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Recent progress of the nuclear reaction calculations at LANL

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What is Hauser-Feshbach-Wolfenstein Theory?

- **Compound nuclear reaction in terms of penetrability**
  - Cross section when many levels are excited in a Compound Nucleus (CN)
  - Statistical decay of CN determined by the average decay width
  - Energy-average cross sections can be factorized by penetration factors for each channel; Γ is replaced by the penetrability P (transmission T)
    - Hauser-Feshbach does not mention if T is calculated by optical model

$$\langle \sigma_{ab} \rangle = \frac{2\pi}{D} \frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\sum \langle \Gamma \rangle}$$

$$\langle \Gamma_a \rangle = \frac{D}{2\pi} T_a$$

$$\langle \sigma_{ab} \rangle = \frac{T_a T_b}{\sum T}$$

- **Problem in the Hauser-Feshbach theory**
  - Average of ratio is different from ratio of averages due to distribution (width fluctuation)
  - Incoming wave exists in the elastic channel (elastic enhancement)
  - Width fluctuation correction factor introduced to fix this problem

$$\frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\sum \langle \Gamma \rangle} \neq \left\langle \frac{\Gamma_a \Gamma_b}{\sum \Gamma} \right\rangle$$

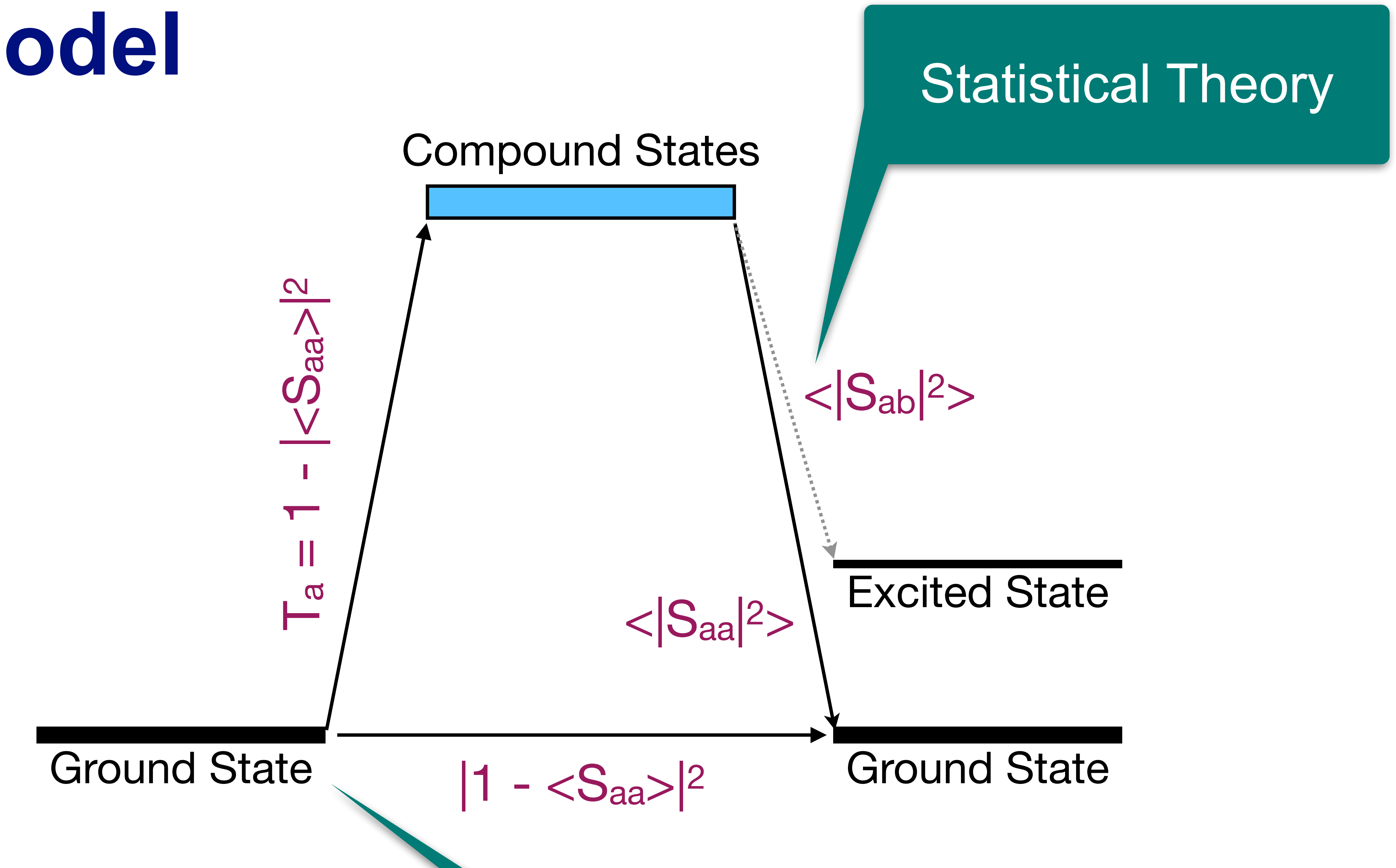
$$\sigma_{ab} = \left| \delta_{ab} - S_{ab} \right|^2$$

$$\langle \sigma_{ab} \rangle = \frac{T_a T_b}{\sum T} W_{ab}$$

Transmission Coefficients by Optical Model

- **Energy average cross section**

$$\begin{aligned}\langle \sigma_{ab} \rangle &= \langle |\delta_{ab} - S_{ab}|^2 \rangle \\ &= |\delta_{ab} - \langle S_{ab} \rangle|^2 + \langle |S_{ab}^{\mathrm{CN}}|^2 \rangle \\ &= \sigma_{ab}^{\mathrm{DI}} + \langle \sigma_{ab}^{\mathrm{CN}} \rangle\end{aligned}$$



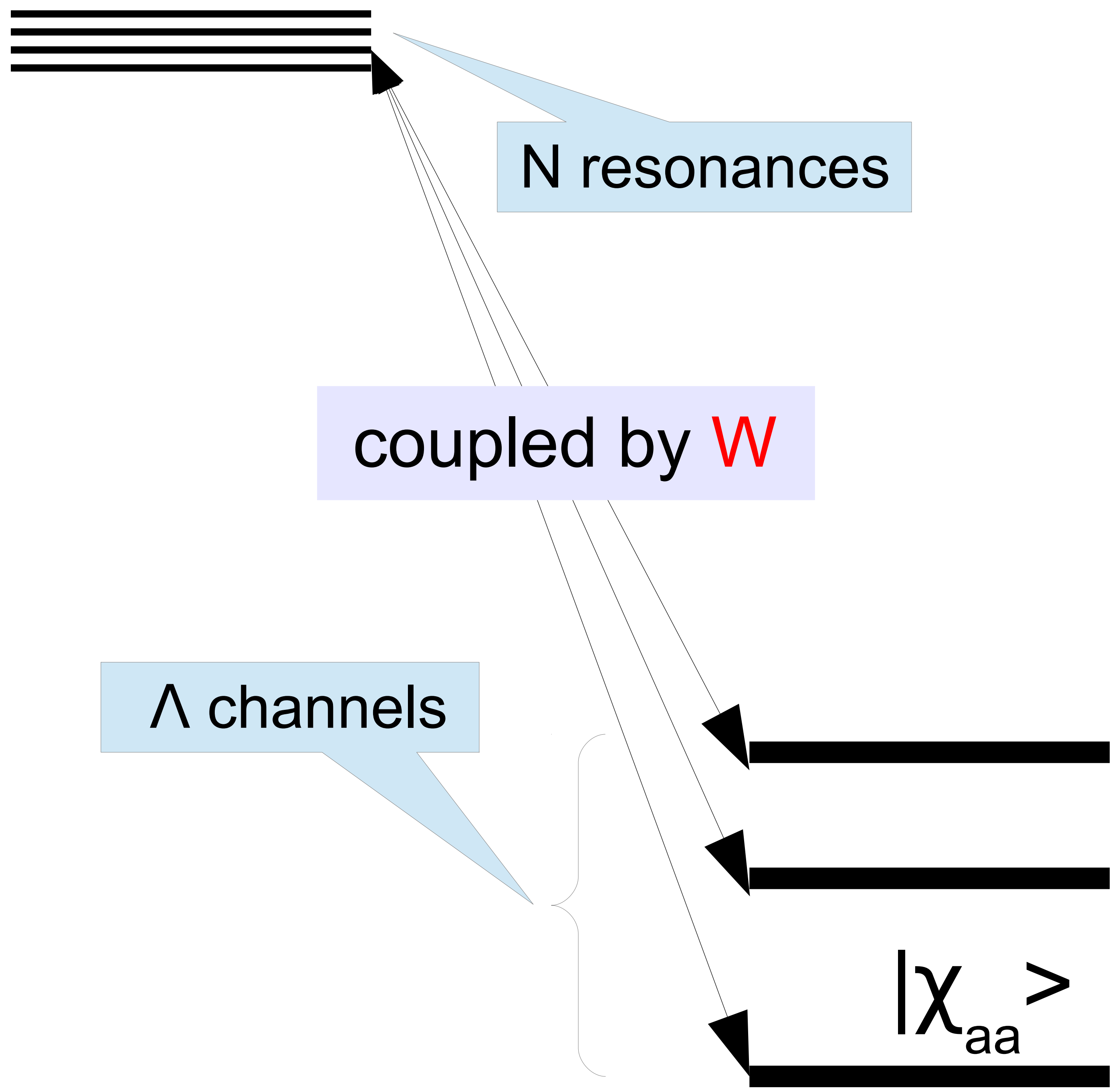
- **Optical model gives energy average S-matrix**

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

  - from which we can calculate $|1 - \langle S_{aa} \rangle|^2$ (direct / shape elastic)
  - but not $\langle | S_{aa} |^2 \rangle$ (compound elastic)

