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Random-matrix approach to the statistical compound nuclear reaction at low energies using the Monte-Carlo technique

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Random Matrix Theory, Integrable Systems, and Topology in Physics,
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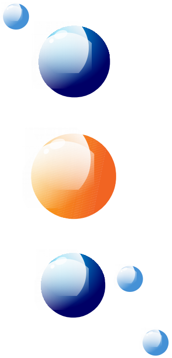
Los Alamos

Compound Nuclear Reaction

- Bohr Hypothesis
  - Incident particle shares its energy with the target nucleons
  - Compound nucleus (CN) attains statistical equilibrium
  - Decay modes of CN are independent of formation
- The hypothesis holds very well at high energies
  - Energy-average cross sections can be factorized by penetration factors for each channel
  - Hauser-Feshbach theory
- but not for isolated or weakly overlapping compound-nucleus resonances
  - Hauser-Feshbach theory corrected by the width fluctuation correction, WFC
    - decay width distribution over the eigenstates (resonances)
    - incoming wave interferes in the elastic channel



TK, P. Talou, H.A. Weidenmüller, PRC **92**, 044617 (2015)

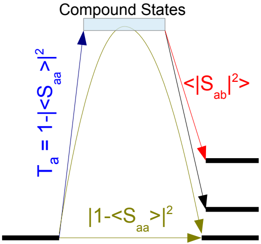
Average Compound Nucleus Cross Section

Reaction cross section from channel a to channel b is written as

$$\sigma_{ab} = \frac{\pi}{k_a^2} g_a |\delta_{ab} - S_{ab}|^2 \tag{1}$$

and the energy average cross section

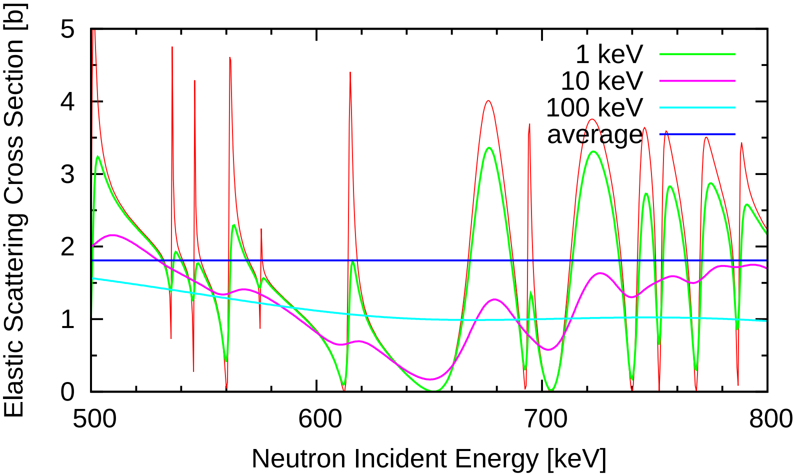
$$\begin{aligned} \langle\sigma_{ab}\rangle &= \frac{\pi}{k_a^2} g_a \langle|\delta_{ab} - S_{ab}|^2\rangle \\ &= \frac{\pi}{k_a^2} g_a \left\{ |\delta_{ab} - \langle S_{ab}\rangle|^2 + \langle|S_{ab}^{\mathrm{fl}}|^2\rangle \right\} \\ &= \sigma_{ab}^{\mathrm{dir}} + \langle\sigma_{ab}^{\mathrm{fl}}\rangle \end{aligned} \tag{2}$$



The aim of various CN reaction theories is to express $\langle\sigma_{ab}\rangle$ in terms of $\langle S_{aa}\rangle$, or the transmission coefficients

$$\langle S_{aa}\rangle = S_{aa}(E + iI), \qquad T_a = 1 - |\langle S_{aa}\rangle|^2 , \qquad 0 \le T_a \le 1 \tag{3}$$

