



Fission reactions

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ICTP-IAEA Workshop on Simulation of Nuclear Reaction Data with the TALYS Code - TRIESTE - October 2023

- 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

- Model ingredients

- Level densities
- Gamma-ray strengths
- Fission transmission coefficients

- Fission reactions

- Generalities about fission
- Fission neutrons and gammas
- Fission yields
- Fission cross sections

- Prospects

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FEW REMINDERS



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Models sequence and required ingredients





Models sequence and required ingredients







Time scales and associated models



Time scales and associated models



Fission reactions



- Generalities about fission

Induced, spontaneous, energy balance, fission yields, PFNS, neutron multiplicities, cross sections, fission chances, Kinetic energies,

- Fission yields

- GEF model
- SPY model
- Microscopic approach

- Neutrons and gammas from fission

- Madland-Nix model
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GENERALITIES



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The fission process





..... Energy (200 MeV)

The fission process : sequence for induced fission





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The fission process : typical energy balance

Fragments kinetic energy	165 MeV
prompt γ	8 MeV
β decay	19 MeV
delayed γ	7 MeV
prompts neutrons	5 MeV
TOTAL :	204 MeV

$n + {}^{235}U \rightarrow {}^{94}Sr + {}^{140}Xe + 2n$	=> Q= 184.68 MeV
\rightarrow ⁹⁴ Kr + ¹³⁹ Ba + 2n	=> Q= 177.46 MeV
\rightarrow ¹¹⁸ Pd + ¹¹⁷ Pd + 1n	=> Q= 192.73 MeV

The fission process : fragments kinetic energies







The fission process : yields variations with energy



 \Rightarrow Well filled with increasing incident energy

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The fission process : yields variations with targets



 \Rightarrow FF distribution strongly modified with different targets

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The fission process : rapid yield variations





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The fission process : emitted neutrons spectrum



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The fission process : mean energy of emitted neutrons



235U

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The fission process : neutron multiplicities



	$\overline{\nu}$		
²⁴⁰ Pu	2.257	+/-	.045
²³⁸ Pu	2.33	+/-	.08
²³⁵ U+n	2.47	+/-	.03
²⁴² Cm	2.65	+/-	.09
²⁴⁴ Cm	2.82	+/-	.05
²⁵² Cf	3.86	+/-	.07
²⁴² Pu	2.18	+/-	.09
²³³ U+n	2.585	+/-	.062

The fission process : neutron multiplicities and incident nrj



Figure 13: Prompt-neutron multiplicity as a function of the pre-neutron fragment mass for the system ${}^{237}Np(n,f)$ for $E_n = 0.8$ MeV and 5.55 MeV



The fission process : sequence for induced fission



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The fission process : fissile vs fertile











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The fission process : fission chances



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Describing all previously mentioned data is a real challenge for theoretical models.

Several phenomenological approaches are usually adopted to describe each type of data because of the flexibility they offer for measured nuclei.

⇒ Many models and parameters : extrapolation at your own risks !

⇒ Clear lack of coherence or deep understanding of the underlying physics !

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Details in Nucl. Data Sheets 131 (2016) 107-221 Code at www.khs-erzhausen.de/home.html

Phenomenological approach not intended to compete with fundamental microscopic approach, but aiming at producing data with the accuracy required for industrial application

 \Rightarrow many empirical laws fitted to data

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Phenomenological approach not intended to compete with fundamental microscopic approach, but aiming at producing data with the accuracy required for industrial application

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The available measured fission barriers were used to deduce the following empirical function, which describes the difference between the inner and the outer barrier height:

 $E_A - E_B = 5.40101 - 0.00666175 \cdot Z^3 / A + 1.52531 \cdot 10^{-6} \cdot (Z^3 / A)^2.$ (10)



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Phenomenological approach not intended to compete with fundamental microscopic approach, but aiming at producing data with the accuracy required for industrial application

 \Rightarrow many empirical laws fitted to data

 \Rightarrow range of application restricted close to experimentally accessible regions



According to the concept of the GEF model, the range of validity is not Details it strictly defined. Technically, the code runs for any heavy nucleus. However, the results of the model are more reliable for nuclei which are not too far Code at v from the region where experimental data exist. It is recommended not to use the code outside the range depicted in figure 1 on the chart of the nuclides. Phenomena microscopi 23411 ²²⁹Th the accurac 226 Th ²¹⁸Th 208 Rn ²⁵⁶Fm many er \Rightarrow \Rightarrow range of <u>Th</u> r 227Ra Z=82 0 ²¹³At mass distributions + Z distributions 201 × Z distributions in N=126 inverse kinematics

> Figure 1: Validity range of the GEF model on a chart of the nuclides, marked in yellow. For a detailed description of the figure see figure 6.

