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Los Alamos National Laboratory

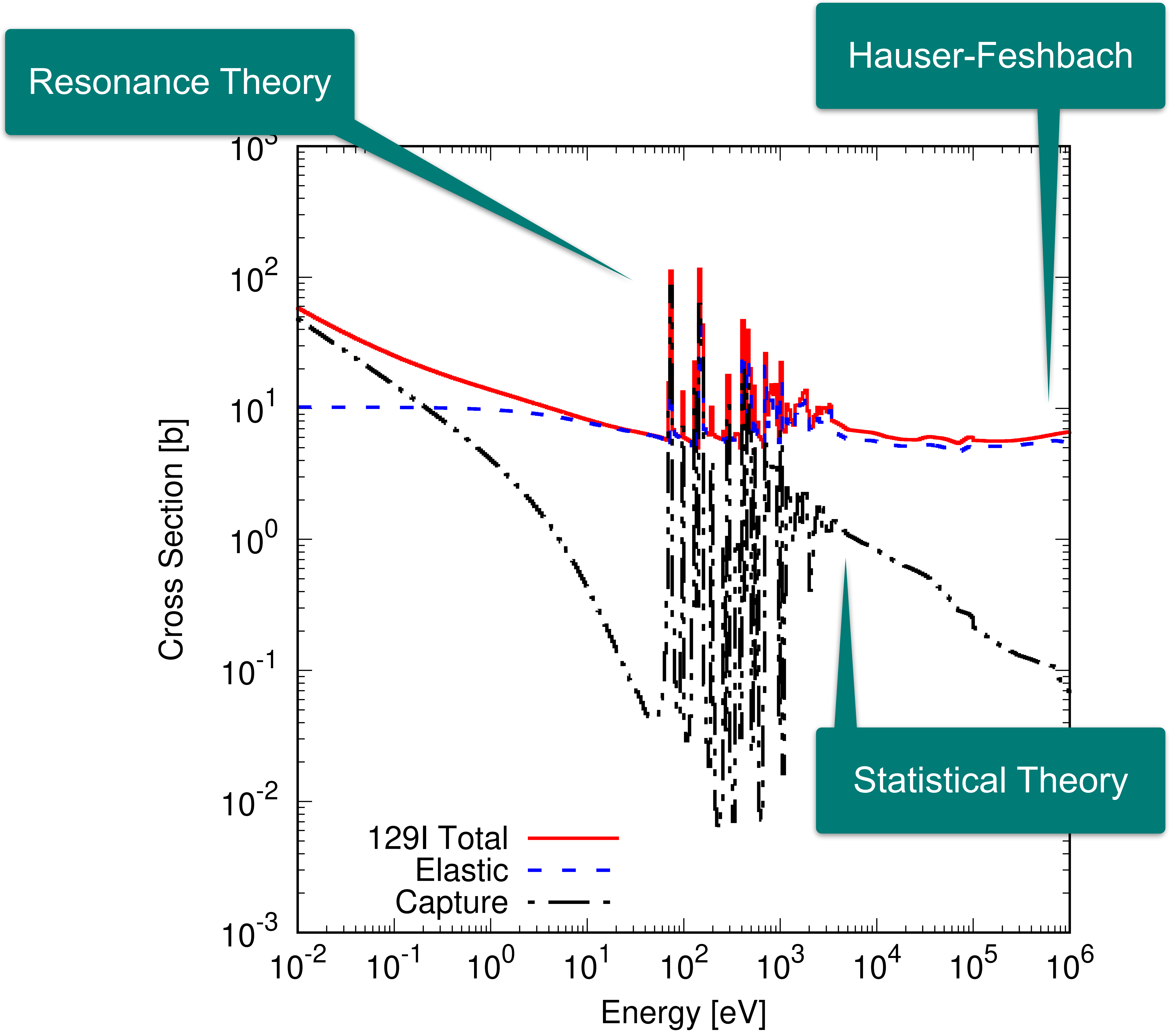
Gaussian Orthogonal Ensemble model for low-energy neutron-induced reaction to excite weakly overlapped compound nucleus states

T. Kawano, A.E. Lovell
Theoretical Division

National Nuclear Security Administration

Introduction: Cross Section Representation

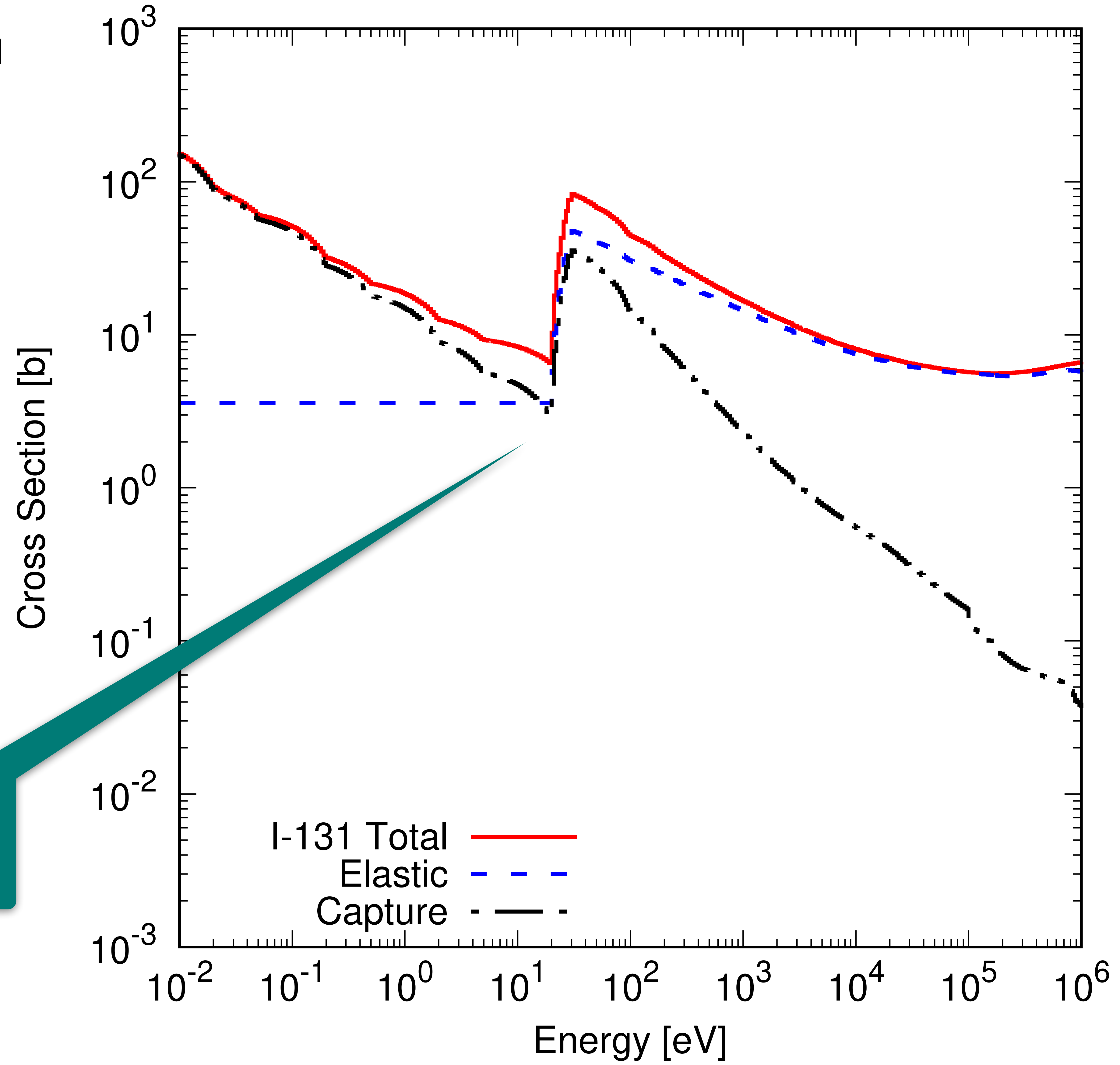
- **Resolved resonance range (RRR)**
  - cross sections are not energy-averaged
- **Unresolved resonance range (URR)**
  - average resonance parameters given and statistical theory applied
  - no fluctuation, but non-smooth behavior may persist if experimental data show
- **Higher energy range**
  - cross sections given by the Hauser-Feshbach model are smooth and energy-averaged



Connecting RRR and HF Energy Regions

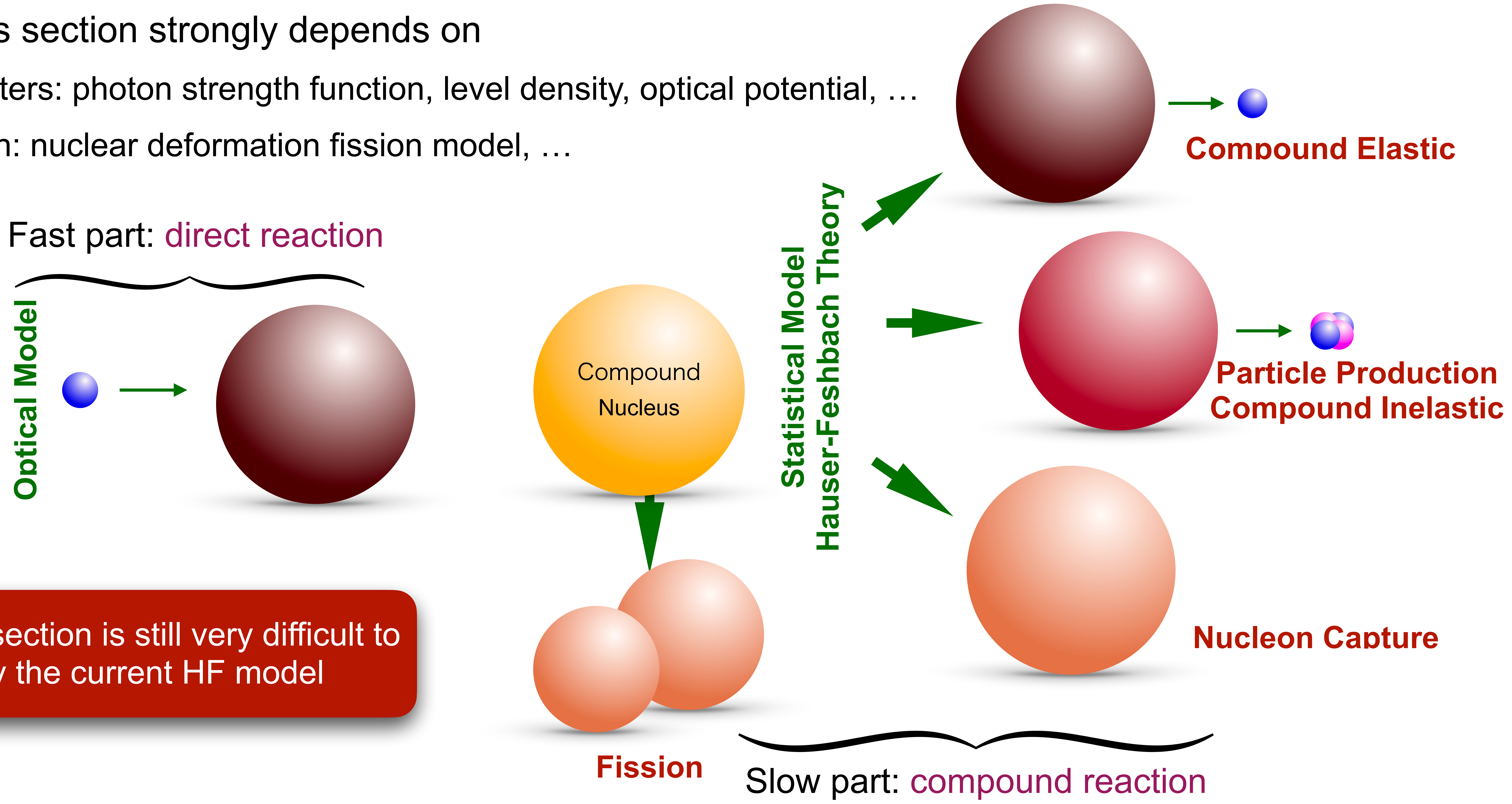
- **Smooth transition from RRR to HF not always guaranteed**
  - URR parameters not given
    - fluctuation in cross sections suddenly disappear at the boundary energy
    - sometimes fluctuation is given based on experimental data, but no predictive model exists
  - URR parameters given, but not used to calculate cross section
    - parameters used for self-shielding calculation only
  - URR parameters given
    - cross sections by the statistical model
    - artificial fluctuation can be added
    - channel degree-of-freedom not so well studied
- **Improvement of statistical theory in URR**
  - direct reaction when deformed nuclei
  - channel d.o.f