Average Over Resonances



Width Fluctuation Correction

Hauser-Feshbach formula for the CN cross section

$$\sigma_{ab}^{\mathrm{HF}} = \frac{\pi}{k_a^2} g_a \frac{T_a T_b}{\sum_c T_c} \tag{4}$$

with the width fluctuation correction (WFC) factor

$$\sigma_{ab}^{\mathrm{CN}} = \frac{\pi}{k_a^2} g_a \frac{T_a T_b}{\sum_c T_c} W_{ab} \tag{5}$$

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

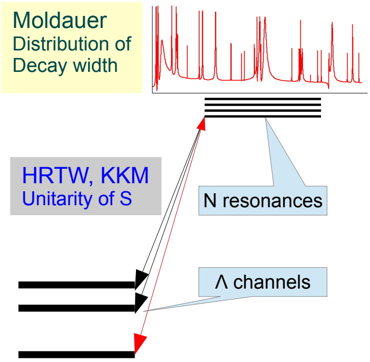
- the elastic enhancement factor W_a
- and the width fluctuation correction factor

For the comparison of various approaches it is convenient to define WFC as

$$W_{ab} = \sigma_{ab}^{\mathrm{CN}} / \sigma_{ab}^{\mathrm{HF}} \tag{6}$$

Statistical Theories for Compound Reactions

- Moldauer (1960 – 1980)
  - based on statistical S or K-matrix simulation
- KKM, Kawai-Kerman-McVoy (1973)
  - projection operator method
- HRTW, Hofmann, Richert, Tepel, Weidenmüller (1975)
  - based on statistical K-matrix
- Mello and Seligman (1980)
  - maximum entropy distribution of S
- Verbaarschot, Weidenmüller, Zirnbauer (1985)
  - analytic expression based on GOE



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

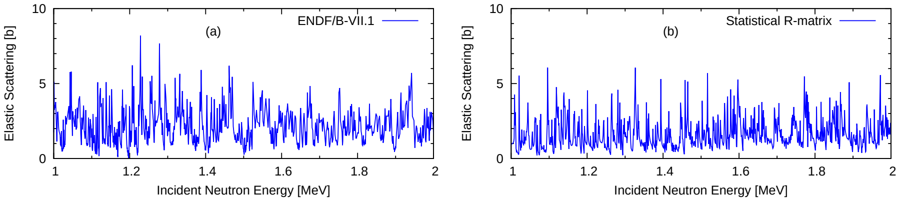
Statistical R and K Matrices for Computer Simulations

Compound nuclear reactions modelled by GOE-inspired ensembles

$$K_{ab}(E) = \pi \sum_{\sigma} \frac{\gamma_{a\mu}\gamma_{\mu b}}{E - E_\mu}, \qquad S_{ab} = \left(\frac{1 - iK}{1 + iK} \right)_{ab} \tag{7}$$

where

- $\gamma_{a\mu}$ is sampled from Gaussian, zero-average and assumed width
- E_μ is sampled from Wigner distribution, $P_W(s) = \pi/2s \exp(-\pi s^2/4)$



HRTW and Moldauer

In HRTW all the channel cross sections are calculated from an effective transmission coefficient V_a

$$\langle \sigma_{ab} \rangle = \frac{\pi}{k_a^2} g_a \frac{V_a V_b}{\sum_c V_c} \{1 + \delta_{ab}(W_a - 1)\}, \quad (8)$$

where the elastic enhancement W_a was estimated by computer simulations. When the χ^2 distribution with the channel degree-of-freedom of ν_a is assumed to $\gamma^2_{\mu a}$, WFC can be evaluated numerically as

$$W_{ab} = (1 + \frac{2\delta_{ab}}{\nu_a}) \int_0^\infty dt \Pi_f \left(1 + \frac{2tT_f}{\nu_f T}\right)^{-\nu_f/2-\delta_{fa}-\delta_{fb}} \quad (9)$$

ν_a were obtained by Monte Carlo simulations.

$$\nu_a = 1.78 + (T_a^{1.212} - 0.78) \exp(-0.228T) \qquad T = \sum_c T_c \quad (10)$$

