

Statistical Theory of Nuclear Reactions, Channel Widths and Level Densities

# S. Hilaire - CEA, DAM, DIF

TRIESTE 2014 – S. Hilaire & The TALYS Team – 23/09/2014

www.cea.fr



## Content

## - Introduction

#### TODAY

## - General features about nuclear reactions

- Time scales and associated models
- Types of data needed
- Data format = f (users)

# - Nuclear Models

- Basic structure properties
- Optical model
- Pre-equilibrium model
- Compound Nucleus model
- Miscellaneous : level densities, fission, capture

# - From in depth analysis to large scale production with TALYS

- General features about TALYS
- Fine tuning and accuracy
- Global systematic approaches
- What remains to be done ?

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### INTRODUCTION





Available online at www.sciencedirect.com



Nuclear Data Sheets 110 (2009) 3107-3214

Nuclear Data Sheets

www.elsevier.com/locate/nds

#### RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

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(Received July 20, 2009)

We describe the physics and data included in the Reference Input Parameter Library, which is devoted to input parameters needed in calculations of nuclear reactions and nuclear data evaluations. Advanced modelling codes require substantial numerical input, therefore the International Atomic Energy Agency (IAEA) has worked extensively since 1993 on a library of validated nuclear-model input parameters, referred to as the Reference Input Parameter Library



# Nuclear data needed for

### Understanding basic reaction mechanism between particles and nuclei

Good accuracy if possible  $\Rightarrow$  good understanding or room for improvements

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Understanding basic reaction mechanism between particles and nuclei Astrophysical applications (Age of the Galaxy, element abundances ...)

Good accuracy if possible  $\Rightarrow$  good understanding or room for improvements Predictive power important  $\Rightarrow$  sound physics (first principles)

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Understanding basic reaction mechanism between particles and nuclei Astrophysical applications (Age of the Galaxy, element abundances ...) Existing or future nuclear reactor simulations

Good (Excellent) accuracy required  $\Rightarrow$  reproduction of data, safety Predictive power less important  $\Rightarrow$  Reproductive power

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Understanding basic reaction mechanism between particles and nuclei Astrophysical applications (Age of the Galaxy, element abundances ...) Existing or future nuclear reactor simulations Medical applications, oil well logging, waste transmutation, fusion, ...

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# Nuclear data needed for

Understanding basic reaction mechanism between particles and nuclei Astrophysical applications (Age of the Galaxy, element abundances ...) Existing or future nuclear reactor simulations Medical applications, oil well logging, waste transmutation, fusion, ...

# But

Finite number of experimental data (price, safety or counting rates) Complete measurements restricted to low energies ( < 1 MeV) to scarce nuclei



Predictive & Robust Nuclear models (codes) are essential

## GENERAL FEATURES ABOUT NUCLEAR REACTIONS



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### TIME SCALES AND ASSOCIATED MODELS (1/4) Typical spectrum shape

62 MeV<sup>56</sup>Fe (p,xp) Double differential cross sections



- Always evaporation peak
- Discrete peaks at forward angles
- Flat intermediate region



**Reaction time** 

## TIME SCALES AND ASSOCIATED MODELS (2/4)



## TIME SCALES AND ASSOCIATED MODELS (2/4)





#### Direct (shape) elastic



TIME SCALES AND ASSOCIATED MODELS (4/4)



# TYPES OF DATA NEEDED

### **Cross sections :**

total, reaction, elastic (shape & compound), non-elastic, inelastic (discrete levels & total) total particle (residual) production all exclusive reactions (n,nd2a) all exclusive isomer production all exclusive discrete and continuum  $\gamma$ -ray production

#### Spectra :

elastic and inelastic angular distribution or energy spectra all exclusive double-differential spectra total particle production spectra compound and pre-equilibrium spectra per reaction stage.

#### **Fission observables :**

cross sections (total, per chance) fission fragment mass and isotopic yields fission neutrons (multiplicities, spectra)

#### Miscellaneous :

recoil cross sections and ddx particle multiplicities astrophysical reaction rates covariances informations



- Trivial for basic nuclear science : x,y,(z) file
- Complicated (even crazy) for data production issues : ENDF file

## **DATA FORMAT : ENDF file**

### **Content nature (**σ**)**

1

6,215100+4 1	1,496234+2	0	0	0	06210	3	16	350
-5,596445+6-5	5,596445+6	0	0	1	1336210	3	16	351
133	2				6210	3	16	352
5,633849+6 (	0+000000+0	5,700000+6	1,580180-3	5,800000+6	6,073681-36210	3	16	353
5,900000+6 1	1,347960-2	6,000000+6	2,690410-2	6,100000+6	4,687551-26210	3	16	354
6,200000+6 7	7,598900-2	6,300000+6	1,119810-1	6,400000+6	1,518520-16210	3	16	355
6.500000+6 2	2.016680-1	6,600000+6	2.528690-1	6,700000+6	3,144490-16210	3	16	356
6,800000+6 3	3,780410-1	6,900000+6	4,433380-1	7,000000+6	5,136740-16210	3	16	357
7,100000+6 5	5.833550-1	7,200000+6	6.576591-1	7,300000+6	7,306390-16210	3	16	358
7,400000+6 8	3.033710-1	7,500000+6	8.746620-1	7,600000+6	9,434911-16210	3	16	359
7,700000+6 1	1,010920+0	7,800000+6	1,078550+0	7,900000+6	1,140340+06210	3	16	360
8.000000+6 1	1,202710+0	8,100000+6	1.257750+0	8,200000+6	1,313880+06210	3	16	361
8,300000+6 1	1,367080+0	8,400000+6	1,416210+0	8,500000+6	1,463580+06210	3	16	362
8,600000+6 1	1.506400+0	8,700000+6	1.546900+0	8,800000+6	1,586770+06210	3	16	363
8,900000+6 1	1,623670+0	9,000000+6	1,656720+0	9,100000+6	1,687830+06210	3	16	364
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9,500000+6 1	1,796050+0	9,600000+6	1,817200+0	9,700000+6	1,837390+06210	3	16	366
9,800000+6 1	1.858090+0	9,900000+6	1.876590+0	1,000000+7	1,893530+06210	3	16	367

