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SMR.1555 - 22

**Workshop on
Nuclear Reaction Data and Nuclear Reactors:
Physics, Design and Safety**

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**RIPL Database +
Statistical Model of Nuclear Reactions**

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These are preliminary lecture notes, intended only for distribution to participants



EMPIRE-II **statistical model**

(version: 2.18 Mondovi)
(version: 2.19beta12 Lodi)

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Contents

- Introduction
- Huser-Feshbach
- Width fluctuations
 - Moldauer
 - HRTW
 - triple integral
- relation to other reaction models
- Implementation in EMPIRE

Statistical theory of nucl. reactions

Compound Nucleus formation

- multiple scattering of a projectile with target nucleons and among target nucleons =>
- many nucleons excited around the Fermi level =>
- relatively low excitation energy per particle =>
- low probability of particle emission =>
- enough time for mixing of configurations

Statistical theory of nucl. reactions

Main features

- long life-time ($\sim 10^{-18}$ sec.)
- initial and final channel factorization (lost memory)
- symmetric angular distributions
- time independence

Formal development

“At the beginning there was chaos”

$$S_{ab}^{fl} = S_{ab} - \langle S_{ab} \rangle$$

$$\langle \sigma_{ab} \rangle = |\delta_{ab} - \langle S_{ab} \rangle|^2 + \langle |S_{ab}^{fl}|^2 \rangle = \sigma_{ab}^{dir} + \sigma_{ab}^{fl}$$

$\langle S_{ab} \rangle$ known from Optical Model

Goal of statistical theory

express: $\langle |S_{ab}^{fl}|^2 \rangle$ in terms of $\langle S_{ab} \rangle$

Elimination of dir. reactions

$$P = 1 - \langle S \rangle \langle S^+ \rangle$$

if U diagonalizes P it does it also for S

$$\tilde{S} = USU^T$$

$$\langle |S_{ab}^{fl}|^2 \rangle = \sum_{efgh} U_{ea}^* U_{fb}^* U_{ga} U_{hb} \langle \tilde{S}_{ef}^{fl} \tilde{S}_{gh}^{fl*} \rangle$$

This elimination is **NOT** performed in EMPIRE

Huaser-Feshbach formula

$$T_a = 1 - | \langle S_{aa} \rangle |^2$$

unitarity of S-matrix

$$T_a = \sum_{b=1}^{\Lambda} \sigma_{ab}^{fl}$$

Bohr's hypothesis

$$\sigma_{ab}^{fl} = \frac{T_a T_b}{\sum_c^{\Lambda} T_c}$$

Width fluctuation correction

elastic channel is correlated

$$\sigma_{ab}^{fl} = \frac{V_a V_b W_{ab}}{\sum_{c=1}^{\Lambda} V_c}$$

pole expansion of S-matrix

$$S_{ab}(E) = S_{ab}^0 - i \sum_{\mu=1}^N \frac{g_{\mu a} g_{\mu b}}{E - \epsilon_{\mu} + i\Gamma_{\mu}/2}$$

Width fluctuation (cont.)

transmission coefficient

$$T_c \simeq 2\pi \langle |g_{\mu c}|^2 \rangle_{\mu} / D$$

Compound Nucleus cross section

$$\sigma_{ab}^{fl} \simeq \frac{T_a T_b W_{ab}}{\sum_c T_c}$$

Width fluctuation (cont.)

the width fluctuation factor is

$$W_{ab} = \left\langle \frac{|g_{\mu a}|^2 |g_{\mu b}|^2}{\Gamma_{\mu}} \right\rangle_{\mu} \left(\frac{\langle |g_{\mu a}|^2 \rangle_{\mu} \langle |g_{\mu b}|^2 \rangle_{\mu}}{\langle \Gamma_{\mu} \rangle_{\mu}} \right)^{-1}$$

Width fluctuation (cont.)