Projection Operator Technique

Feshbach's projection operators P and $Q = 1 - P$

$$(E - H_{PP})P\Psi = H_{PQ}Q\Psi \tag{11}$$

$$(E - H_{QQ})Q\Psi = H_{QP}P\Psi \tag{12}$$

P space scattering wave function $\psi_a^{(+)}$

$$(E - H_{PP})\psi_a^{(+)} = 0 \tag{13}$$

The unitary and symmetric S matrix is given by

$$S_{ab} = S_{ab}^{(0)} - 2\pi i \left(\psi_a^{(-)} | H_{PQ} \frac{1}{E - \mathcal{H}_{QQ}} H_{QP} | \psi_b^{(+)} \right) \tag{14}$$

Effective Hamiltonian in Q space

$$\mathcal{H}_{QQ} = H_{QQ} + H_{QP} \frac{1}{E^{+} - H_{PP}} H_{PQ} \tag{15}$$

Stochastic S-Matrix Based on GOE

Orthonormal basis of states labeled μ in Q space

$$W_{\mu a} = (\mu|H_{QP}|\psi_a) = W_{a\mu} = W_{a\mu}^* \quad (16)$$

$$\left(\mu|H_{QP}\frac{1}{E^+ - H_{PP}}H_{PQ}|\nu\right) = \Delta_{\mu\nu} - i\pi\sum_c W_{\mu c}W_{c\nu} \simeq -i\pi\sum_c W_{\mu c}W_{c\nu} \quad (17)$$

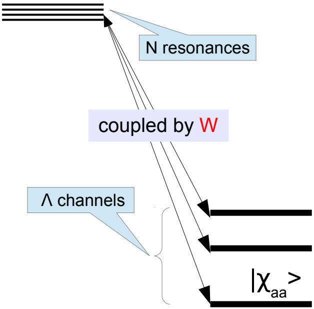
$$(\mu|H_{QQ}|\nu) = H_{\mu\nu} \Rightarrow H_{\mu\nu}^{(\mathrm{GOE})} \quad (18)$$

Scattering matrix that includes GOE

$$S_{ab} = \delta_{ab} - 2i\pi\sum_{\mu\nu} W_{a\mu}(D^{-1})_{\mu\nu}W_{\nu b} \quad (19)$$

$$D_{\mu\nu} = E\delta_{\mu\nu} - H_{\mu\nu}^{(\mathrm{GOE})} + i\pi\sum_c W_{\mu c}W_{c\nu} \quad (20)$$

Compound Nucleus Cross Section



$$S_{ab}^{(\mathrm{GOE})} = \delta_{ab} - 2i\pi \sum_{\mu\nu} W_{a\mu} \left(D^{-1}\right)_{\mu\nu} W_{\nu b} \quad (21)$$

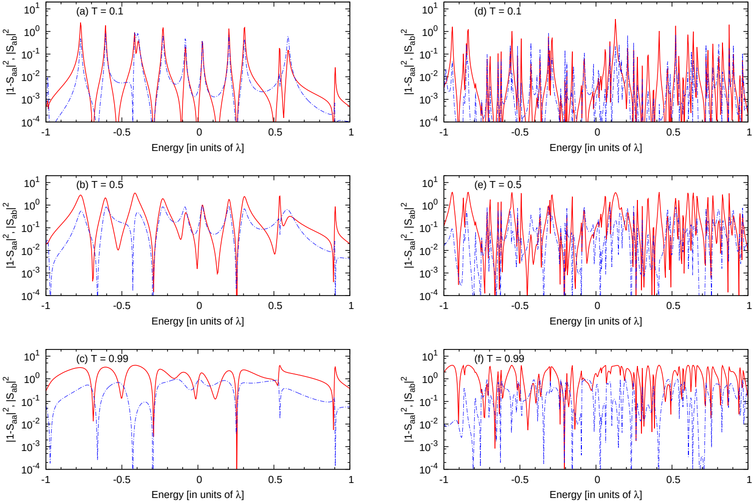
$$D_{\mu\nu} = E\delta_{\mu\nu} - H_{\mu\nu}^{(\mathrm{GOE})} + i\pi \sum_{c} W_{\mu c} W_{c\nu} \quad (22)$$

$$\overline{H_{\mu\nu}^{(\mathrm{GOE})} H_{\rho\sigma}^{(\mathrm{GOE})}} = \frac{\lambda^2}{N} (\delta_{\mu\rho}\delta_{\nu\sigma} + \delta_{\mu\sigma}\delta_{\nu\rho}) \quad (23)$$