- **Statistical model is to express the CN part by Transmission Coefficient**

Stochastic S-matrix (K-matrix) based on GOE



GOE S-Matrix

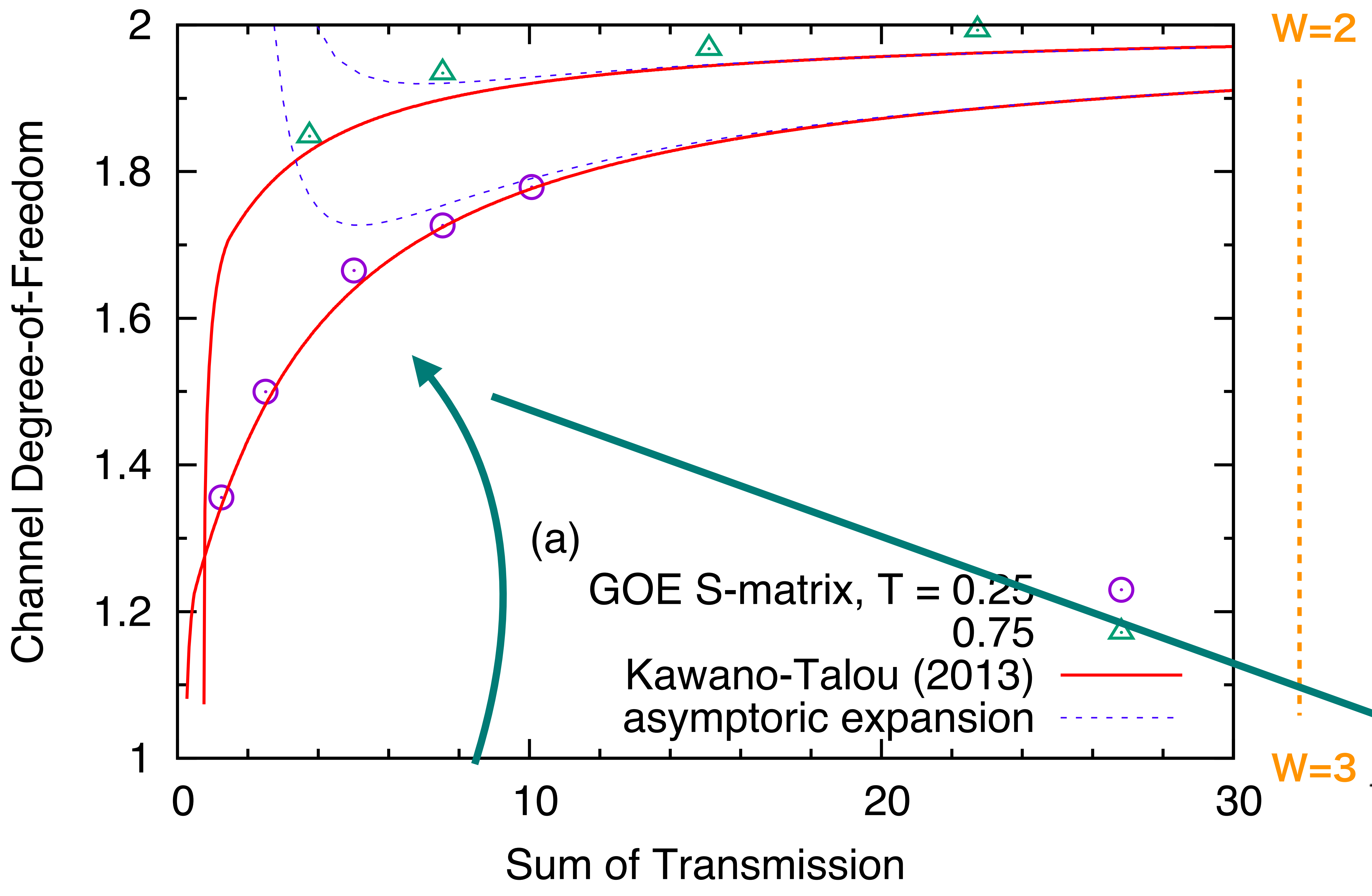
$$S_{ab}^{(\mathrm{GOE})} = \delta_{ab} - 2i\pi \sum_{\mu\nu} W_{a\mu} \left(D^{-1}\right)_{\mu\nu} W_{\nu b}$$

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

$$\overline{H_{\mu\nu}^{(\mathrm{GOE})} H_{\rho\sigma}^{(\mathrm{GOE})}} = \frac{1}{N}\left(\delta_{\mu\rho}\delta_{\nu\sigma} + \delta_{\mu\sigma}\delta_{\nu\rho}\right)$$

- Perform ensemble average $\overline{|S_{aa}|^2}$ by realization of $H^{(\mathrm{GOE})}$
- T_a given by eigenvalues of WW^T
- Model parameters are T_a (transmission), N (number of resonance), and Λ (channel)

Width Fluctuation Correction Factor by GOE Monte Carlo Simulation



Elastic enhancement factor, and Channel degree-of-freedom

- **Realization of GOE**
  - for various T and different number of channels

$$T = \sum_c T_c$$

  - parameterize elastic enhancement (or channel degree-of-freedom) by *T*
- **Width fluctuation for each channel**

$$W_{ab} = \left(1 + \frac{2\delta_{ab}}{\nu_a}\right) \int_0^\infty \frac{dt}{F_a(t)F_b(t)\prod_k F_k(t)^{\nu_k/2}}$$

$$F_k(t) = 1 + \frac{2}{\nu_k}\frac{T_k}{\sum_c T_c}t$$

Kawano, Talou, Weidenmuller PRC92, 044617 (2015)

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Engelbrecht-Weidenmuller Transformation for CC S-matrix

- **Width fluctuation calculation requires single-channel transmission T_a**
  - Unitary transformation of Satchler's penetration matrix, P

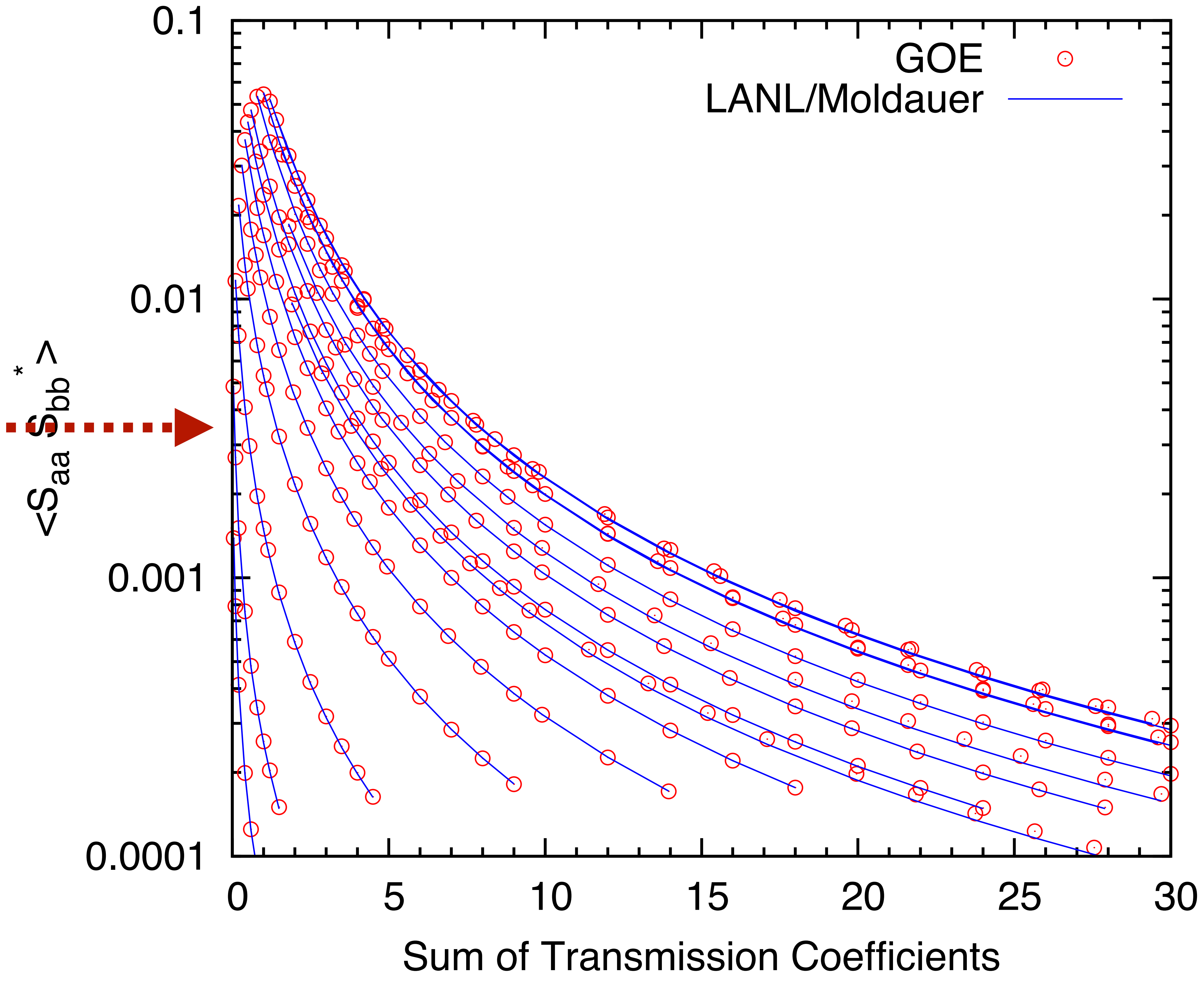
use this for transmission coefficients

$$P_{ab} = \delta_{ab} - \sum_c S_{ac} S^*_{bc} \qquad (UPU^\dagger)_{\alpha\beta} = \delta_{\alpha\beta} p_\alpha, \quad 0 \le p_\alpha \le 1$$

$$\sigma_{ab} = \sum_\alpha |U_{\alpha a}|^2 |U_{\alpha b}|^2 \sigma_{\alpha\alpha} + \sum_{\alpha\neq\beta} U^*_{\alpha a} U^*_{\beta b} (U_{\alpha a} U_{\beta b} + U_{\beta a} U_{\alpha b}) \sigma_{\alpha\beta} + \sum_{\alpha\neq\beta} U^*_{\alpha a} U^*_{\alpha b} U_{\beta a} U_{\beta b} \left\langle \tilde{S}_{\alpha\alpha} \tilde{S}^*_{\beta\beta} \right\rangle$$

$$\overline{\tilde{S}_{\alpha\alpha} \tilde{S}^*_{\beta\beta}} \simeq e^{i(\phi_\alpha - \phi_\beta)} \left(\frac{2}{\nu_\alpha} - 1 \right)^{1/2} \left(\frac{2}{\nu_\beta} - 1 \right)^{1/2} \sigma_{\alpha\beta}$$