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GEF model





Figure 1: Validity range of the GEF model on a chart of the nuclides, marked in yellow. For a detailed description of the figure see figure 6.

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The fission process : GEF results





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The fission process : GEF results





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Details in Phys. Rev. C92 (2015) 034617 & Phys. Rev. C99 (2019)

Approach based on absolute energy balance based on HFB potential energy surfaces as function of axial deformation ⇒ Available energy at scission

Available energy (AE) shared between fragments : x (AE) and (1-x) (AE)

$$\pi(Z_{1}, N_{1}, Z_{2}, N_{2}, \tilde{q}_{1}, \tilde{q}_{2}, x) = \rho_{1}(x |AE|) \rho_{2}((1-x) |AE|) \delta E^{2}$$

$$\Pi(Z_{1}, N_{1}, Z_{2}, N_{2}, \tilde{q}_{1}, \tilde{q}_{2}) = \int_{0}^{1} \pi(Z_{1}, N_{1}, Z_{2}, N_{2}, \tilde{q}_{1}, \tilde{q}_{2}, x) dx$$

$$P(Z_{1}, N_{1}, Z_{2}, N_{2}) = \iint \Pi(Z_{1}, N_{1}, Z_{2}, N_{2}, \beta_{1}, \beta_{2}) d \tilde{q}_{1} d \tilde{q}_{2}$$

SPY : available energy





$$\mathbf{AE} = \left| \mathbf{E}_{\text{ind1}} + \mathbf{E}_{\text{ind2}} + \mathbf{E}_{\text{coul}} + \mathbf{E}_{\text{nucl}} - \mathbf{E}_{\text{CN}} \right|$$

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1

The fission process : energy sharing & level densities



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SPY model : raw results





 \Rightarrow Less accurate than GEF (only one parameter fixed !)

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SPY model : raw results



 \Rightarrow Can be improved with smoothing methods (much more parameters)

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SPY model : systematic predictions rather easy



\Rightarrow Rather good qualitative description



SPY model : systematic predictions rather easy





1) PES calculation as function of elongation-asymmetry



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- 1) PES calculation as function of elongation-asymmetry
- 2) Quantum mechanical Wave packet propagation in the computed PES (FELIX code)





- 1) PES calculation as function of elongation-asymmetry
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- 1) PES calculation as function of elongation-asymmetry
- 2) Quantum mechanical Wave packet propagation in the computed PES (FELIX code)
- 3) Extraction of the flux through a scission line (whose definition is not trivial)



- \Rightarrow Not accurate enough for applications
- \Rightarrow Time consuming (10000 h per nucleus on single CPU)
- \Rightarrow Extrapolations and systematics manageable with HPC
- \Rightarrow Limited to even-even

Neutrons and gammas from fission

Fission reactions



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Details in Nucl. Sci. Eng. 81 (1982) 213.

- Fission yields reduced to a light and a heavy fragment whose temperatures are distributed according to a triangular law
- For each temperature, each fragment neutron emission is modeled by the corresponding Weisskopf spectrum normalized by the fragment formation cross section by induced neutron reaction
- Multiple fission chances accounted for using fission cross sections -
- Final neutron spectrum defined by an average of light and heavy fragment spectra

 \Rightarrow model with parameters designed to fit data







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Electric Fission reactions

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mean gamma energy parameterized (several options)

 \Rightarrow model with parameters designed to fit data



mean gamma energy parameterized (several options)

$$\overline{\nu_{p\,i}} = \frac{\langle E_i^* \rangle - \langle E_\gamma^{tot} i \rangle}{\langle S_{n\,i} \rangle + \langle \epsilon_i \rangle}$$

 $\langle E_{\gamma}^{tot} \rangle$ mean prompt gamma energy $\langle S_n \rangle$ mean neutron binding energy

 $\langle \epsilon \rangle$ mean emitted neutron energy

 \Rightarrow model with parameters designed to fit data



mean gamma energy parameterized (several options)



- $\langle \epsilon \rangle$ mean emitted neutron energy

$$\sigma_{f\,i}$$
: ith fission chance cross section.