Artificial transition from RRR to statistical model calculation



Nuclear Reaction Rates by Statistical Hauser-Feshbach

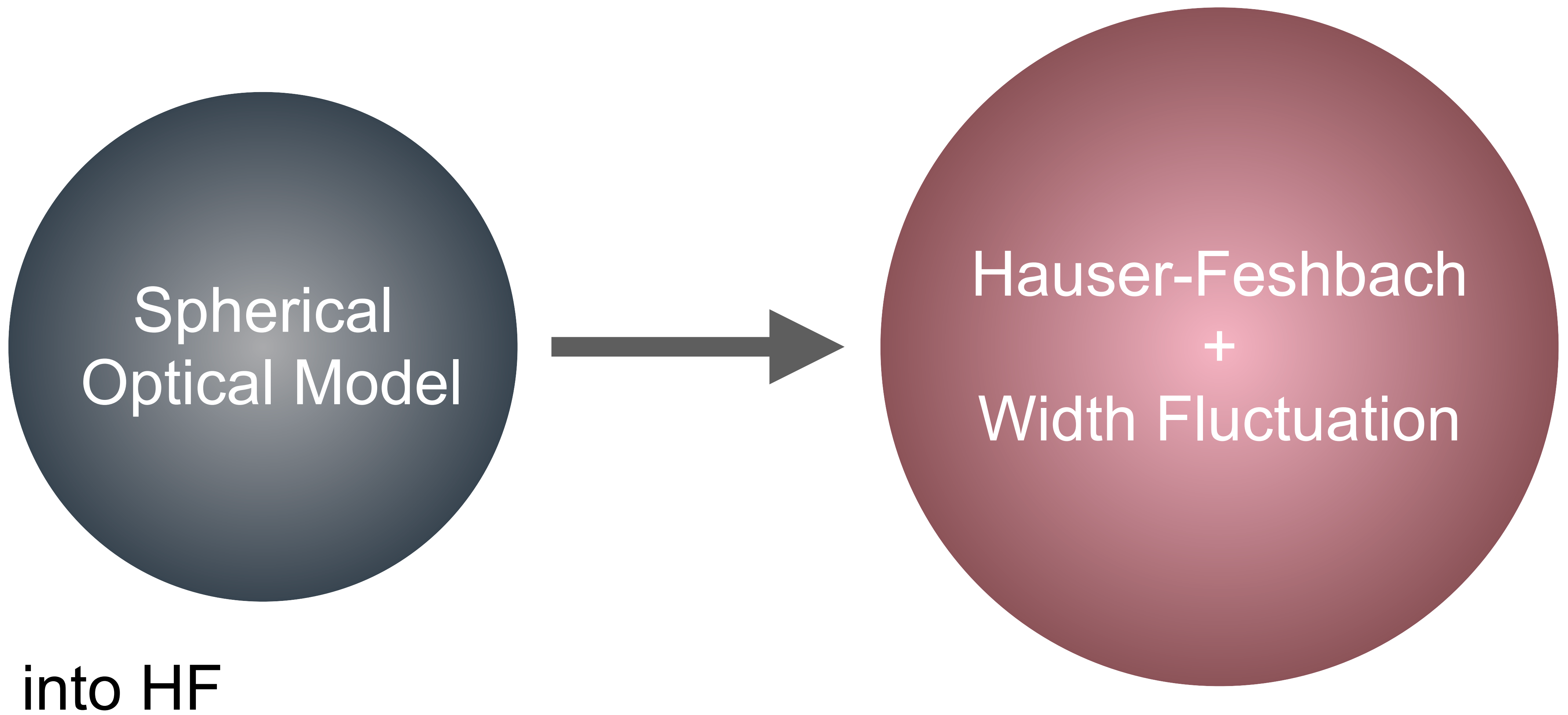
- **Statistical Hauser-Feshbach theory for nuclear reactions in the keV to MeV energy range**
  - Widely employed for applications such as nuclear technology, astrophysics, etc
  - Calculated cross section strongly depends on
    - model parameters: photon strength function, level density, optical potential, …
    - implementation: nuclear deformation fission model, …



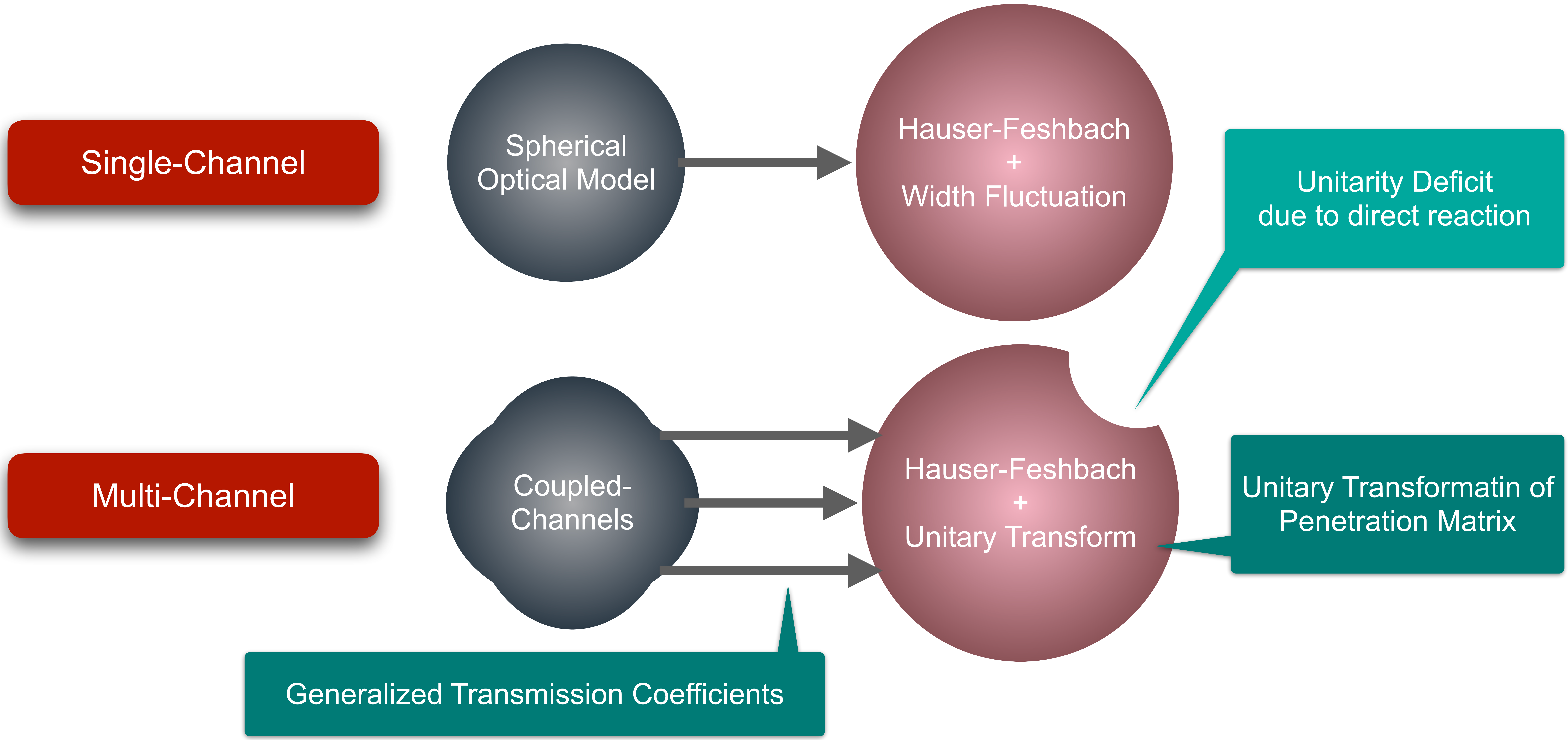
Fission cross section is still very difficult to predict by the current HF model

Ingredients for Statistical Hauser-Feshbach

- **Phenomenological and/or microscopic models**
  - Optical potential for entrance channel
    - global parameterization or individual fit to data
    - microscopic approaches, yet not generally accepted
  - Level density in the residual nuclei
    - phenomenological models, Gilbert-Cameron, BSFG, …
    - mean-field single-particle spectrum + combinatorial calculation (+ phenomenological corrections)
    - large-scale shell model
  - Photon strength function for gamma-ray emission
    - Giant Dipole Resonance (GDR) models
    - quasi-particle random phase approximation (QRPA)
  - Fission barriers
    - simple penetration model
    - microscopic potential energy landscape not yet incorporated into HF



Unification of Coupled-Channels and Hauser-Feshbach Theories



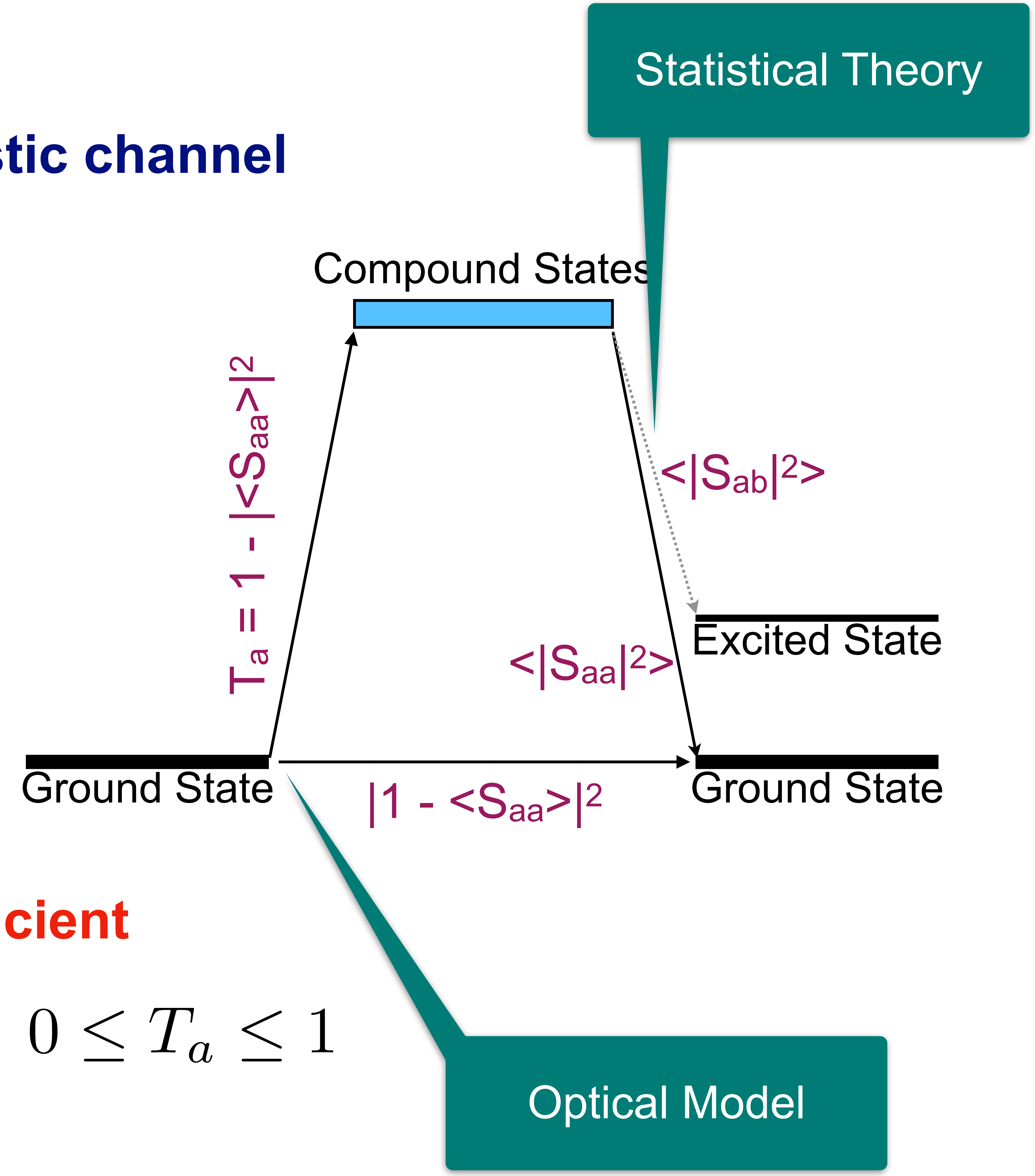
Are the Slow and Fast Processes Independent?