### **DATA FORMAT : ENDF file**

6,215100+4	1,496234+2	0	0	0	06210	3	16	350
-5,596445+6	-5,596445+6	0	0	1	1336210	3	16	351
133	2				6210	3	16	352
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8,600000+6	1.506400+0	8,700000+6	1.546900+0	8,800000+6	1,586770+06210	3	16	363
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9,800000+6	1.858090+0	9,900000+6	1.876590+0	1.000000+7	1,893530+06210	3	16	367

**Content type (n,2n)** 

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6,215100+4	1,496234+2	0	0	0	<b>0</b> 62	210	3 16	350
-5,596445+6	-5,596445+6	0	0	1	133 <mark>62</mark>	210	3 16	351
133	2				62	210	3 16	352
5,633849+6	0,000000+0	5,700000+6	1,580180-3	5,800000+6	-6₊073681- <mark>36</mark> 2	210	3 16	353
5,900000+6	1.347960-2	6,000000+6	2,690410-2	6,100000+6	4.687551-2 <mark>62</mark>	210	3 16	354
6,200000+6	7,598900-2	6,300000+6	1,119810-1	6,400000+6	1.518520-1 <mark>62</mark>	210	3 16	355
6,500000+6	2,016680-1	6,600000+6	2,528690-1	6,700000+6	3,144490-1 <mark>6</mark> 2	210	3 16	356
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7,700000+6	1,010920+0	7,800000+6	1,078550+0	7,900000+6	1,140340+0 <mark>6</mark> 2	210 -	3 16	360
8,000000+6	1,202710+0	8,100000+6	1,257750+0	8,200000+6	1.313880+0 <mark>6</mark> 2	210 -	3 16	361
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8,600000+6	1.506400+0	8,700000+6	1.546900+0	8,800000+6	1.586770+0 <mark>6</mark> 2	210 -	3 16	363
8,900000+6	1,623670+0	9,000000+6	1,656720+0	9,100000+6	1.687830+0 <mark>62</mark>	210	3 16	364
9,200000+6	1.717430+0	9,300000+6	1.745200+0	9,400000+6	1.771480+0 <mark>6</mark> 2	210 -	3 16	365
9,500000+6	1,796050+0	9,600000+6	1,817200+0	9,700000+6	1 <sub>+</sub> 837390+0 <mark>62</mark>	210	3 16	366
9,800000+6	1,858090+0	9,900000+6	1,876590+0	1.000000+7	1.893530+0 <mark>6</mark> 2	210 -	3 16	367

Material number

### **Target identification (**<sup>151</sup>**Sm)**

-								
6,215100+4	1,496234+2	0	0	0	06210	3	16	350
-5,596445+6-	-5,596445+6	0	0	1	1336210	3	16	351
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**Target mass** 

		_						
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6,215100+4	1,496234+2	0	0	0	06210	3	16	350
-5,5964 <u>45+6</u>	-5,596445+6	0	0	1	1336210	3	16	351
133	2				6210	3	16	352
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9,800000+6	1.858090+0	9,900000 /3	1.876590+0	1,000000+7	1,893530+06210	3	16	367

Number of values

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	8,000000+6	1,202710+0	8,100000+6	1,257750+0	8,200000+6	1,313880+06210	3	16	361
	8,300000+6	1,367080+0	8,400000+6	1,416210+0	8,500000+6	1,463580+06210	3	16	362
	8,600000+6	1,506400+0	8,700000+6	1.546900+0	8,800000+6	1,586770+06210	3	16	363
	8,900000+6	1,623670+0	9,000000+6	1,656720+0	9,100000+6	1,687830+06210	3	16	364
	9,200000+6	1.717430+0	9.300000+6	1.745200+0	9,400000+6	1.771480+06210	3	16	365
	9.500000+6	1.796050+0	9.600000+6	1.817200+0	9.700000+6	1.837390+06210	3	16	366
	9.800000+6	1.858090+0	9.900000+6	1.876590+0	1.000000+7	1.893530+06210	3	16	367
	•	• • •	•	• •		••	-		

**Values** 

### NUCLEAR MODELS



- Introduction

## - General features about nuclear reactions

- Time scales and associated models
- Types of data needed
- Data format = f (users)

# - Nuclear Models

- Basic structure properties
- Optical model
- Pre-equilibrium model
- Compound Nucleus model
- Miscellaneous : level densities, fission, capture
- From in depth analysis to large scale production with TALYS
  - General features about TALYS
  - Fine tuning and accuracy
  - Global systematic approaches
- What remains to be done ?