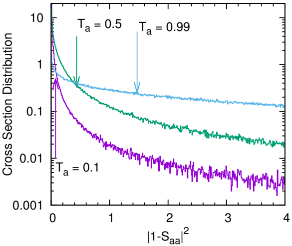
- We assume that the energy average $\langle |S_{aa}|^2 \rangle$ can be replaced by the ensemble average $\overline{|S_{aa}|^2}$ (to be considered later)
- T_a given by eigenvalues of WW^T
- Our model parameters are T_a, N, and Λ

GOE Generated Cross Sections

$N = 20$ and 100, $T_a = 0.1$, 0.5, and 0.99



Ensemble Average Cross Section



Ensemble average over Monte Carlo generated cross sections at the center of GOE

- when $N = 100$, $\Lambda = 2$, and $T_a \simeq 1$
- Hauser-Feshbach $\sigma = T_a^2/(T_a + T_b) = T_a/2 = 0.5$
- while ensemble average $\overline{\sigma}_{aa}^{\mathrm{fl}} = \overline{\sigma}_{aa} - \sigma_{aa}^{\mathrm{SE}} = 0.66$
- $W_{aa} = 1.32$

Analytical expression by Verbaarschot, Weidenmüller, Zirnbauer (1985) reads

$$\overline{\sigma}_{ab}^{\mathrm{fl}} = \frac{T_a T_b}{8} \int_0^\infty d\lambda_1 \int_0^\infty d\lambda_2 \int_0^1 d\lambda\, \mu(\lambda, \lambda_1, \lambda_2) \prod_c \frac{1 - T_c \lambda}{\sqrt{(1 + T_c\lambda_1)(1 + T_c\lambda_2)}} J_{ab}(\lambda, \lambda_1, \lambda_2) \quad (24)$$

which yields $\overline{\sigma}_{aa}^{\mathrm{fl}} = 0.66$.

Why Monte Carlo Approach?

- We know the exact solution for the average cross section. However,
  - the VWZ triple-integral formula is an analytical form of the ensemble average in the limit of $N \rightarrow \infty$
  - It is, unfortunately, inconvenient in realistic cross section calculation cases
    - triple-integral is time-consuming when Λ is large
    - the final state could be in a continuum; individual channel is not well-defined
- MC approach enables us to explore various realistic cases
  - such as photon width distribution for neutron capture reaction
- Various models proposed such as Moldauer's are practically useful for nuclear reaction cross section calculations
- However, these models should be verified by rigorous GOE calculations

GOE Monte Carlo Approach vs Models

Comparison of numerical average $\overline{|S^{\text{fl}}_{aa}|^2}$ with the statistical models

$N = 100,\ \Lambda = 2$

T_a	0.1		0.5		0.99	
	Elastic	Inelastic	Elastic	Inelastic	Elastic	Inelastic
MC simulation	0.0733	0.0261	0.351	0.149	0.660	0.330
VWZ	0.0734	0.0260	0.351	0.148	0.661	0.330
Hauser-Feshbach	0.0500	0.0500	0.250	0.250	0.495	0.495
KKM	0.0662	0.0332	0.333	0.167	0.660	0.330
HRTW	0.0737	0.0257	0.352	0.147	0.661	0.330
Moldauer	0.0734	0.0260	0.349	0.150	0.665	0.325
Ernebjerg-Herman	0.0742	0.0252	0.366	0.134	0.681	0.310
Kawano-Talou	0.0735	0.0259	0.351	0.148	0.661	0.330

Hauser-Feshbach (1952), Kawai-Kerman-MacVoy (1973), HRTW (1980), Moldauer (1980), Ernebjerg-Herman (2004), and Kawano-Talou (2014)

VWZ agrees even for small N!

