



*The Abdus Salam  
International Centre for Theoretical Physics*



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**Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced  
Reactor Technologies**

*19 - 30 May 2008*

**Neutron induced resonance reactions.**

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# Neutron induced resonance reactions

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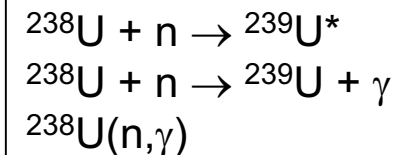
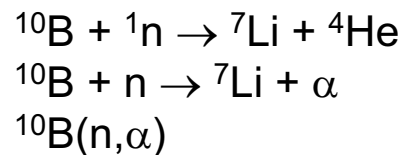
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## Neutron-nucleus reactions

Reaction:

- $X + a \rightarrow Y + b$
- $X(a,b)Y$
- $X(a,b)$

Examples of  
equivalent notations:



Reaction cross section  $\sigma$ , expressed in barns,  $1 \text{ b} = 10^{-28} \text{ m}^2$

Neutron induced nuclear reactions:

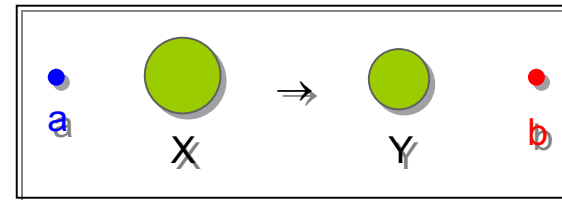
- elastic scattering  $(\text{n},\text{n})$
- inelastic scattering  $(\text{n},\text{n}')$
- capture  $(\text{n},\gamma)$
- fission  $(\text{n},\text{f})$
- particle emission  $(\text{n},\alpha)$ ,  $(\text{n},\text{p})$ ,  $(\text{n},\text{xn})$

Total cross section  $\sigma_{\text{tot}}$ : sum of all reactions

# Neutron-nucleus reactions

Reaction:

- $X + a \rightarrow Y + b$
- $X(a,b)Y$



**Cross section:**

function of the kinetic energy of the particle **a**

$$\sigma(E_a) = \int \int \frac{d^2\sigma(E_a, E_b, \Omega)}{dE_b d\Omega} dE_b d\Omega$$

**Differential cross section:**

function of the kinetic energy of the particle **a**  
and function of the kinetic energy **or** the angle  
of the particle **b**

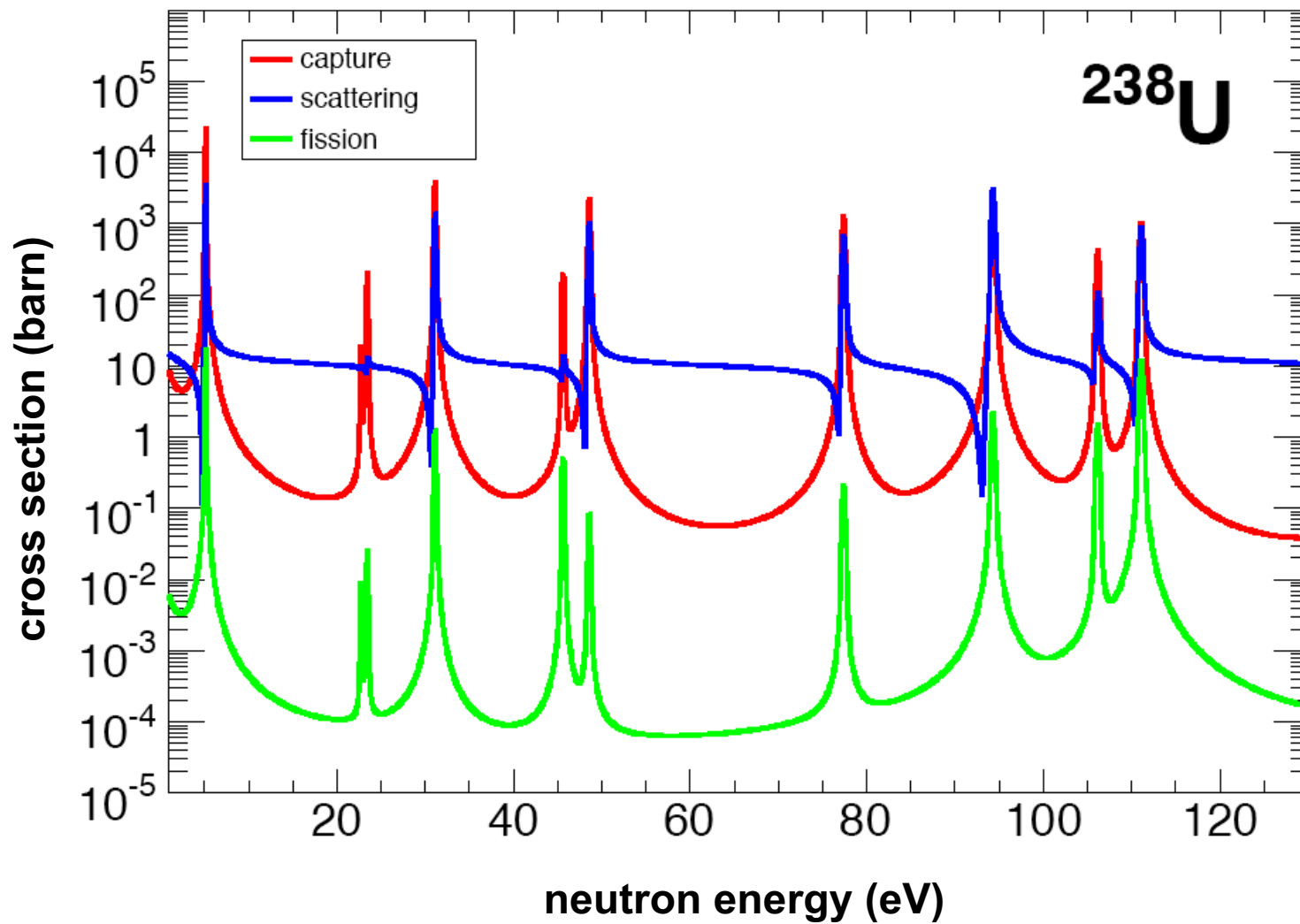
$$\frac{d\sigma(E_a, E_b)}{dE_b} \quad \frac{d\sigma(E_a, \Omega)}{d\Omega}$$

**Double differential cross section:**

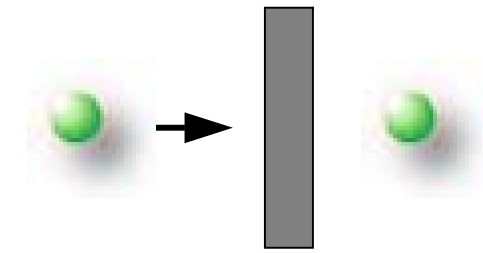
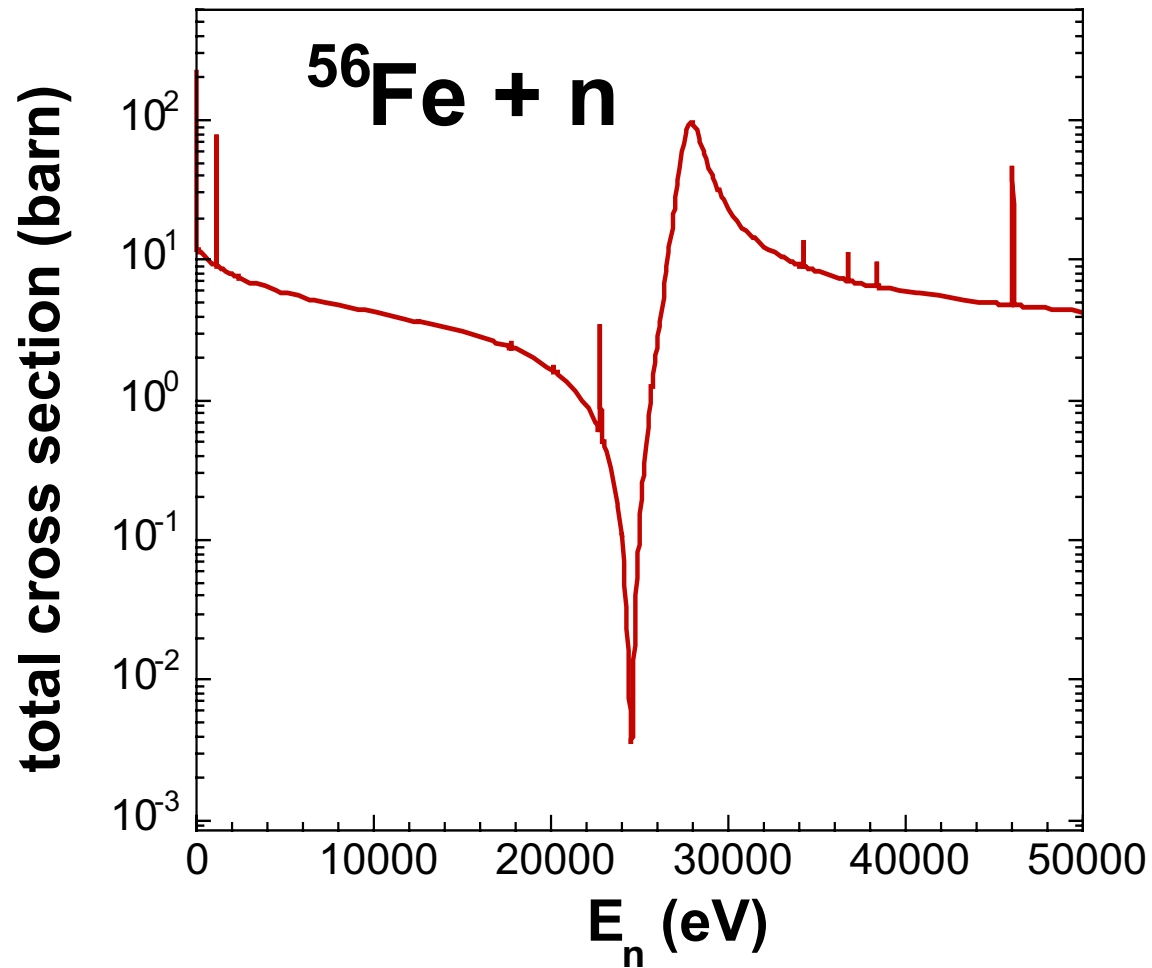
function of the kinetic energy of the particle **a**  
and function of the kinetic energy **and** the angle  
of the particle **b**

