.754$

Output

- $\overline{|1 - S_{aa}|^2} = 2.85$
- $\sigma^{\rm dir} = |1 - \overline{S_{aa}}|^2 = 2.37$
- $\sigma^{\rm fl} = \overline{|1 - S_{aa}|^2} - \sigma^{\rm dir} = 0.477$

Model Prediction

- $\sigma^{\rm HF} = 0.343$
- $\sigma^{\rm Moldauer} = 0.478$
- $\sigma^{\rm HRTW} = 0.480$
- $\sigma^{\rm GOE} = 0.480$

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
  - Hauser-Feshbach is performed in the direct-eliminated cross-section space (detailed balance)
  - many HF codes employ this method
- Rigorous Method — Engelbrecht-Weidenmüller transformation
  - diagonalize S-matrix to eliminate the direct channels
  - Hauser-Feshbach is performed in the channel space
  - transform back to the cross section space

Diagonalization of S-Matrix

Satchler's Transmission Matrix — Hermitian

$$P_{ab} = \delta_{ab} - \sum_c \langle S_{ac} \rangle \langle S^*_{bc} \rangle \tag{11}$$

The Hermitian matrix P can be diagonalized by unitary transformation

$$(UPU^\dagger)_{ab} = \delta_{ab} p_a, \qquad 0 \le p_a \le 1 \tag{12}$$

and the same U diagonalizes the scattering matrix

$$\langle \tilde{S} \rangle = U \langle S \rangle U^T \tag{13}$$

Statistical Model in Channel Space

New transmission coefficients are defined as

$$T_p = 1 - |\tilde{S}_{pp}|^2 \tag{14}$$

Perform GOE triple-integral in the channel space to calculate $\langle \tilde{S}_{pq} \tilde{S}^*_{rs} \rangle$, and finally a back-transformation from the channel space to the cross-section space reads

$$\langle |S_{ab}|^2 \rangle = \sum_{pqrs} U^*_{pa} U^*_{qb} U_{ra} U_{sb} \langle \tilde{S}_{pq} \tilde{S}^*_{rs} \rangle . \tag{15}$$

Note that ECIS calculates $\langle \tilde{S} \tilde{S}^* \rangle$ using Moldauer

Implementation of Direct Channel in Stochastic S-Matrix

$$S_{ab} = S_{ab}^{(0)} - i \sum_{\mu} \frac{\gamma_{\mu a}\gamma_{\mu b}}{E - E_\mu - (i/2)\Gamma_\mu} \tag{16}$$

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.

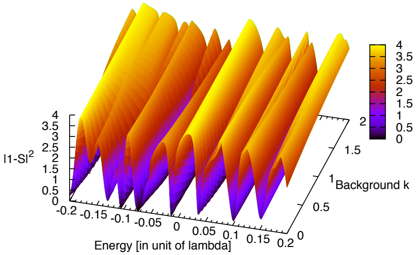
$$K_{ab}(E) = K^{(0)} + \sum_{\mu} \frac{\tilde{W}_{a\mu}\tilde{W}_{\mu b}}{E - E_\mu}. \tag{17}$$

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

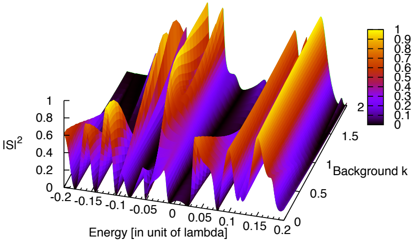
Generated Elastic/Inelastic Cross Sections

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

Elastic



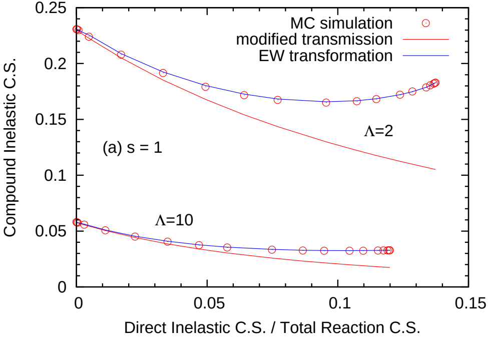
Inelastic



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

Classical Pre-Equilibrium Model

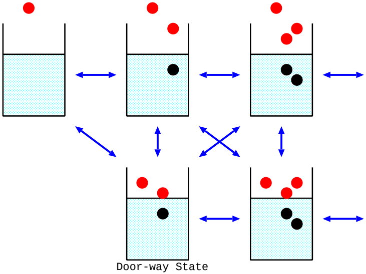
Exciton Model

- Nuclear state — n-particle $(n-1)$-hole state
- Transition rate — $\lambda_{nn'} = \frac{2\pi}{\hbar^2}|M|^2\rho_{n'}$
- Solve a master equation for the occupation probability $P(p,h)$
- or a closed form expression using the never-come-back approximation
- The matrix element $|M|^2$ is regarded as an adjustable parameter
- ρ is calculated from a single-particle state density model
- Pros:
  - calculation very quick
  - generally the exciton model give a good fit to the energy distribution of emitted particles
  - phenomenological model input parameters available
- Cons:
  - cannot calculate angular distributions nor spin-transfer