Ensemble Average and Energy Average

- Ensemble average in the limit $N \to \infty$
  - analytical form given by the VWZ triple integral formula
  - it can be performed by MC simulation
- While, we wan to know the energy-average cross section
- Do these averages agree?

$$\int_{-\infty}^{+\infty} w(E_0, E, I) S(E) dE = \overline{S}(E_0), \qquad w(E_0, E, I) = \frac{I}{\pi} \frac{1}{(E - E_0)^2 + I^2} \tag{25}$$

where width I specified in units of d/π, or weaker condition

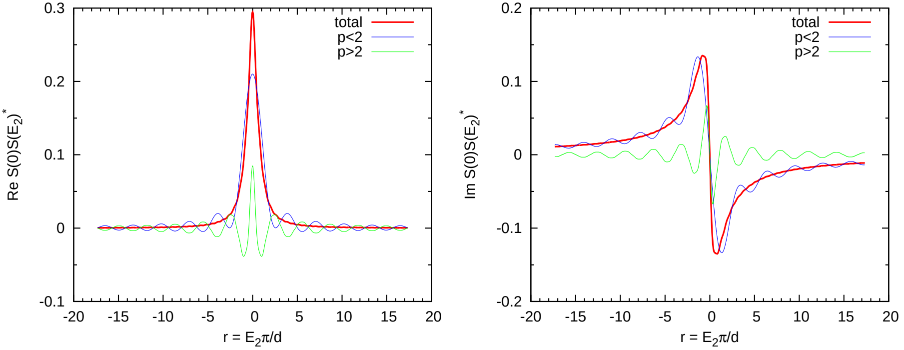
$$\overline{\left| \langle S \rangle - \overline{S} \right|^2} = 0 \tag{26}$$

which is equivalent to

$$\int_{-\infty}^{+\infty} dE_1 w(E_0, E_1, I) \int_{-\infty}^{+\infty} dE_2 w(E_0, E_2, I) \overline{S^{\rm fl}(E_1) S^{\rm fl *}(E_2)} = 0 \tag{27}$$

Two-Point Function, $\overline{S^{\mathrm{fl}} S^{\mathrm{fl}*}}$

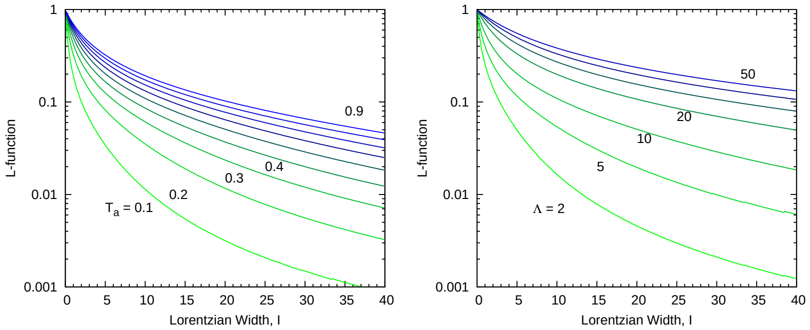
$$
\begin{aligned}
&\overline{S^{\mathrm{fl}}_{ab}(E_1) S^{\mathrm{fl}*}_{cd}(E_2)} \\
= \quad & \frac{1}{8} \int_0^\infty d\lambda_1 \int_0^\infty d\lambda_2 \int_0^1 d\lambda\, \mu(\lambda, \lambda_1, \lambda_2) e^{-ir(\lambda_1 + \lambda_2 + 2\lambda)} \prod_c \frac{1 - T_c \lambda}{\sqrt{(1 + T_c \lambda_1)(1 + T_c \lambda_2)}} J(\lambda, \lambda_1, \lambda_2)
\end{aligned}
$$