$$\frac{d^2\sigma(E_a, E_b, \Omega)}{dE_b d\Omega}$$

# Cross sections $\sigma_\gamma$ , $\sigma_n$ et $\sigma_f$



# Interference of $\sigma_{\text{potential}}$ and $\sigma_n$

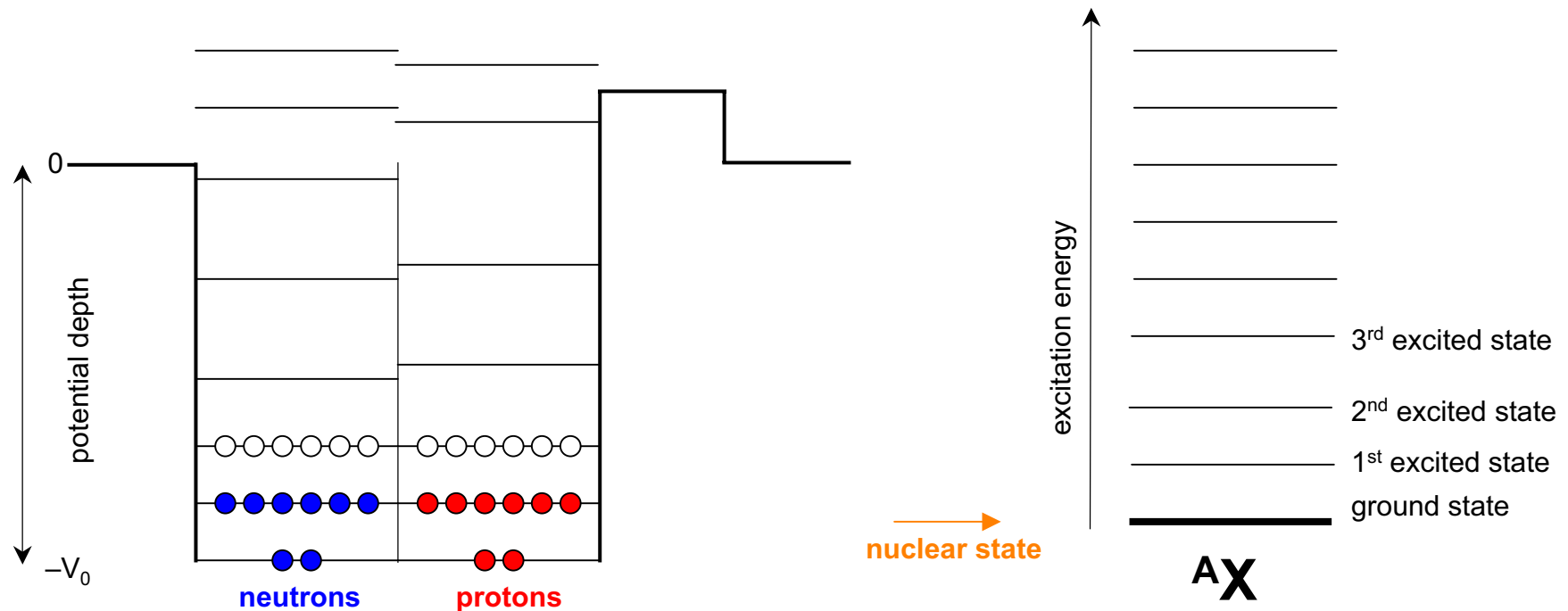


transmission  
 $T = \exp(-n \cdot \sigma_T)$   
 $0 < T < 1$

# The nucleus as a quantum system

**shell model representation:**  
configuration of nucleons in their potential

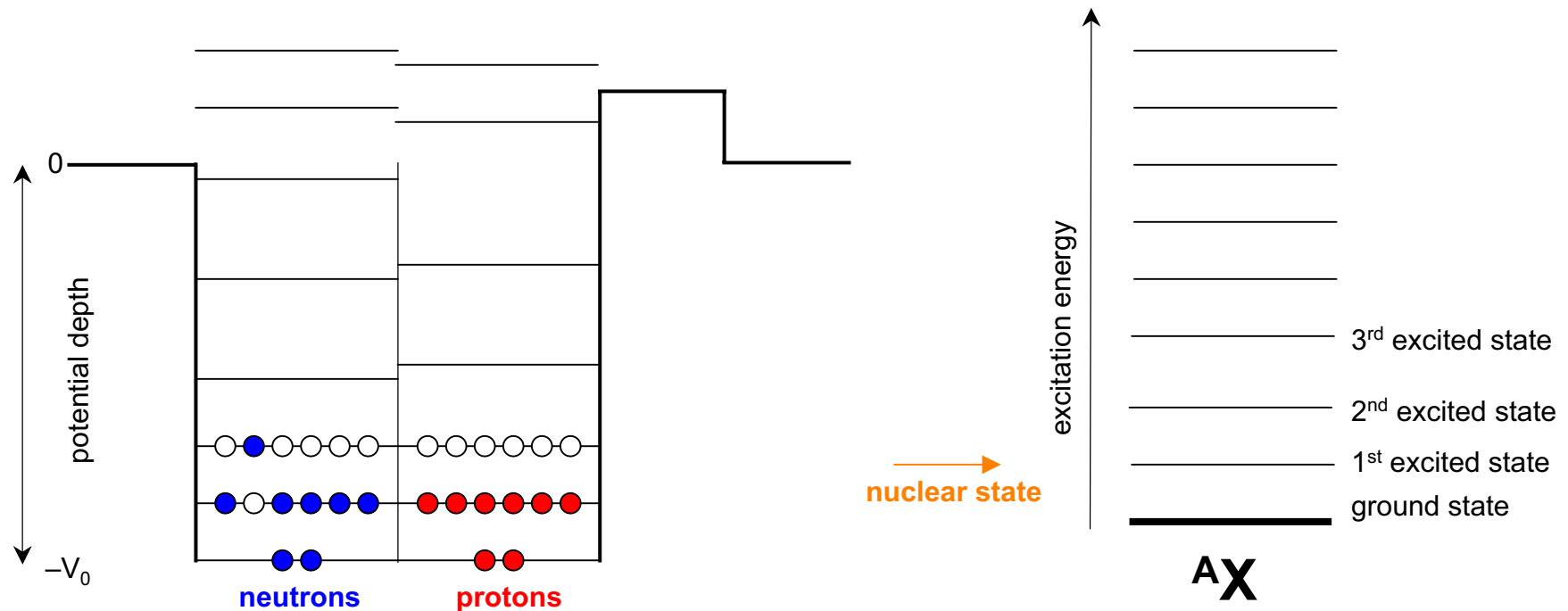
**level scheme representation:**  
excited states of a nucleus  
(shell model and other states)



# The nucleus as a quantum system

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configuration of nucleons in their potential

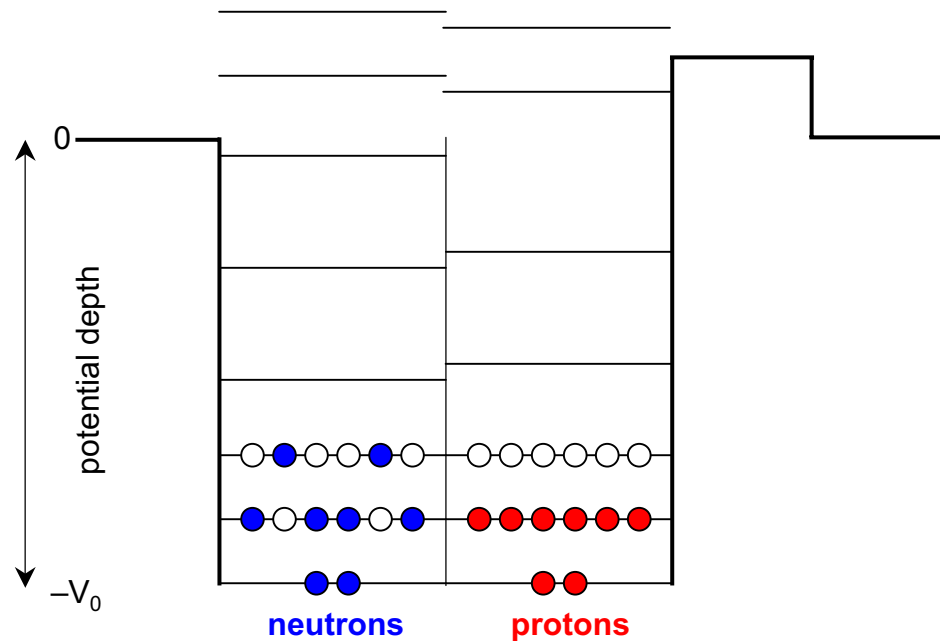
**level scheme representation:**  
excited states of a nucleus  
(shell model and other states)



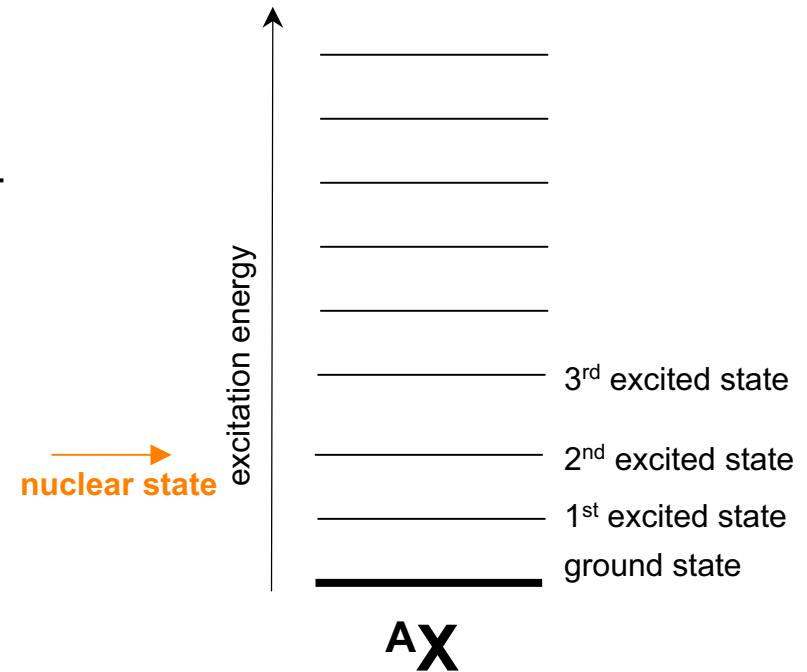


# The nucleus as a quantum system

**shell model representation:**  
configuration of nucleons in their potential



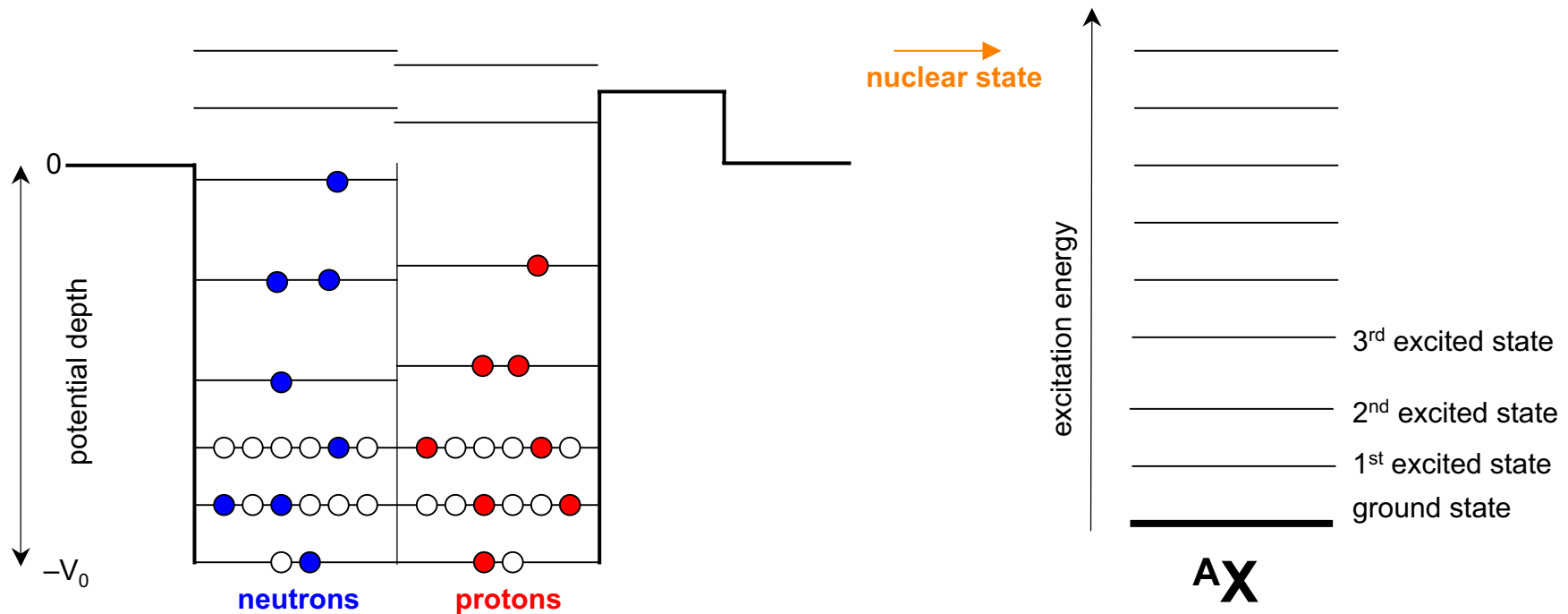
**level scheme representation:**  
excited states of a nucleus  
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# The nucleus as a quantum system

**shell model representation:**  
configuration of nucleons in their potential

**level scheme representation:**  
excited states of a nucleus  
(shell model and other states)



## Decay of a nuclear state

state with a life time  $\tau$ :

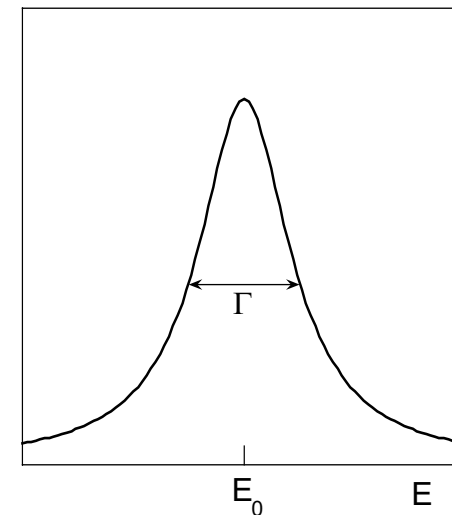
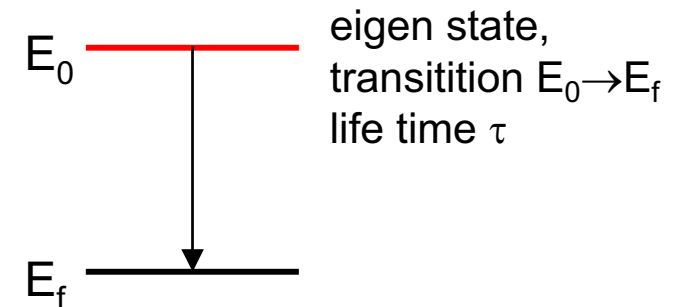
$$\Psi(t) = \Psi_0 e^{-iE_0 t / \hbar} e^{-t / 2\tau}$$

definition (Heisenberg):

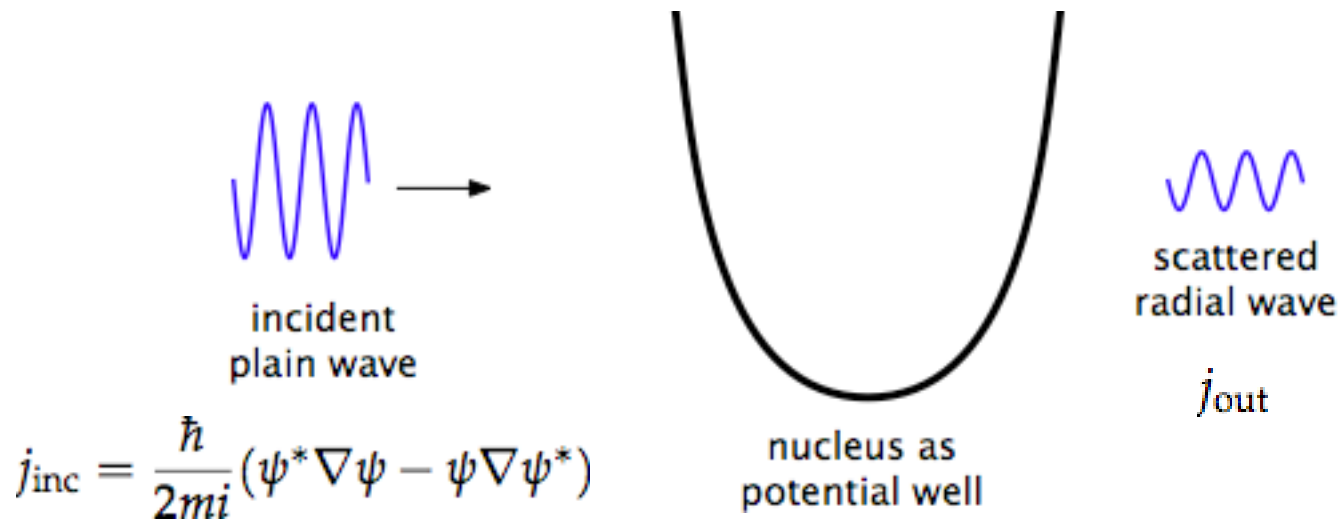
$$\Gamma = \frac{\hbar}{\tau}$$

Fourier transform gives energy profile:

$$I(E) = \frac{\Gamma / 2\pi}{(E - E_0)^2 + \Gamma^2 / 4}$$



## Neutron-nucleus reactions



Conservation of probability density: 
$$\sigma(\Omega) = \frac{r^2 j_{out}(r, \Omega)}{j_{inc}}$$

Solve Schrödinger equation of system to get cross sections.