if fluctuations of Γ_μ are neglected elastic enhancement reads

$$W_a = \frac{\langle |g_{\mu a}|^4 \rangle}{\langle |g_{\mu a}|^2 \rangle \langle |g_{\mu a}|^2 \rangle}$$

and

$$W_a = 3 \text{ for } T_a \ll 1$$

$$W_a = 2 \text{ for } T_a \simeq 1$$

WF - Moldauer approach

$$W_{ab} = (1 + 2\delta_{ab}/\nu_a) \times \int_0^\infty dt \prod_{c=1}^N \left(1 + \frac{2tT_c}{\nu_c \sum_d T_d} \right)^{-\frac{1}{2} - \delta_{ca} - \delta_{cb}}$$

Moldauer had found

$$\nu_c = 1.78 + (T_c^{1.212} - 0.78) e^{-0.228 \sum_a T_a}$$

Moldauer approach is **NOT** used in EMPIRE-II

WF - the HRTW approach

In the case of no direct reactions

$$\langle S \rangle_{ab} = \delta_{ab} e^{i\zeta_{ab}} (1 - T_a)^{1/2}$$

$$T_a = 1 - |\langle S \rangle_{aa}|^2$$

HRTW model assumes cross sections
factorization

$$\langle \sigma_{ab}^{fl} \rangle = \xi_a \xi_b \quad a \neq b \quad \text{and} \quad \langle \sigma_a^{fl} \rangle = W_a \xi_a^2$$

WF - the HRTW approach

Setting

$$\xi_a = \frac{V_a}{\sqrt{\sum_c V_c}}$$

we get for the CN cross section

$$\sigma_{ab}^{CN} = [1 + \delta_{ab} (W_a - 1)] \frac{V_a V_b}{\sum_c V_c}$$

WF - the HRTW approach

Taking into account flux conservation (unitarity condition)

$$V_a = T_a \left[1 + \frac{V_a}{(\sum_c V_c)} (W_a - 1) \right]^{-1}$$

Can be solved for V_a by iteration once all W_a are known

WF - the HRTW approach

K-matrix representation

$$S = \frac{(1 + iK)}{(1 - iK)}$$

$$K_{ab} = K_{ab}^0 + \sum_{\mu=1}^N \frac{\gamma_{\mu a} \gamma_{\mu b}}{E_{\mu} - E}$$

$\gamma_{\mu a}$ and E_{μ} are real and uncorrelated, K_0 - direct reactions

WF - the HRTW approach

Numerical experiment:

$\gamma_{\mu a}$ - drawn randomly with normal distribution

E_{μ} - spacing ($x = E_{\mu} - E_{\mu+1}$) according to the Wigner distribution

$$Q_W(x)dx = \frac{\pi}{2} \exp\left(-\frac{\pi x^2}{4}\right) dx$$

$$T = \frac{4\pi \langle \gamma^2 \rangle / D}{(1 + \pi \langle \gamma^2 \rangle / D)^2}$$

Generate ensemble of K-matrices \Rightarrow S-matrices

$\Rightarrow \langle S \rangle \Rightarrow \sigma_{ab}$

HRTW (cont.)

V_a can be found by iteration with W_a given by:

$$W_a = 1 + 2 \left[1 + T_a^F \right]^{-1} + 87 \left(\frac{T_a - T_{ave}}{\sum_c T_c} \right)^2 \left(\frac{T_a}{\sum_c T_c} \right)^5$$

with

$$F = 4 \frac{T_{ave}}{\sum_c T_c} \left(1 + \frac{T_a}{\sum_c T_c} \right) \left(1 + 3 \frac{T_{ave}}{\sum_c T_c} \right)^{-1}$$

By default, the HRTW model is applied below 5 MeV incident energy. Users have the option to apply it at all energies or to turn it off.