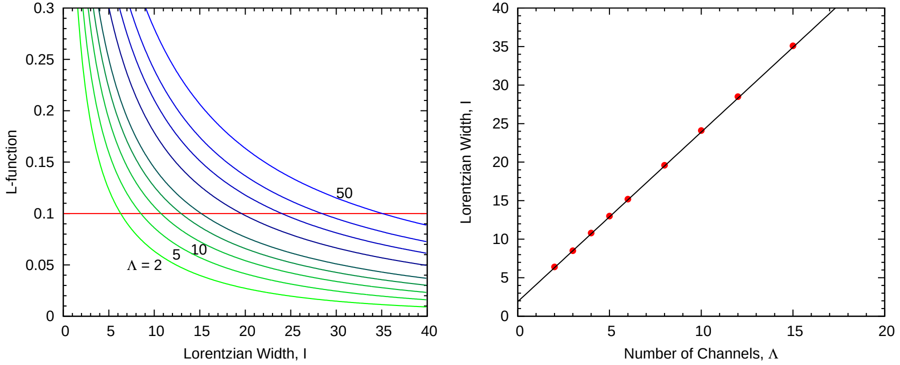
Definition of L-Function

$$L(T_a, \Lambda, I) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} w(E_1, 0, I) w(E_2, 0, I) R(E_2 - E_1; T_a, \Lambda)\, dE_1 dE_2 \tag{28}$$

$$R(E_2 - E_1; T_a, \Lambda) = \frac{\Re \left\{ \overline{S^{\text{fl}} S^{\text{fl}*}}(|E_2 - E_1|) \right\}}{\overline{|S|^2}(0)} \tag{29}$$



Required Lorentzian Average Width

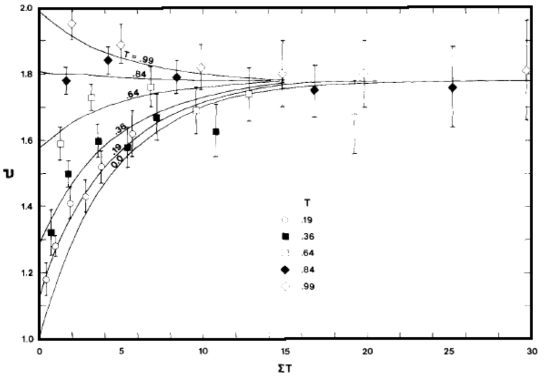


$I = 100$ corresponds to $100d/\pi \sim 30d$.
L-function will be sufficiently small when the energy-averaging interval is one or two orders of magnitude larger than the average resonance spacing d.

Strong Absorption Limit

$$\langle\sigma_{ab}\rangle = \frac{(1+\delta_{ab})T_a T_b}{\sum_c T_c} + \dots\ . \quad (30)$$

- Almost al models predict the elastic enhancement factor W_a of two, when $\sum_a T_a \gg 1$
- While, Moldauer's model gives the asymptotic value of $\nu_a = 1.78$.

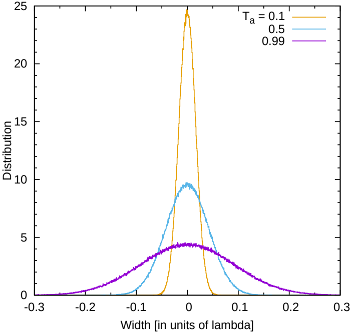


P.A. Moldauer, NPA **344**, 185 (1980)

$$\nu_a = \frac{2}{W_a - 1}, 1 \le \nu_a \le 2, \quad 2 \le W_a \le 3 \qquad (31)$$

Moldauer obtained this result by performing a similar Monte Carlo simulation based on GOE.