Shape of wave functions of in- and outgoing particles are known, potential is unknown. Two approaches:

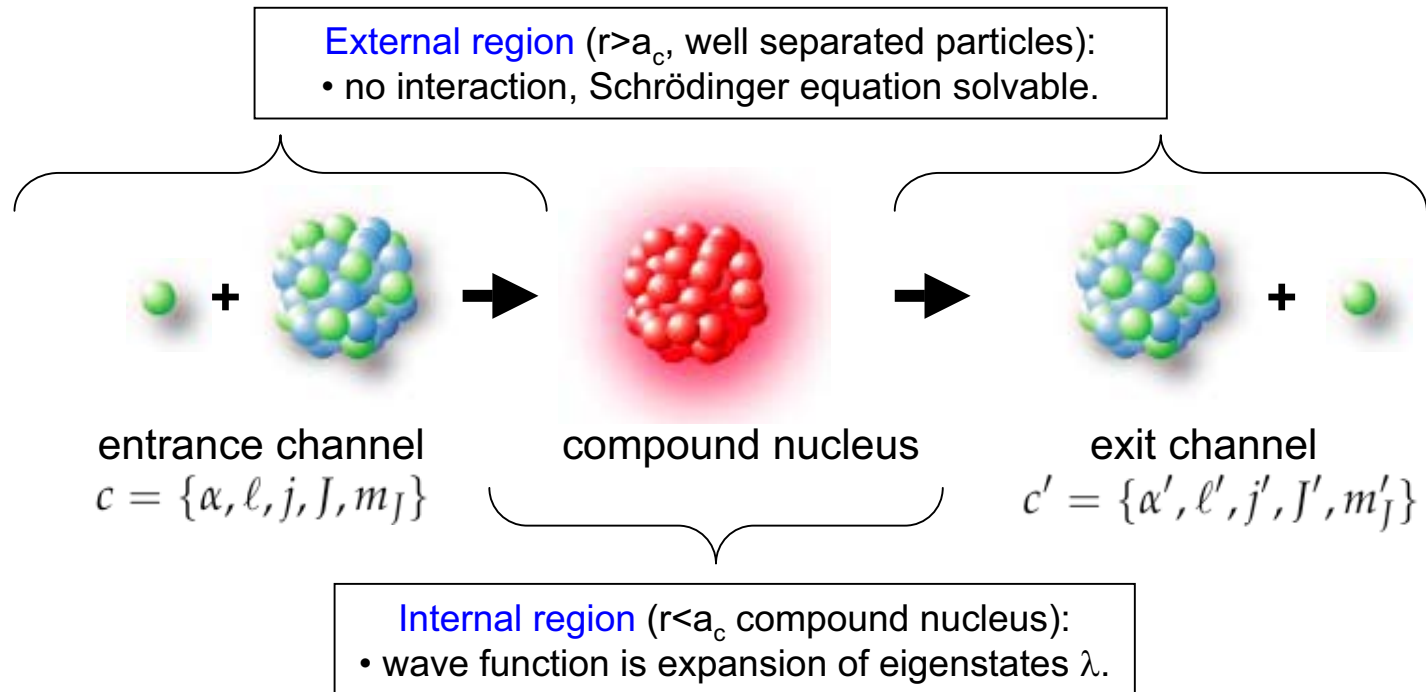
- calculate potential (optical model calculations, smooth cross section)
- use eigenstates (R-matrix, resonances)

## R-matrix formalism

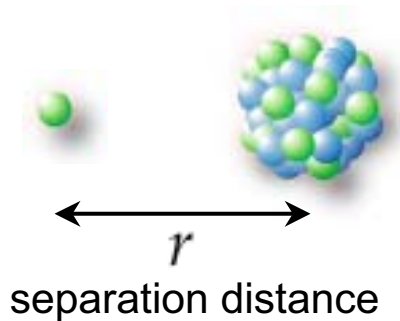
partial incoming wave functions:  $\mathcal{I}_c$   
 partial outgoing wave functions:  $\mathcal{O}_{c'}$   
 related by collision matrix:  $U_{cc'}$

cross section:  

$$\sigma_{cc'} = \pi \lambda_c^2 |\delta_{c'c} - U_{c'c}|^2$$



## Find the wave functions



$r > a_c$  external region

$r < a_c$  internal region

$r = a_c$  match value and derivative of

$$\left[ \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2m_c}{\hbar^2} (V(r) - E) \right] R(r) = 0$$

External region: **easy**, solve Schrödinger equation

central force, separate radial and angular parts.

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

**solution:** solve Schrödinger equation of relative motion:

- Coulomb functions
- special case of neutron particles (neutrons): fonctions de Bessel

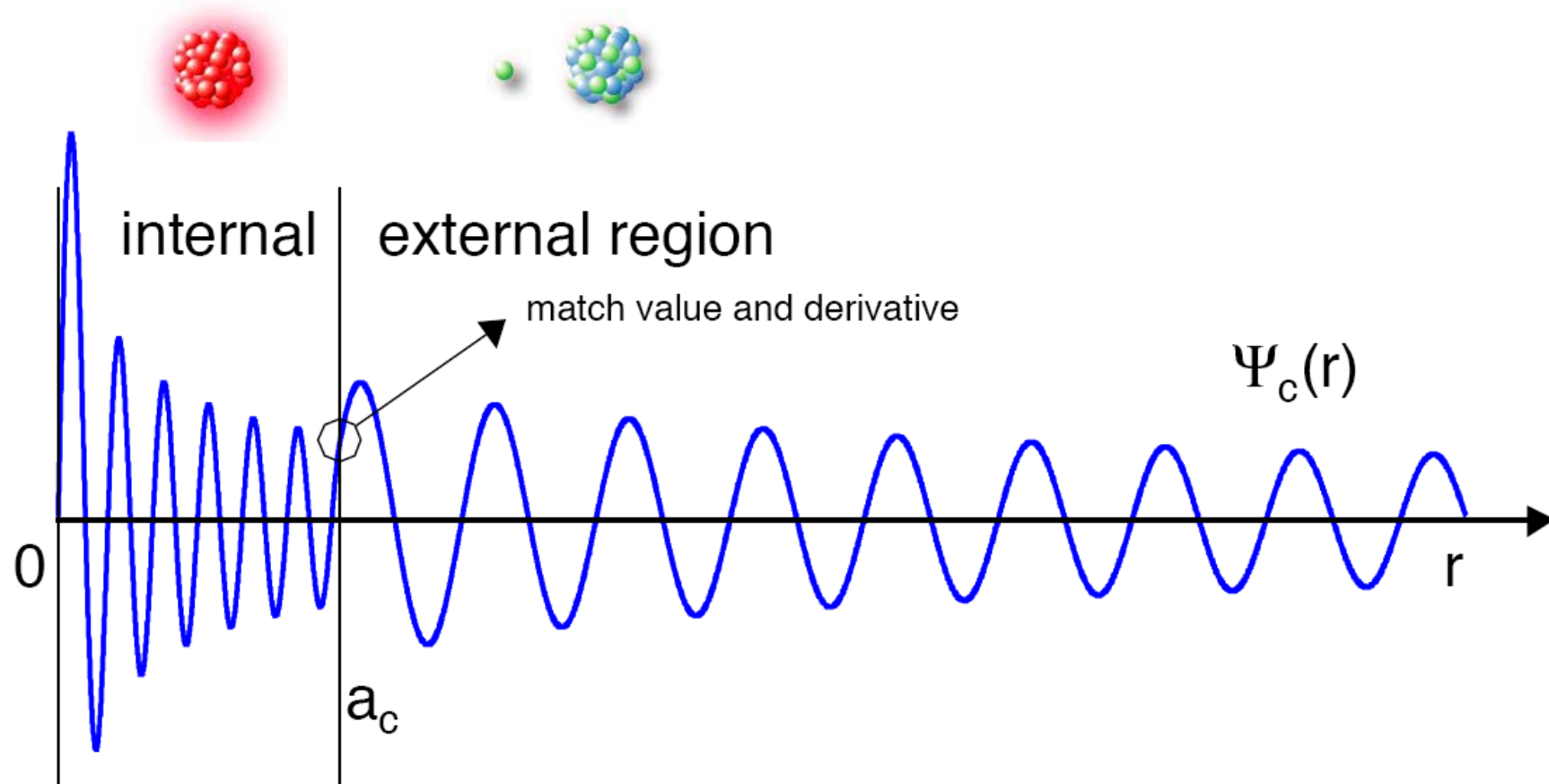
Internal region: **very difficult**, Schrödinger equation cannot be solved directly

**solution:** expand the wave function as a linear combination of its eigenstates.

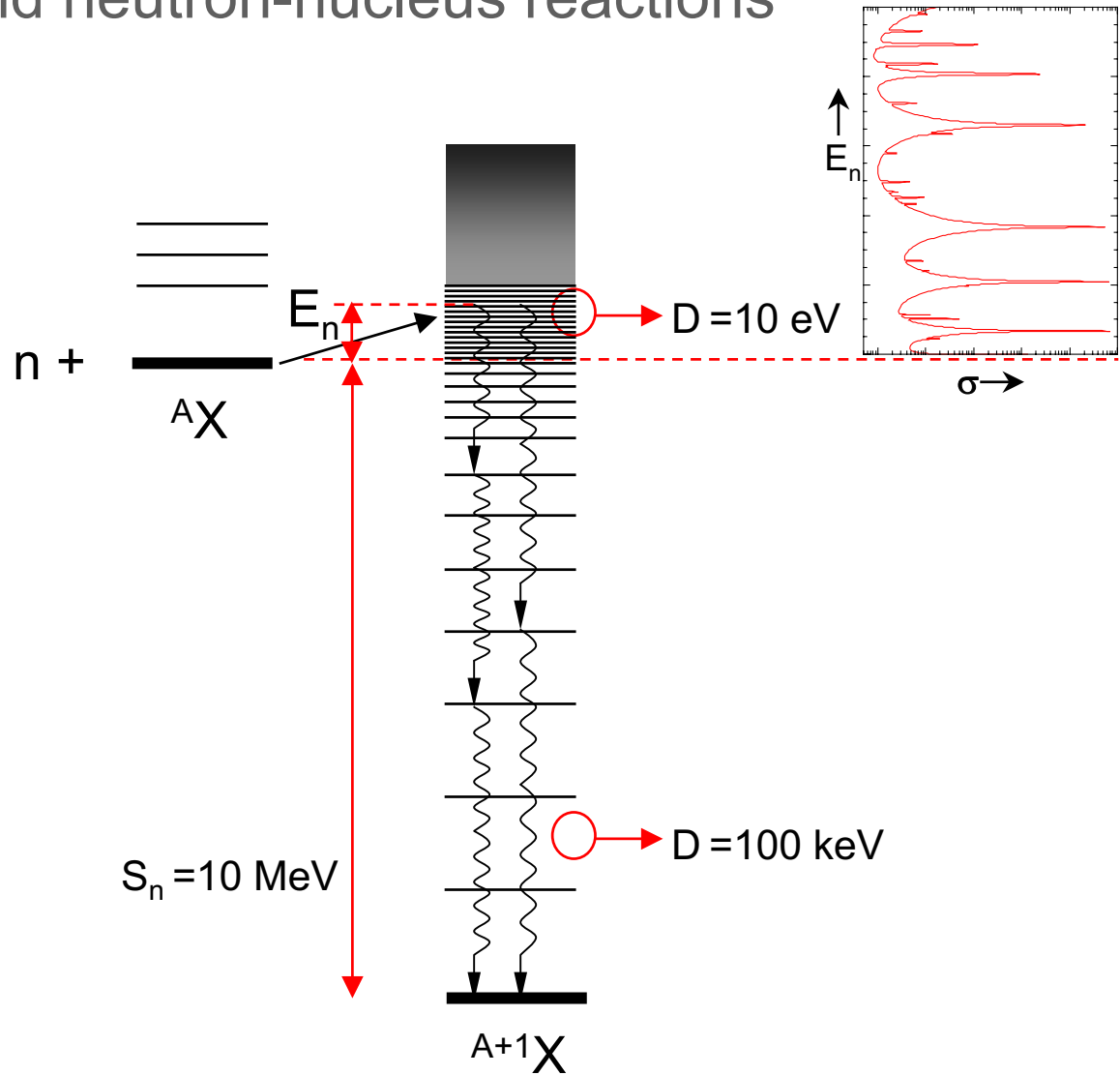
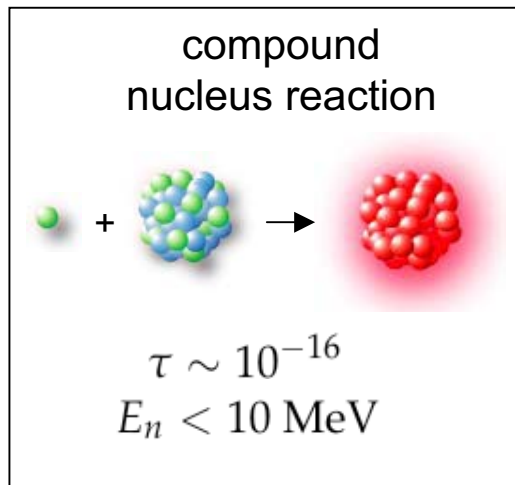
using the **R-matrix**:

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E}$$

# The R-matrix formalism



# Compound neutron-nucleus reactions





## The R-matrix formalism

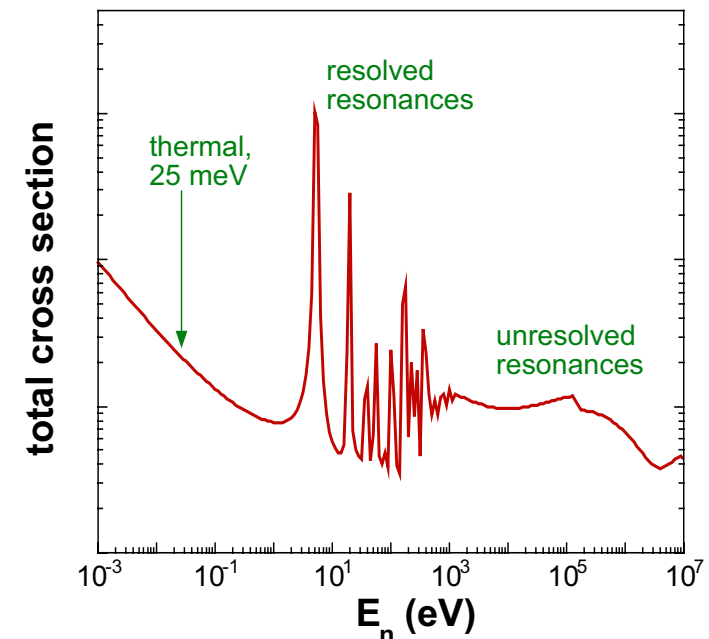
- The R-matrix formalism is adapted to describe compound nucleus reactions.
- Typically used for neutron-induced reactions at low energy ( $E_n < 10$  MeV, resonance region).
- The resonance parameters are properties of the excited nuclear levels:

- in the **resolved** resonance region (RRR),  
to each level (resonance) corresponds a  
set of parameters:

$$E, J^\pi, \Gamma_n, \Gamma_\gamma$$

- in the **unresolved** resonance region (URR)  
average parameters are used:

$$\langle D_l \rangle, \langle \Gamma_n^l \rangle, \langle \Gamma_\gamma^l \rangle$$



## Resonance parameters

- A same set of resonance parameters is used to produce all resonant reactions,
- at low energies mainly elastic scattering and capture (and fission).

$$\sigma_{r,t} = \sigma_{r,t}(\text{resonance parameters})$$

- In a measurement, one does not measure a cross section, but a reaction yield or transmission factor.

$$Y_r = (1 - e^{-n\sigma_t}) \frac{\sigma_r}{\sigma_t} \quad 0 < Y_r < 1$$

$$T = e^{-n\sigma_t} \quad 0 < T < 1$$

- The measured reaction yield is not equally sensitive to all parameters, additional
- constraints can be necessary to extract RP from measurement.