- **Strong constraint by S-matrix unitarity**
- **Incoming wave interferes with out-going wave in the elastic channel**

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

- **Statistical theory gives energy average cross section**

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



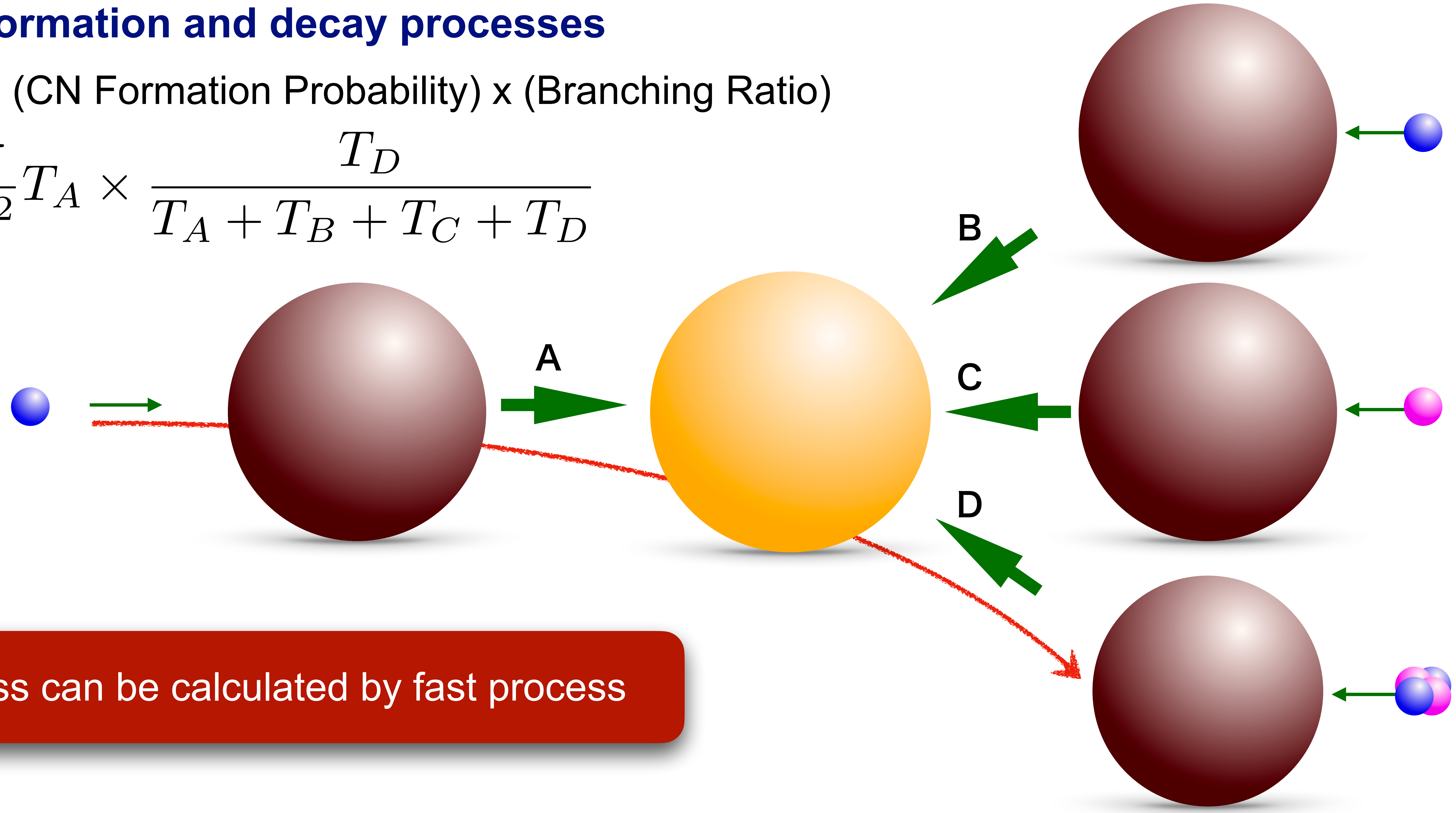
We want to express the CN part by Transmission Coefficient

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

Detailed Balance: Statistical Theory

- **Time-reversal process**
- **Factorizing CN formation and decay processes**
  - Cross section = (CN Formation Probability) x (Branching Ratio)

$$\sigma_D = \frac{\pi}{k^2} T_A \times \frac{T_D}{T_A + T_B + T_C + T_D}$$



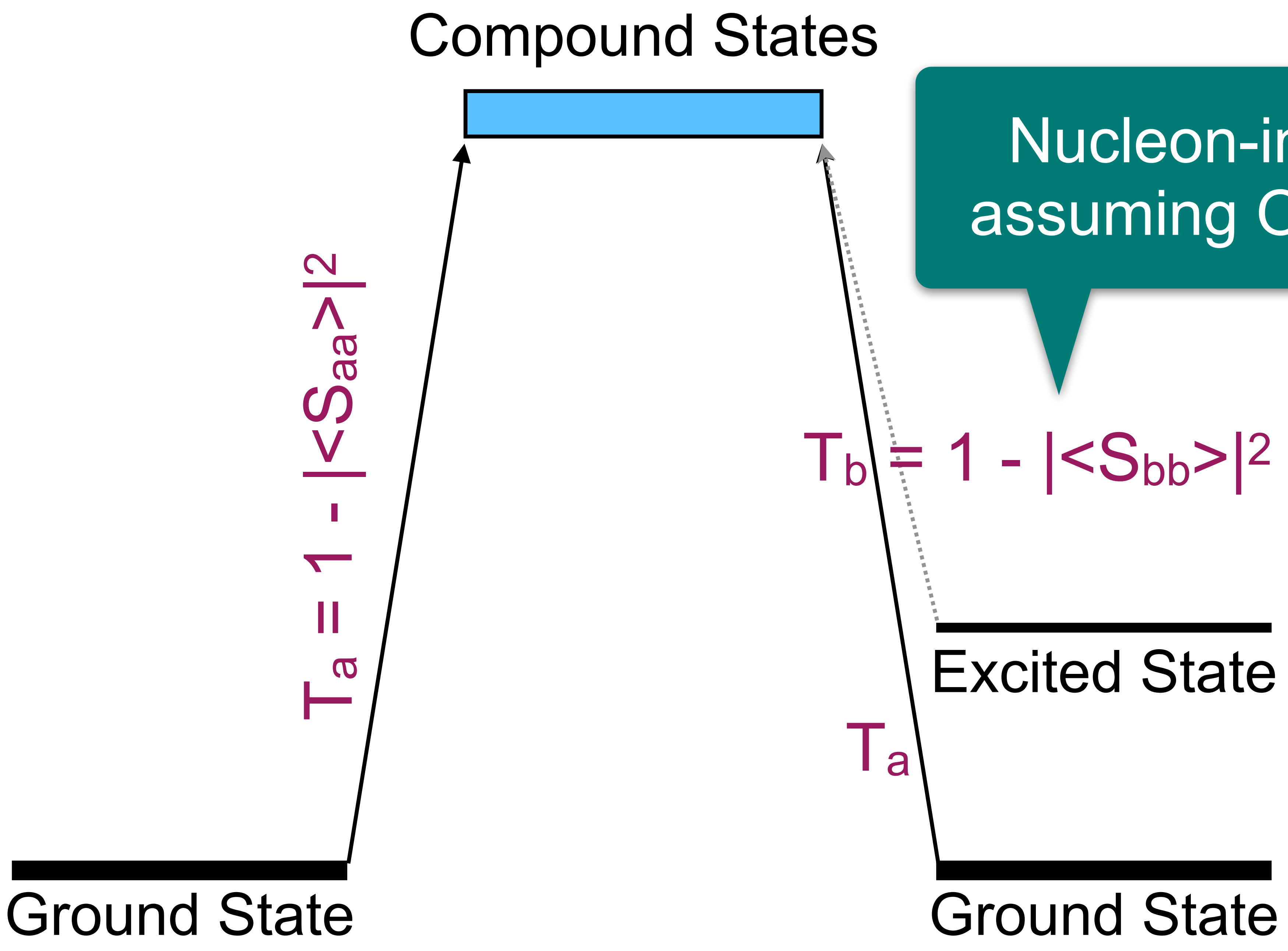
Slow process can be calculated by fast process

Spherical and Deformed Targets

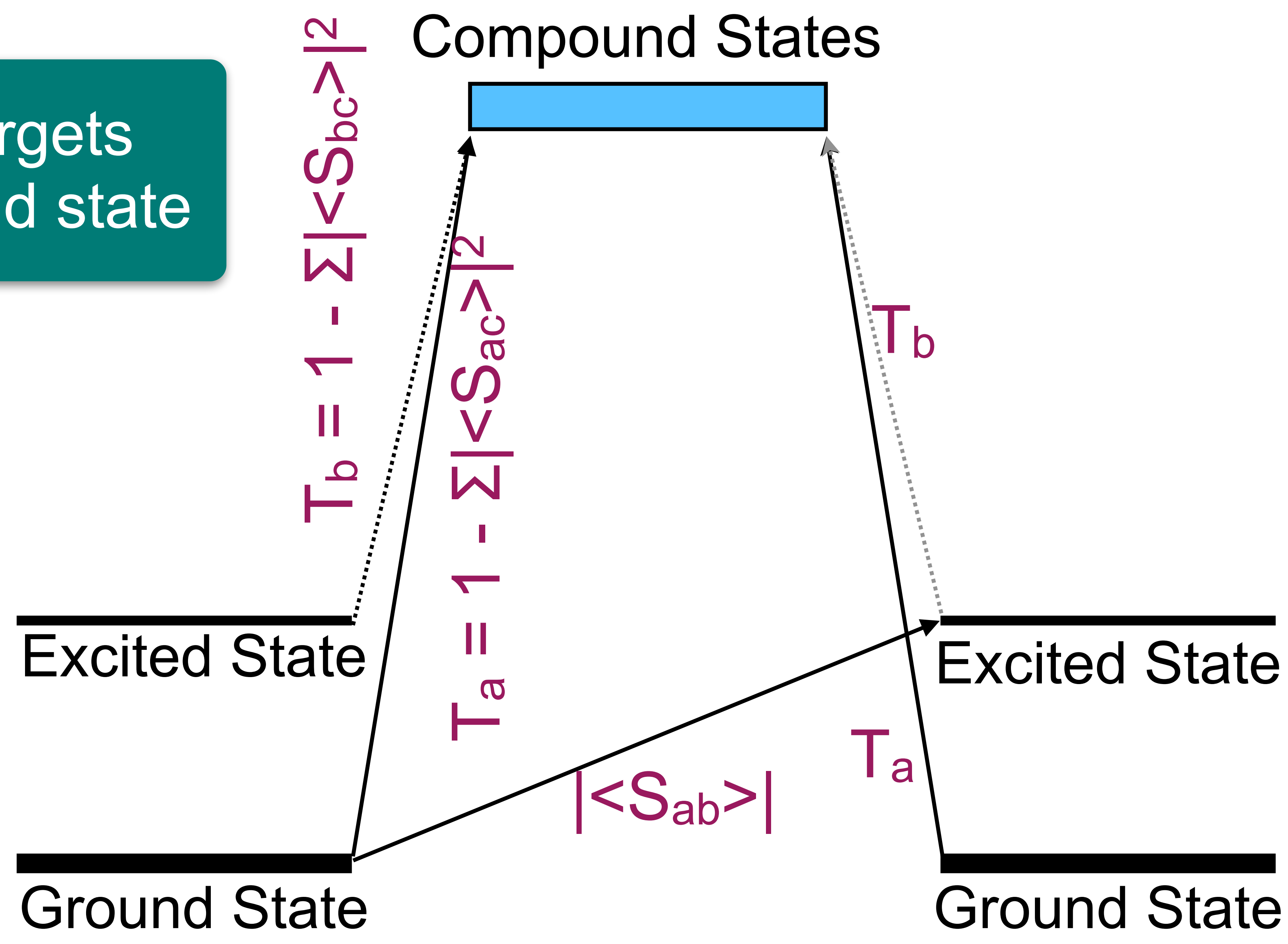
- **Single channel optical model**
  - target is spherical, S-matrix is diagonal
- **Coupled-channels optical model**
  - target is deformed, Include off-diagonal elements

Generalized transmission coefficients in the coupled-channels formalism

$$T_{lj}^{(n)} = \sum_{J\Pi} \sum_{a} \frac{2s+1}{2j_a+1} g_J \left(1 - \sum_{b} |S_{ab}^{J\Pi}|^2 \right) \delta_{n_a,n} \delta_{l_a,l} \delta_{j_a,j}$$



Nucleon-induced reaction on excited targets assuming OMP is the same as the ground state