## BASIC STRUCTURE PROPERTIES (1/5) What is needed

### Nuclear Masses :

 $\Rightarrow$  basic information to determine reaction threshold

### **Excited levels :**

- ⇒ Angular distributions (depend on spin and parities)
- $\Rightarrow$  Decay properties (branching ratios)
- $\Rightarrow$  Excitation energies (reaction thresholds)

#### **Target levels' deformations :**

- $\Rightarrow$  Required to select appropriate optical model
- $\Rightarrow$  Required to select appropriate coupling scheme

# Many different theoretical approaches if experimental data is missing Recommended databases (RIPL !)







 $rms(M) = 600-700 \text{ keV on } 2149 \text{ (} Z \ge 8\text{)}$  experimental masses



### **BASIC STRUCTURE PROPERTIES (3/5)** Mass models predictive power

Comparison between several mass models adjusted with 2003 exp and tested with 2012 exp masses



### BASIC STRUCTURE PROPERTIES (4/5) HFB Mass models

**Most advanced theoretical approach = multireference level** 

• Methodology : E =  $E_{mf} + \delta E_{\infty} + \delta E_{bmf}$ 



### \* Additional filters

- Collective properties (0+,2+, BE2), RPA modes, backbending properties, pairing properties, fission properties, gamma strength functions, level densities


## BASIC STRUCTURE PROPERTIES (5/5) HFB-Gogny Mass model

Cez





#### Direct (shape) elastic









Direct interaction of a projectile with a target nucleus considered as a whole Quantum model  $\rightarrow$  Schrödinger equation





Direct interaction of a projectile with a target nucleus considered as a whole Quantum model  $\rightarrow$  Schrödinger equation





## The optical model yields :



## **TWO TYPES OF APPROACHES**

#### Phenomenological

Adjusted parameters Weak predictive power Very precise ( ≈ 1%) Important work

## (Semi-)microscopic

No adjustable parameters Usable without exp. data Less precise (  $\approx$  5-10 %) Quasi-automated





## PHENOMENOLOGICAL OPTICAL MODEL

- $\approx$  20 adjusted parameters
- Very precise (1%)

92

- Weak predictive power





# SEMI-MICROSCOPIC OPTICAL MODEL

- No adjustable parameters
- Based on nuclear structure properties
  - $\Rightarrow$  usable for any nucleus
- Less precise than the phenomenological approach



## SEMI-MICROSCOPIC OPTICAL MODEL







Unique description of elastic scattering



Unique description of elastic scattering (n,n)





Unique description of elastic scattering (n,n), (p,p)





Unique description of elastic scattering (n,n), (p,p) and (p,n)



## SEMI-MICROSCOPIC OPTICAL MODEL

07

Enables to give predictions for very exotic nuclei for which there exist no experimental data







THE PRE-EQUILIBRIUM MODEL

#### Shape elastic

/





## THE PRE-EQUILIBRIUM MODEL



## TIME SCALES AND ASSOCIATED MODELS (1/4) Typical spectrum shape

62 MeV<sup>56</sup>Fe (p,xp) Double differential cross sections



- Always evaporation peak
- Discrete peaks at forward angles
- Flat intermediate region

## THE PRE-EQUILIBRIUM MODEL (quantum vs semi-classical approaches)

## Semi-classical approaches

- called « exciton model »
- « simple » to implement
- initially only able to describe angle integrated spectra (1966 & 1970)
- extended to ddx spectra in 1976
- link with Compound Nucleus established in 1987
- systematical underestimation of ddx spectra at backward angles
- complemented by Kalbach systematics (1988) to improve ddx description
- link with OMP imaginary performed in 2004

## Quantum mechanical approaches

- distinction between MSC and MSD processes
  - MSC = bound p-h excitations, symetrical angular distributions
  - MSD = unbound configuration, smooth forward peaked ang. dis.
- MSD dominates pre-equ xs above 20 MeV
- 3 approaches : FKK (1980)
  - TUL (1982)
  - NWY (1986)
- ddx spectra described as well as with Kalbach systematics

1





1/







C22





 $\mathbb{C}\mathbb{P}$ 



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P(n,E,t) = Probability to find for a given time t the composite system with an energy E and an exciton number n.

 $\lambda_{a, b}$  (E) = Transition rate from an initial state a towards a state b for a given energy E.

P(n,E,t) = Probability to find for a given time t the composite system with an energy E and an exciton number n.

λ<sub>a, b</sub> (E) = Transition rate from an initial state a towards a state b for a given energy E.

## **Evolution equation**

 $\frac{dP(n,E,t)}{dt} = Apparition$ 

- **Disparition** 

P(n,E,t) = Probability to find for a given time t the composite system with an energy E and an exciton number n.

 $\lambda_{a, b}$  (E) = Transition rate from an initial state a towards a state b for a given energy E.

# **Evolution equation**

 $\frac{dP(n,E,t)}{dt} = P(n-2, E, t) \lambda_{n-2, n}(E) + P(n+2, E, t) \lambda_{n+2, n}(E)$ 

- **Disparition** 

P(n,E,t) = Probability to find for a given time t the composite system with an energy E and an exciton number n.

 $\lambda_{a, b}$  (E) = Transition rate from an initial state a towards a state b for a given energy E.

# **Evolution equation**

 $\frac{dP(n, E, t)}{dt} = P(n-2, E, t) \lambda_{n-2, n}(E) + P(n+2, E, t) \lambda_{n+2, n}(E)$  $- P(n, E, t) \left[\lambda_{n, n+2}(E) + \lambda_{n, n-2}(E) + \lambda_{n, emiss}(E)\right]$
P(n,E,t) = Probability to find for a given time t the composite system with an energy E and an exciton number n.