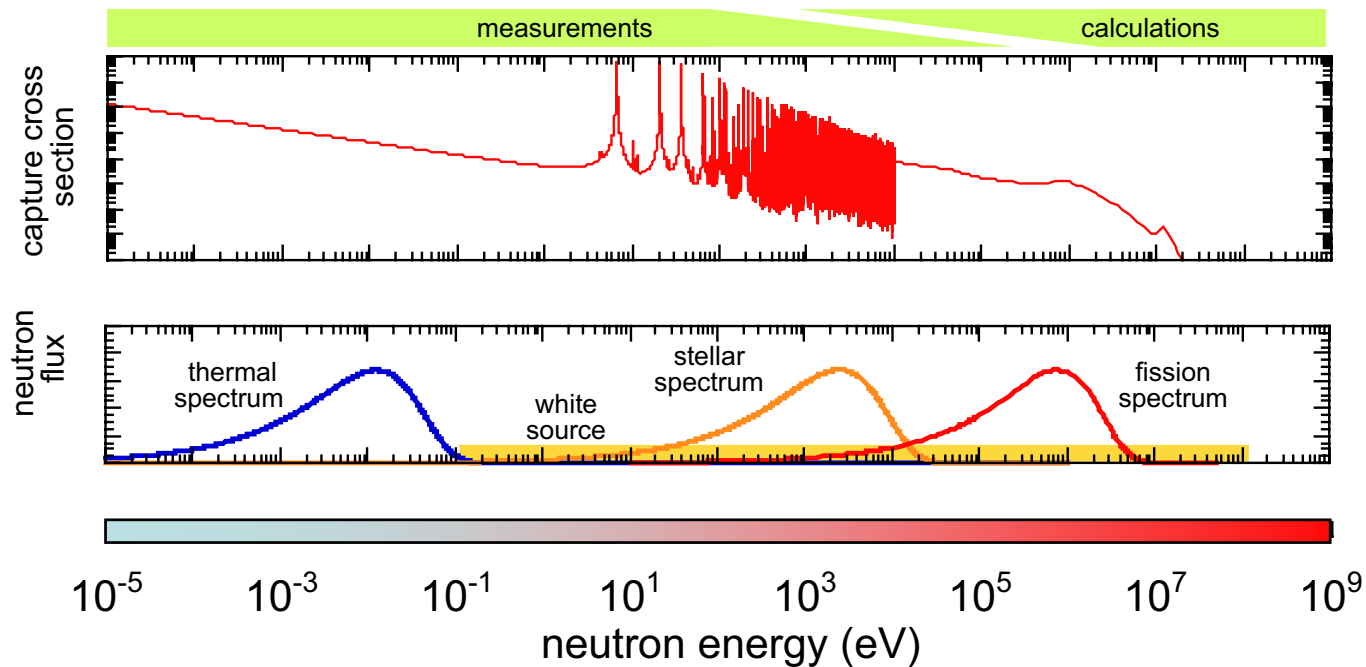
# Neutron-nucleus reactions

## R-matrix resonance description

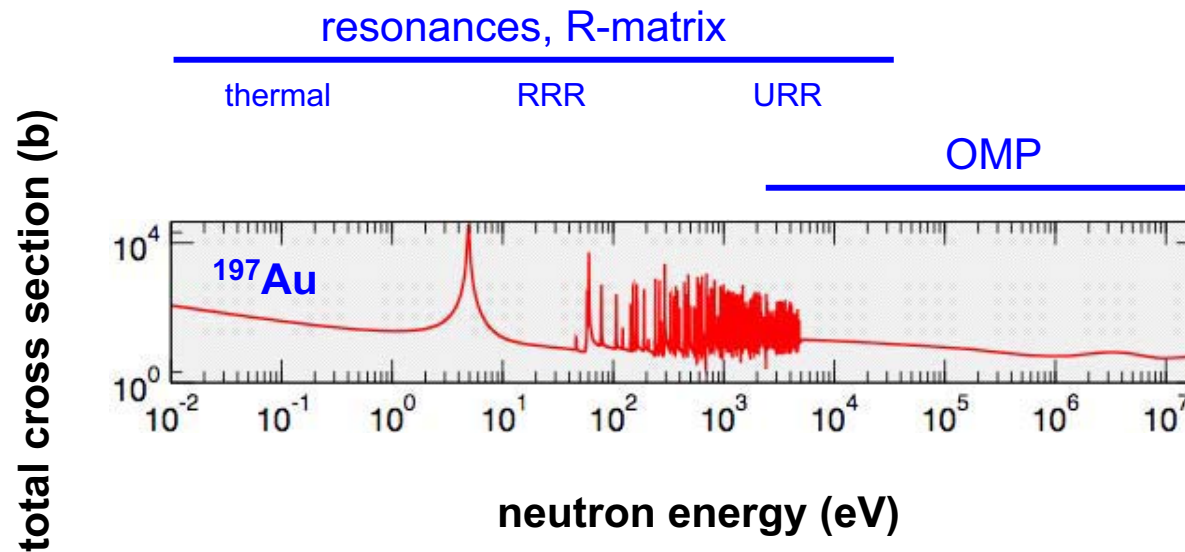
- fine structure (resonances)
- highly fluctuating cross sections
- resonance parametrization
- low energy, few channels

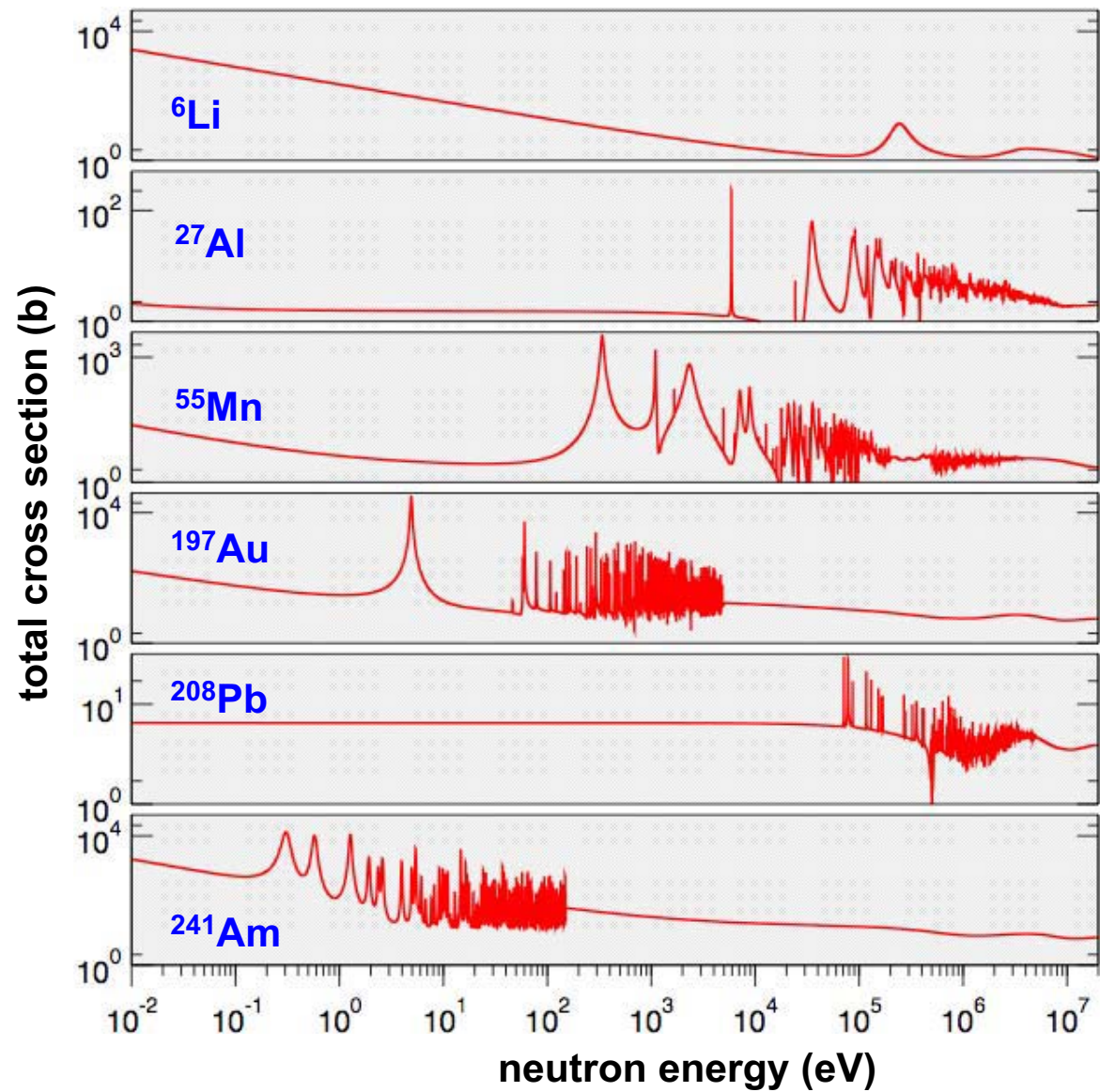
## Optical model calculations

- gross structure
- average cross sections
- optical model potential
- high energy, many channels



# Compound nucleus reactions



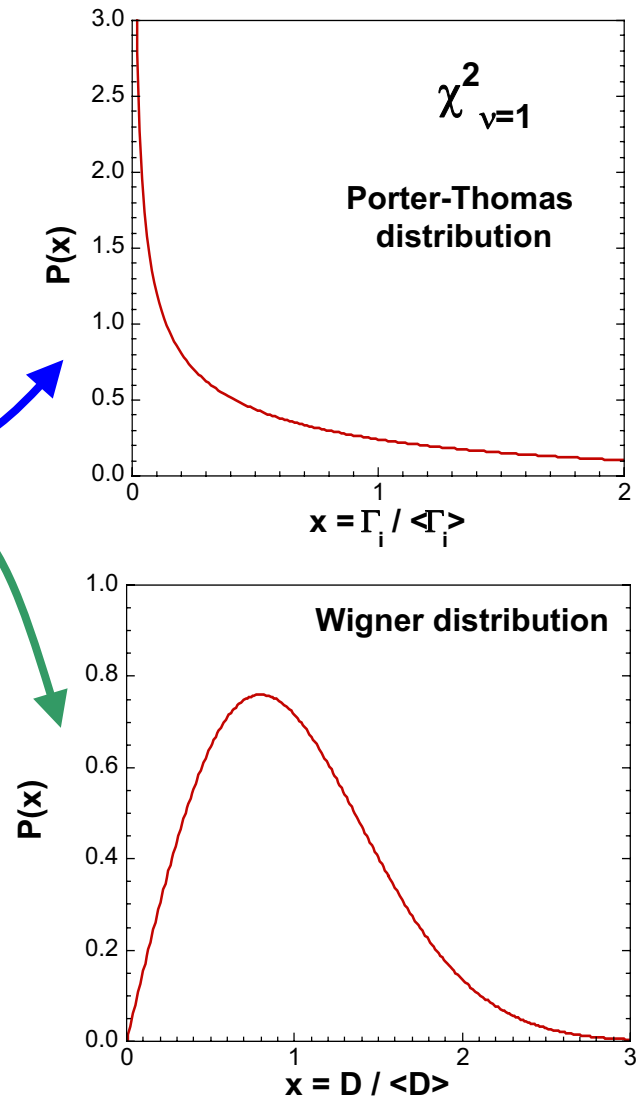
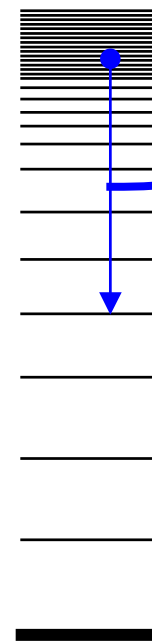


# Statistical model

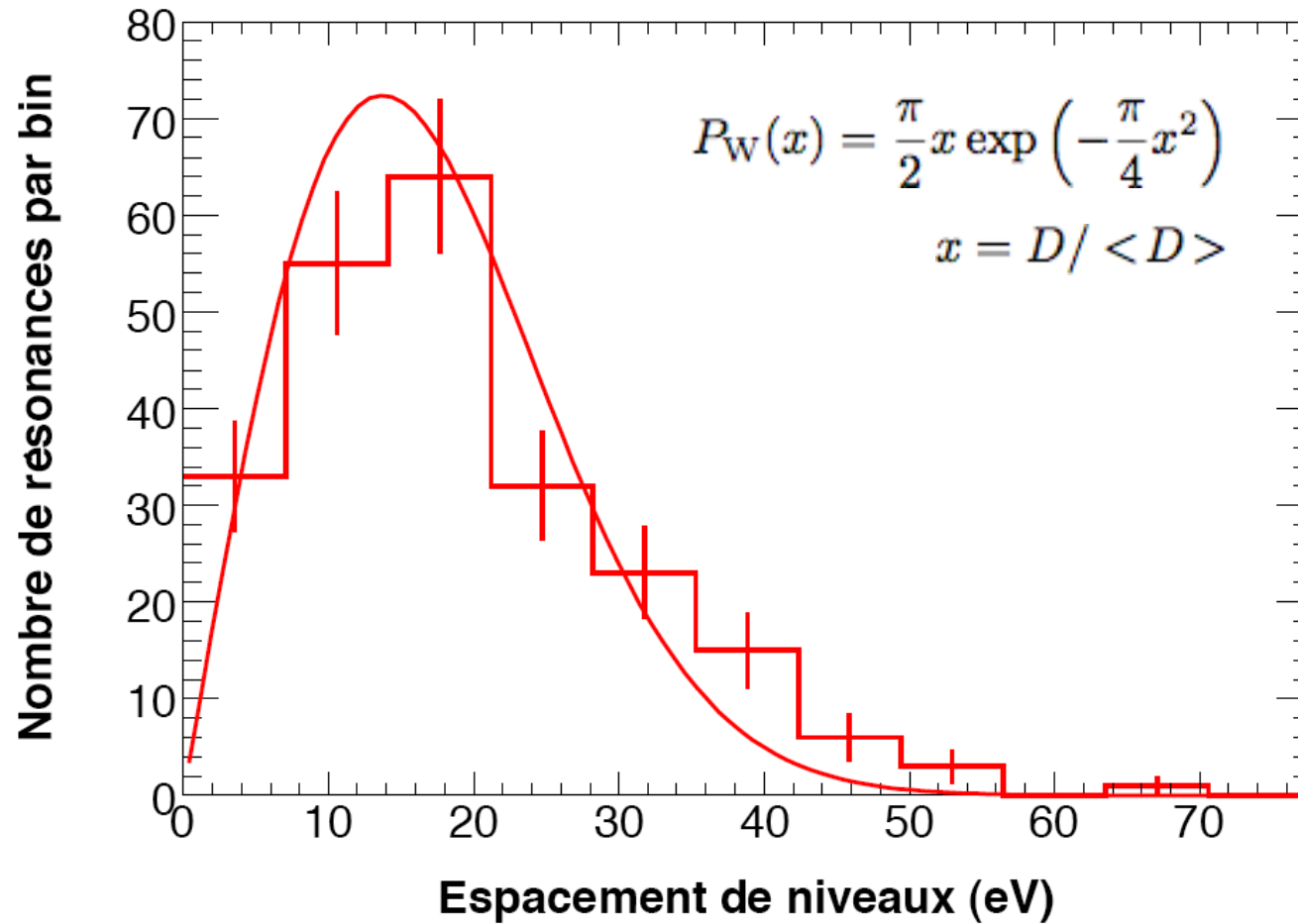
The nucleus in the vicinity of  $S_n$  is described by the **Gaussian Orthogonal Ensemble (GOE)**

The matrix elements are random variables with a Gaussian distribution.