Width fluctuation corrected cross section in the diagonal space



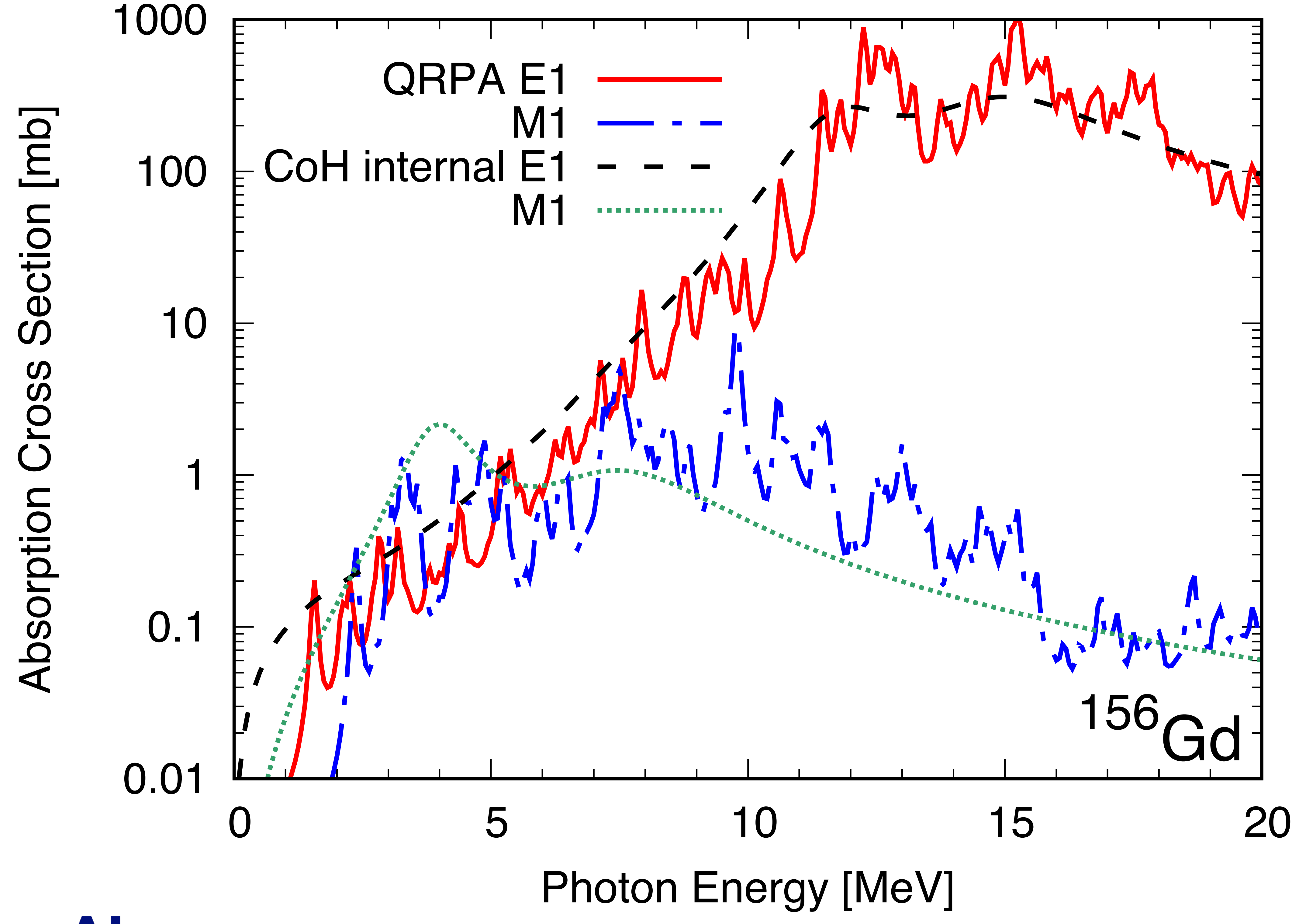
Kawano et al, PRC94, 014612 (2016)

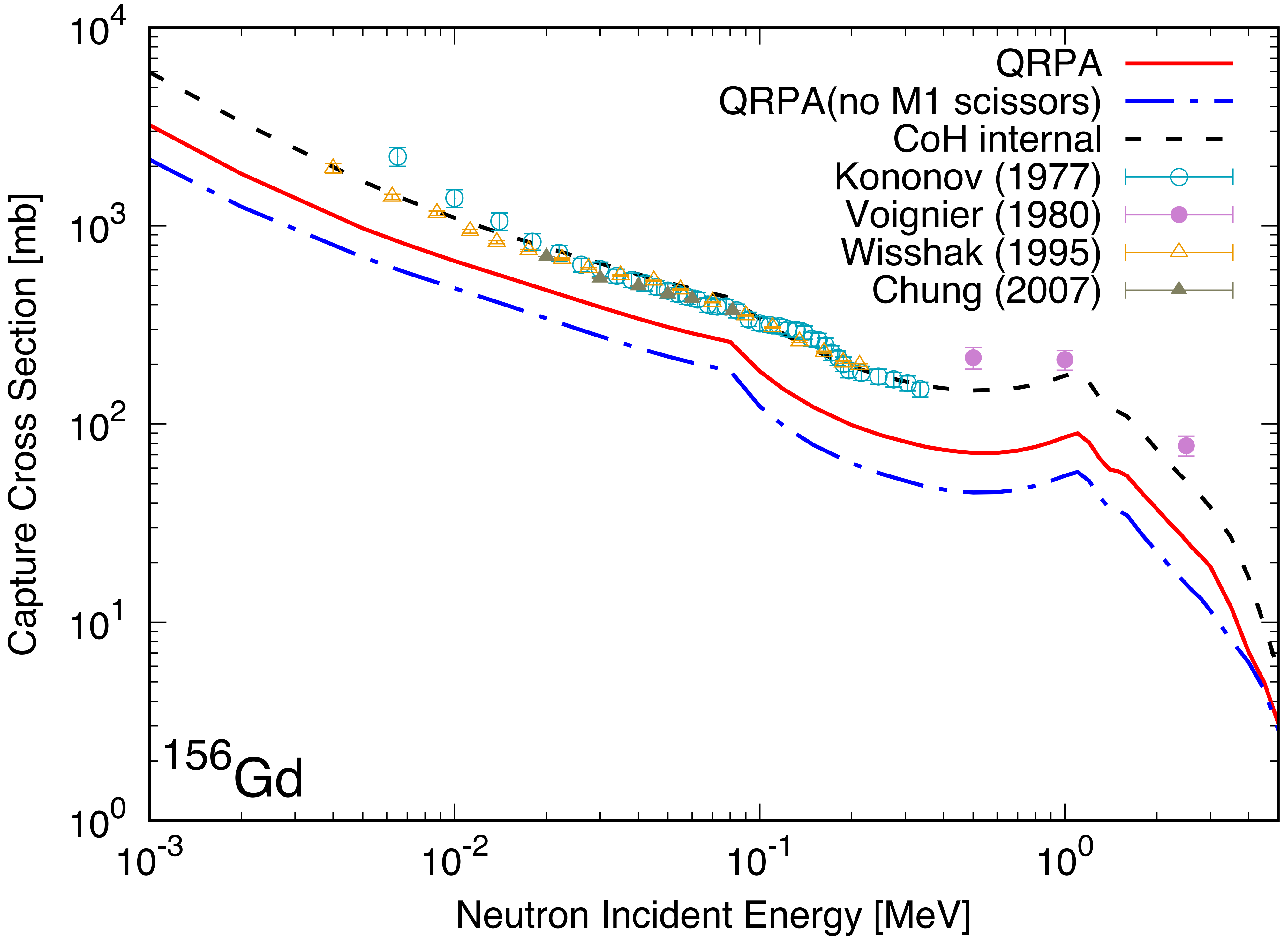
Beyond Optical Model + Hauser-Feshbach Theory

- **Photon channel**
  - Neutron capture reaction as an inverse process of photo-nuclear reaction
  - Transmission coefficient of photon is calculated by the photo-absorption cross section
    - Macroscopic Giant (Dipole etc) Resonances
    - Microscopic models - QRPA or FAM approaches
- **Fission channel**
  - Fission is not a simple inverse process of heavy ion fusion
  - Calculation of fission transmission coefficient strongly model dependent
- **Direct reactions**
  - Coupled-channels, DWBA, Direct/SemiDirect capture, composite particle interactions, ...
- **Pre-equilibrium emission**
  - Exciton model widely used, but no quantum mechanical effects
  - MSC/MSD calculation still expensive

Non-Iterative Finite Amplitude Method (Photons and Pre-Equilibrium)