 $\lambda_{a, b}$  (E) = Transition rate from an initial state a towards a state b for a given energy E.

# **Evolution equation**

$$\frac{dP(n, E, t)}{dt} = P(n-2, E, t) \lambda_{n-2, n}(E) + P(n+2, E, t) \lambda_{n+2, n}(E)$$
$$- P(n, E, t) \left[\lambda_{n, n+2}(E) + \lambda_{n, n-2}(E) + \lambda_{n, emiss}(E)\right]$$

# Emission cross section in channel c

$$d\sigma_{c}(E, \varepsilon_{c}) = \sigma_{R} \int_{0}^{\infty} \sum_{n, \Delta n=2} P(n, E, t) \lambda_{n, c}(E) dt d\varepsilon_{c}$$

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THE PRE-EQUILIBRIUM MODEL (Initialisation & transition rates)

### THE PRE-EQUILIBRIUM MODEL (Initialisation & transition rates)

## Initialisation

 $P(n, E, 0) = \delta_{n, n_0}$  with  $n_0=3$  for nucleon induced reactions

## **Transition rates**

$$\lambda_{n, n-2} (E) = \frac{2\pi}{\hbar} \langle M^2 \rangle \quad \omega(p,h,E) \text{ with } p+h=n-2$$

$$\lambda_{n, n+2} (E) = \frac{2\pi}{\hbar} \langle M^2 \rangle \quad \omega(p,h,E) \text{ with } p+h=n+2$$

$$\lambda_{n, n+2} (E) = \frac{2s_c+1}{\hbar} \langle M^2 \rangle \quad \omega(p,h,E) \text{ with } p+h=n+2$$

$$\lambda_{n, c} (E) = \frac{2s_c+1}{\pi^2 \hbar^3} \mu_c \quad \varepsilon_c \quad \sigma_{c,inv} (\varepsilon_c) \frac{\omega(p-p_b,h,E-\varepsilon_c-B_c)}{\omega(p,h,E)}$$
Original formulation

### THE PRE-EQUILIBRIUM MODEL (Initialisation & transition rates)

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Corrections for proton-neutron distinguishability & complex particle emission

### THE PRE-EQUILIBRIUM MODEL (Initialisation & transition rates)

# Initialisation

 $P(n, E, 0) = \delta_{n, n_0}$  with  $n_0 = 3$  for nucleon induced reactions

# **Transition rates**

$$\lambda_{n, n-2} (E) = \frac{2\pi}{\hbar} \langle M^2 \rangle \quad \omega(p,h,E) \text{ with } p+h=n-2$$

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$$\lambda_{n, c} (E) = \frac{2s_c+1}{\pi^2 \hbar^3} \mu_c \, \varepsilon_c \, \sigma_{c,inv} \, (\varepsilon_c) \frac{\omega(p-p_b,h,E-\varepsilon_c-B_c)}{\omega(p,h,E)} \, Q_c(n) \, \Phi_c$$

### **State densities**

 $\omega(\mathbf{p},\mathbf{h},\mathbf{E}) =$  number of ways of distributing  $\mathbf{p}$  particles and  $\mathbf{h}$  holes on among accessible single particle levels with the available excitation energy  $\mathbf{E}$ 



### THE PRE-EQUILIBRIUM MODEL (State densities)

### State densities in ESM

- Ericson 1960 : no Pauli principle
- Griffin 1966 : no distinction between particles and holes
- Williams 1971 : distinction between particles and holes as well as between neutrons and protons but infinite number of accessible states for both particle and holes

$$\omega_{p_{\pi}h_{\pi}p_{\nu}h_{\nu}}(U) = g_{\pi}^{p_{\pi}+h_{\pi}}g_{\nu}^{p_{\nu}+h_{\nu}}\frac{(U-B)^{M-1}}{p_{\pi}!p_{\nu}!h_{\pi}!h_{\nu}!(M-1)!},$$

where M is the total number of particles and holes of both kinds and

$$B = \frac{1}{4} \left( \frac{p_{\pi}^2 + h_{\pi}^2 + p_{\pi} - h_{\pi}}{g_{\pi}} + \frac{p_{\nu}^2 + h_{\nu}^2 + p_{\nu} - h_{\nu}}{g_{\nu}} \right) - \frac{1}{2} \left( \frac{h_{\pi}}{g_{\pi}} + \frac{h_{\nu}}{g_{\nu}} \right)$$



### THE PRE-EQUILIBRIUM MODEL (State densities)

### State densities in ESM

- Ericson 1960 : no Pauli principle
- Griffin 1966 : no distinction between particles and holes
- Williams 1971 : distinction between particles and holes as well as between neutrons and protons but infinite number of accessible states for both particle and holes
- Běták and Doběs 1976 : account for finite number of holes' states
- Obložinský 1986 : account for finite number of particles' states (MSC)
- Anzaldo-Meneses 1995 : first order corrections for increasing number of p-h
- Hilaire and Koning 1998 : generalized expression in ESM