\Rightarrow model with parameters designed to fit data





 \Rightarrow model with parameters designed to fit data

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GEF model : neutron multiplicities



Details in Nucl. Data Sheets 131 (2016) 107-221 Code at www.khs-erzhausen.de/home.html



GEF model



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Fission reactions

GEF model : neutron multiplicities distributions



Details in Nucl. Data Sheets 131 (2016) 107-221 Code at www.khs-erzhausen.de/home.html





GEF model : neutron and gamma spectra

 \Rightarrow GEF very efficient to fit data and fill the gaps for applications

FIFRELIN



Monte Carlo approach designed to deal with fission fragment decay

- \Rightarrow fragment's mass sampled from exp. or theory (GEF)
- \Rightarrow fragment's kinetic energy sampled from exp. or theory
- \Rightarrow fragment's charge sampled from Wahl model (Z=Z_{CN}/A_{CN} * A)
- \Rightarrow fragment's spin distribution sampled from level density law
- \Rightarrow excitation energy sharing following temperature ratio law adjusted on saw tooth



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FIFRELIN : neutron multiplicities

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Fission reactions





Courtesy O. Litaize

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150

160

 $< \epsilon_v > (MeV)$

 0.85 ± 0.02

FIFRELIN : PFGS and spontaneous fission

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FIFRELIN : PFGS and neutron induced fission



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FIFRELIN : PFNS and neutron induced fission



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FIFRELIN : neutron multiplicities and incident energy



MICROSCOPIC APPROACH



Details in Phys. Rev. C 77 (2008) 014310.



FIG. 15. ²⁵⁶Fm. Neutron multiplicity versus fragment mass. Comparison between predictions (solid symbols) and data [47] (empty symbols).

 \Rightarrow Not yet at the level

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Fission cross sections

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Fission barriers and fission paths





Fissile or fertile

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Fissile or fertile





Incident energy (MeV)

Incident neutron data / ENDF/B-VI.8 / U235 / MT=19 : (n,f) / Cross section

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Fission transmission coefficient :Hill-Wheeler penetrability



Fission transmission coefficient :Hill-Wheeler penetrability



Fission transmission coefficient :Hill-Wheeler penetrability



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+ 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 !

Fission reactions



+ class II states in the intermediate well !

Two barriers A et B

$$T_{f} = \frac{T_{A} T_{B}}{T_{A} + T_{B}}$$

Electric Fission reactions

Two barriers A et B

$$\mathbf{T}_{\mathbf{f}} = \frac{\mathbf{T}_{\mathbf{A}} \mathbf{T}_{\mathbf{B}}}{\mathbf{T}_{\mathbf{A}} + \mathbf{T}_{\mathbf{B}}}$$

Three barriers A, B and C

$$T_{f} = \frac{\frac{T_{A} T_{B}}{T_{A} + T_{B}} \times T_{C}}{\frac{T_{A} T_{B}}{T_{A} + T_{B}} + T_{C}}$$

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



Two barriers A et B

Three barriers A, B and C

$$T_{f} = \frac{\frac{T_{A} T_{B}}{T_{A} + T_{B}} \times T_{C}}{\frac{T_{A} T_{B}}{T_{A} + T_{B}} + T_{C}}$$

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

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

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T_f =

Fission transmission coefficient : role of class II states



²³⁹Pu (n,f)



Fission transmission coefficient : role of class II states



²³⁹Pu (n,f)



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Bjornholm and Lynn, Rev. Mod. Phys. 52 (1980) 725.

Fission transmission coefficient : class II and class III states

Case of a fertile nucleus

Partially damped class II states. No class III states



Fission transmission coefficient : class II and class III states

Case of a fertile nucleus

Class II + III states. Partial damping.