- **Consequences:**
  - The partial width have a **Porter-Thomas** distribution.
  - The spacing of levels with the same  $J^\pi$  have approximately a **Wigner** distribution.

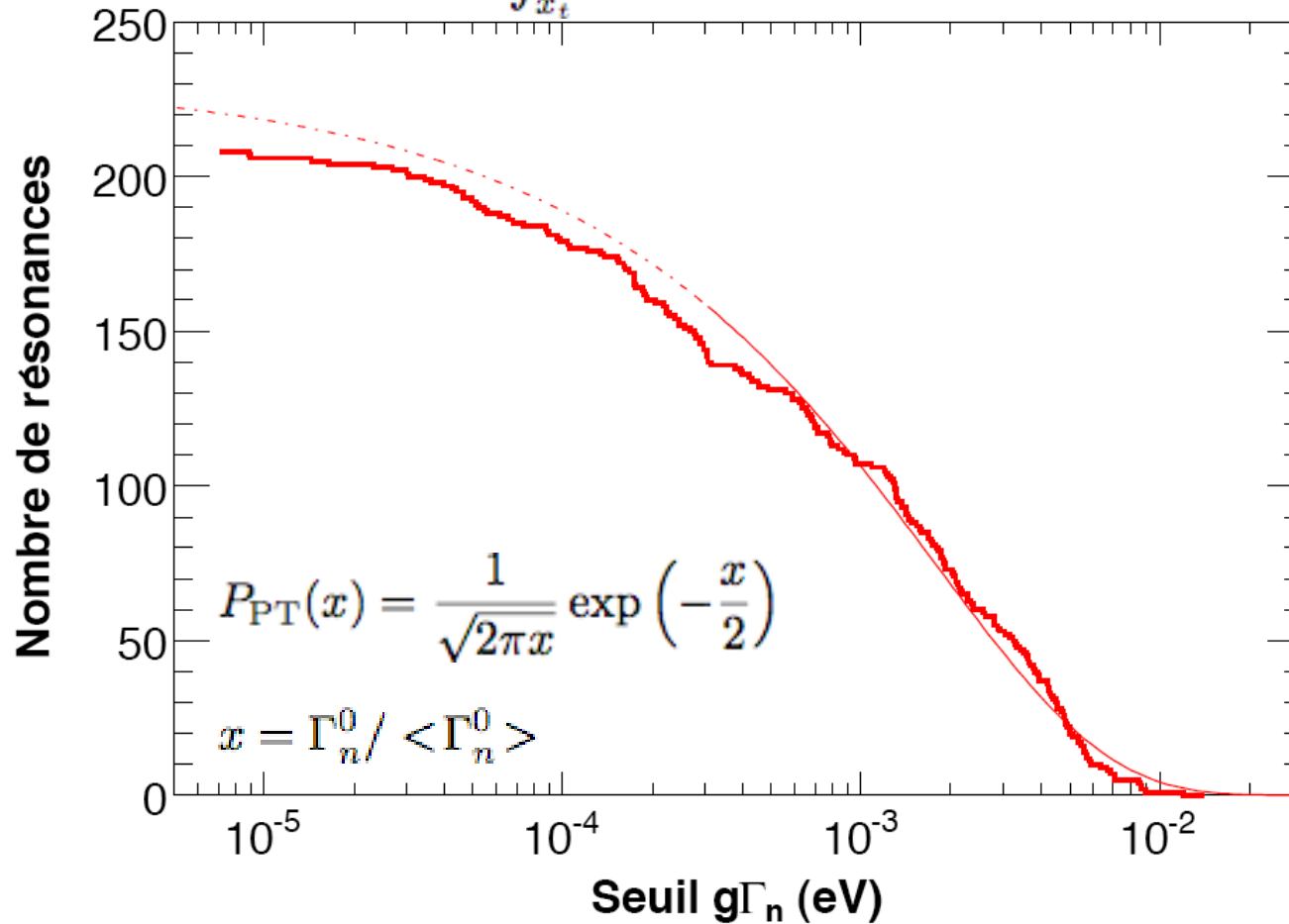


## Distribution of the spacing of two consecutive levels



## Distribution of neutron widths

$$N(x_t) = N_0 \int_{x_t}^{\infty} P_{PT}(x) dx = N_0(1 - \text{erf}\sqrt{x_t/2})$$