THE PRE-EQUILIBRIUM MODEL

### **Cross section**

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### **Outgoing energy**



THE PRE-EQUILIBRIUM MODEL



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• p-h level density tables



#### Shape elastic







### THE COMPOUND NUCLEUS MODEL (initial population)

After direct and pre-equilibrium emission







After direct and pre-equilibrium emission





### THE COMPOUND NUCLEUS MODEL (initial population)

After direct and pre-equilibrium emission





### THE COMPOUND NUCLEUS MODEL (basic formalism)

#### **Compound nucleus hypothesys**

- Continuum of excited levels
- Independence between incoming channel a and outgoing channel b



 $\Rightarrow$  Hauser- Feshbach formula

$$\sigma_{ab} = \frac{\pi}{k_a^2} \qquad \frac{T_a T_b}{\sum_c T_c}$$

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### THE COMPOUND NUCLEUS MODEL (qualitative feature)

**Compound** angular distribution & **direct** angular distributions





THE COMPOUND NUCLEUS MODEL (complete channel definition)

### **Channel Definition**

Incident channel a =  $(\vec{l}_a, \vec{j}_a = \vec{l}_a + \vec{s}_a, \vec{J}_A, \pi_A, E_A, E_a)$ 

### **Conservation equations**

- Total energy :  $E_a + E_A = E_{CN} = E_b + E_B$
- Total momentum :  $\vec{p}_a + \vec{p}_A = \vec{p}_{CN} = \vec{p}_b + \vec{p}_B$
- Total angular momentum :  $\vec{l}_a + \vec{s}_a + \vec{J}_A = \vec{J}_{CN} = \vec{l}_b + \vec{s}_b + \vec{J}_B$
- Total parity :  $\pi_{A}$  (-1)<sup>I</sup><sub>a</sub> =  $\pi_{CN} = \pi_{B}$  (-1)<sup>I</sup><sub>b</sub>



### THE COMPOUND NUCLEUS MODEL (loops over all quantum numbers)

In realistic calculations, all possible quantum number combinations have to be considered





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In realistic calculations, all possible quantum number combinations have to be considered





### THE COMPOUND NUCLEUS MODEL (width fluctuation correction factor)

Breit-Wigner resonance integrated and averaged over an energy width Corresponding to the incident beam dispersion





### THE COMPOUND NUCLEUS MODEL (main methods to calculate WFCF)

• Tepel method

Simplified iterative method

Moldauer method

Simple integral

• GOE triple integral

« exact » result

Elastic enhancement with respect to the other channels Inelastic enhancement sometimes in very particular situations ? DE LA RECHERCHE À L'INDUSTRIE

### THE COMPOUND NUCLEUS MODEL (the GOE triple integral)

$$W_{a,l_a,j_a,b,l_b,j_b} = \int_0^{+\infty} d\lambda_1 \int_0^{+\infty} d\lambda_2 \int_0^1 d\lambda \frac{\lambda(1-\lambda)|\lambda_1-\lambda_2|}{\sqrt{\lambda_1(1+\lambda_1)\lambda_2(1+\lambda_2)}(\lambda+\lambda_1)^2(\lambda+\lambda_2)^2}$$

$$\prod_{c} \frac{(1 - \lambda T_{c,l_{c},j_{c}}^{J})}{\sqrt{(1 + \lambda_{1} T_{c,l_{c},j_{c}}^{J})(1 + \lambda_{2} T_{c,l_{c},j_{c}}^{J})}} \quad \left\{ \delta_{ab} (1 - T_{a,l_{a},j_{a}}^{J}) \right\}$$

$$\left[\frac{\lambda_1}{1+\lambda_1 T^J_{a,l_a,j_a}} + \frac{\lambda_2}{1+\lambda_2 T^J_{a,l_a,j_a}} + \frac{2\lambda}{1-\lambda T^J_{a,l_a,j_a}}\right]^2 + (1+\delta_{ab})$$

$$\left[\frac{\lambda_1(1+\lambda_1)}{(1+\lambda_1 T^J_{a,l_a,j_a})(1+\lambda_1 T_{b,l_b,j_b})} + \frac{\lambda_2(1+\lambda_2)}{(1+\lambda_2 T^J_{a,l_a,j_a})(1+\lambda_2 T_{b,l_b,j_b})}\right]$$

$$+ \frac{2\lambda(1-\lambda)}{(1-\lambda T^J_{a,l_a,j_a})(1-\lambda T_{b,l_b,j_b})} \bigg] \bigg\}$$

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### THE COMPOUND NUCLEUS MODEL (flux redistribution illustration)



### THE COMPOUND NUCLEUS MODEL (multiple emission)



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#### **REACTION MODELS & REACTION CHANNELS**

 $n + {}^{238}U$ 



Cea

THE COMPOUND NUCLEUS MODEL (compact expression)

$$\mathbf{\sigma}_{\mathbf{NC}} = \sum_{\mathbf{b}} \mathbf{\sigma}_{\mathbf{ab}} \quad \text{où } \mathbf{b} = \gamma, \mathbf{n}, \mathbf{p}, \mathbf{d}, \mathbf{t}, \dots, \text{ fission}$$

$$\mathbf{\sigma}_{\mathbf{ab}} = \frac{\pi}{\mathbf{k}_{\mathbf{a}}^{2}} \sum_{\mathbf{J}, \pi} \sum_{\alpha, \beta} \frac{(2\mathbf{J}+1)}{(2\mathbf{s}+1)(2\mathbf{I}+1)} \mathbf{T}_{\mathbf{lj}}^{\mathbf{J}\pi}(\alpha) \quad \frac{\langle \mathbf{T}_{\mathbf{b}}^{\mathbf{J}\pi}(\beta) \rangle}{\sum_{\delta} \langle \mathbf{T}_{\mathbf{d}}^{\mathbf{J}\pi}(\delta) \rangle} \quad W_{\alpha\beta}$$
with  $\mathbf{J} = \mathbf{l}_{\alpha} + \mathbf{s}_{\alpha} + \mathbf{I}_{\mathbf{A}} = \mathbf{j}_{\alpha} + \mathbf{I}_{\mathbf{A}} \text{ and } \pi = (-1)^{\mathbf{l}_{\alpha}} \pi_{\mathbf{A}}$ 

and  $\langle T_b(\beta) \rangle$  = transmission coefficient for outgoing channel  $\beta$  associated with the outgoing particle b