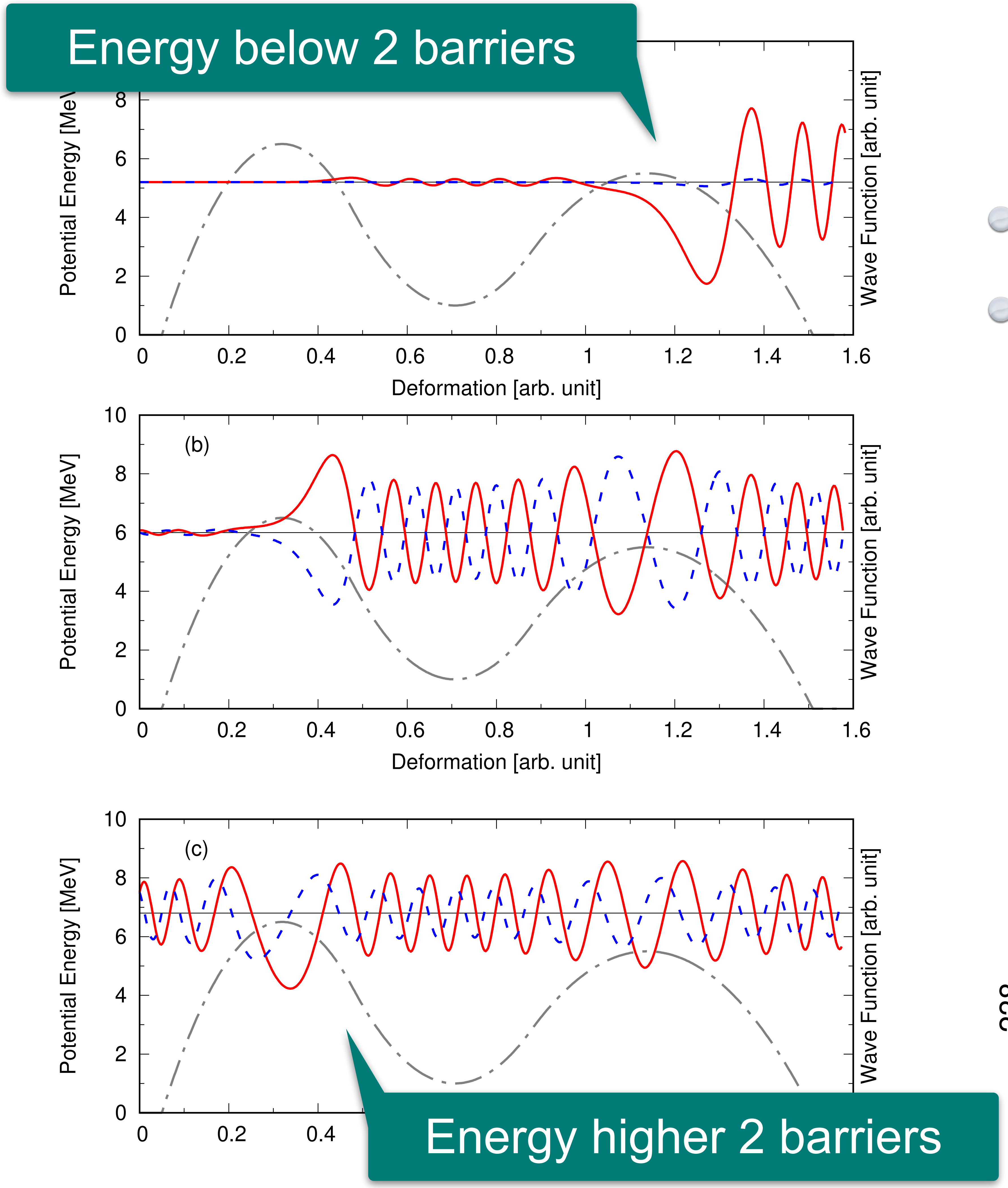
- **Fast calculation of QRPA developed by H. Sasaki**
  - Iteration procedure not required
  - So far applied to photo-absorption (gamma-ray transmission coefficient)
  - Neutron inelastic scattering under development
    - study spin-transfer in the pre-equilibrium process





H. Sasaki, PRC107, 054312 (2023)

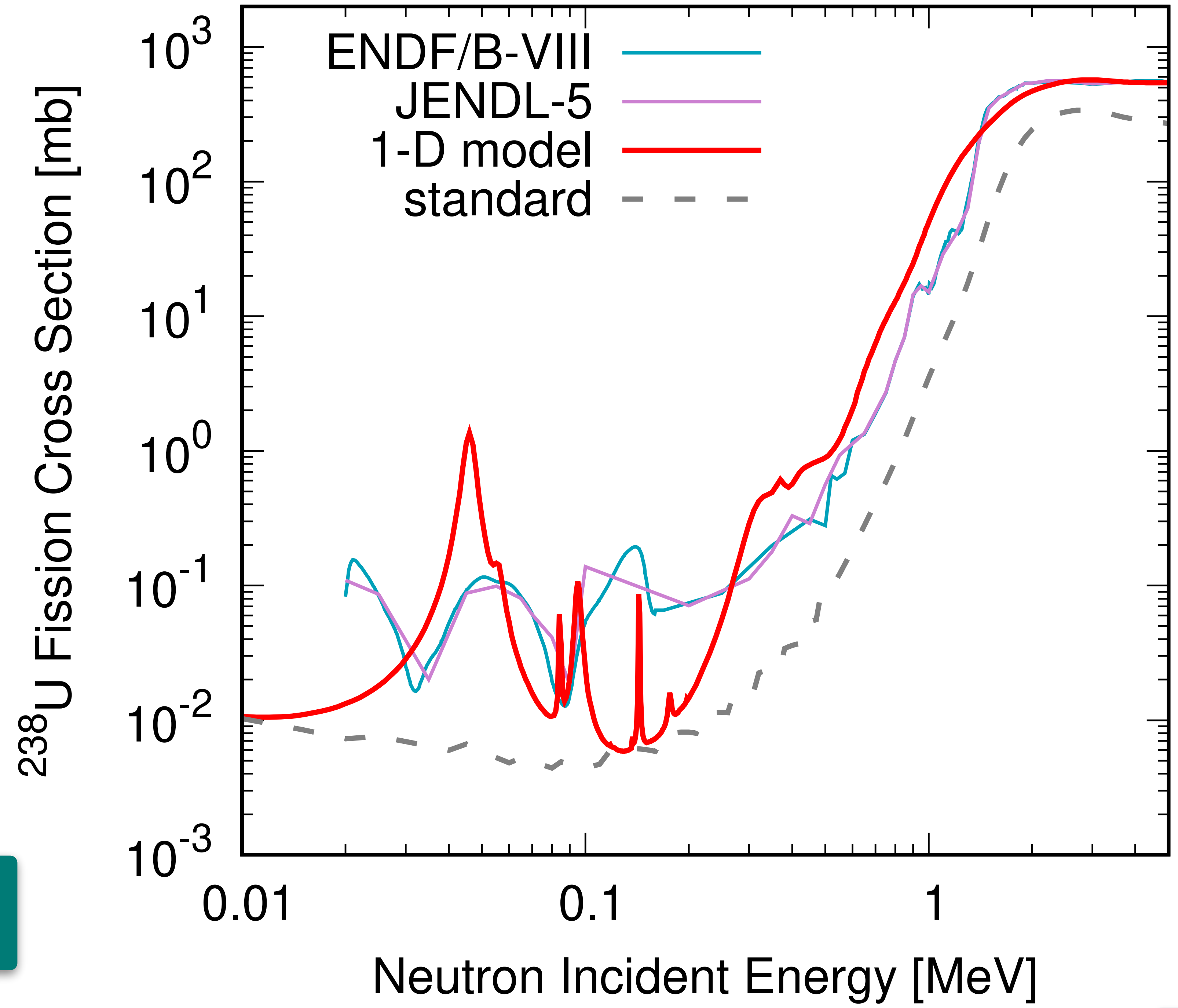
One-Dimensional Penetration Calculation for Fission