T. Kawano, PRC80, 024611 (2009)

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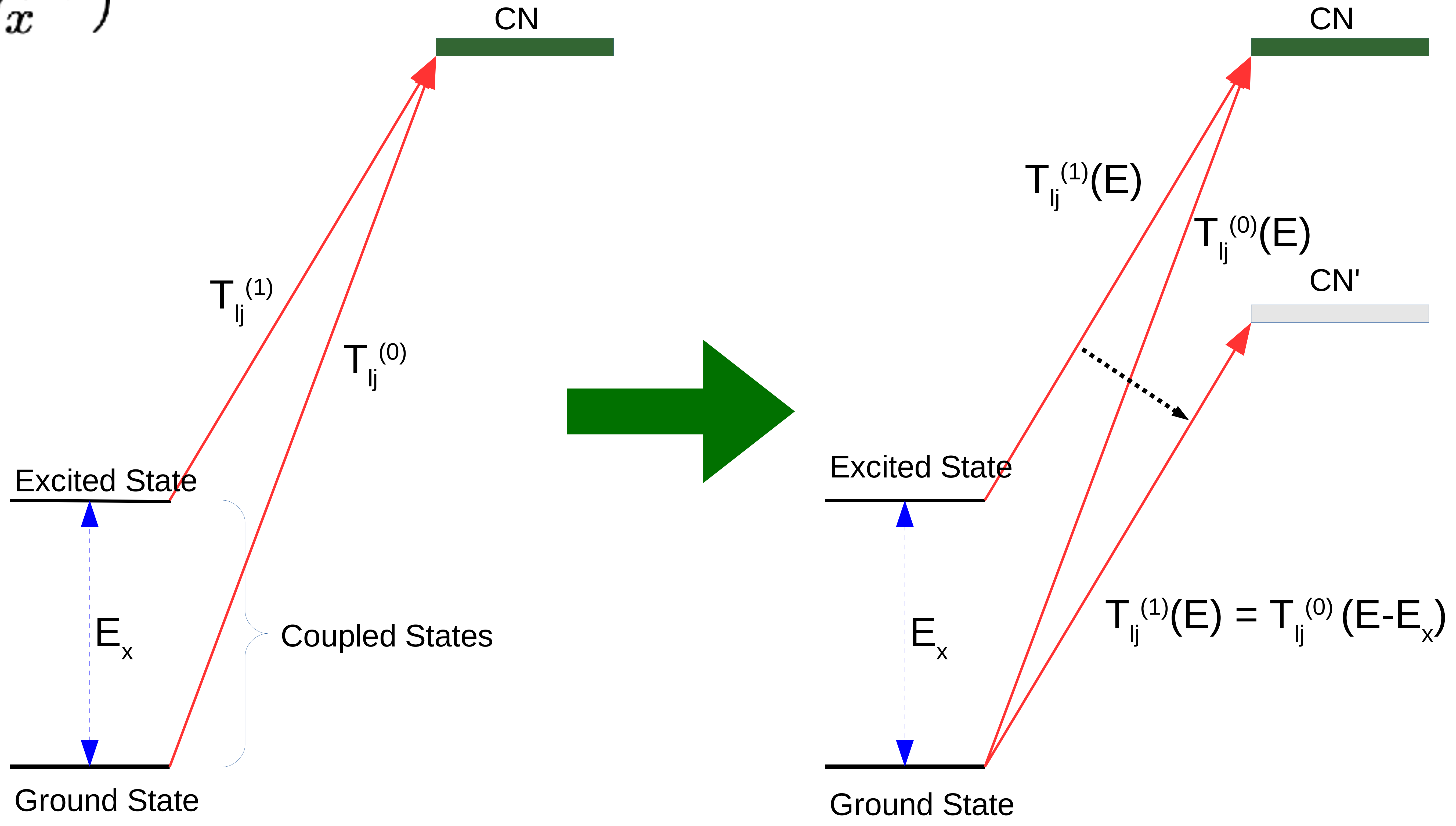
Conventional HF Calculation for Deformed Targets

- **CC and HF calculations are often fully decoupled**
  - Many of HF codes do not use generalized transmission coefficients for the excited states,
  - but approximated by T for the ground state shifted by excitation energy

$$T_{lj}^{(n)}(E) \simeq T_{lj}^{(0)}(E - E_x^{(n)})$$

  - This approximation never validated

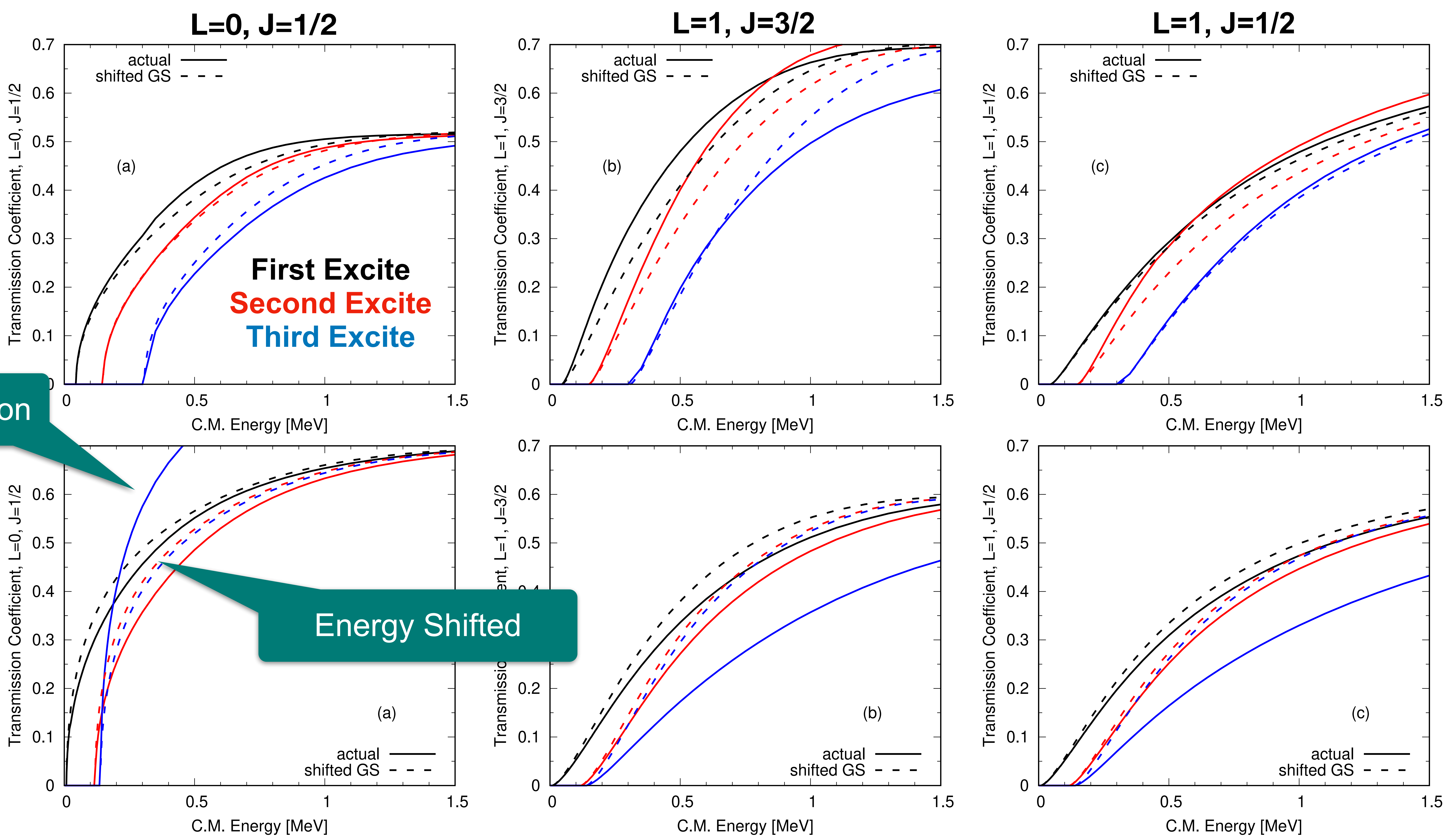


T. Kawano, EPJA 57, 16 (2021)

Generalized Transmission and Energy-Shifted Transmission

Even-Even Target
^{238}U

Even-Odd Target
^{169}Tm



T. Kawano, EPJA 57, 16 (2021)

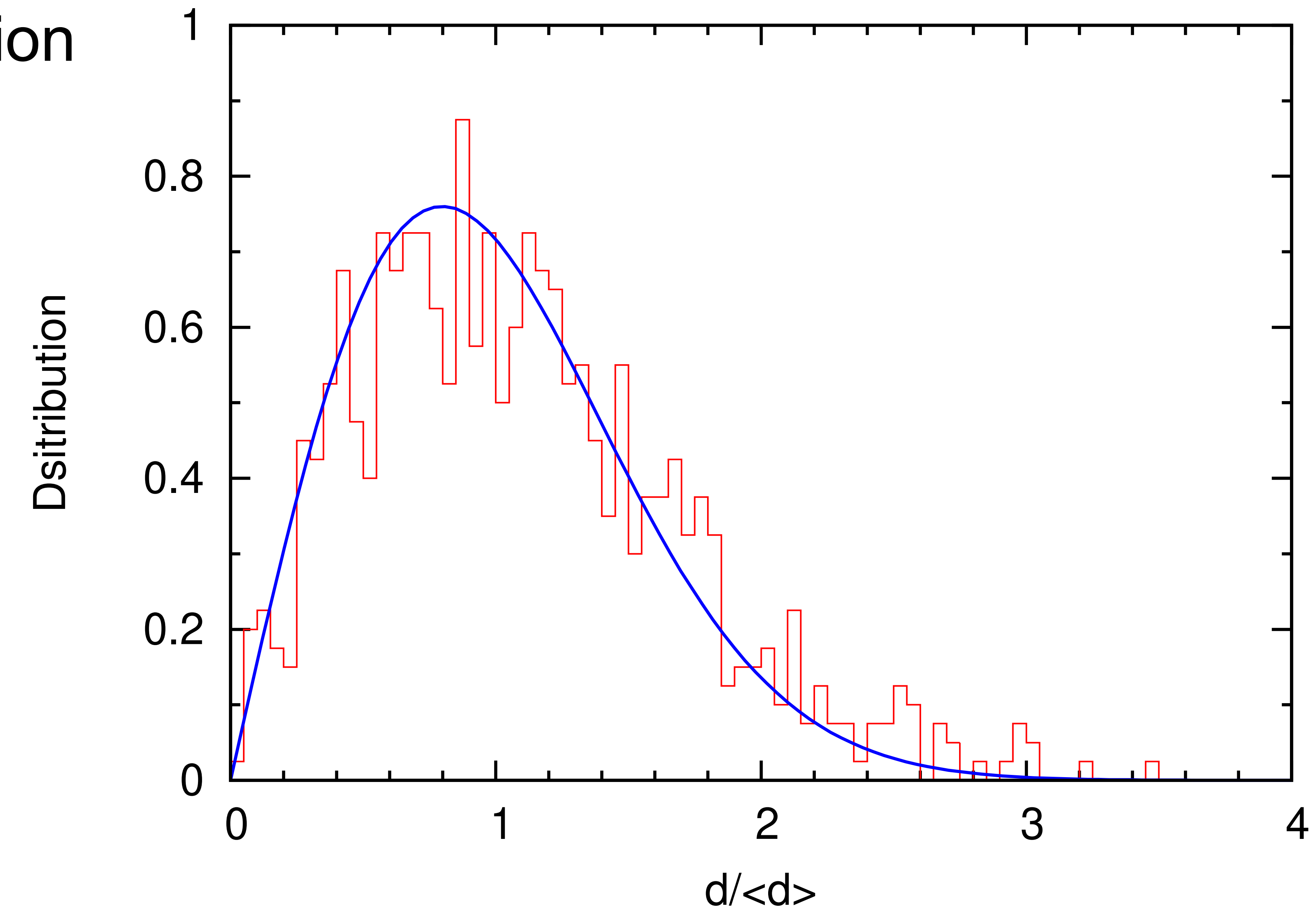
Correction to HF: Elastic Enhancement and Width Fluctuation

- **Compound cross section defined by average resonance properties**

$$\sigma_{ab}^{\mathrm{CN}} = \frac{2\pi}{D}\left\langle \frac{\Gamma_a \Gamma_b}{\sum_c \Gamma_c} \right\rangle = \frac{2\pi}{D}\frac{\langle\Gamma_a\rangle\langle\Gamma_b\rangle}{\sum_c \langle\Gamma_c\rangle} W_{ab} = \frac{T_a T_b}{\sum_c T_c} W_{ab}$$