### THE COMPOUND NUCLEUS MODEL (various decay channels)

### **Possible decays**

• Emission to a discrete level with energy E<sub>d</sub>

$$\langle T_{b}(\beta) \rangle = T_{lj}^{J\pi}(\beta)$$
 given by the O.M.P.

Emission in the level continuum

$$\langle T_{b}(\beta) \rangle = \int_{E}^{E + \Delta E} T_{lj}^{J\pi}(\beta) \rho(E, J, \pi) dE$$

 $\rho(E,J,\pi)$  density of residual nucleus' levels (J, $\pi$ ) with excitation energy E

Emission of photons, fission

**Specific treatment** 



Two types of strength functions :



Two types of strength functions :

- the « upward » related to photoabsorption

$$\overrightarrow{f}_{\rm XL}(\epsilon_{\gamma}) = \frac{\epsilon_{\gamma}^{-2L+1}}{(\pi\hbar c)^2} \frac{\langle \sigma_{\rm XL}(\epsilon_{\gamma}) \rangle}{2L+1}.$$

 $\overleftarrow{f}_{\rm XL}(\epsilon_{\gamma}) = \epsilon_{\gamma}^{-(2L+1)} \frac{\langle \Gamma_{\rm XL}(\epsilon_{\gamma}) \rangle}{D_l}$ 

- the « downward » related to  $\gamma$ -decay



$$T^{k\lambda}(E,\varepsilon_{\gamma}) = 2\pi \int \Gamma^{k\lambda}(\varepsilon_{\gamma}) \rho(E) dE$$
$$= 2\pi f(k,\lambda,\varepsilon_{\gamma}) \varepsilon_{\gamma}^{2\lambda+1}$$
$$f(k,\lambda,\varepsilon_{\gamma}) : gamma strength fur$$

k : transition type EM (E ou M)

 $\boldsymbol{\lambda}$  : transition multipolarity

 $\varepsilon_{\gamma}$ : outgoing gamma energy

 $f(k,\lambda, \varepsilon_{\gamma})$ : gamma strength function (several models)

Decay selection rules from a level  $J_i^{\pi}$  to a level  $J_f^{\pi}$ :

Pour E $\lambda$ :  $\pi_f = (-1)^{\lambda} \pi_i$ Pour M $\lambda$ :  $\pi_f = (-1)^{\lambda+1} \pi_i$   $|J_i - \lambda| \le J_f \le J_i + \lambda$  (E1  $\approx 10^2$  M1) (XL  $\approx 10^{-3}$  XL-1)

Renormalisation method for thermal neutrons

$$<\mathbf{T}_{\gamma}>=\sum_{\mathbf{J}_{i},\pi_{i}}\sum_{\mathbf{k}\lambda}\sum_{\mathbf{J}_{f},\pi_{f}}\int_{0}^{\mathbf{B}_{n}}\mathbf{T}_{\mathbf{k}\lambda}(\varepsilon)\rho(\mathbf{B}_{n}-\varepsilon,\mathbf{J}_{f},\pi_{f})\mathbf{S}(\lambda,\mathbf{J}_{i},\pi_{i},\mathbf{J}_{i},\pi_{f}) d\varepsilon = \mathbf{2\pi} <\mathbf{\Gamma}_{\gamma}>\rho(\mathbf{B}_{n})$$

$$T^{k\lambda}(E,\varepsilon_{\gamma}) = 2\pi \int_{\Gamma}^{E+\Delta E} \Gamma^{k\lambda}(\varepsilon_{\gamma}) \rho(E) dE$$
$$= 2\pi f(k,\lambda,\varepsilon_{\gamma}) \varepsilon_{\gamma}^{2\lambda+1}$$
$$f(k,\lambda,\varepsilon_{\gamma}) : gamma strength func-$$

k : transition type EM (E ou M)

- $\boldsymbol{\lambda}$  : transition multipolarity
- $\varepsilon_{\gamma}$ : outgoing gamma energy

 $f(k,\lambda, \varepsilon_{\gamma})$ : gamma strength function (several models)

Decay selection rules from a level  $J_i^{\pi}$  to a level  $J_f^{\pi}$ :