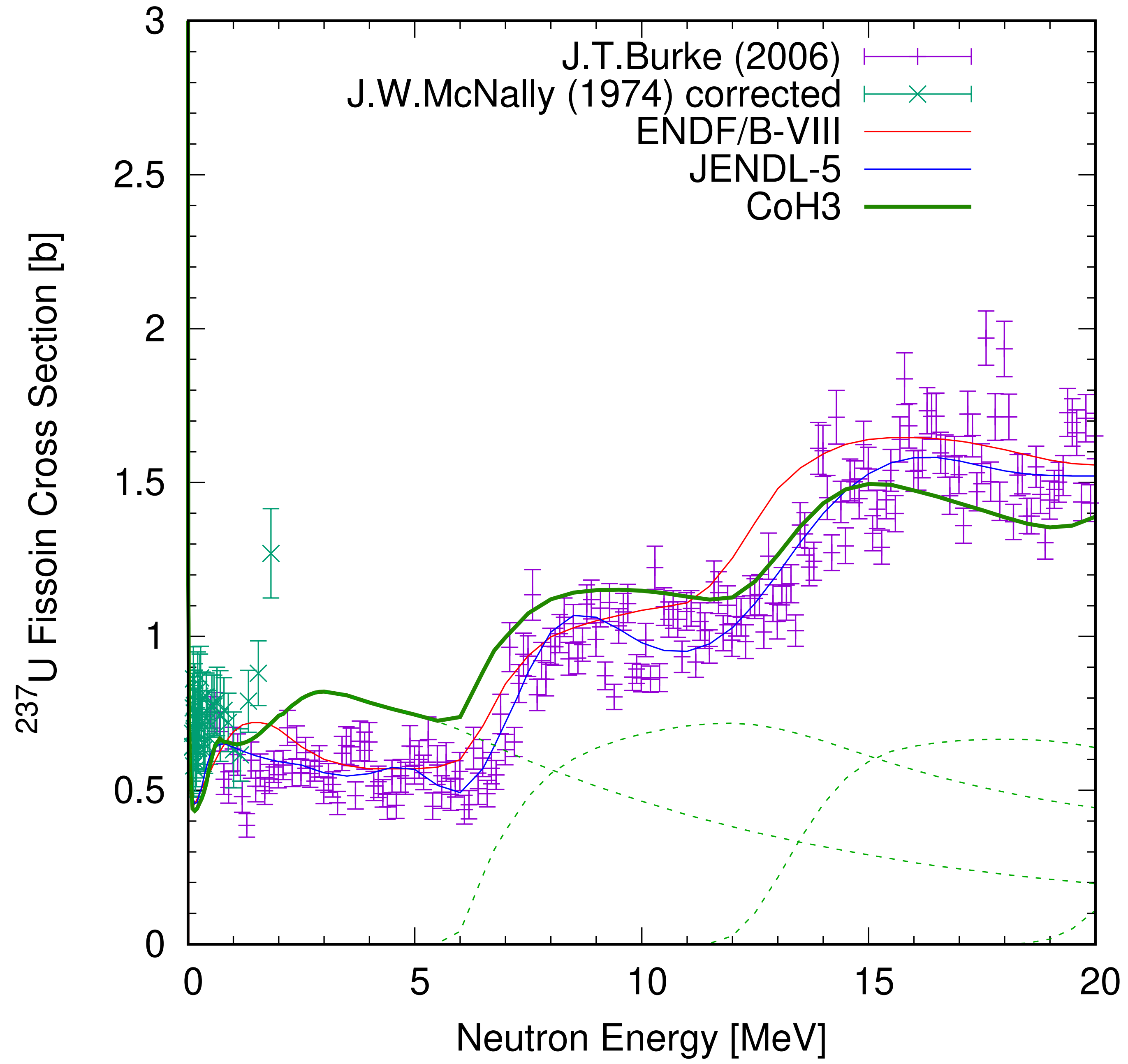


- **Solving Schrodinger equation to calculate fission penetration**

$$\frac{d^2}{dx^2}\phi(x) + \frac{2\mu}{\hbar^2}\left\{E - (V(x) + iW(x))\right\}\phi(x) = 0$$

- can be performed for arbitrary shape of potential energy
- might be extended to higher dimensions





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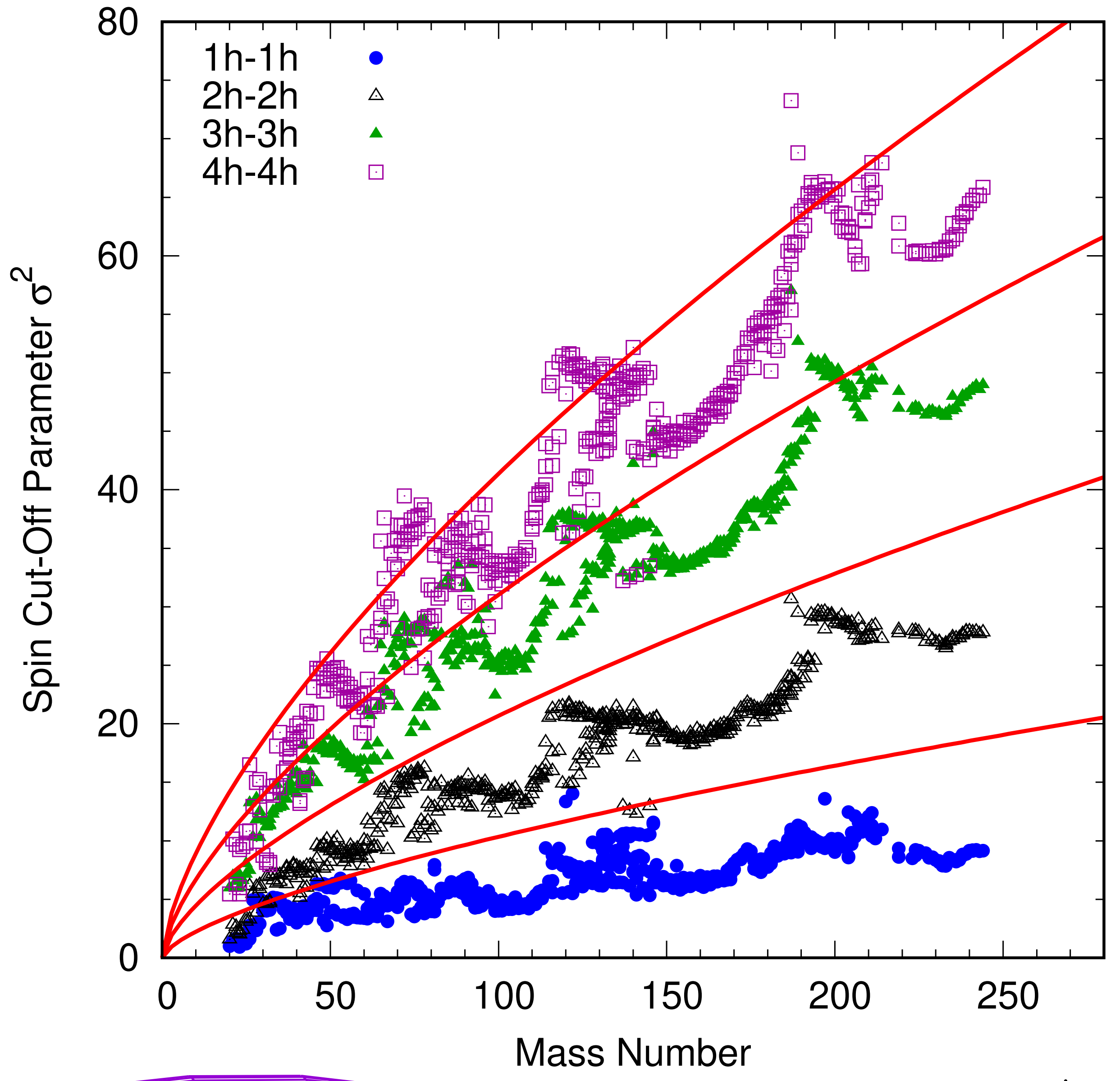
Kawano, Talou, Hilaire PRC 107, 044610 (2024)

Number of Configurations in Pre-Equilibrium — Partial Level Density

- **1-Step MSD double differential cross section**

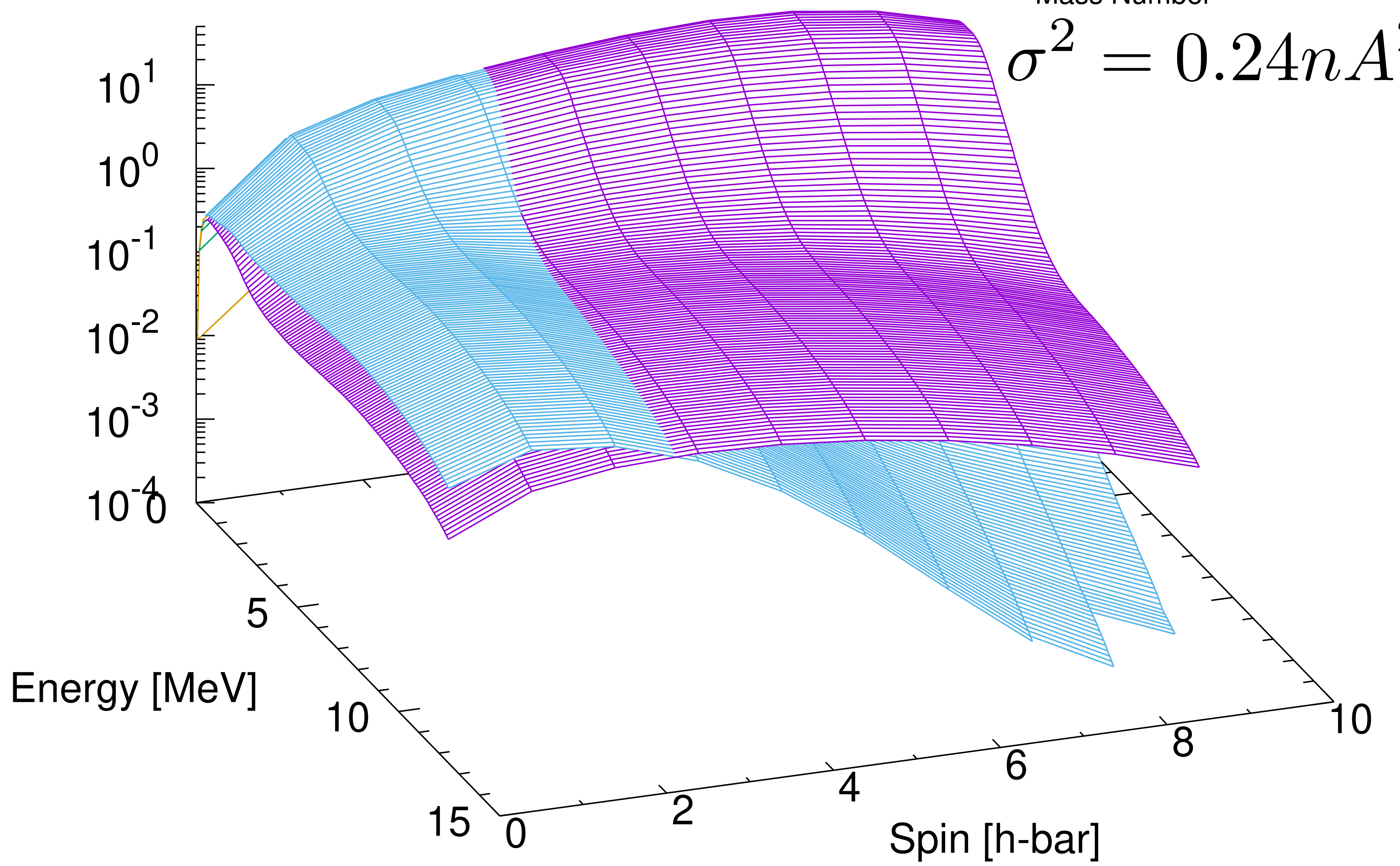
$$\left(\frac{d^2\sigma}{d\Omega dE}\right)_m = \sum_\mu |\langle \chi^{(-)} u_{m\mu} | \mathcal{V} | \chi^{(+)} u_0 \rangle|^2 \rho_{m\mu}(E_x)$$