Triple integral

$$\begin{aligned} & \langle S_{ab}(E_1) S_{cd}^*(E_2) \rangle & = \\ & \langle S_{ab}(E_1) \rangle \langle S_{cd}^*(E_2) \rangle & + \\ & \frac{1}{8} \int_0^\infty d\lambda_1 \int_0^\infty d\lambda_2 \int_0^1 d\lambda & \times \\ & \frac{(1-\lambda)\lambda|\lambda_1-\lambda_2|}{[(1+\lambda_1)\lambda_1(1+\lambda_2)\lambda_2]^{1/2}(\lambda+\lambda_2)^2(\lambda+\lambda_2)^2} & \times \\ & \exp[-i\pi(E_2^* - E_1)(\lambda_1 + \lambda_2 + 2\lambda)/d] & \times \\ & \prod_{e=1}^{\Lambda} \frac{(1-T_e\lambda)}{[(1+T_e\lambda_1)(1+T_e\lambda_2)]^{1/2}} & \times \end{aligned}$$

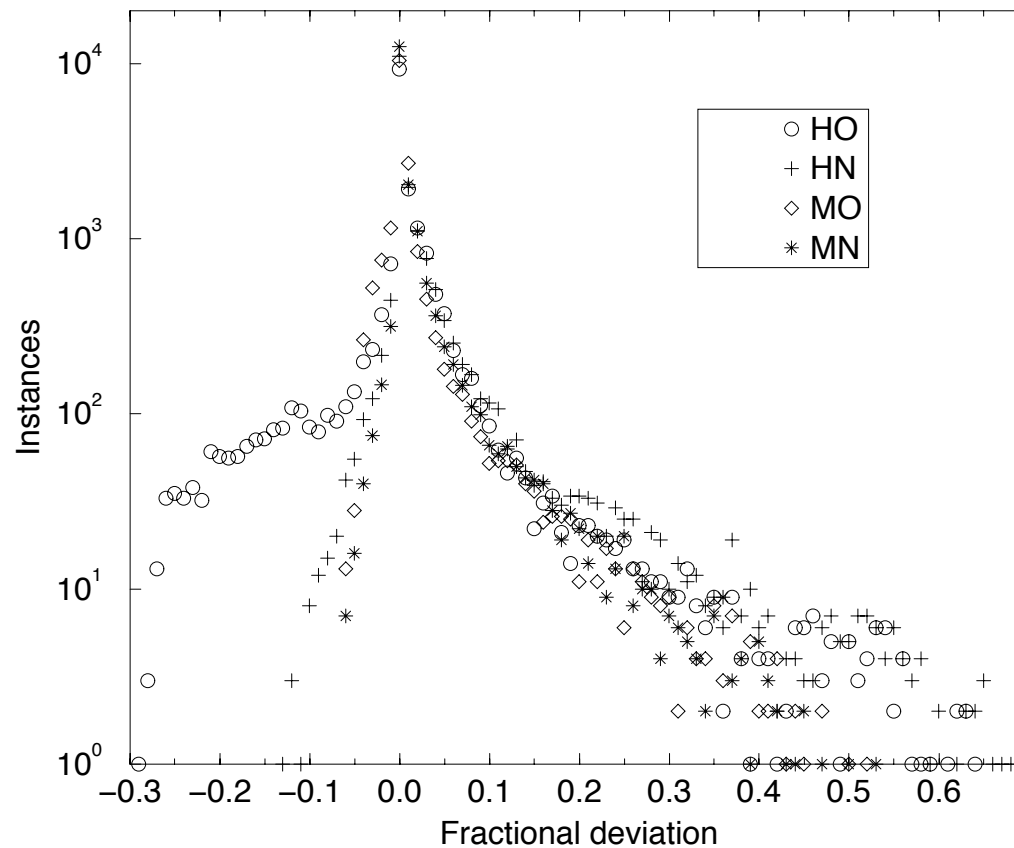
Triple integral (cont.)