Decay Width Distribution



$\tilde{W}$ for the case $N = 100$, $\Lambda = 2$, and three values of $T_a = 0.1$, 0.5, and 0.99

Using the eigenvalue of $H^{(\mathrm{GOE})}$, E_σ

$$K_{ab}(E) = \sum_\sigma \frac{\tilde{W}_{a\sigma}\tilde{W}_{\sigma b}}{E - E_\sigma} , \quad (32)$$

$$\tilde{W}_{\sigma a} = \sqrt{\pi} \sum_\nu O_{\sigma\nu} W_{\nu a} , \quad (33)$$

$$O^{-1} H^{(\mathrm{GOE})} O = \mathrm{diag}(E_\sigma) , \quad (34)$$

In this form the width amplitudes $\tilde{W}_{a\sigma} = \sqrt{\pi}\gamma_{a\sigma}$ are uncorrelated Gaussian-distributed random variables with zero mean values and the standard deviation.

Emulating Moldauer's MC Method

Moldauer's K matrix can be written as

$$K^{\mathrm{M}}_{ab}(E) = \delta_{ab}\Re K^0_a + \sum_\sigma \frac{w_{a\sigma} w_{\sigma b}}{E - E_\sigma} \tag{35}$$

where the elements K^0_a of the elastic background matrix and the variances of the amplitudes w are determined by the energy-averaged S matrix.

$$K^0 = i\frac{1 - S^{(\mathrm{GOE})}(E + iI)}{1 + S^{(\mathrm{GOE})}(E + iI)} \tag{36}$$

Ensemble average of Eq. (35)

- Generate S^{GOE}, then convert it into K
- $K^0 = K(E + iI)$ and

$$\sigma^2_a = 2\pi\overline{\gamma^2_a} = \frac{d}{\pi}\left|\Im K^0_a\right|$$

- The decay amplitudes sampled from Gaussians with widths σ_a, independently of the GOE eigenvalues.

Moldauer's Channel Degree-of-Freedom

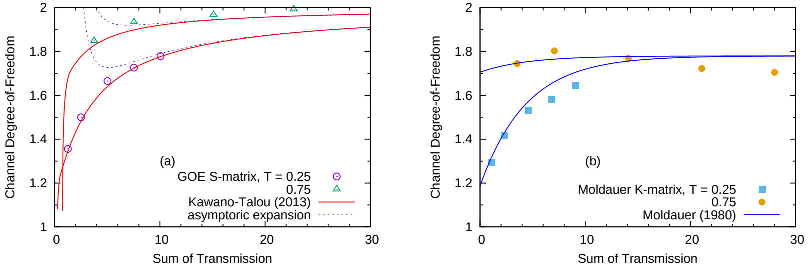
$$\nu_a(\text{Moldauer}) = 1.78 + (T_a^{1.212} - 0.78)\exp(-0.228T) \quad (37)$$

$$\nu_a(\text{LANL}) = 2 - \frac{1}{1 + \alpha \frac{T_a + T}{1 - T_a}} \quad (38)$$

$$\alpha = (0.0288T_a + 0.246)\,(1 + 2.5T_a(1 - T_a)\exp(-2T)) \quad (39)$$

standard GOE

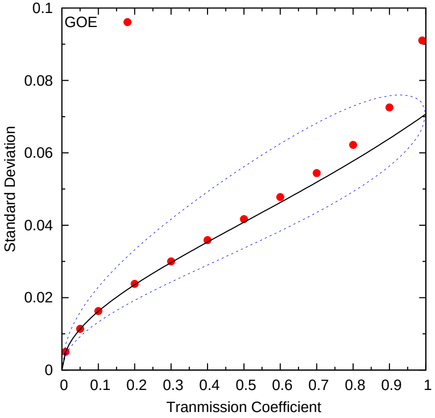
Moldauer

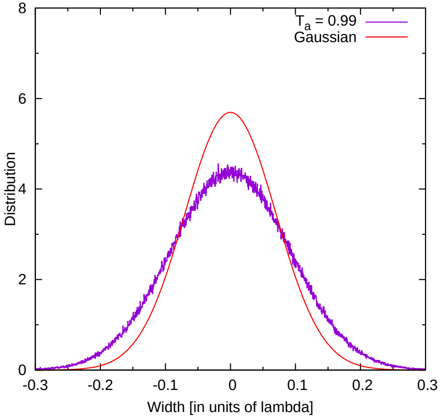


Moldauer's Decay Width Distribution

In the case of Moldauer's simulation, the width will be

$$\sigma_a^2 = \frac{d}{\pi} \left| \Im K_a^0 \right| = \frac{d}{\pi} \frac{T_a}{2 - T_a} \tag{40}$$