Correlation appears in the width fluctuation correction factor

- **Stochastic R-matrix employed in the past**
  - Monte Carlo technique for generating fluctuating cross section by
    - sampling resonance spacing D from Wigner distribution, and
    - sampling decay width Gamma from Porter-Thomas distribution
- **Caveats**
  - Hidden correlation
  - Actual width distribution not so obvious
    - Study CN reaction by random matrix
    - Verbaarschot, Weidenmueller, Zirnbauer
    - implemented GOE in Hamiltonian



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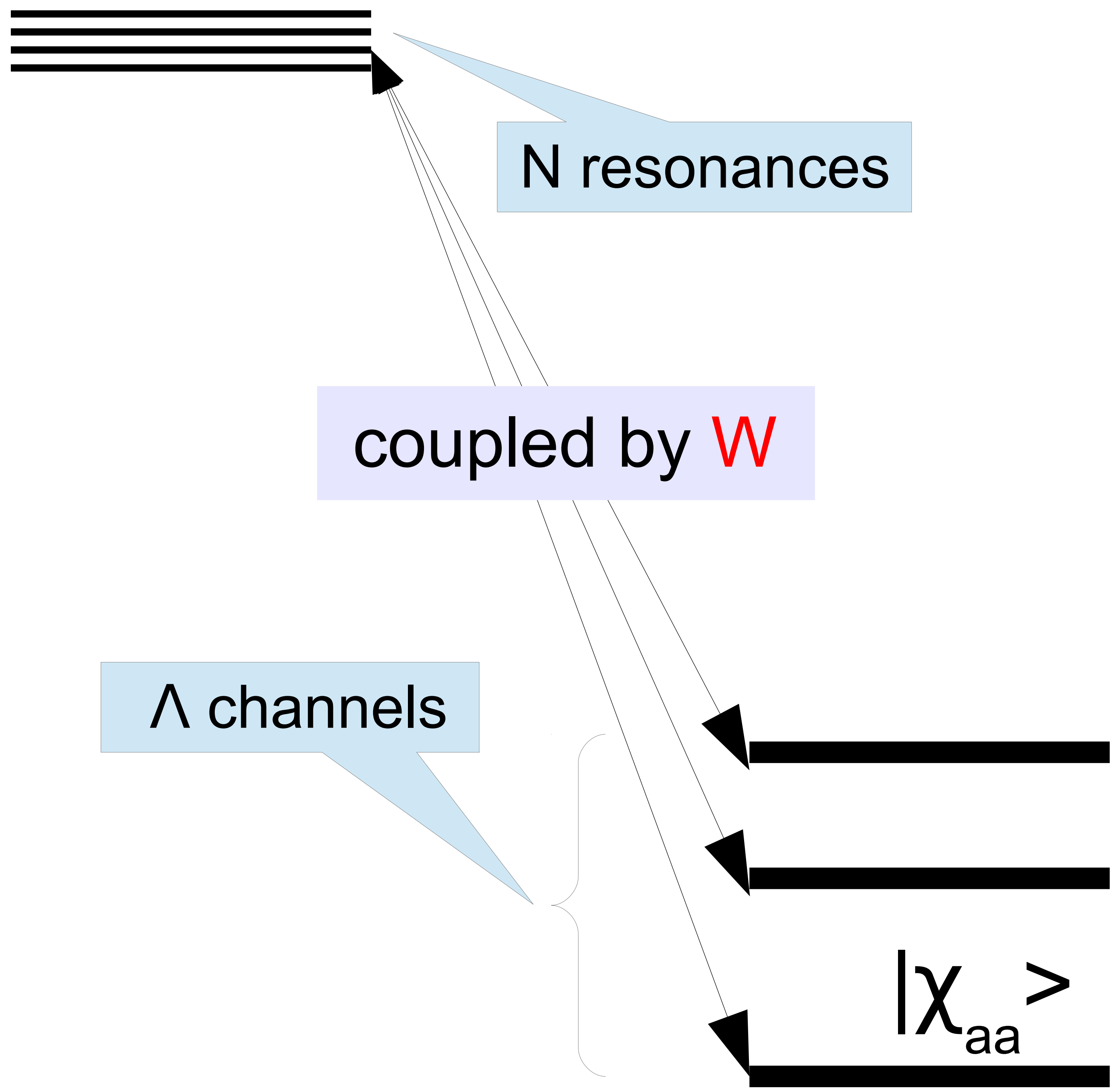
Stochastic S-matrix (K-matrix) based on GOE



GOE S-Matrix

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

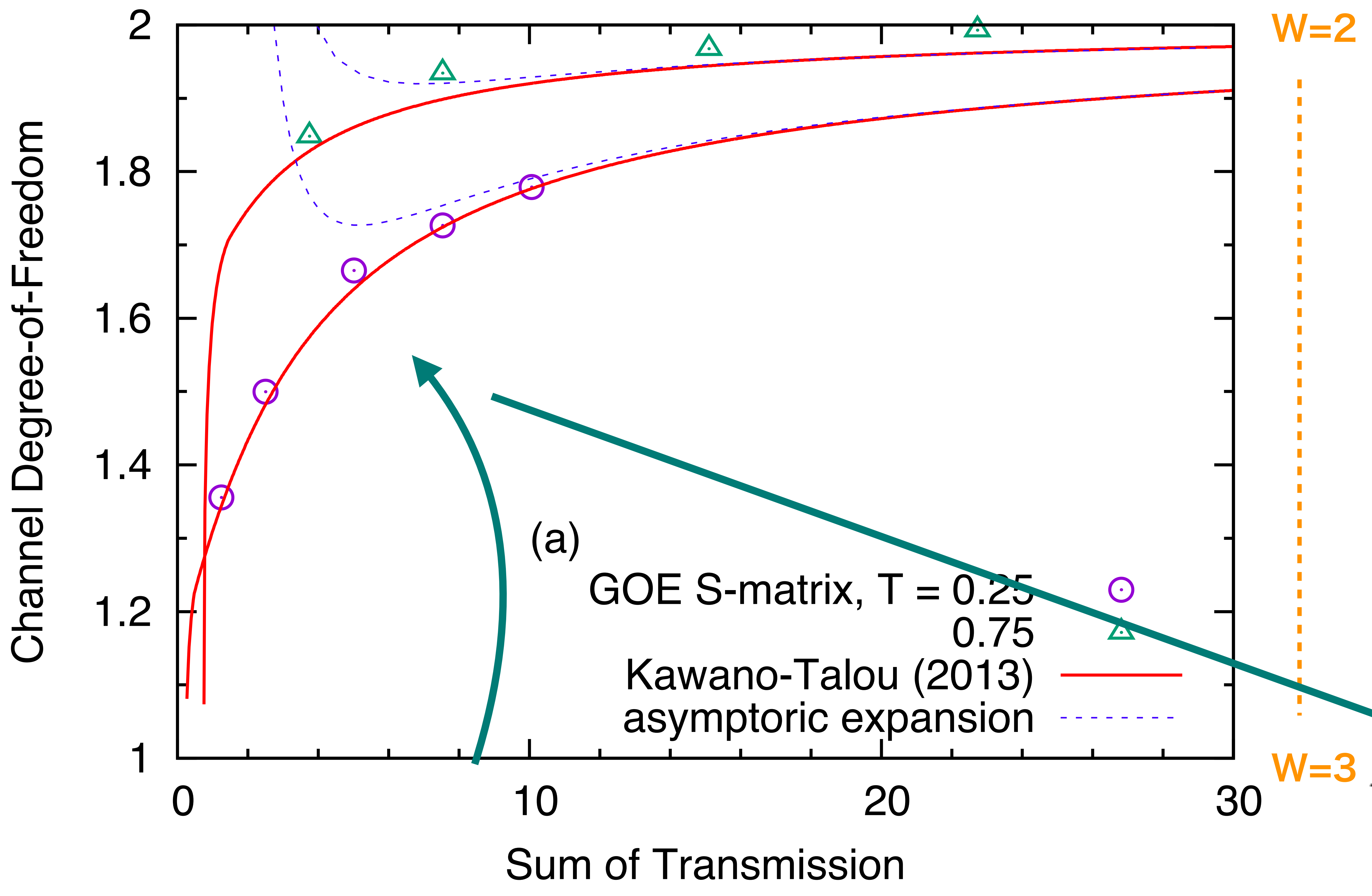
$$D_{\mu\nu} = E\delta_{\mu\nu} - H^{(\mathrm{GOE})}_{\mu\nu} + i\pi \sum_{c} W_{\mu c} W_{c\nu}$$

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

- 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)

T. Kawano, PRC92, 044617 (2015)

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**

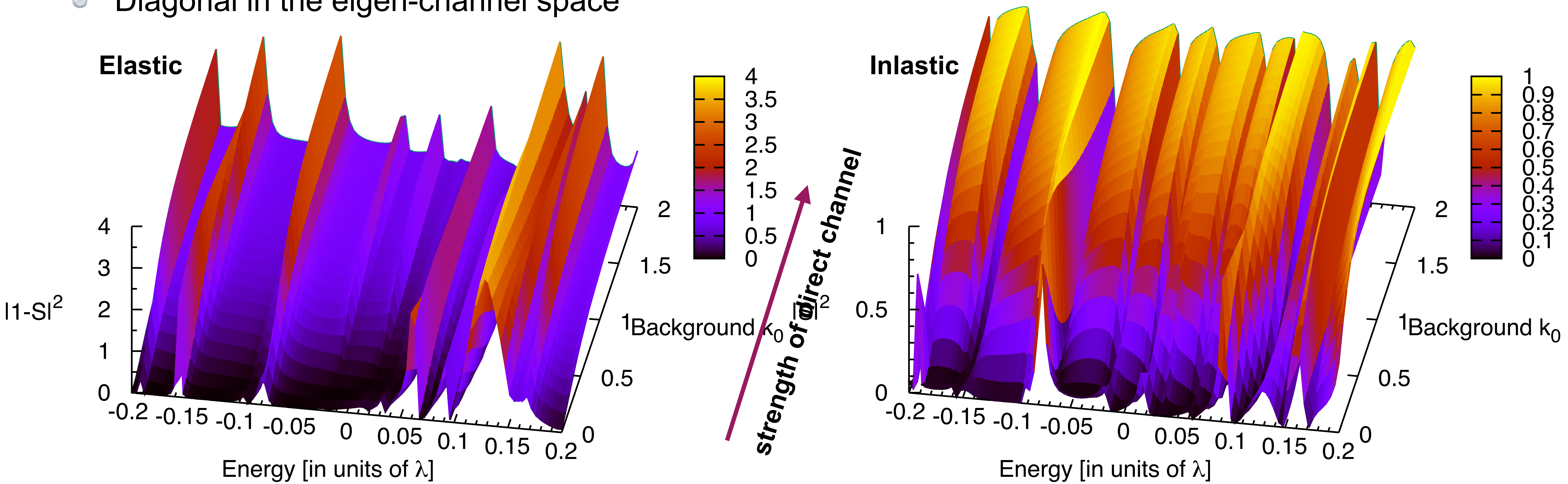
$$W_{ab} = \left(1 + \frac{2\delta_{ab}}{\nu_a}\right) \int_0^\infty \frac{dt}{F_a(t) F_b(t) \prod_k F_k(t)^{\nu_k/2}}$$

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

T. Kawano, PRC92, 044617 (2015)

Influence of Direct Reaction Channels

- **Direct reaction channels introduced as a background in K-matrix**
- **Generalization is not so straightforward**
  - How width fluctuation correction changes by the strength of direct channels
- **The direct contribution can be eliminated by unitary transformation**
  - Diagonal in the eigen-channel space