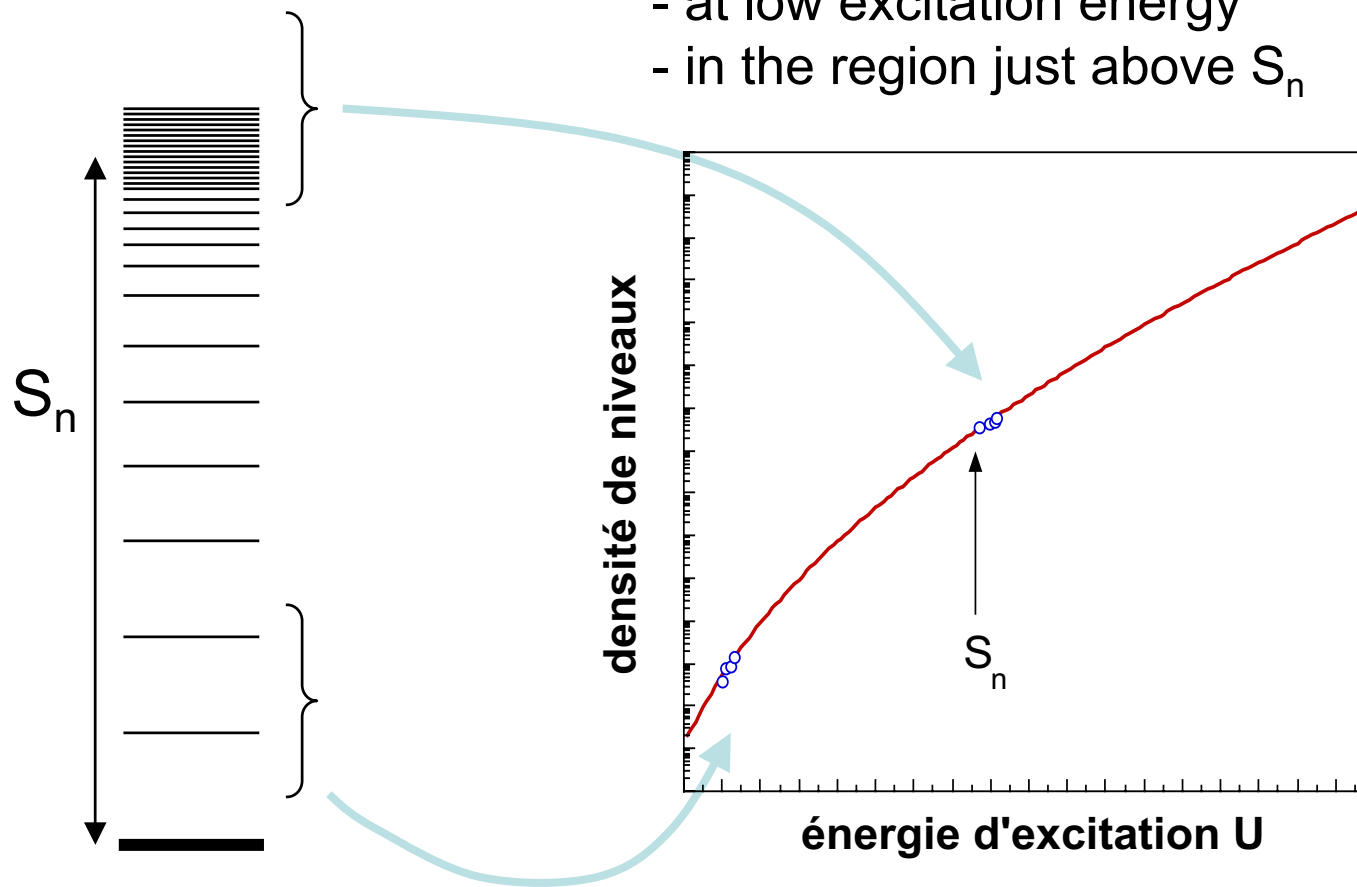




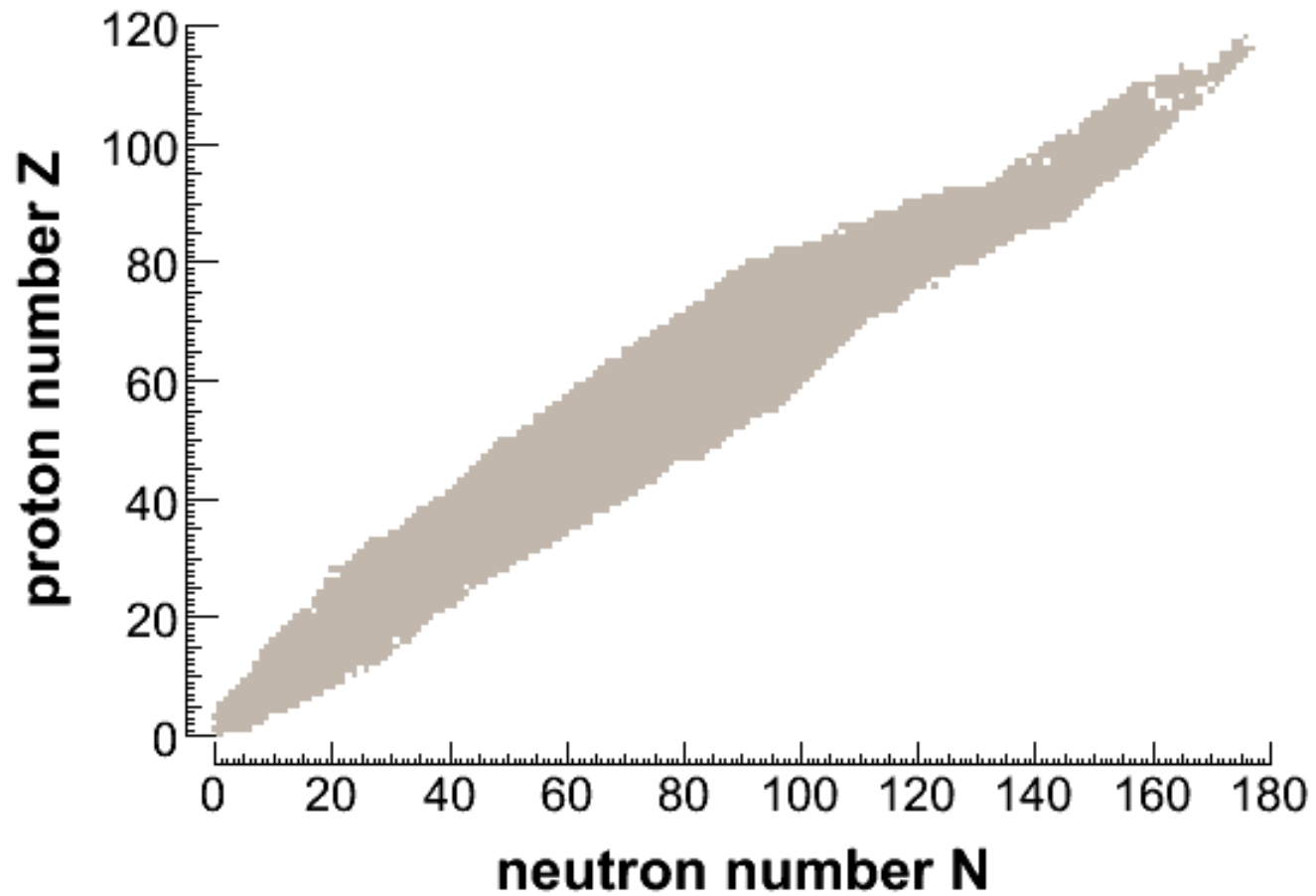
# Level density

Separated states are available

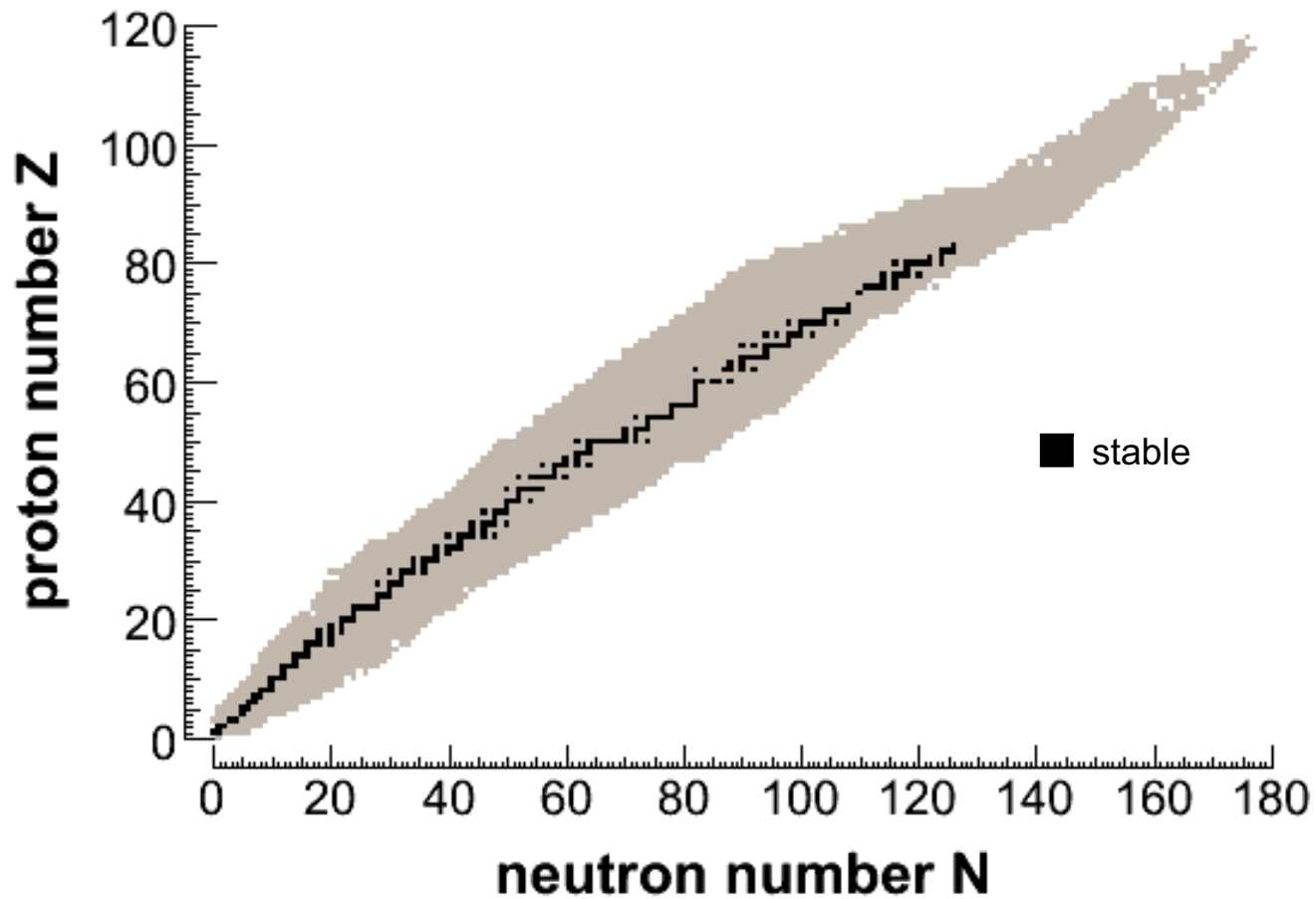
- at low excitation energy
- in the region just above  $S_n$