  - microscopic approach (FAM) under development
- **Combinatorial calculation for intrinsic level density**
  - single-particle spectra generated in folding Yukawa potential
  - J-dependence is almost pure Fermi gas spin distribution



$$\sigma^2 = 0.24nA^{2/3}$$

- **Recent experiments**
  - gamma-ray production data suggest that states are strongly suppressed by the PE degree-of-freedom
  - 0.04 required instead of 0.24 when classical exciton model employed
  - spin-dependence in the two-body matrix elements is missing in the exciton model

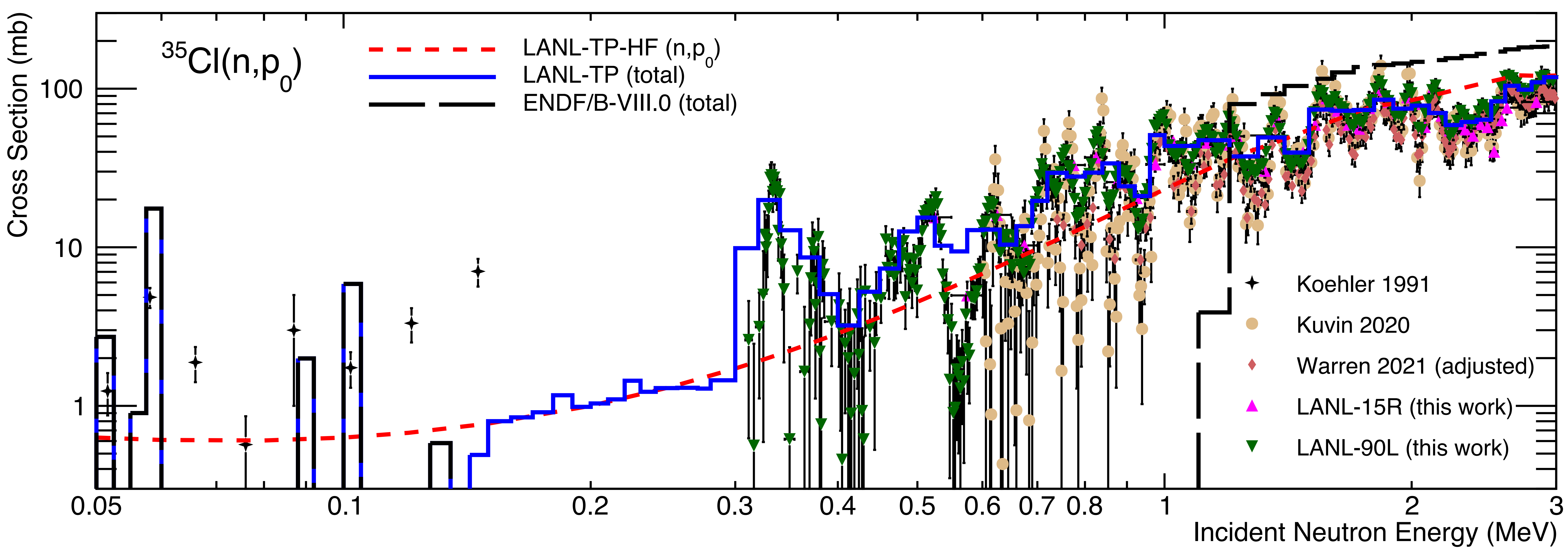


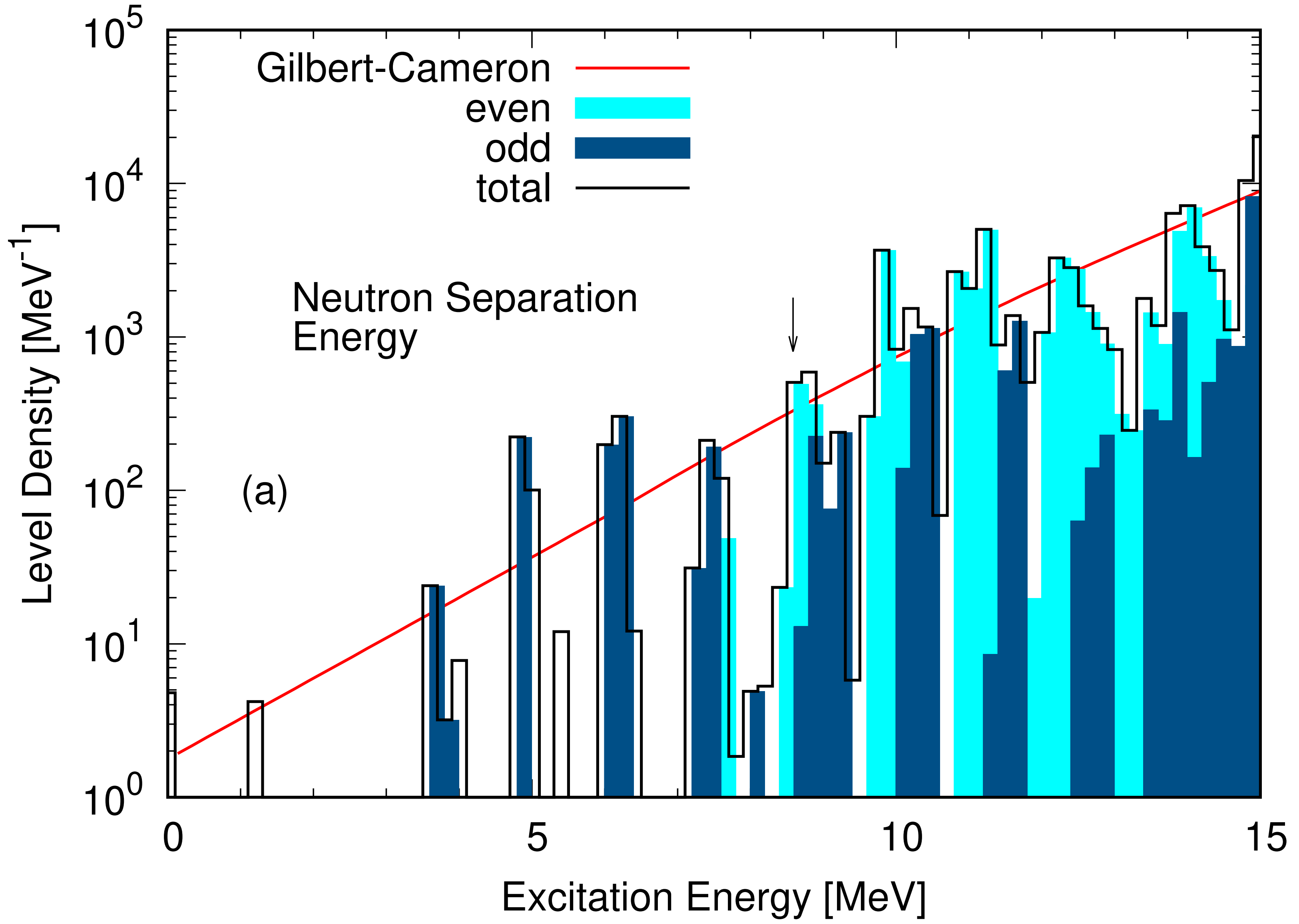
Non-Statistical Behavior in CN Reaction

- **Reaction cross section affected by the distribution of resonances near the CN state**
  - Optical model has no CN state information

$$-\frac{d^2}{dr^2}\phi(r) + \left\{ \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}[V(r) + iW(r)] - k^2 \right\} \phi(r) = 0$$

  - while cross sections often fluctuate strongly due to non-uniform distribution of CN states