Quantum Mechanical Pre-Equilibrium Theory

- Feshbach, Kerman, and Koonin (1980)
- An extension of DWBA to the continuum state
- Particle-Hole excitation

- $\mathcal{P}$-space (Multistep Direct, MSD)
  - Final state is unbound
  - Residual System: $1p$-$1h$, $2p$-$2h$, $3p$-$3h$, $\ldots$
  - Green's Function for matrix elements involved
- $\mathcal{Q}$-space (Multistep Compound, MSC)
  - Final state is bound
  - Residual System: $2p$-$1h$, $3p$-$2h$, $4p$-$3h$, $\ldots$



Multistep Direct MSD Theories

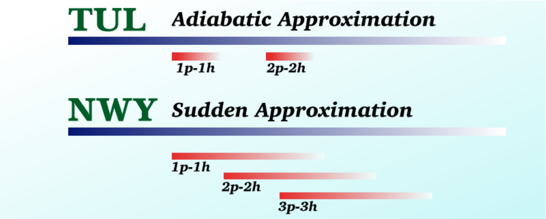
- FKK: Feshbach, Kerman, Koonin (1980)
  - On-Shell Approximation for Green's Function
- TUL: Tamura, Udagawa, Lenske (1982)
  - Adiabatic Approximation for the Second Step
- NWY: Nishioka, Weidenmüller, Yoshida (1988)
  - GOE for residual interaction
  - Sudden Approximation for the Second Step
- SCDW: Luo, Kawai, Weidenmüller (1991,1992)
  - Eikonal Approximation for the Second Step

- One-step process is dominant below 20 MeV
- The one-step expression of FKK, TUL, and NWY is the same (in principle), but modeling could be different.

Comparison of FKK, TUL, and NWY 2-Step

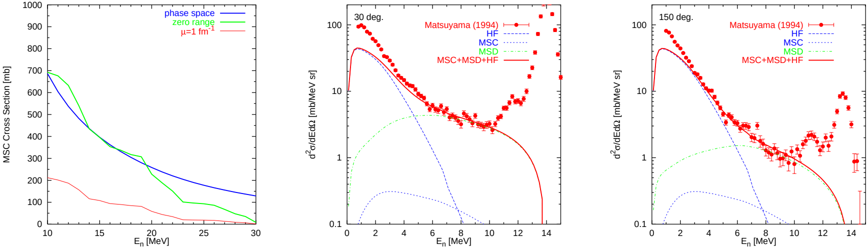
	FKK	TUL	NWY
Approximation	on-shell	Adiabatic	Sudden
Statistical Average	Each	Each	Final
State density	$\rho_{1p1h} \otimes \rho_{1p1h}$	$\rho_{1p1h} \otimes \rho_{1p1h}$	ρ_{2p2h}
Model	Equidistant	RPA	GOE
Interference	No	No	Yes

Time Scale



FKK MSC/MSD Calculation Example

Strength of $2p$-$1h$ Formation and MSC/MSD Emissions for n + ^{93}Nb



- Microscopic calculation of doorway state formation cross section
- Phase-space approximation of Chadwick and Young

TK, Phys. Rev. C, **59**, 865 (1999).

GOE One-Step Cross Section

$$\frac{d^2\sigma_{ba}}{dEd\Omega} = \frac{(2\pi)^4}{k_a^2} \sum_\mu |\langle \chi_b^{(-)} u_{m\mu} | \mathcal{V} | \chi_a^{(+)} u_0 \rangle|^2 \rho_{m\mu}(E_x) \tag{18}$$

Unperturbed State Density

$$\rho_m^{(0)}(E) = \sum_\mu \delta(E - \epsilon_{m\mu}) \tag{19}$$

Exciton State Density for fixed $J\pi$

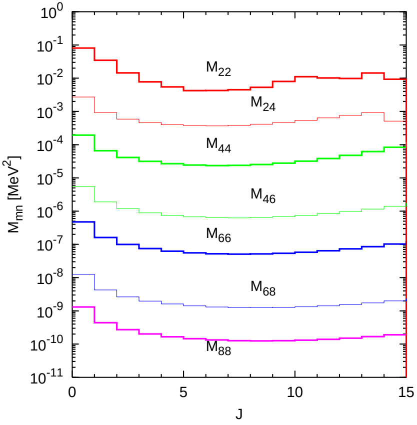
$$\rho_m(E) = -\sum_\mu \frac{1}{\pi} \mathrm{Im} \frac{1}{E - \epsilon_{m\mu} - \sigma_m(E)} \tag{20}$$