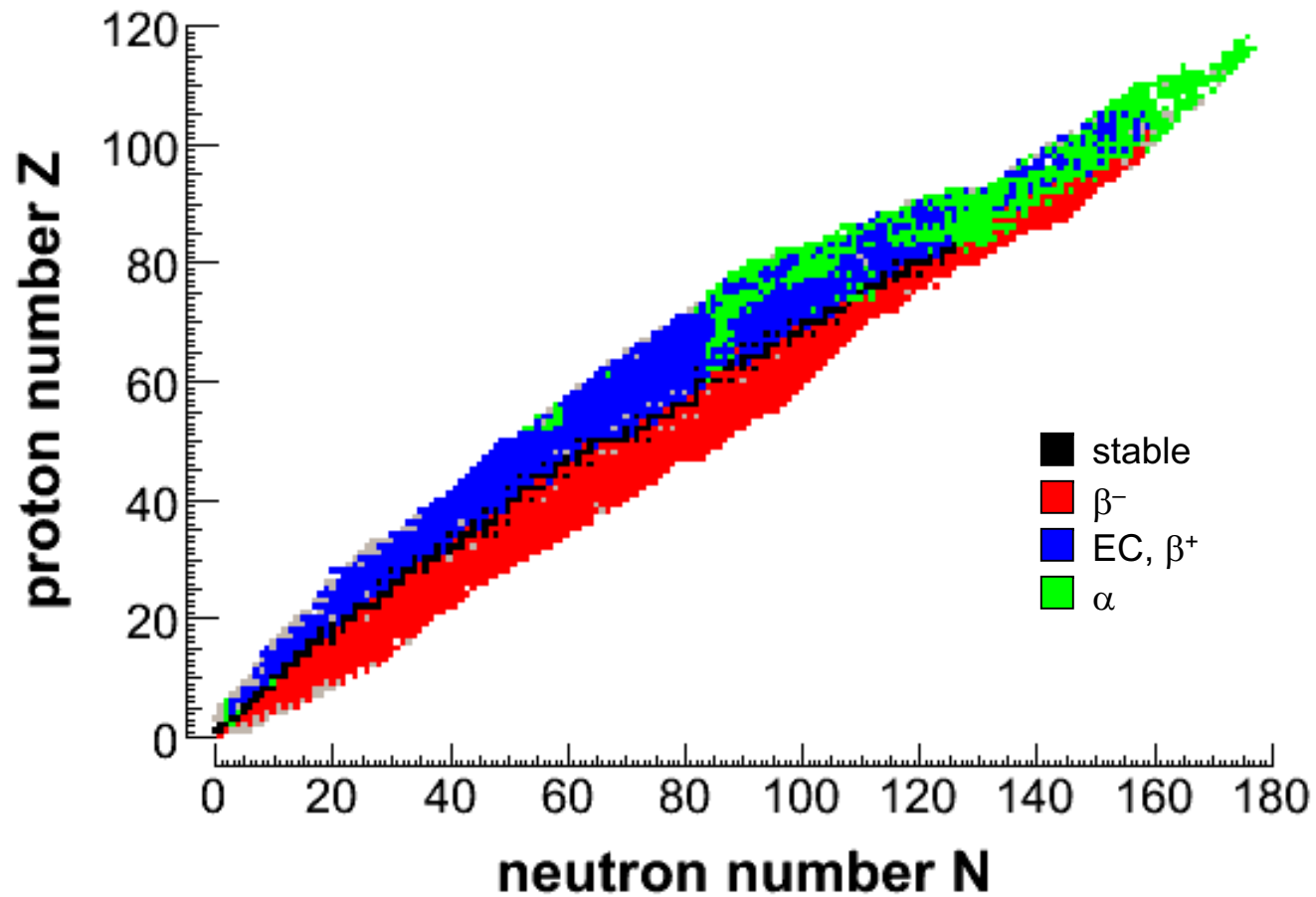
## Known nuclei



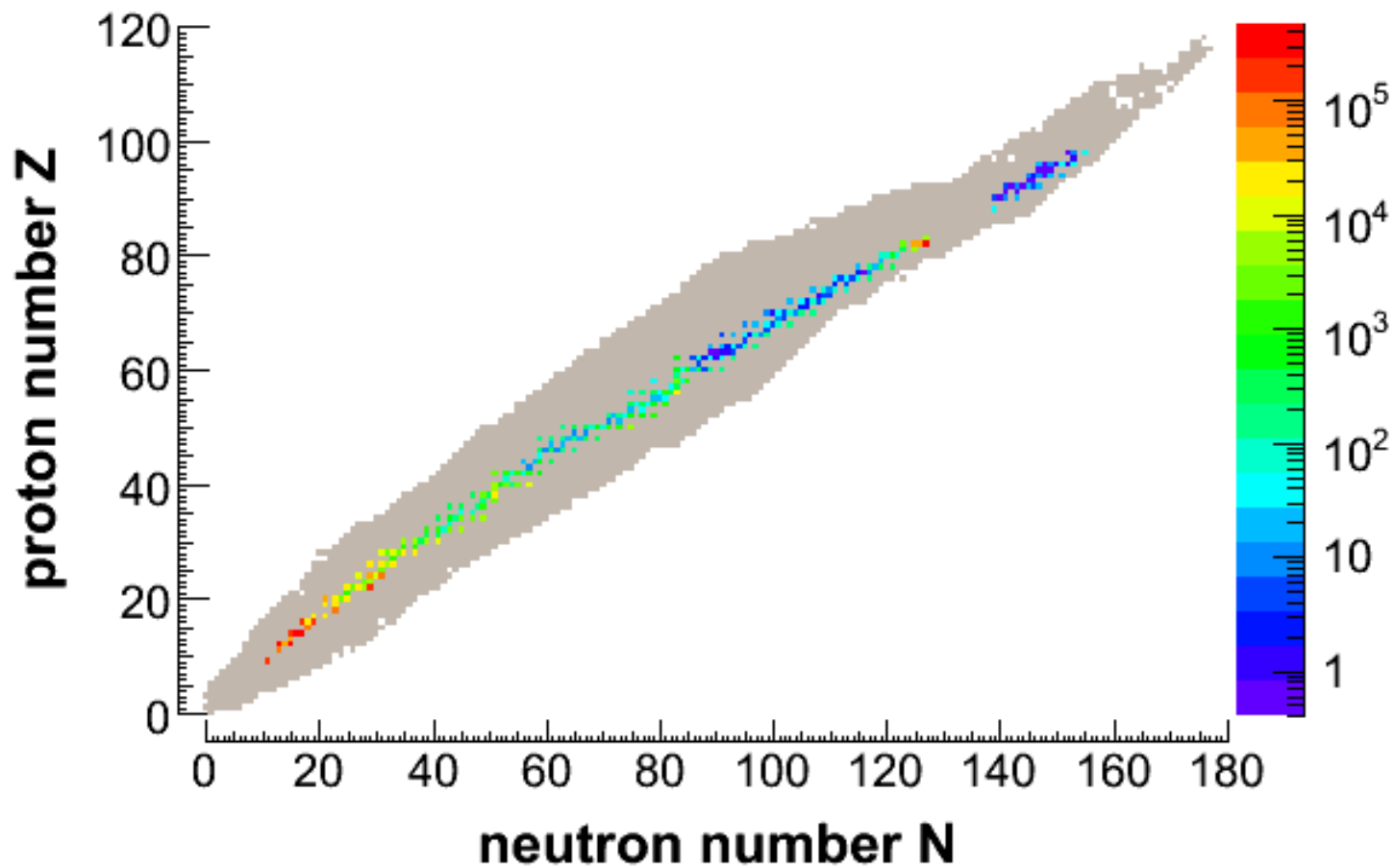
## Known nuclei



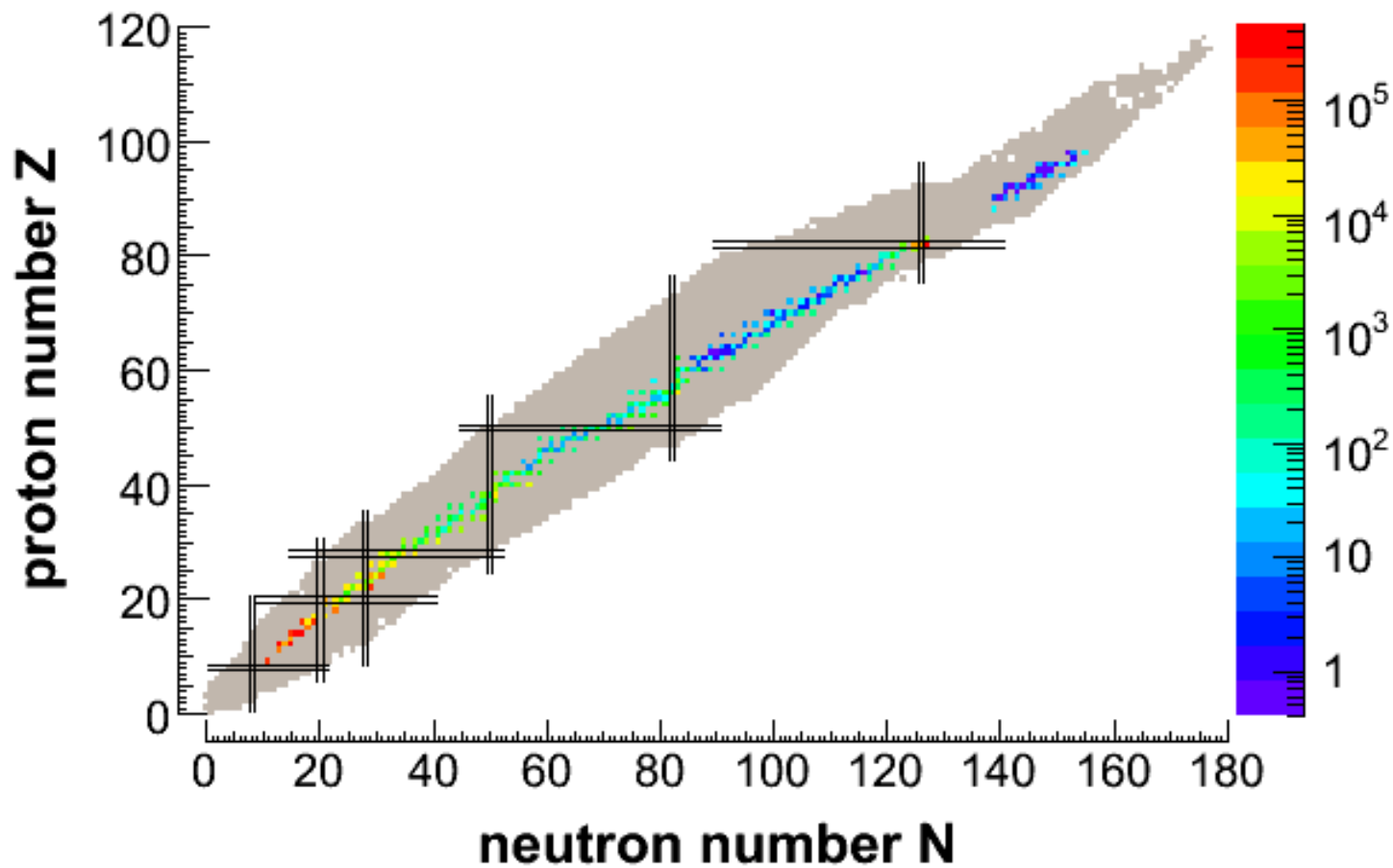
## Known nuclei



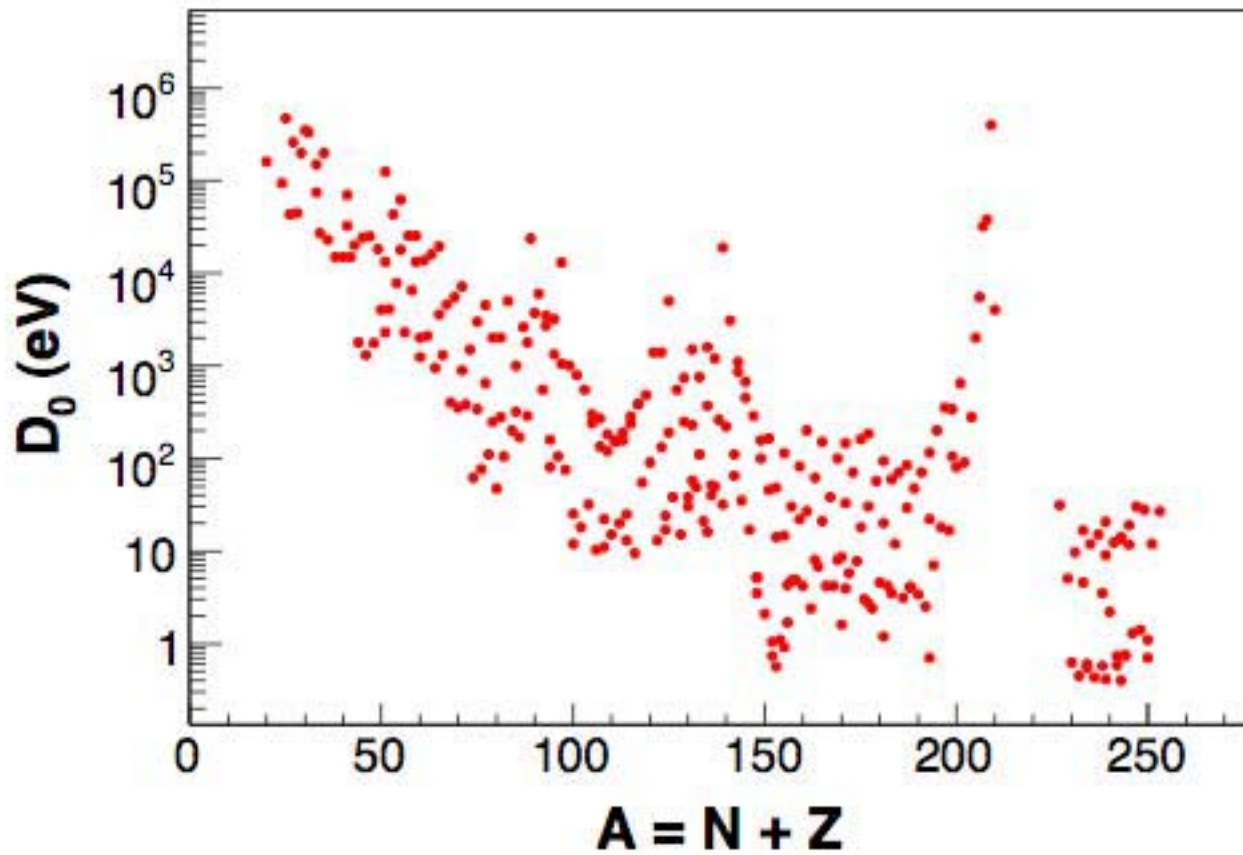
## Level spacing $D_0$



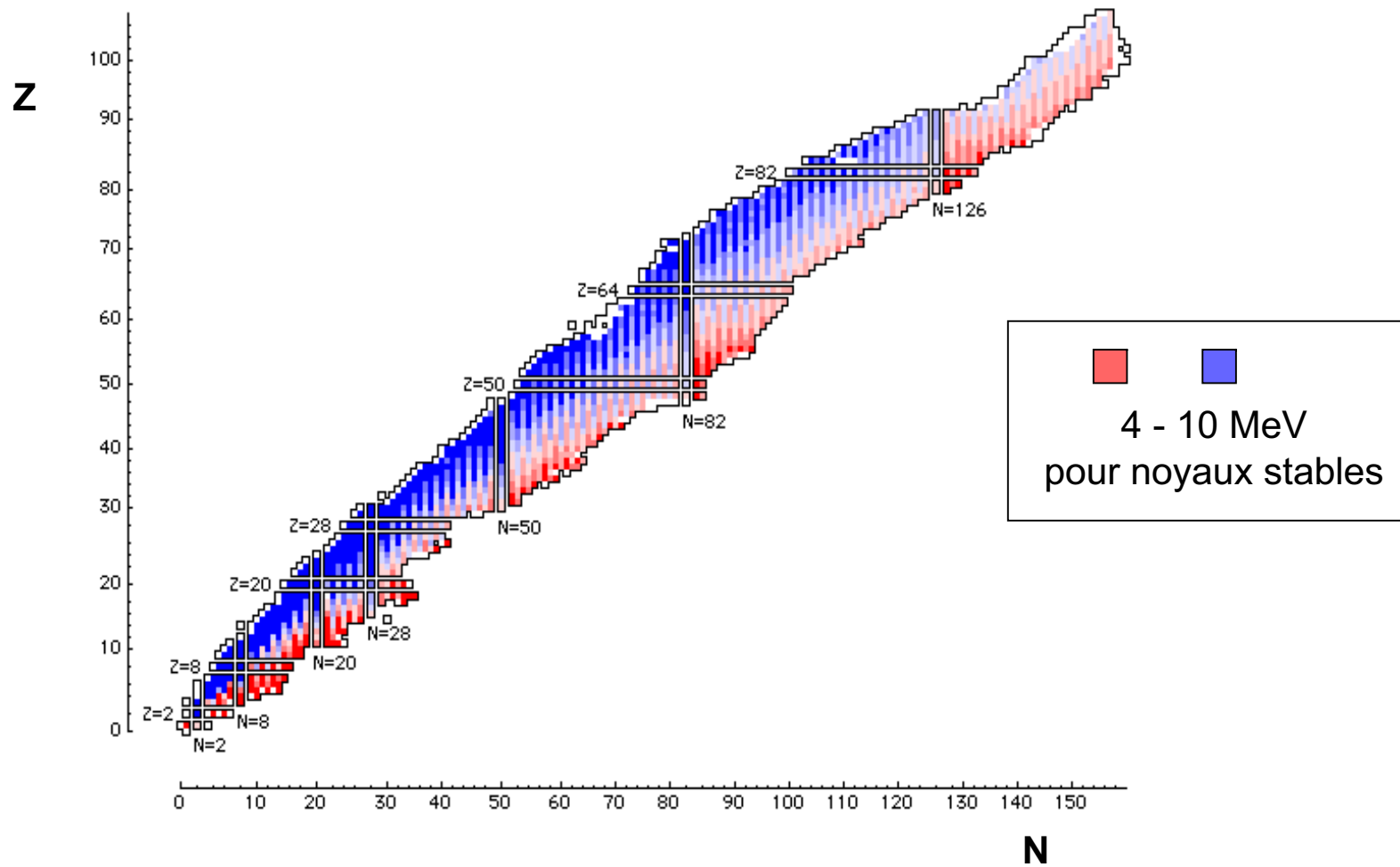
## Level spacing $D_0$



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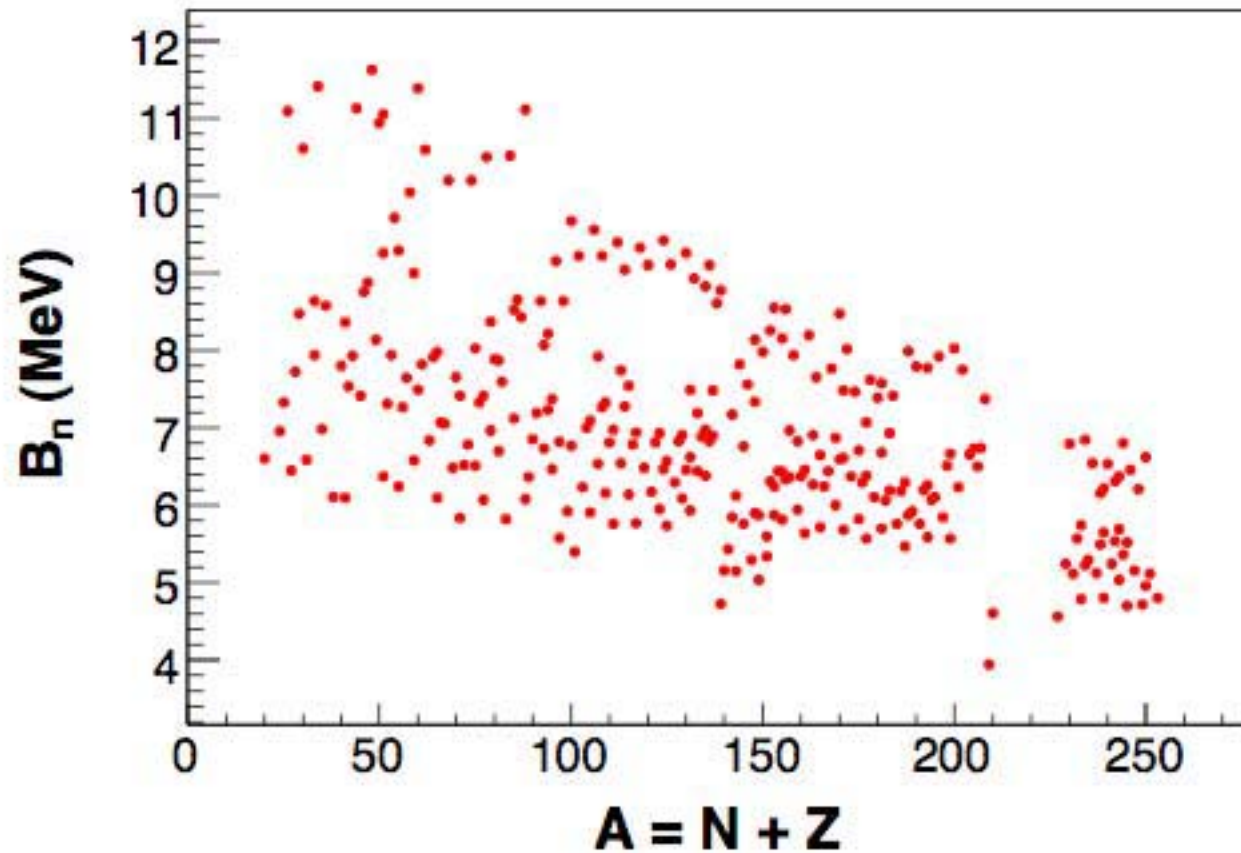


# Neutron separation energy

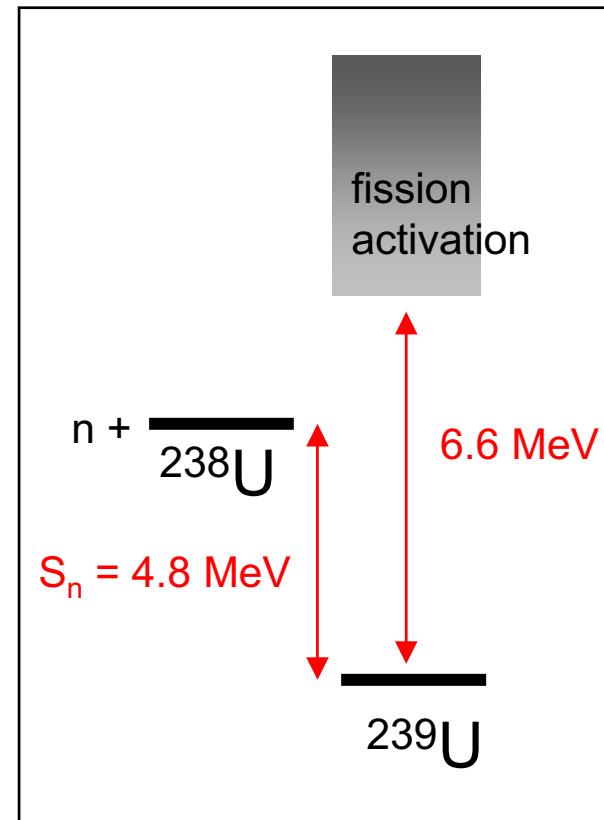
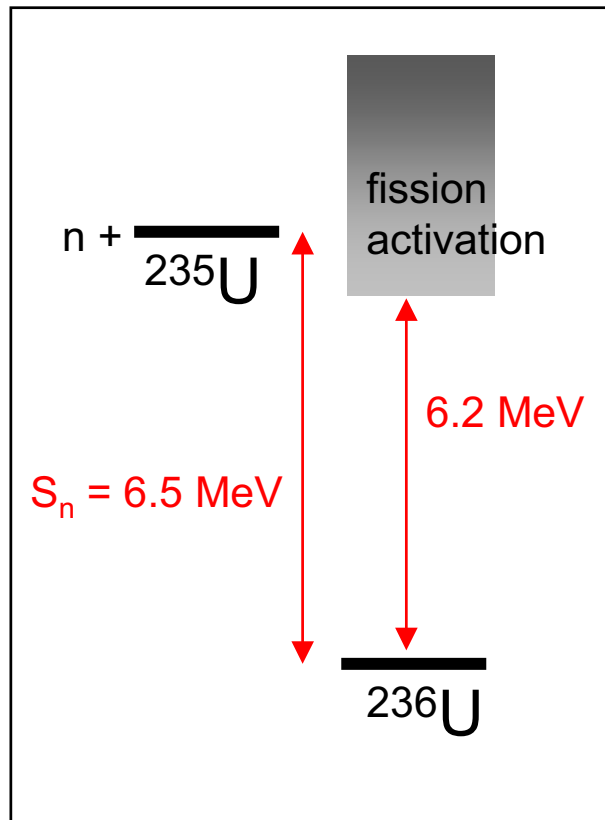