Pour E $\lambda$ :  $\pi_{f}$ =(-1)<sup> $\lambda$ </sup>  $\pi_{i}$ Pour M $\lambda$ :  $\pi_{f}$ =(-1)<sup> $\lambda$ +1</sup>  $\pi_{i}$ IJ<sub>i</sub>- $\lambda$ |  $\leq$  J<sub>f</sub>  $\leq$  J<sub>i</sub>+ $\lambda$ 



experiment

Renormalisation method for thermal neutrons

$$<\mathbf{T}_{\gamma}>=\mathbf{C}\sum_{\mathbf{J}_{i},\pi_{i}}\sum_{\mathbf{k}\lambda}\sum_{\mathbf{J}_{f},\pi_{f}}\int_{0}^{\mathbf{B}_{n}}\mathbf{T}^{\mathbf{k}\lambda}(\varepsilon)\rho(\mathbf{B}_{n}-\varepsilon,\mathbf{J}_{f},\pi_{f})\mathbf{S}(\lambda,\mathbf{J}_{i},\pi_{i},\mathbf{J}_{i},\pi_{f})\,\mathbf{d}\varepsilon=\mathbf{2\pi}<\mathbf{\Gamma}_{\gamma}>\mathbf{1}$$



#### Improved analytical expressions :

- 2 Lorentzians for deformed nuclei
- Account for low energy deviations from standard Lorentzians for E1
  - . Kadmenskij-Markushef-Furman model (1983)
    - $\Rightarrow$  Enhanced Generalized Lorentzian model of Kopecky-Uhl (1990)
    - $\Rightarrow$  Hybrid model of Goriely (1998)
    - $\Rightarrow$  Generalized Fermi liquid model of Plujko-Kavatsyuk (2003)
- Reconciliation with electromagnetic nuclear response theory
  - $\Rightarrow$  Modified Lorentzian model of Plujko et al. (2002)
  - $\Rightarrow$  Simplified Modified Lorentzian model of Plujko et al. (2008)



FIG. 42: E1  $\gamma$ -decay strength function plotted against energy  $\epsilon_{\gamma}$  for <sup>90</sup>Zr; experimental data are taken from Ref. [327].



#### Improved analytical expressions :

- 2 Lorentzians for deformed nuclei
- Account for low energy deviations from standard Lorentzians for E1
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  - $\Rightarrow$  Simplified Modified Lorentzian model of Plujko et al. (2008)

#### Microscopic approaches : RPA, QRPA

« Those who know what is (Q)RPA don't care about details, those who don't know don't care either », private communication

 $\Rightarrow$  Systematic QRPA with Skm force for 3317 nuclei performed by Goriely-Khan (2002,2004)

 $\Rightarrow$  Systematic QRPA with Gogny force under work (300 Mh!!!)
#### MISCELLANEOUS : THE PHOTON EMISSION (phenomenology vs microscopic)





#### MISCELLANEOUS : THE PHOTON EMISSION (phenomenology vs microscopic)



 $\Rightarrow$  Weak impact close to stability but large for exotic nuclei



#### **MISCELLANEOUS : THE FISSION PROCESS** (static picture exhibiting fission barriers)



## MISCELLANEOUS : THE FISSION PROCESS (fissile or fertile ?)



Fertile target (<sup>238</sup>U)

## MISCELLANEOUS : THE FISSION PROCESS (fissile or fertile ?)



MISCELLANEOUS : THE FISSION PROCESS (fissile or fertile ?)



Incident neutron data / ENDF/B-VI.8 / U238 / MT=19 : (n,f) / Cross section



















#### MISCELLANEOUS : THE FISSION PROCESS (Fission transmission coefficients)







+ transition states on top of the barrier !



+ transition states on top of the barrier !



+ transition states on top of each barrier !



+ transition states on top of each barrier !
+ class II states in the intermediate well !



+ transition states on top of each barrier !
+ class II states in the intermediate well !





+ transition states on top of each barrier !
+ class II states in the intermediate well !



More exact expressions in Sin et al., PRC 74 (2006) 014608

#### MISCELLANEOUS : THE FISSION PROCESS (multiple humped barriers with maximum complexity)



See in Sin et al., PRC 74 (2006) 014608 Bjornholm and Lynn, Rev. Mod. Phys. 52 (1980) 725.

## MISCELLANEOUS : THE FISSION PROCESS (Impact of class II states)

<sup>239</sup>Pu (n,f)





## MISCELLANEOUS : THE FISSION PROCESS (impact of class II and class III states)

# **Case of a fertile nucleus**

Partially damped class II states. No class III states





## MISCELLANEOUS : THE FISSION PROCESS (impact of class II and class III states)

## **Case of a fertile nucleus**

Class II + III states. Partial damping.



## MISCELLANEOUS : THE FISSION PROCESS (Hill-Wheeler ?)

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 $\Rightarrow$  For exotic nuclei : strong deviations from Hill-Wheeler.

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## MISCELLANEOUS : THE FISSION PROCESS (Microscopic fission cross sections)

MISCELLANEOUS : THE LEVEL DENSITIES (Principle)

Cez



#### MISCELLANEOUS : THE LEVEL DENSITIES (Qualitative aspects 1/2)



• Exponential increase of the cumulated number of discrete levels N(E) with energy

- $\Rightarrow \rho(E) = \frac{dN(E)}{dE}$  increases exponentially
- $\Rightarrow$  odd-even effects

Mean spacings of s-wave neutron resonances at  $B_n$  of the order of few eV

 $\Rightarrow \rho(B_n)$  of the order of  $10^4 - 10^6$  levels / MeV

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#### MISCELLANEOUS : THE LEVEL DENSITIES (Qualitative aspects 2/2)



MISCELLANEOUS : THE LEVEL DENSITIES (Quantitative analysis 1/2)