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Coherent fission modeling : single target / several fissions $n + {}^{238}U$ $\sigma_{n,f}$ 1.8 Section efficace (barn) ⇒(n,3nf) **U6** 0.2 3n 0 $\frac{10}{20} \frac{20}{10} \frac{10}{10} \frac{10$ 50 **U7** >(n,2nf) **2n U8** ⇒(n,nf) \sqrt{n} **U9** ⇒ (n,f) ► MeV 12 24 **Fission reactions** 72 19/10/2023 cea 6

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Ingredients of relevance to estimate fission properties

$$T(E, J, \pi) = \int_0^E P(E - \varepsilon)\rho(\varepsilon, J, \pi)d\varepsilon \begin{cases} P(E) = \frac{1}{1 + \exp(2K)} \\ K = \pm \int_a^b [2\mu(E - V(\beta))/\hbar^2]^{1/2}d\beta \end{cases}$$
Hill-Wheeler approximation: $P^{HW} = \frac{1}{1 + \exp[2\pi(V_0 - E)/\hbar\omega]}$

Fundamental ingredients:

- Fission barrier heightsFission barrier widths Fission path
- Nuclear Level Densities at saddle points

MAJOR CHALLENGE: COHERENT PREDICTIONS OF ALL INPUTS



Determination of the fission path performing HFB calculation as function of appropriate deformation (collective) variables using ideally an effective interaction also adjusted on experimental masses



Also use the same effective interaction to calculate level densities (GS and top of each barrier)



Microscopic approach : fission paths



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

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Microscopic approach : Fission level densities



Nuclear level densities at the saddle points

HFB model provides at each deformation (including saddle points) all nuclear properties needed to estimate the NLD



Possibility to estimate NLD at the saddle point within the HFB+Combinatorial model



Microscopic approach : summary

Nuclear Level Density at Saddle Points

- Fission Barriers and saddle point deformations (Q,O,H) determined within HFB method
- Nuclear properties (spl, pairing) at the inner and outer saddle points with constrained HFB model
- NLD in the framework of the microscopic combinatorial model based on HFB single-particle level and pairing predictions at the HFB saddle points (plus collective rotational and vibrational enhancement)

All ingredients described on the basis of the

same Skyrme effective interaction (BSk14) at GS and Saddle Points

NLD in a table format at inner and outer saddle points (~2000 nuclei : 2/3 saddle points & 1/2 shape isomers)

For inner barrier, usually predicted to be triaxial: $\rho_{triax} = \sqrt{\frac{\pi}{2}} \sigma_{\perp} \times \rho_{Comb}$ Bjornholm & Lynn (1980) For outer barrier, usually predicted to be left-right asymmetric: $\rho_{asym} = 2 \times \rho_{Comb}$



Microscopic approach : results



 $\Rightarrow Default \ calculations \ not \ sufficient \ for \ applications.$

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Microscopic approach : results



Fission barriers adjusted for each target

Fission barriers adjusted for each type of target - odd-odd - odd-even - even-odd

- even-even

 $\Rightarrow Not ridiculous after few adjustments.$

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Coherent fission cross sections with phenomenological approach

Neutron induced fission on ²³⁸U

- several hundreds of parameters
- unique set for all fission chances or U targets









Can we do the same with microscopic ingredients ?



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HFB-14 predictions of fission barriers and NLD at saddle points,

including renormalization (max 5 parameters) of

- fission path height: $B_f'(\beta_2) = B_f(\beta_2) \ge v_{corr}$
- NLD at 1st and 2^d saddle points:

$$\rho'(U,J,P) = \rho(U - \delta,J,P) e^{\alpha \sqrt{U \cdot \delta}}$$

Additional nuclear inputs:

- Nuclear structure properties: HFB-14 (Goriely et al. 2007)
- Optical potential: Soukhovitskii et al. (2004)
- γ-ray strength: Hybrid model (Goriely, 1998)
- NLD: HFB-14 plus combinatorial model (Goriely et al., 2008) normalized on s-wave spacings and discrete excited levels

Note:

- 1 UNIQUE set of nuclear ingredients for all U isotopes
- no class 2 states included
- no discrete transition states included









Coherence = more constraints = slightly worse fit

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²³⁹Pu (n,f)



-20 keV sur V_A ≈ 0.34% !!

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²³⁹Pu (n,f)



-20 keV sur V_A ≈ 0.34% !!



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Conclusions and Prospects

Conclusions



Nuclear reaction modeling : 2 complementary paths



Empirical / Analytical approaches

- Good (very) fitting power
- Weak (modest) computing time
- Weak predictive power
- Important human optimization
- ⇒ accurate evaluated files for applications (ENDF, JEFF, JENDL ...)

Microscopic (semi-) approaches

- Weak fitting power
- Important computing time
- Good predictive power
- Weak human optimization
- \Rightarrow astrophysical applications
- \Rightarrow fundamental research
- \Rightarrow guide for empical approaches

Phenomelogical approach : fitting loop

















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