$$\begin{aligned}
 & \{ \delta_{ab} \delta_{cd} \langle S_{aa} \rangle \langle S_{cc} \rangle T_a T_c \quad \times \\
 & \left(\frac{\lambda_1}{1+T_a \lambda_1} + \frac{\lambda_2}{1+T_a \lambda_2} + \frac{2\lambda}{1+T_a \lambda} \right) \quad \times \\
 & \left(\frac{\lambda_1}{1+T_c \lambda_1} + \frac{\lambda_2}{1+T_c \lambda_2} + \frac{2\lambda}{1+T_c \lambda} \right) + (\delta_{ac} \delta_{bd} + \delta_{ad} \delta_{bc}) T_a T_c \quad \times \\
 & \left[\frac{\lambda_1(1+\lambda_1)}{(1+T_a \lambda_1)(1+T_b \lambda_1)} + \frac{\lambda_2(1+\lambda_2)}{(1+T_a \lambda_2)(1+T_b \lambda_2)} \right. \\
 & \left. \frac{2\lambda(1+\lambda)}{(1+T_a \lambda)(1+T_b \lambda)} \right] \quad +
 \end{aligned}$$

NOT used in EMPIRE

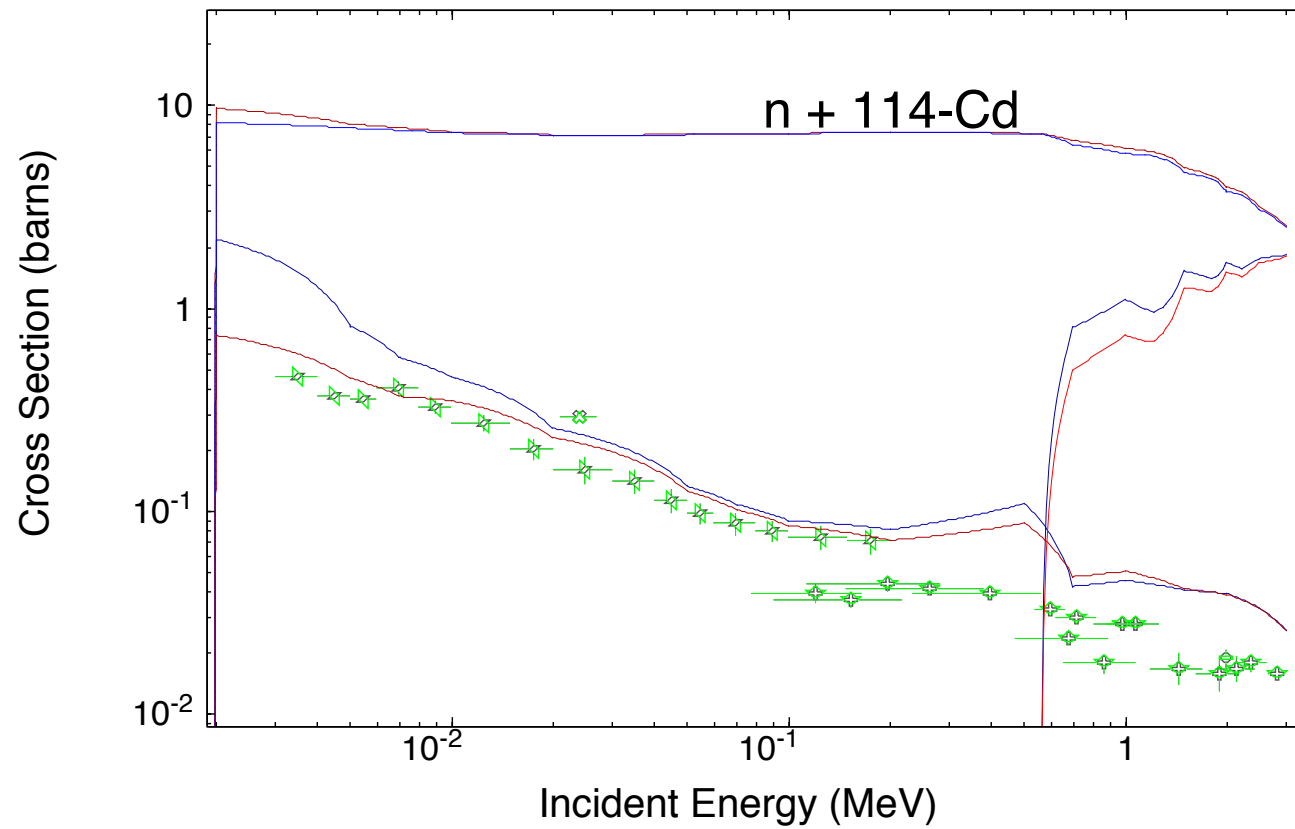
Validation of approx. approaches

Deviations of HRTW & Moldauer from the Triple Integral (≈ 8000 cases)



Effect of HRTW

elastic, inelastic, capture



CN and other nuclear models

- **Optical Model** - provides averaged S-matrix (transmission coefficients)
- **Direct Reaction Models** - provides averaged S-matrix including off-diagonal elements
- **Preequilibrium emission** - CN formation mechanism, reduction of the CN absorption cross section

CN and other nuclear models

- **Shell Model** - basis for the CN development
- **Fermi Gas and BCS** - determination of level densities
- **Nuclear Structure** - discrete level schemes, γ -transition probabilities
- **Liquid Drop + Shell Model** - binding energies, shell corrections, fission barriers, nuclear shape

Hauser-Feshbach in EMPIRE

- Each Compound Nucleus state contributes with a cross section

$$\sigma_b(E, J, \pi) = \sigma_a(E, J, \pi) \frac{\Gamma_b(E, J, \pi)}{\sum_c \Gamma_c(E, J, \pi)}$$