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$$\rho(\mathbf{U}, \mathbf{J}, \pi) = \frac{1}{2} \frac{\sqrt{\pi}}{12} \frac{\exp(2\sqrt{aU})}{a^{1/4}U^{5/4}} \frac{2\mathbf{J}+1}{2\sqrt{2\pi}\sigma^3} \exp\left[\frac{(\mathbf{J}+1/2)^2}{2\sigma^2}\right] + \sigma^2 = \mathbf{I}_{rig} \sqrt{\frac{\mathbf{U}}{a}}$$

MISCELLANEOUS : THE LEVEL DENSITIES (Quantitative analysis 1/2)



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MISCELLANEOUS : THE LEVEL DENSITIES (Quantitative analysis 2/2)



### **MISCELLANEOUS : THE LEVEL DENSITIES** (Summary of most simple analytical description)


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## MISCELLANEOUS : THE LEVEL DENSITIES (More sophisticated approaches)

Superfluid model & Generalized superfluid model

Ignatyuk et al., PRC 47 (1993) 1504 & RIPL3 paper (IAEA)

 $\Rightarrow$  More correct treatment of pairing for low energies

- $\Rightarrow$  Fermi Gas + Ignatyuk beyond critical energy
- $\Rightarrow$  Explicit treatment of collective effects



 $\Rightarrow$  Collective enhancement only if  $\rho_{int}(U) \neq 0$  not correct for vibrational states



## MISCELLANEOUS : THE LEVEL DENSITIES (More sophisticated approaches)

Superfluid model & Generalized superfluid model

Ignatyuk et al., PRC 47 (1993) 1504 & RIPL2 Tecdoc (IAEA)

- $\Rightarrow$  More correct treatment of pairing for low energies
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- $\Rightarrow$  Explicit treatment of collective effects

#### **Shell Model Monte Carlo approach**

Agrawal et al., PRC 59 (1999) 3109

- $\Rightarrow$  Realistic Hamiltonians but not global
- $\Rightarrow$  Coherent and incoherent excitations treated on the same footing
- $\Rightarrow$  Time consuming and thus not yet systematically applied

#### **Combinatorial approach**

S. Hilaire & S. Goriely, NPA 779 (2006) 63 & PRC 78 (2008) 064307.

- $\Rightarrow$  Direct level counting
- $\Rightarrow$  Total (compound nucleus) and partial (pre-equilibrium) level densities
- $\Rightarrow$  Non statistical effects
- $\Rightarrow$  Global (tables)



# THE LEVEL DENSITIES (The combinatorial method 1/3)

See PRC 78 (2008) 064307 for details

- HFB + effective nucleon-nucleon interaction  $\Rightarrow$  single particle level schemes
- Combinatorial calculation  $\Rightarrow$  intrinsic p-h and total state densities  $\omega$  (U, K,  $\pi$ )

## THE LEVEL DENSITIES (The combinatorial method 1/3)

Level density estimate is a counting problem:  $\rho(U)=dN(U)/dU$ 

N(U) is the number of ways to distribute the nucleons among the available levels for a fixed excitation energy U



## THE LEVEL DENSITIES (The combinatorial method 1/3)

See PRC 78 (2008) 064307 for details

- HFB + effective nucleon-nucleon interaction  $\Rightarrow$  single particle level schemes
- Combinatorial calculation  $\Rightarrow$  intrinsic p-h and total state densities  $\omega$  (U, K,  $\pi$ )
- Collective effects  $\Rightarrow$  from state to level densities  $\rho(U, J, \pi)$

folding of intrinsic and vibrational state densities
construction of rotational bands for deformed nuclei

$$\rho(\mathbf{U}, \mathbf{J}, \pi) = \sum_{\mathbf{K}} \omega \left(\mathbf{U} - \mathbf{E}_{\text{rot}}^{\mathbf{JK}}, \mathbf{K}, \pi\right)$$

2) spherical nuclei

$$\rho(\mathbf{U}, \mathbf{J}, \pi) = \omega (\mathbf{U}, \mathbf{K}=\mathbf{J}, \pi) - \omega (\mathbf{U}, \mathbf{K}=\mathbf{J}+1, \pi)$$

- Phenomenological transition for deformed/spherical nucleus

#### THE LEVEL DENSITIES (The combinatorial method 2/3)



→ Structures typical of non-statistical feature

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## THE LEVEL DENSITIES (The combinatorial method 3/3)



$$f_{\rm rms} = \exp\left[\frac{1}{\bar{N}_e}\sum_{i=1}^{5}\ln^2\frac{D_{\rm th}^i}{D_{\rm exp}^i}\right]$$

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## THE LEVEL DENSITIES (The combinatorial method 3/3)



Description similar to that obtained with other global approaches

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# **CONCLUSIONS & PROPECTS**

- Nuclear reaction modeling complex and no yet fully satisfactory
  - $\Rightarrow$  pre-equilibrium phenomenon must be improved
  - $\Rightarrow$  fission related phenomena (fission, FF yields & decay) must be improved
- Formal and technical link between structure and reactions has to be pushed further
  - $\Rightarrow$  pre-equilibrium and OMP efforts already engaged
  - $\Rightarrow$  computing time is still an issue
- Fundamental v-v interaction knowledge (and treatment) has to be improved
  - $\Rightarrow$  Ab-initio not universal (low mass or restricted mass regions)
  - $\Rightarrow$  Relativistic aspects not included systematically
  - $\Rightarrow$  Human & computing time is still an issue