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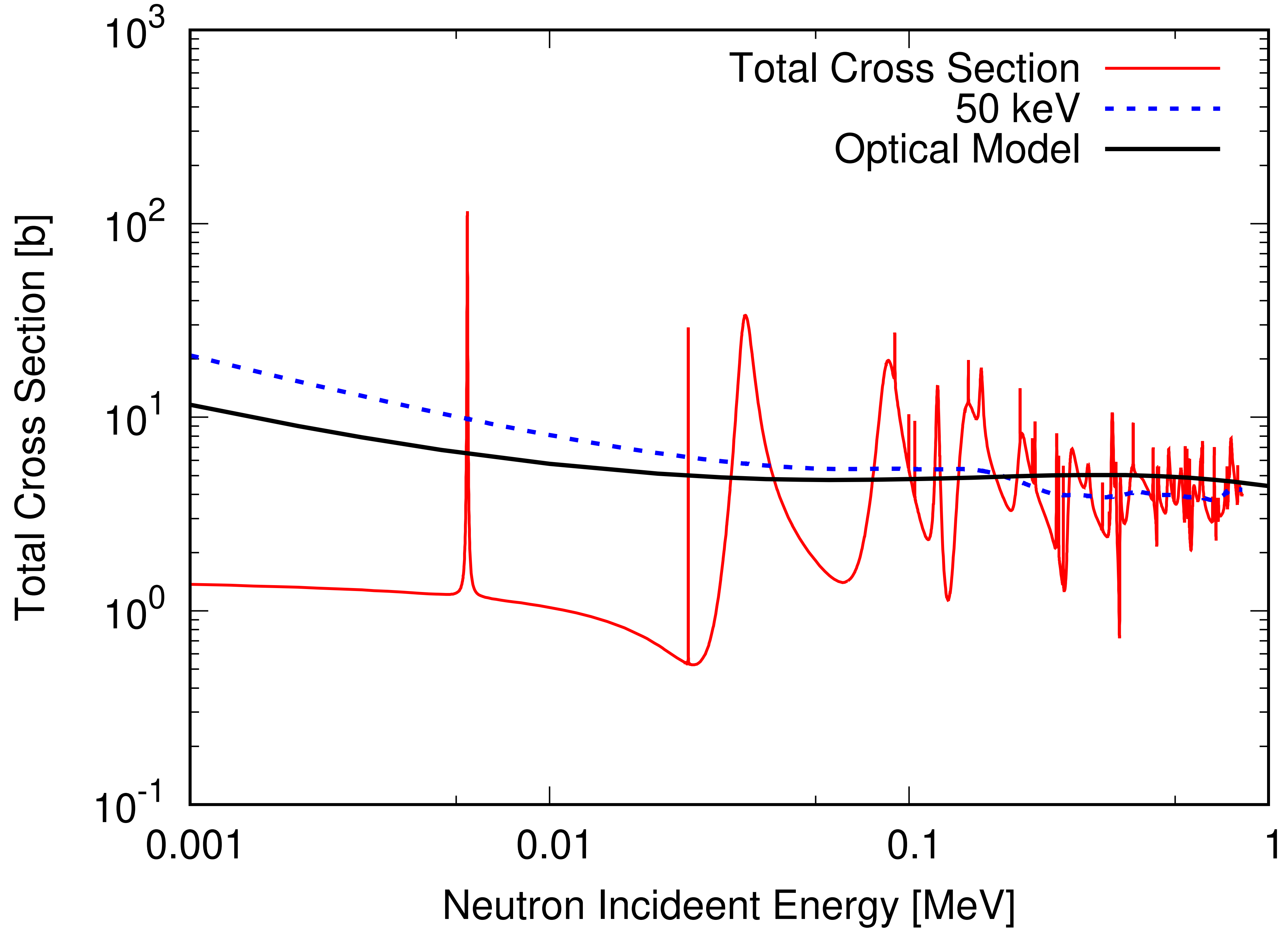
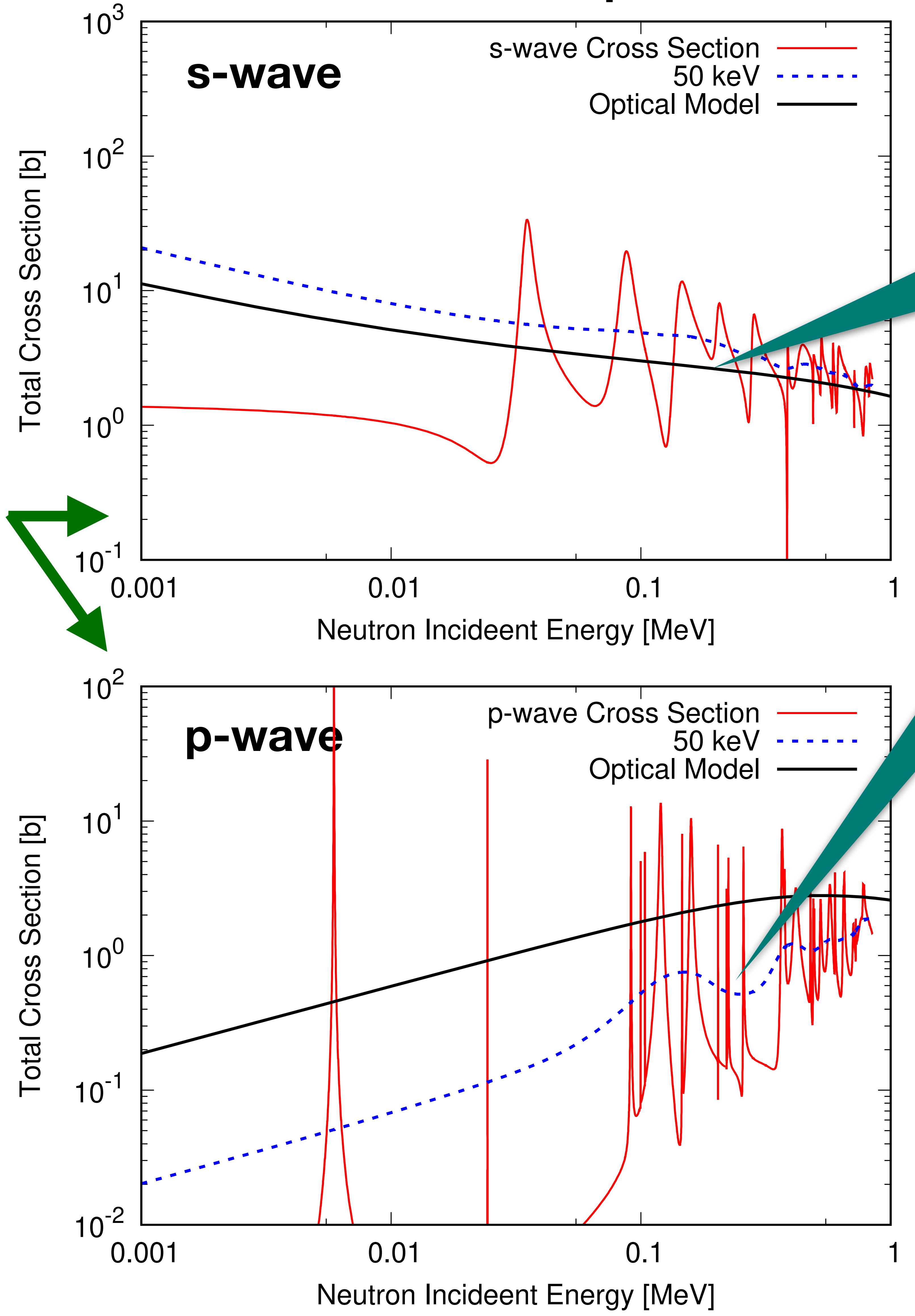
Hanselman et al, PRC110, 024609(2024)

Relation between Resonances and Optical Model



Partial Wave Decomposition



The s-wave strength function might be too low

This implies there are less number of p-wave resonances, which hinders the penetration of L=1 component

If both of the partial waves cannot be reproduced simultaneously, the standard optical model does not capture this nuclear structure effect (L-dependence)

- **Lorentzian average can be evaluated in the complex plane**
  - Energy average R-matrix

$$R(E+iI)=\overline{R}(E)\rightarrow\overline{S}(E)\simeq S^{\mathrm{OM}}(E)$$

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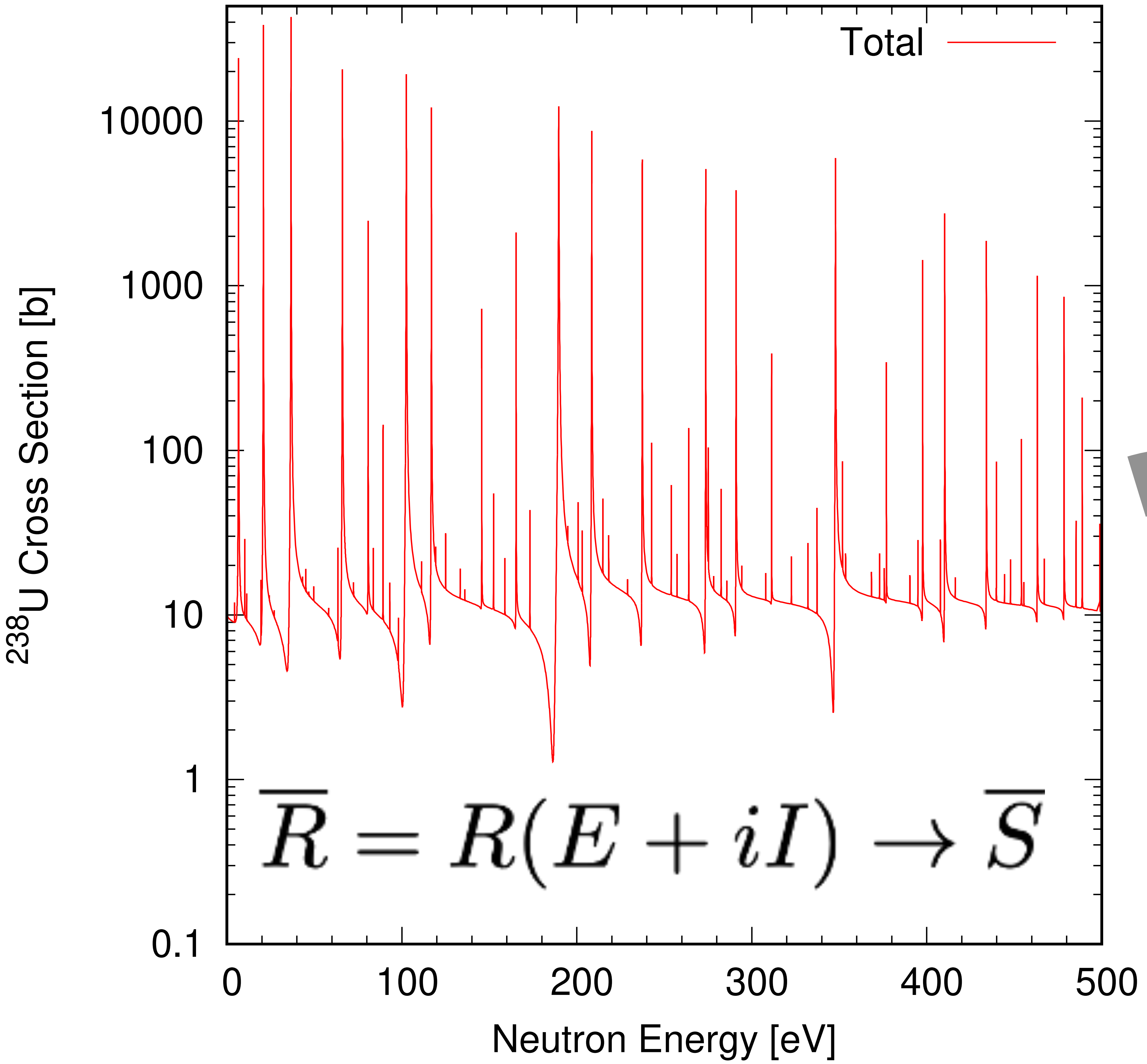
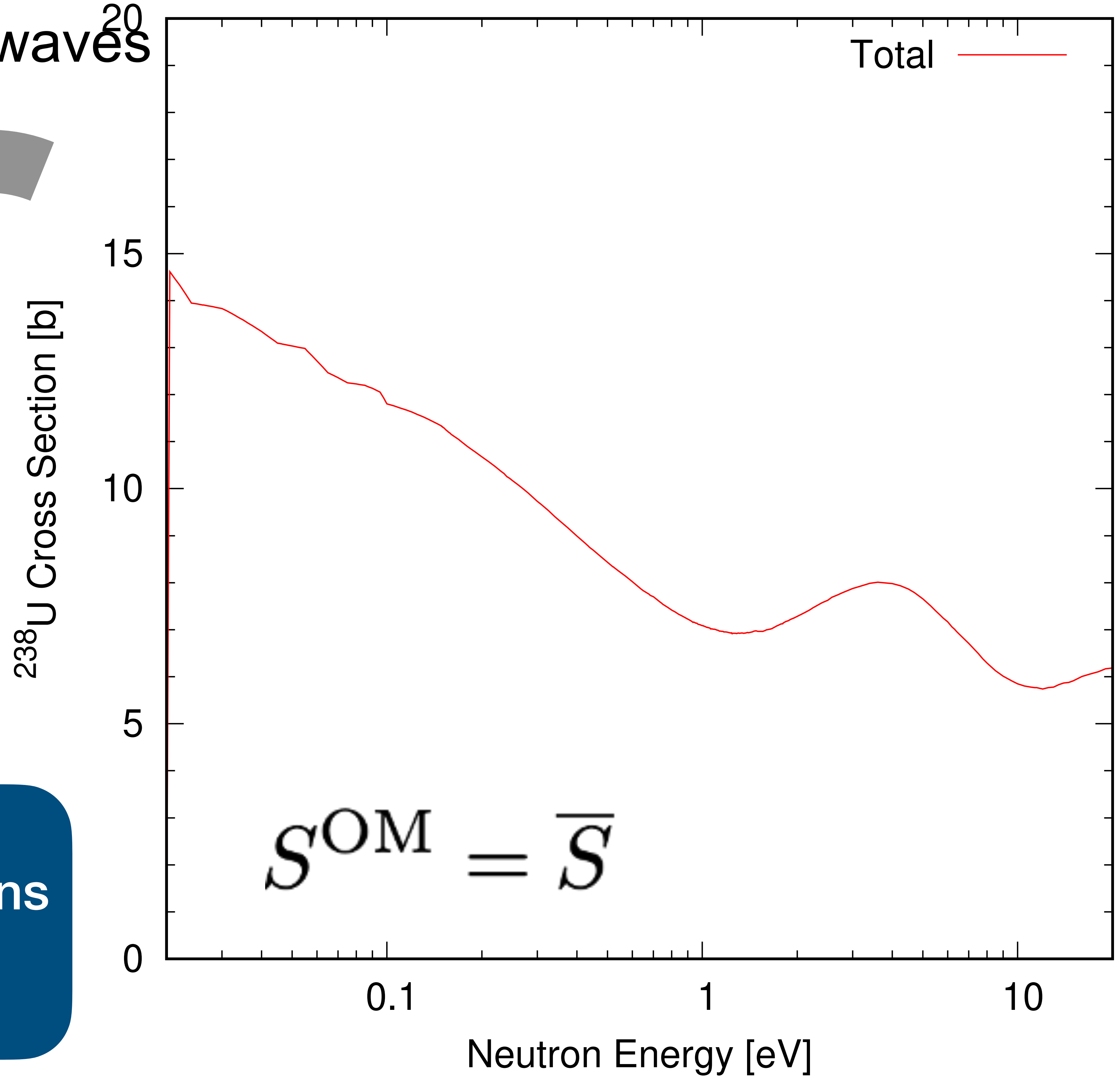
Random Matrix Approach to Smoothly Connect 2 Regions