These have to be summed over spin J and parity π , and integrated over excitation energy E (in case of daughter CN)

HF in EMPIRE (cont.)

- Particle decay width

$$\Gamma_c(E, J, \pi) = \frac{1}{2\pi\rho_{CN}(E, J, \pi)} \sum_{J'=0}^{\infty} \sum_{\pi'} \sum_{j=J'-J}^{J+J'} \int_0^{E-B_c} \rho_c(E', J', \pi') T_c^{l,j}(E - B_c - E') dE',$$

B_c - binding energy of particle c ,

ρ - level density (for discrete levels

$$\rho = \delta(E - E_i) \delta_{(J', J_i)} \delta_{(\pi', \pi_i)}$$

$T_c^{l,j}(\epsilon)$ - transmission coefficient,

HF in EMPIRE (cont.)

- Gamma decay width assumed to be a mixture of single-particle estimate and Giant Resonance contributions

$$T_{Xl} = (1 - t)T_{Xl}^{Weiss} + tT_{Xl}^{GMR}$$

Single-particle estimates (Weisskopf):

$$T_{E1}^{Weiss} = C_{E1} 4.599^{-7} A^{2/3} E_{\gamma}^3 [MeV^{-3}]$$

$$T_{M1}^{Weiss} = C_{M1} 1.3^{-7} E_{\gamma}^3 [MeV^{-3}]$$

HRTW implementation

HRTW is applied to each J^π state in the highest energy bin in the first CN

- fusion cross section to J^π has to be decomposed into its l components
- first sweep: T_l for all channels are stored and elastic channels are recorded
- second sweep: V_l and HF-type denominator are calculated, elastic channels enhanced
- third sweep: partial widths are normalized

Conclusions

EMPIRE contains a fairly complete implementation of statistical model

- angular momentum coupling (although T_l scheme is used rather than T_{lj})
- Width fluctuation correction
- multiple emission of n, p, α , γ , and optionally one light ion (d, ^3He , t, etc.)
- full γ -cascade
- treatment of discrete levels (isomeric cross sections)