T. Kawano, PRC92, 044617 (2015)

Engelbrecht-Weidenmuller Transformation for CC S-matrix

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

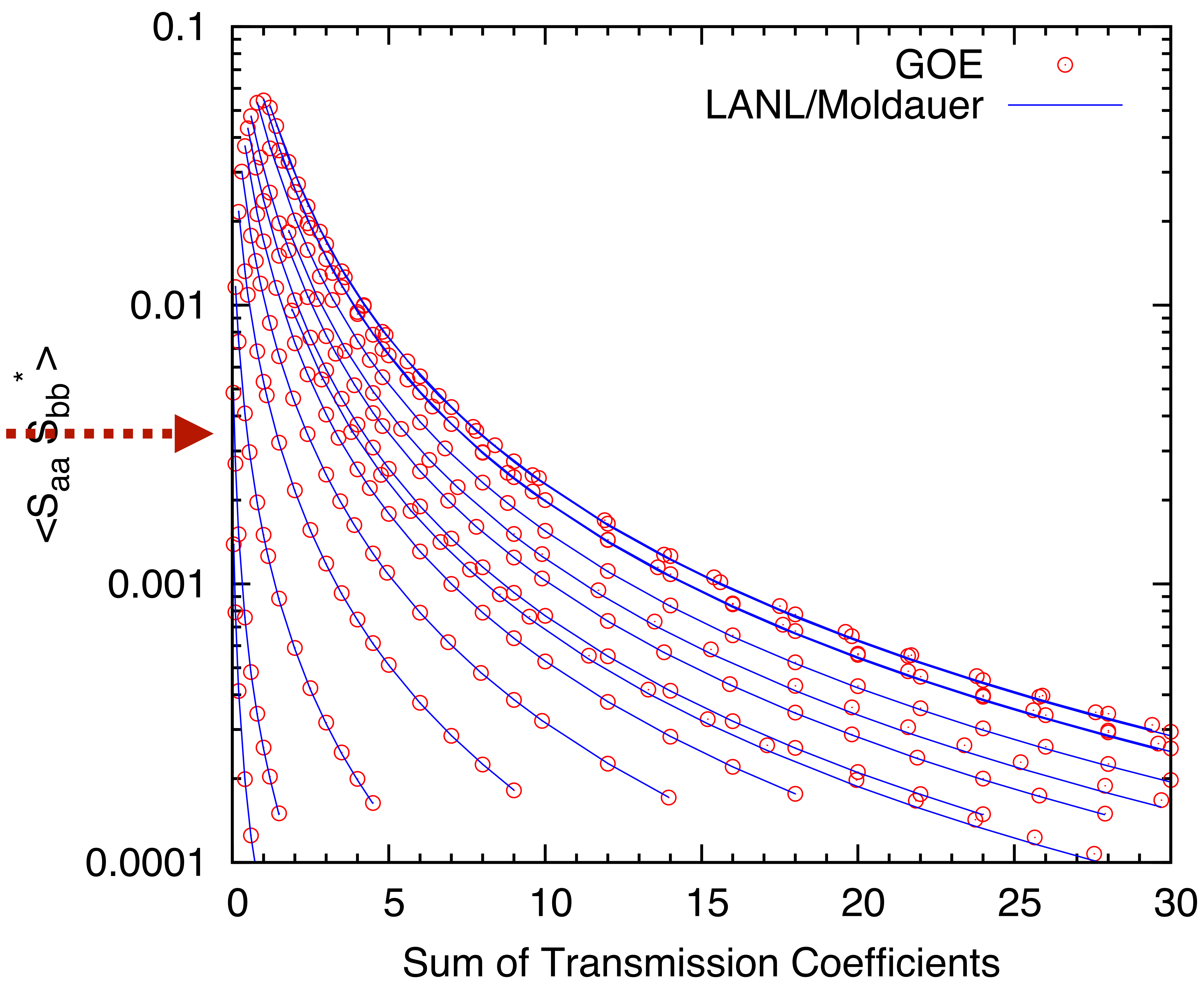
use this for transmission coefficients

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

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

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

Width fluctuation corrected cross section in the diagonal space



T. Kawano, PRC94, 014612 (2016)

Inclusion of Uncoupled Channels

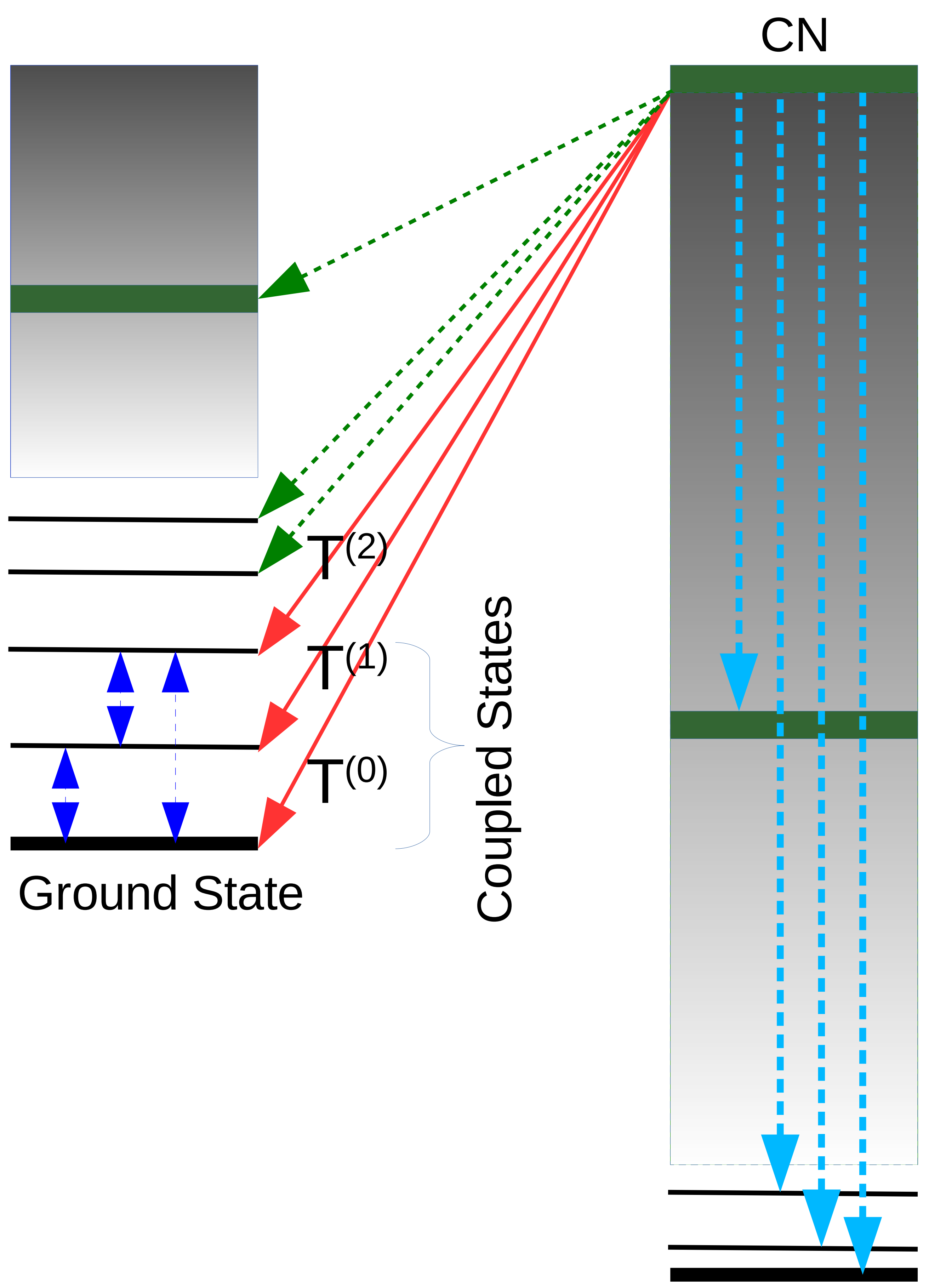
- **The whole S-matrix includes more channels than treated in the CC formalism**
  - capture (gamma-ray emission), fission, compound inelastic scattering, etc
  - Spherical optical model for uncoupled inelastic scattering channels
  - Strength function for gamma-ray emission channel

$$T_\gamma = \sum_{XL} \int_0^{E_n+S_n} T_{XL}(E_\gamma)\rho(E_x)dE_x$$

  - Hill-Wheeler WKB transmission for fission channel, if open

$$P = \begin{pmatrix} P_C & & & \\ & T_n & & \\ & & T_\gamma & \\ & & & T_f \end{pmatrix}$$

$$\sigma_{ab} = \sum_\alpha |U_{\alpha a}|^2 \sigma_{\alpha\beta}\delta_{\beta b}$$



Decay Amplitude from GOE Hamiltonian

K-Matrix Representation

$$K = \pi W^T \frac{1}{E - H^{\mathrm{GOE}}} W, \qquad K_{cc'} = \frac{1}{2} \sum_{\mu} \frac{\tilde{\gamma}_{\mu c} \tilde{\gamma}_{\mu c'}}{E - E_{\mu}}$$

S-Matrix Pole Expansion

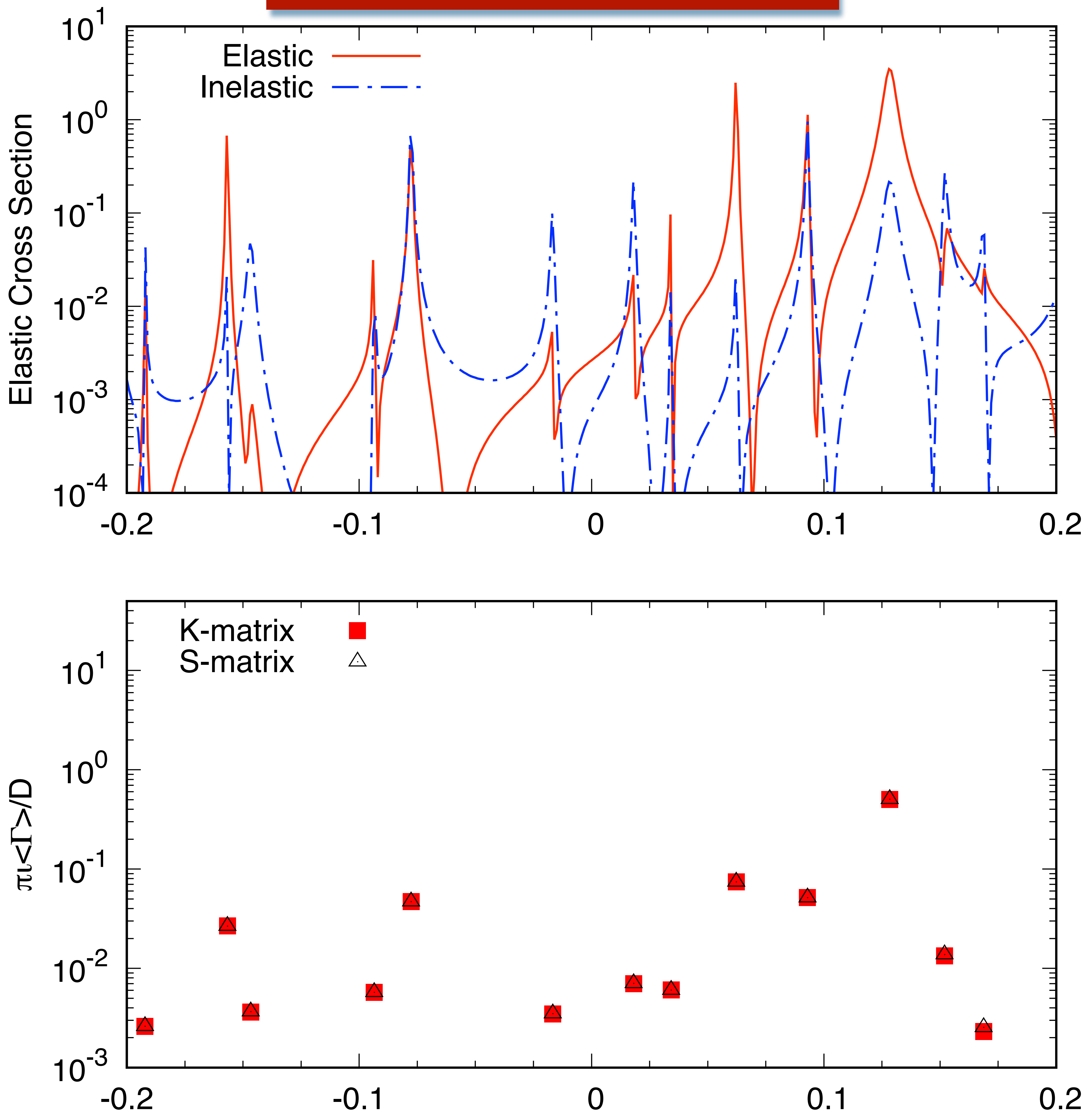
$$S = 1 - 2\pi i (CW)^T \frac{1}{E - C(H^{\mathrm{GOE}} - i\pi W W^T) C^T} CW, \qquad C^T C = 1$$

$$S_{cc'} = \delta_{cc'} - i \sum_{\nu} \frac{\gamma_{\nu c} \gamma^*_{\nu c'}}{E - E_{\nu} + i\Gamma_{\nu}/2}$$