- **Transmission coefficients in both regions**
  - it guarantees smoothly connected cross sections
  - but limited to s-wave (and p-wave) only
- **Optical model**
  - for higher partial waves

$$T = 1 - |\overline{S}|^2$$

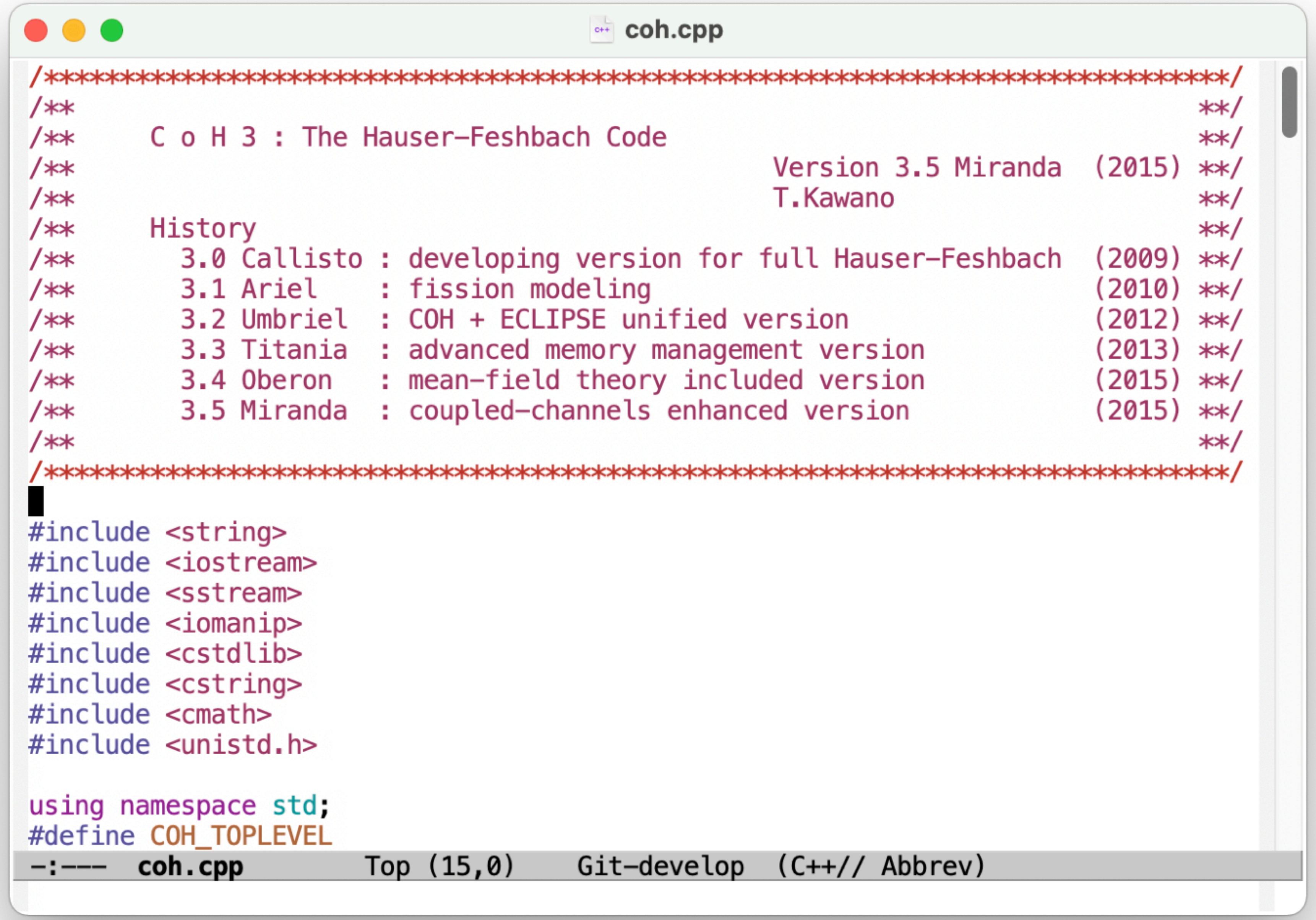


GOE model provides average cross sections as well as their realistic distribution

Coupled-Channels and Hauser-Feshbach Code CoH_3

- **Hauser-Feshbach-Moldauer theory for compound reaction**
  - 60k+ lines C++ code, including ~180 source and ~70 header files
  - written in OOP style, ~ 80 classes defined
  - GNU Autotools package for building
- **Some special features**
  - Internal optical model / coupled-channels solver
  - Unified description of coupled-channels and statistical model
  - Compound nucleus decay by deterministic or Monte Carlo method
  - Accurate exclusive reaction cross sections and spectra
  - Mean-field models included (FRDM, Hartree-Fock-BCS)
  - Subsidiary code BeoH

https://github.com/toshihikokawano/coh3


coh.cpp

```
/*************************************************************************************/
/**                                                                               **/
/**     C o H 3 : The Hauser-Feshbach Code                                        **/
/**                                         Version 3.5 Miranda  (2015) **/
/**                                         T.Kawano                    **/
/**                                                                               **/
/**     History                                                                   **/
/**       3.0 Callisto : developing version for full Hauser-Feshbach  (2009) **/
/**       3.1 Ariel    : fission modeling                              (2010) **/
/**       3.2 Umbriel  : COH + ECLIPSE unified version                 (2012) **/
/**       3.3 Titania  : advanced memory management version            (2013) **/
/**       3.4 Oberon   : mean-field theory included version            (2015) **/
/**       3.5 Miranda  : coupled-channels enhanced version             (2015) **/
/**                                                                               **/
/*************************************************************************************/

#include <string>
#include <iostream>
#include <sstream>
#include <iomanip>
#include <cstdlib>
#include <cstring>
#include <cmath>
#include <unistd.h>

using namespace std;
#define COH_TOPLEVEL
-:---  coh.cpp        Top (15,0)     Git-develop  (C++// Abbrev)
```

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Concluding Remarks

- **Statistical Hauser-Feshbach theory for compound nucleus reactions**
  - GOE model finally solved the problem to express the reaction cross section in terms of transmission coefficients for both spherical and deformed cases
  - Connection with the resonance theory by the GOE formalism underway
- **Beyond Hauser-Feshbach**
  - Microscopic approaches for the photon strength function and the level density commonly employed
  - Fission still less predictive, but under progress
  - Pre-equilibrium renaissance informed by gamma-ray production experiments, which are more sensitive to quantum effects