Inclusion of Direct Channel in Hauser-Feshbach

Cross section calculations for strongly deformed systems

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

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

  - $\sum_a T_a$ gives correct compound formation cross section
  - HF performed in the direct-eliminated cross-section space
- Engelbrecht-Weidenmüller (EW) transformation
  - diagonalize S-matrix to eliminate the direct channels
  - HF performed in the diagonal channel space
  - transform back to the cross section space
- Theory of Kawai-Kerman-McVoy (KKM)
  - correct at the limit of channel degree of freedom $\nu = 2.0$

Implementation of Direct Channel in Stochastic S-Matrix

Unitary background matrix $S_{ab}^{(0)}$

$$S_{ab} = S_{ab}^{(0)} - i \sum_{\mu} \frac{\gamma_{\mu a}\gamma_{\mu b}}{E - E_\mu - (i/2)\Gamma_\mu} \tag{41}$$

Since generating a unitary matrix including off-diagonal elements is cumbersome, we employ a K-matrix method.

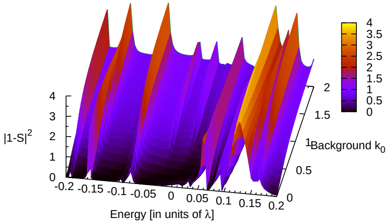
$$K_{ab}(E) = K^{(0)} + \sum_{\mu} \frac{\tilde{W}_{a\mu}\tilde{W}_{\mu b}}{E - E_\mu}. \tag{42}$$

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

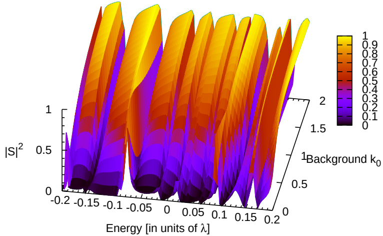
Generated Elastic/Inelastic Cross Sections

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

Elastic



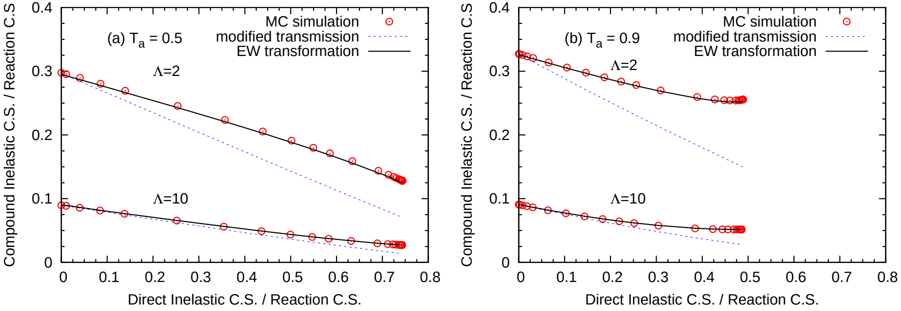
Inelastic



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 largely underestimates the compound inelastic scattering cross sections.

Concluding Remarks

We have investigated the statistical properties of the scattering matrix containing a GOE Hamiltonian in the propagator.

- For all parameter values studied, the numerical average of MC-generated cross sections coincides with the result of the VWZ triple-integral formula.
- Energy average and ensemble average agree reasonably well when I is one or two orders of magnitude larger than d
- In the strong-absorption limit, the channel degree-of-freedom ν_a is 2.
- We find that the direct reaction increases the inelastic cross sections while the elastic cross section is reduced

Work performed with P. Talou (LANL) and H.A. Weidenmüller (MPI)