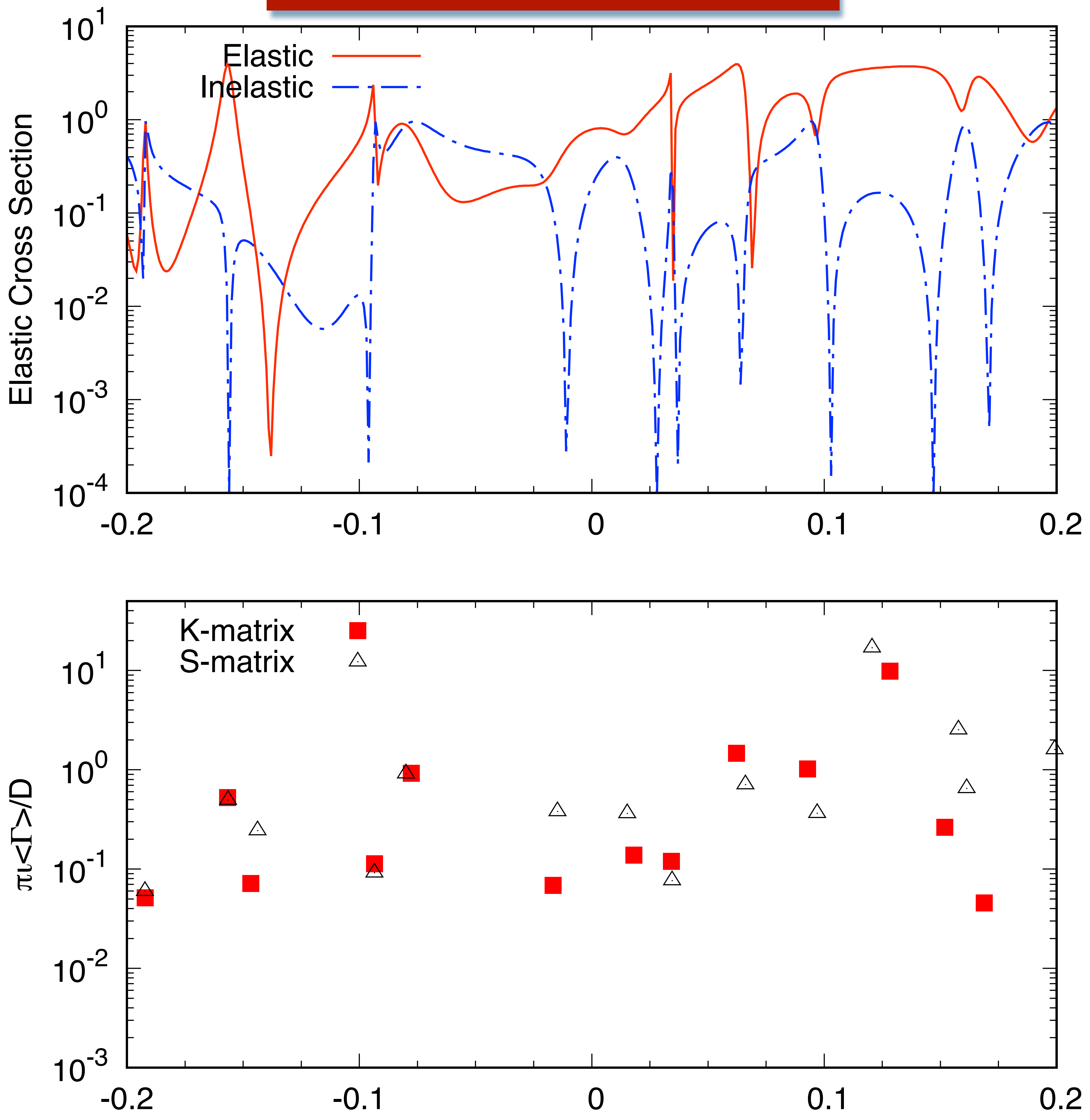
Average decay width is given by the ensemble average of these decay amplitudes

GOE Poles and Decay Widths, 2-Channel and 100-Resonance Case

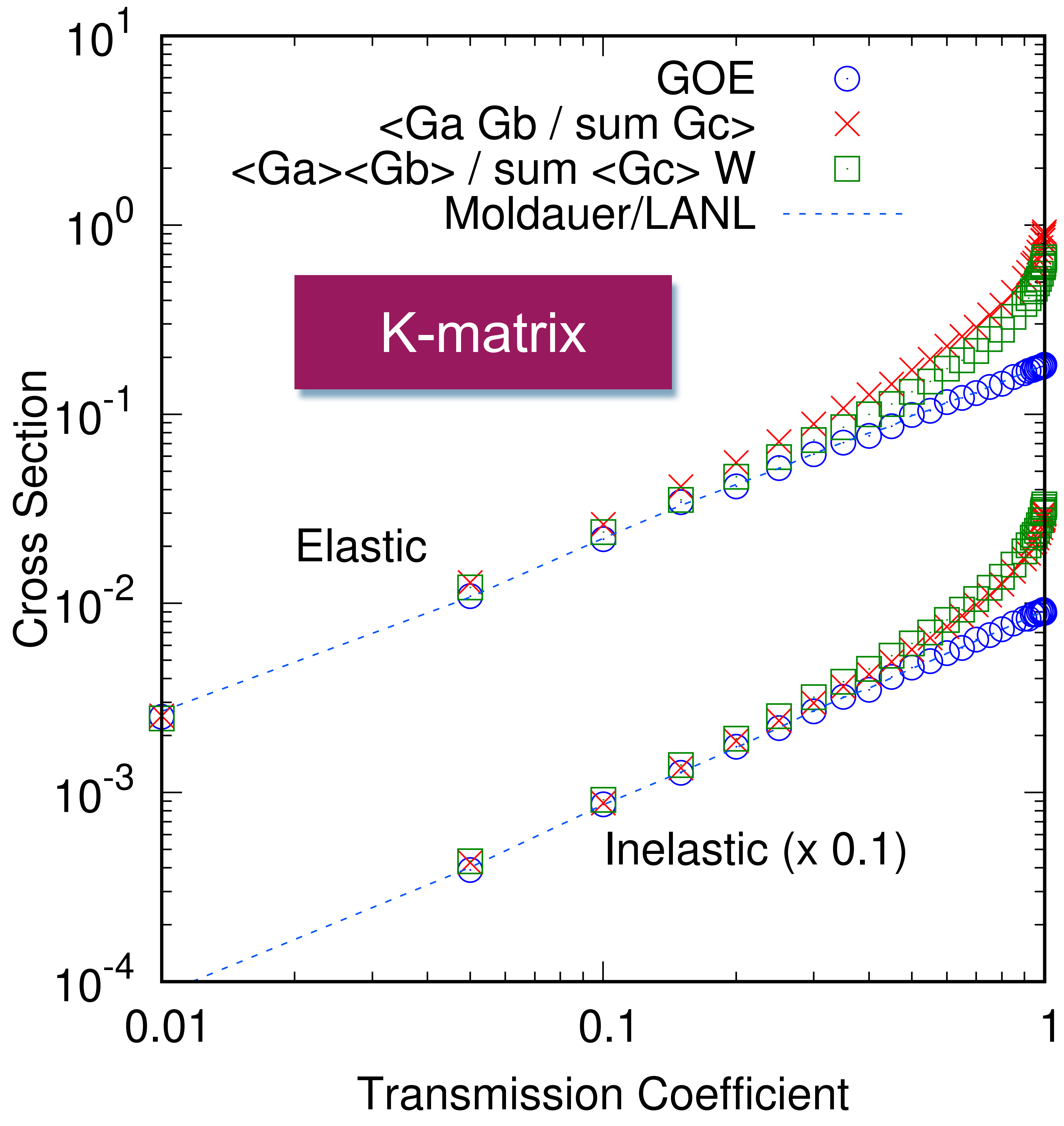
weak coupling case

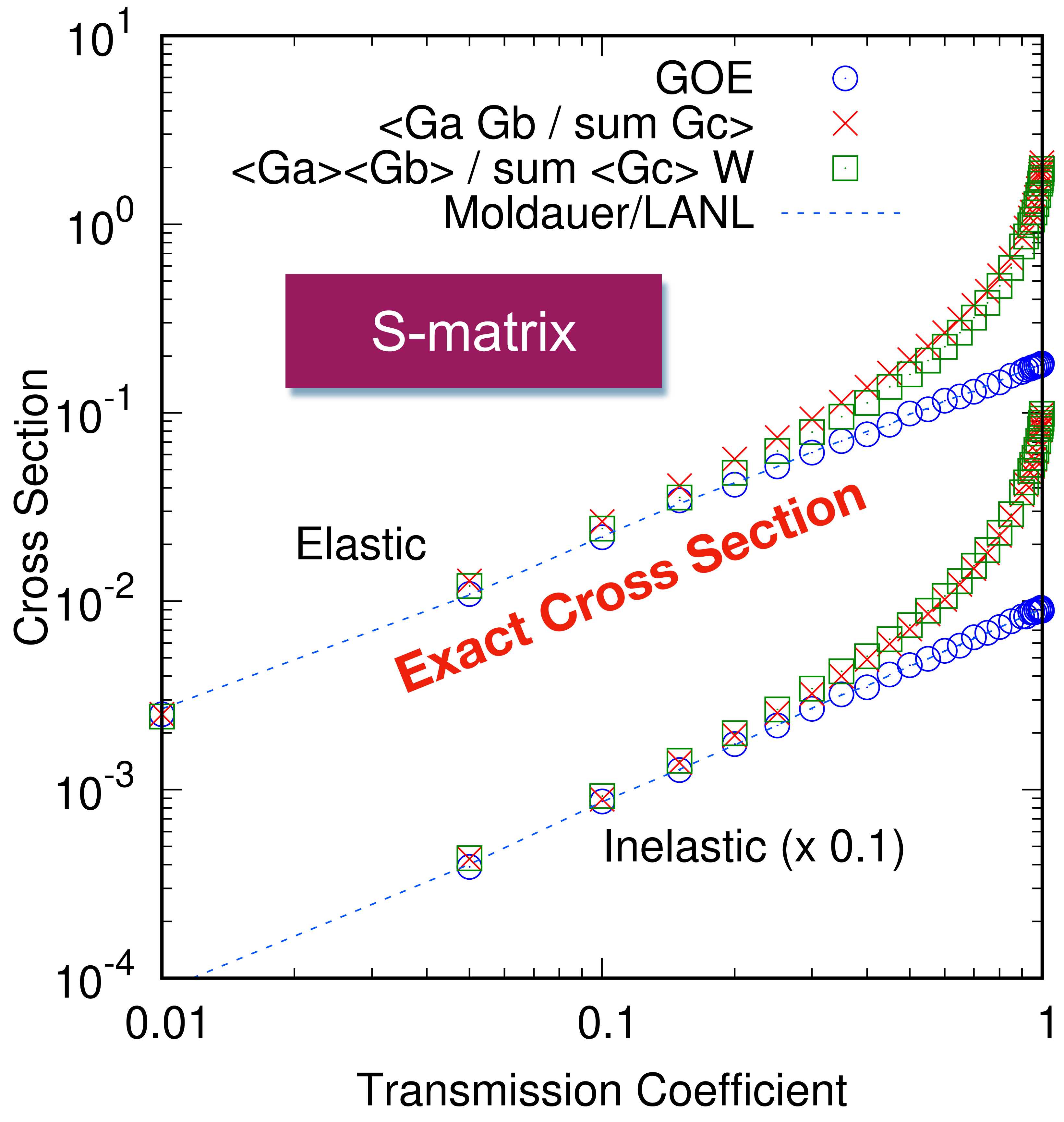


strong coupling case



Can We Express Cross Section in Terms of <Γ> ?





$$\sigma_1 = \frac{2\pi}{D}\left\langle \frac{\Gamma_a \Gamma_b}{\sum_c \Gamma_c} \right\rangle$$

$$\sigma_2 = \frac{2\pi}{D}\frac{\langle\Gamma_a\rangle\langle\Gamma_b\rangle}{\sum_c \langle\Gamma_c\rangle} W_{ab}$$

$$\sigma_3 = \frac{T_a T_b}{\sum_c T_c} W_{ab}$$

$$\frac{2\pi}{D}\left\langle \frac{\Gamma_a \Gamma_b}{\sum_c \Gamma_c} \right\rangle = \frac{2\pi}{D}\frac{\langle\Gamma_a\rangle\langle\Gamma_b\rangle}{\sum_c \langle\Gamma_c\rangle} W_{ab} \neq \frac{T_a T_b}{\sum_c T_c} W_{ab}$$

The compound cross section derived from the decay widths is ambiguous when the transmission coefficient is large (strong coupling