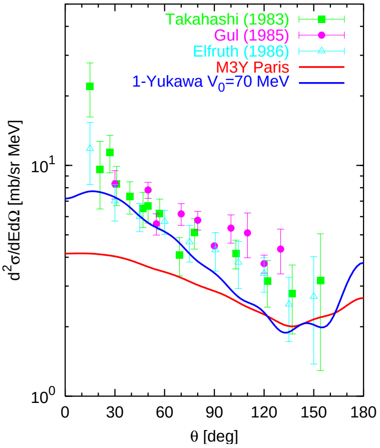
Saddle Point Equation

$$\sigma_m(E) = \sum_n \mathcal{M}_{mn} \int \rho_n^{(0)}(\epsilon) \frac{1}{E - \epsilon - \sigma_n(E)} d\epsilon \tag{21}$$

Calculated One-Step MSD DDX

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





TK and S. Yoshida, Phys. Rev. C, **64**, 024603 (2001).

Notes on Practical Application of MSC/MSD

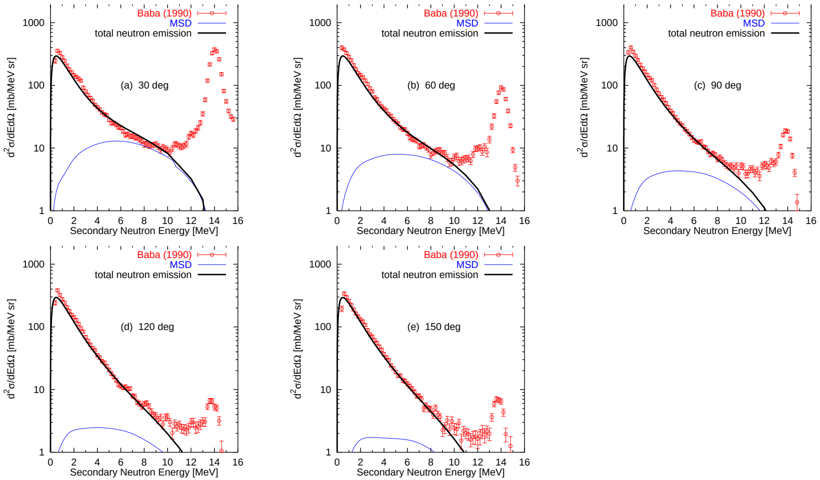
- They tend to be lengthy calculations, and not so practical in the nuclear data evaluation.
- Simplification applied
  - replace DWBA particle-hole matrix elements by the collective ones
  - TUL in Empire, or Koning and Akkermans [PRC **47**, 724 (1993)]
  - second-step takes place on the ground state, rather than the excited state in the adiabatic approximation (TUL).
  - random sample of particle-hole pairs by Kawano and Yoshida (2001).
- Composite particle emissions is difficult to formulate.
- There is very little progress in this area nowadays, except for at CEA.
- Dupuis first time implemented QRPA in the MSD (see his talk).

FKK One-Step, Bonetti Approach

$$
\begin{aligned}
\frac{d^2\sigma_{ba}}{dEd\Omega} &= \frac{(2\pi)^4}{k_a^2}\sum_{\mu} |\langle \chi_b^{(-)} u_{m\mu}|\mathcal{V}|\chi_a^{(+)} u_0\rangle|^2 \rho_{m\mu}(E_x) \\
&= \sum_j \frac{(2\pi)^4}{k_a^2} \overline{|\langle \chi_b^{(-)} u_{m\mu}|\mathcal{V}|\chi_a^{(+)} u_0\rangle|^2} (2j+1)\hat{\rho}_{1p1h}(E_x, j) \\
&= \sum_j \left\langle \left(\frac{d\sigma_{ba}}{d\Omega}\right)_{DWBA} \right\rangle_j \hat{\rho}_{1p1h}(E_x, j) \qquad (22)
\end{aligned}
$$

- Averaged DWBA cross section
  - particle-hole excitation, with angular momentum transfer of j
- Phenomenological level density $\hat{\rho}_{1p1h}(E_x, j)$

Neutron Inelastic Scattering from U-238



TK, et al. Phys. Rev. C, **63**, 034601 (2001).

Notes on Neutron Inelastic Scattering from Actinides

The model

- The phenomenological state density $\rho(E_x)$ drops sharply at the high side due to a pairing correction.
- QRPA calculation is required to take the embedded collective strength into account properly.

The experimental data

- The double-differential cross section data are not pure data with which we can compare the model calculations directly
  - background determination by MC required
  - energy broadening may not be a simple Gaussian

Concluding Remarks

- Direct calculation of cross section average by using the stochastic scattering matrix model that includes GOE
  - K-matrix background cross section given as the direct channel
  - unitarity of the total S-matrix ensured
  - comparison of two methods
    - generalized transmission coefficients, where direct reaction is subtracted
    - Engelbrecht-Weidenmüller transformation
  - looks both methods give very similar cross sections when the direct cross section is small.
  - however, the compound inelastic scattering might be largely underestimated when the direct channels are strong.
- Quantum mechanical pre-euqilibrium 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