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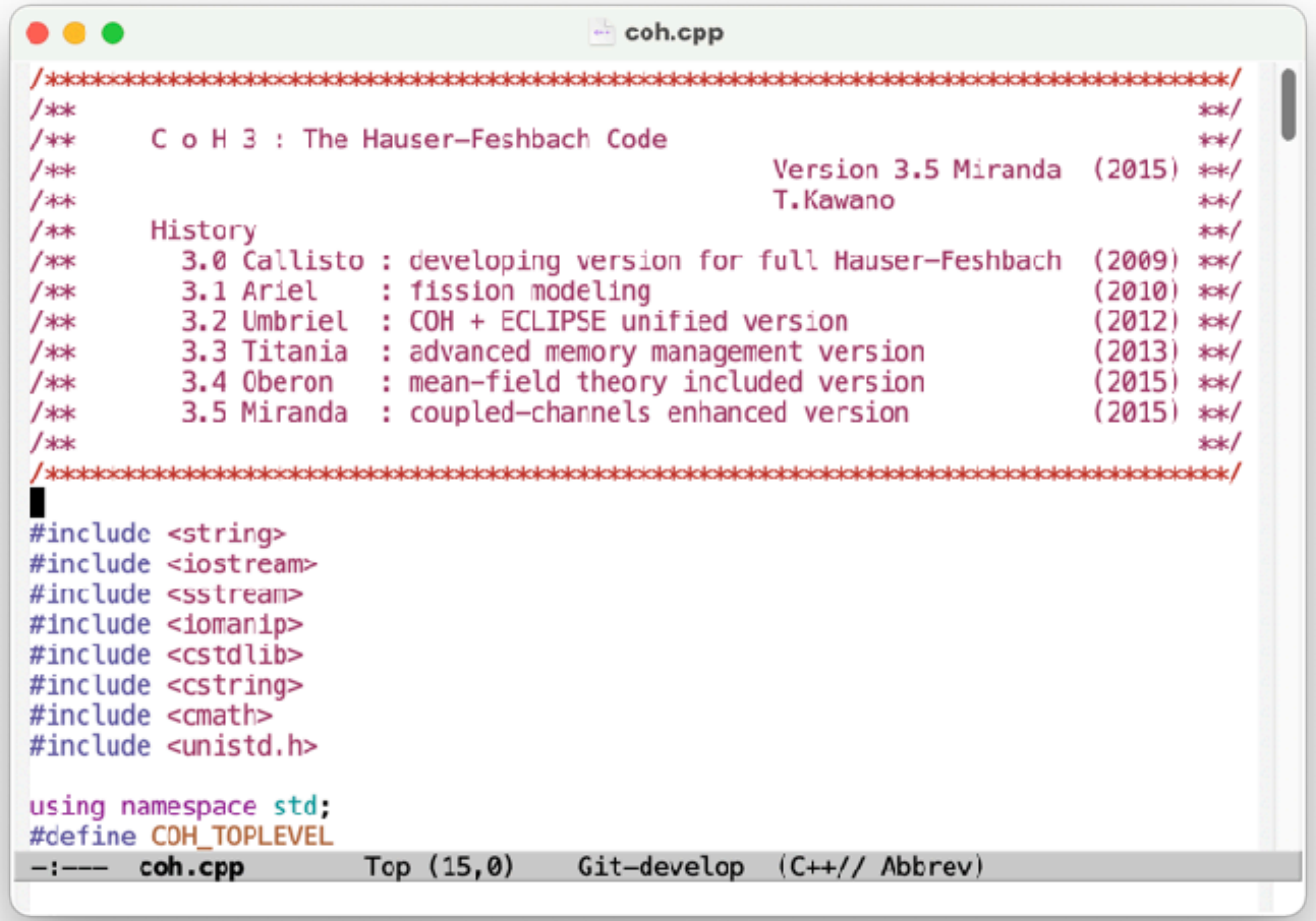
Coupled-Channels and Hauser-Feshbach Code CoH_3

- **Hauser-Feshbach-Moldauer theory for compound reaction**
  - 50k+ lines C++ code, including ~140 source and ~60 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



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Modules and Models in CoH$_3$

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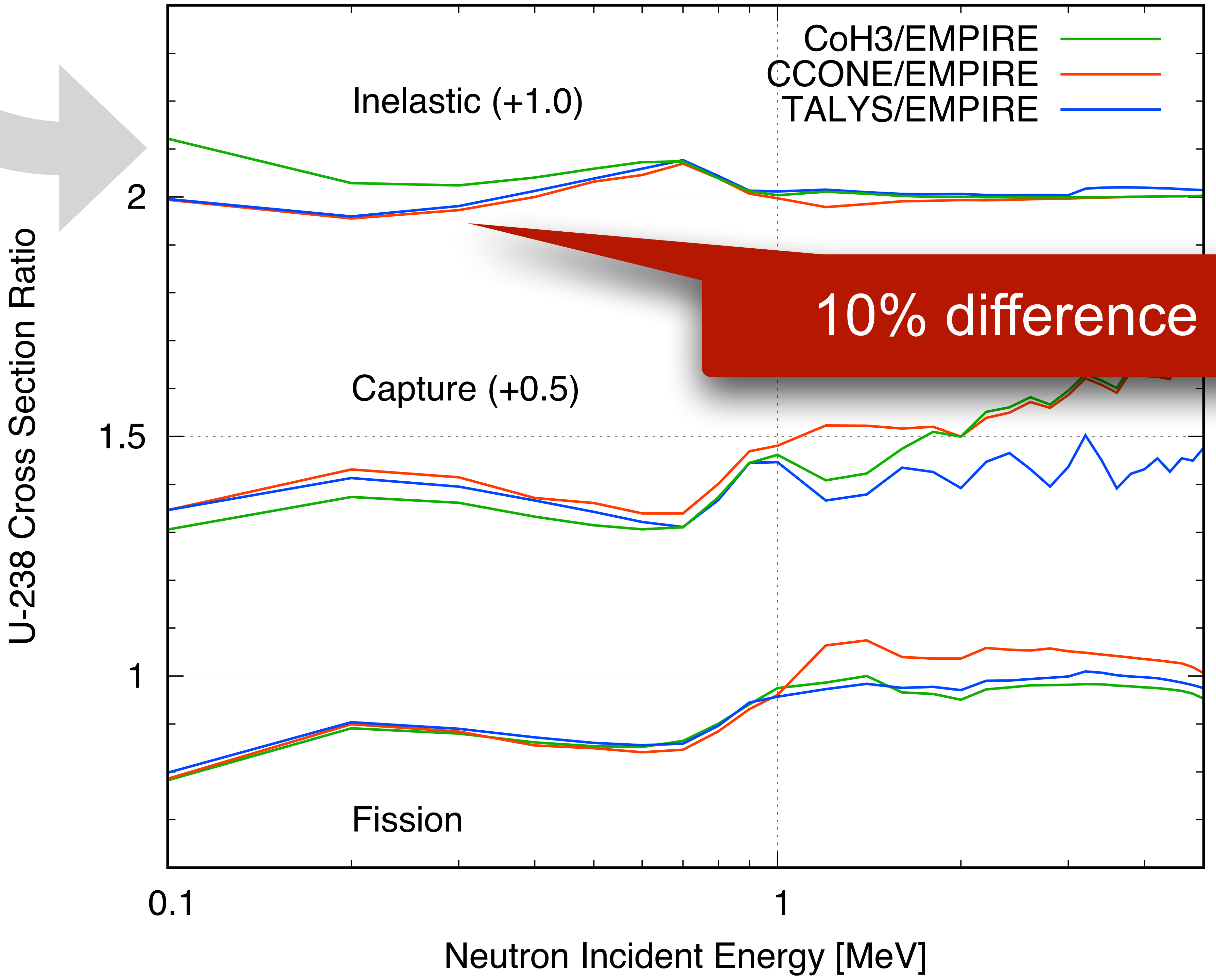
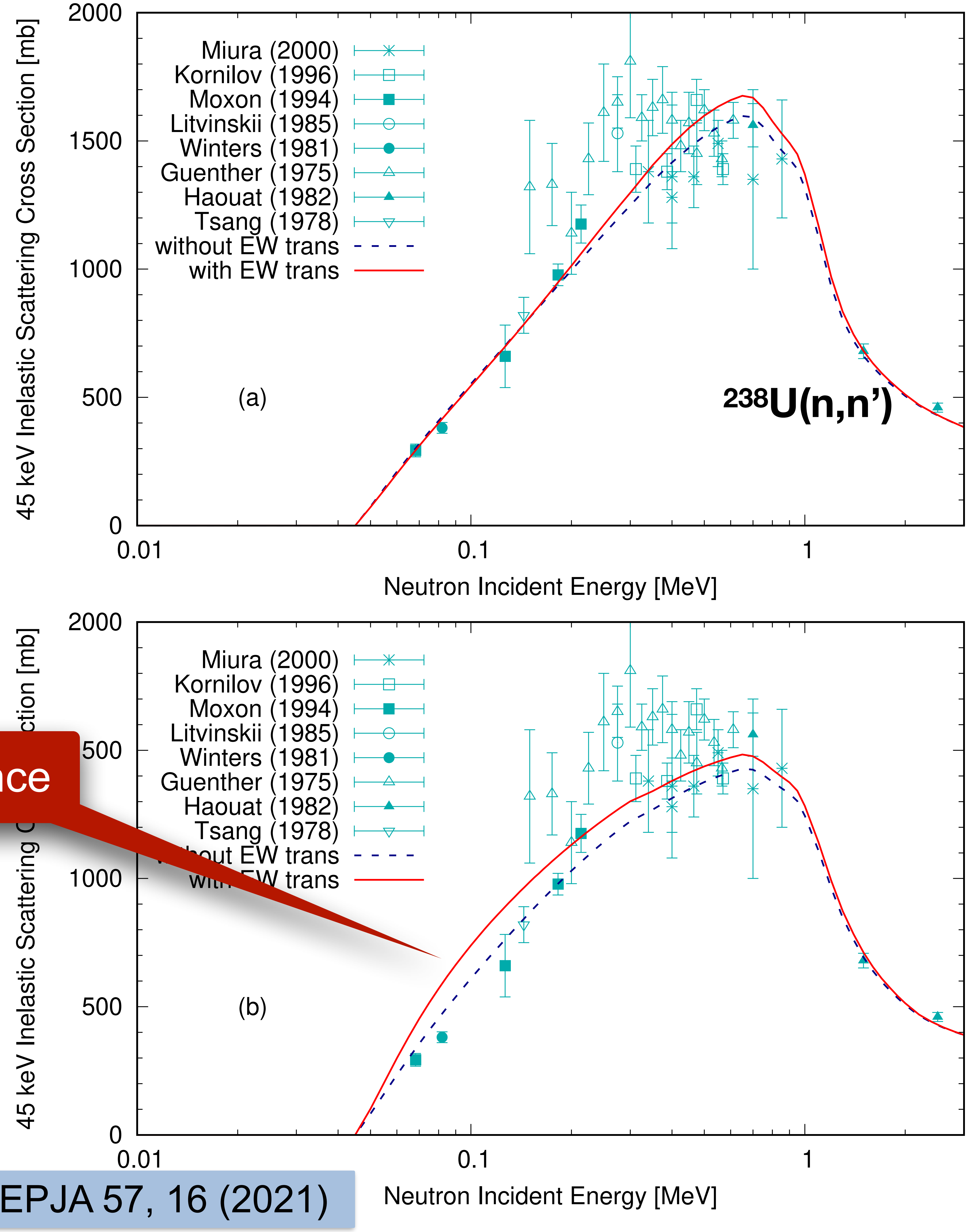
Inelastic Scattering Calculation for ^{238}U at Low Energies

- **Coupled-channels optical model provides S-matrix including off-diagonal elements**
  - Generalized transmission coefficients from P-matrix
  - Engelbrecht-Weidenmueller transformation for the width fluctuation correction





Code comparison at ND2016

T. Kawano, EPJA 57, 16 (2021)

Concluding Remarks

- **Unification of the coupled-channels optical model and the statistical Hauser-Feshbach theory**
  - Calculate generalized transmission coefficients from the coupled-channels S-matrix
  - Width fluctuation calculation in the diagonalized channel space
    - by performing Engelbrecht-Weidenmuller (EW) transformation
    - GOE model for studying relation between transmission coefficient and cross section
    - explicit inclusion of uncoupled channels
- **Applied to deformed nuclei - ^{169}Tm (even-odd) and ^{238}U (even-even)**
  - CoH$_3$ code includes these new developments
  - Both the generalized transmission coefficients and the EW transformation increase the neutron inelastic scattering cross section when strongly coupled direct reaction channels exist
  - This happens due to the fact that contributions from each partial wave are different, and that constraints by the unitarity of S-matrix is somewhat relaxed