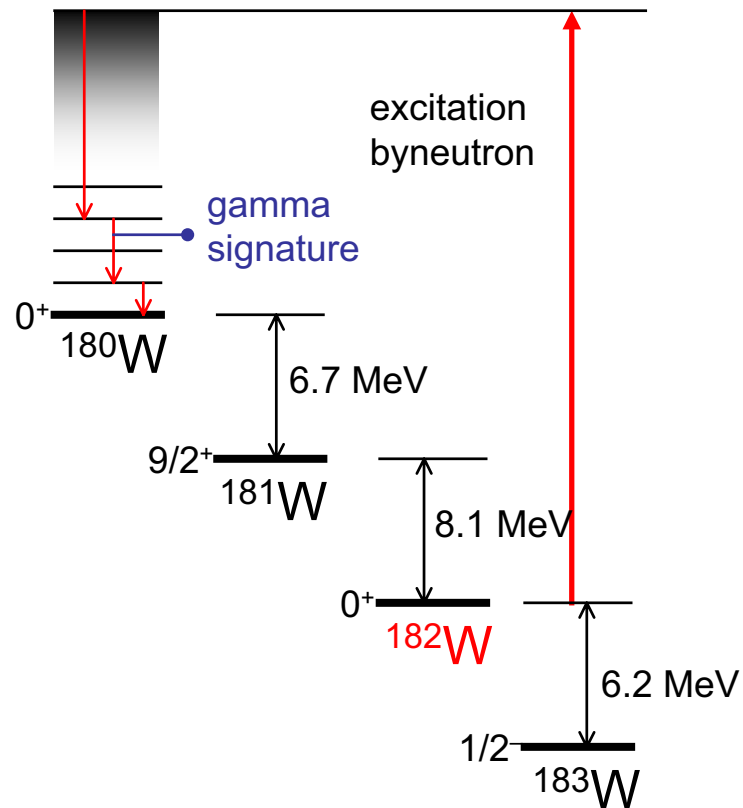
## Neutron separation energy



## Fission of $^{235}\text{U}+n$ and $^{238}\text{U}+n$

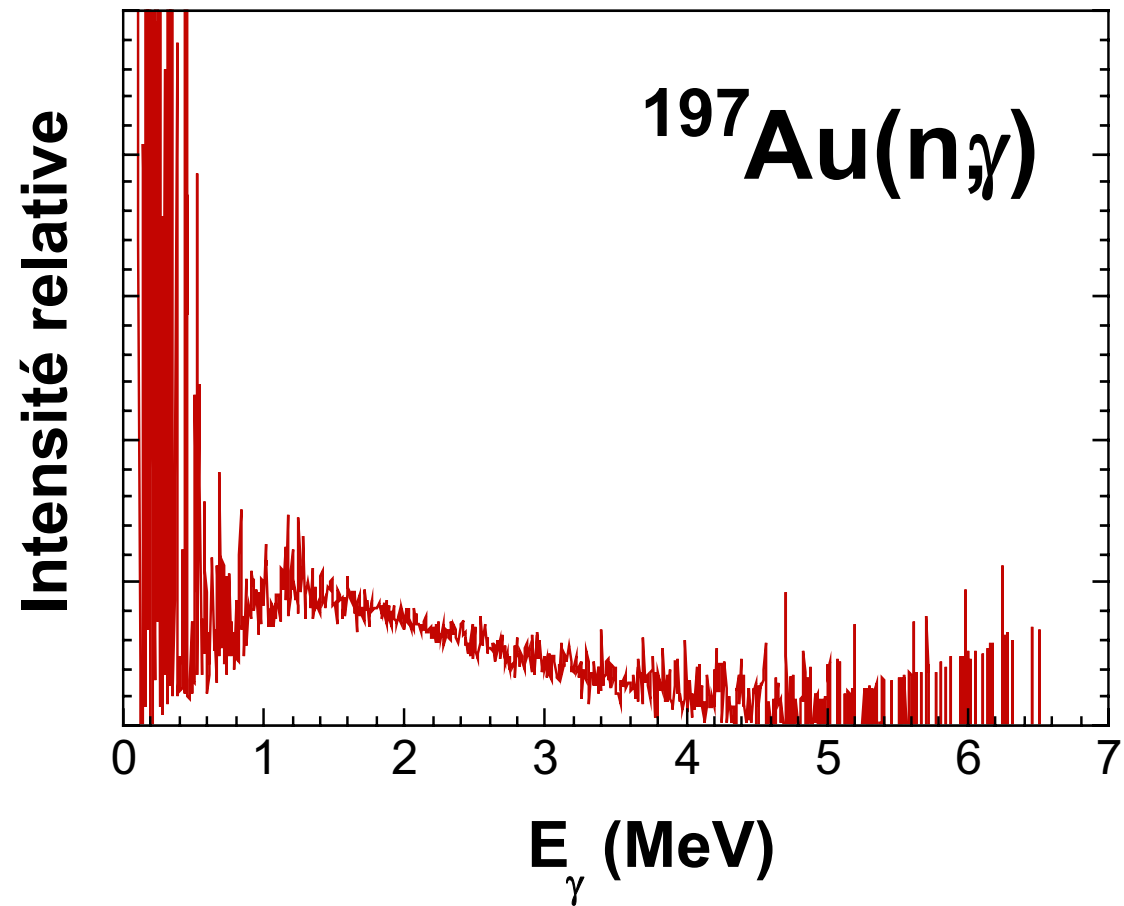


# Measurement of (n,xn) by gamma-ray spectroscopy



example:  $^{182}\text{W}(n,3n)^{180}\text{W}$

## Simulated gamma-ray spectrum



## Moderation of neutrons

Maxwell-Boltzmann velocity distribution:

$$\frac{dn}{dv} \sim v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)$$

$$v_{\max} = \sqrt{2k_B T/m}$$

$$E_{\max} = \frac{1}{2}mv^2 = k_B T$$

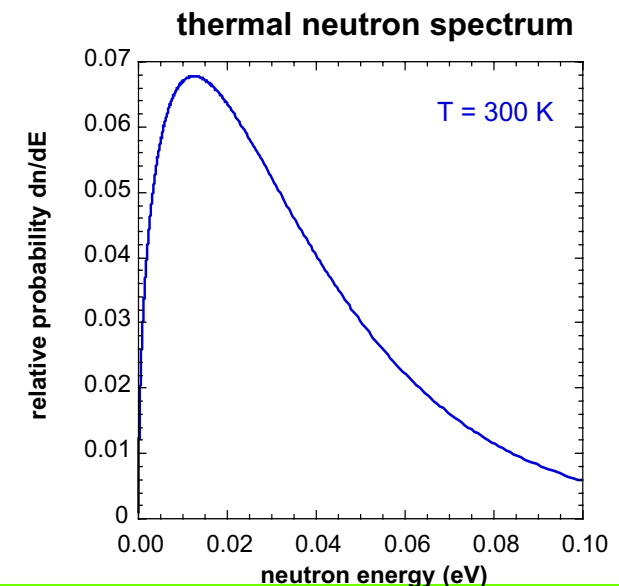
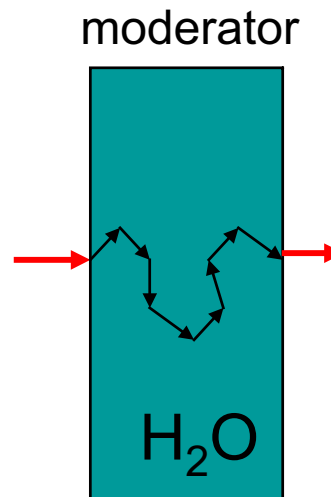
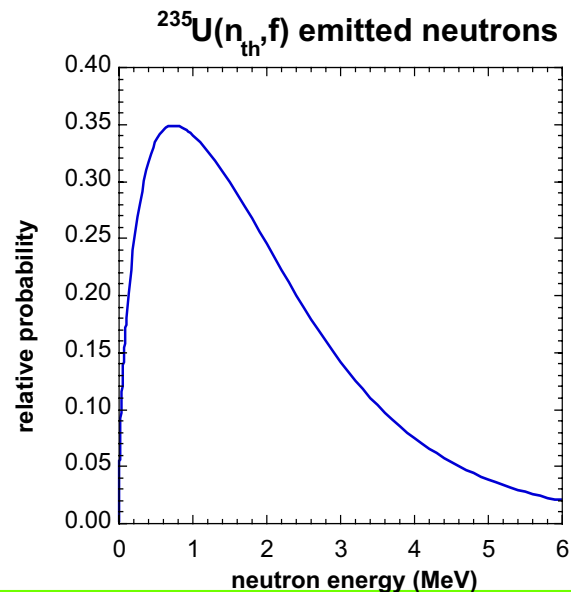
thermal neutrons:

$$v_{\max} = 2200 \text{ m/s (def.)}$$

$$E_{\max} = 25.3 \text{ meV}$$

$$T = \frac{1}{2}mv^2/k_B = 293.6 \text{ K}$$

$$\frac{dn}{dE_n} \rightarrow E_{\max} = \frac{1}{2}k_B T$$



## Evaluated nuclear data libraries

### Libraries

- JEFF - Europe
- JENDL - Japon
- ENDF/B - US
- BROND - Russia
- CENDL - China

### Common format:

ENDF-6

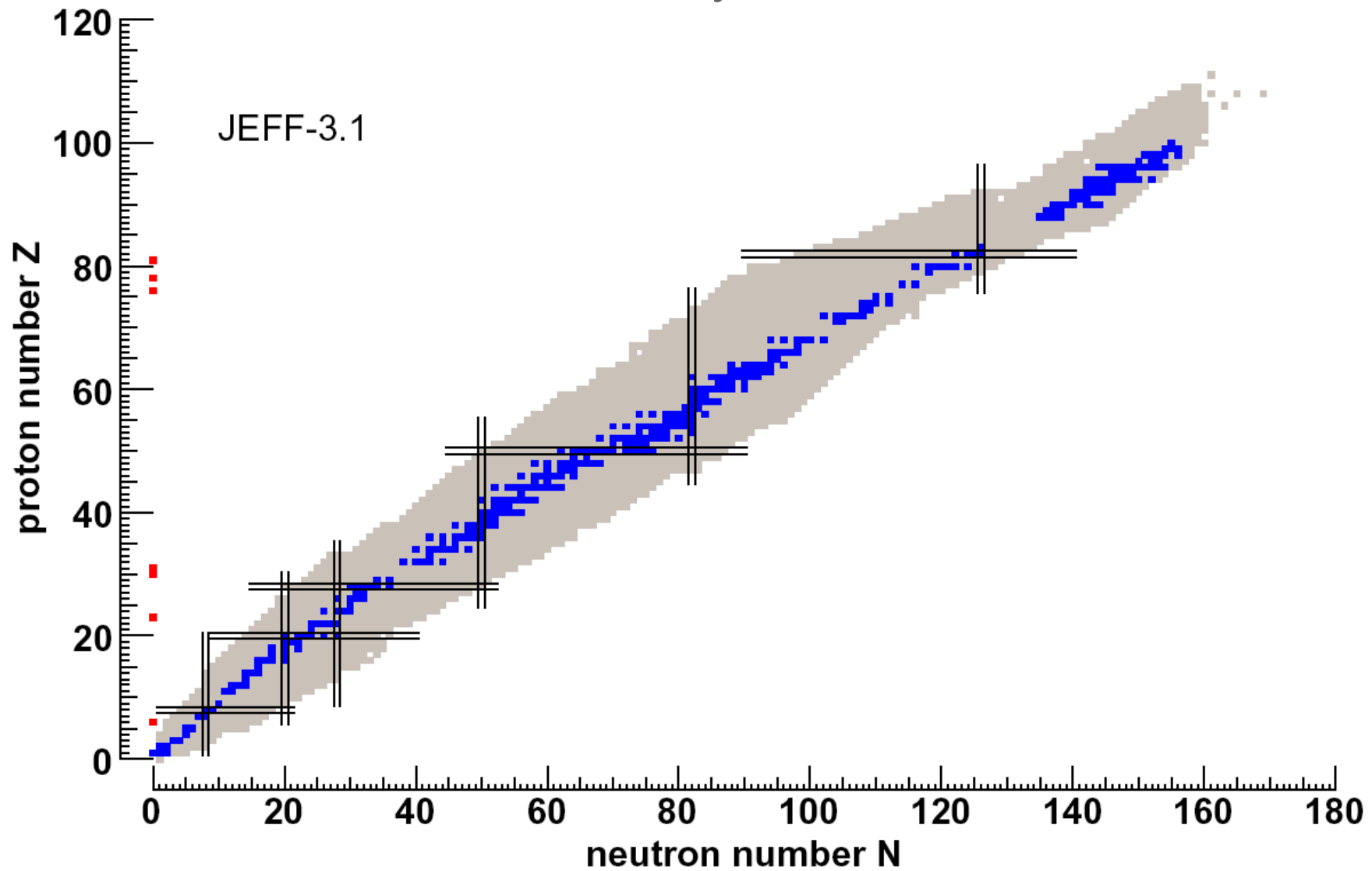
### Contents:

Data for particle-induced reactions (neutrons, protons, gamma, other)  
but also radioactive decay data

Data are identified by “materials”  
(isotopes, isomeric states, (compounds) )

ex.            $^{16}\text{O}$ :       mat = 825  
              natV:       mat = 2300  
               $^{242\text{m}}\text{Am}$ : mat = 9547

## The library JEFF-3.1



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# Files for a material

from report ENDF-102

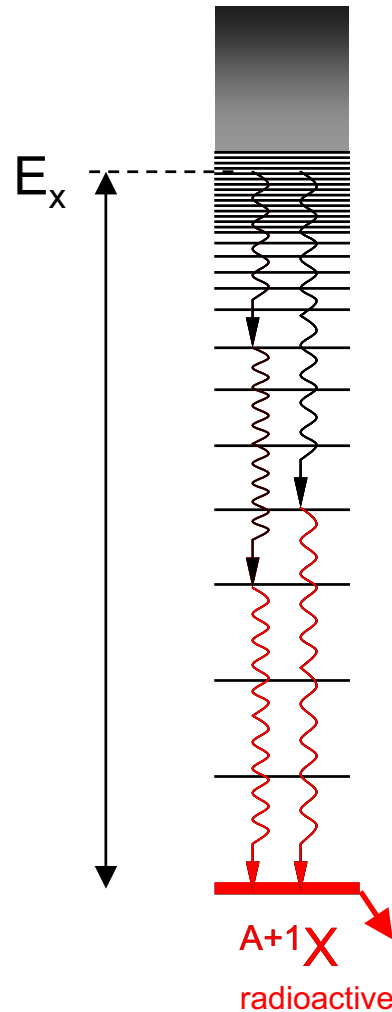
- 1 General information
- 2 Resonance parameter data
- 3 Reaction cross sections
- 4 Angular distributions for emitted particles
- 5 Energy distributions for emitted particles
- 6 Energy-angle distributions for emitted particles
- 7 Thermal neutron scattering law data
- 8 Radioactivity and fission-product yield data
- 9 Multiplicities for radioactive nuclide production
- 10 Cross sections for photon production
- 12 Multiplicities for photon production
- 13 Cross sections for photon production
- 14 Angular distributions for photon production
- 15 Energy distributions for photon production
- 23 Photo-atomic interaction cross sections
- 27 Atomic form factors or scattering functions for photo-atomic interactions
- 30 Data Covariances obtained from parameter covariances and sensitivities
- 31 Data covariances for nubar
- 32 Data covariances for resonance parameters
- 33 Data covariances for reaction cross sections
- 34 Data covariances for angular distributions
- 35 Data covariances for energy distributions
- 39 Data covariances for radionuclide production yields
- 40 Data covariances for radionuclide production cross sections



## Example: part of an evaluated data file

Z and A values	nuclear mass		formalism flag	number of resonances	material number	MF number	MT number
7.919700+4	1.952740+2	0	0	1	07925	2151	1
7.919700+4	1.000000+0	0	0	1	07925	2151	2
1.000000-5	5.000000+3	1	2	0	07925	2151	3
1.500000+0	9.800000-1	0	0	1	07925	2151	4
1.952740+2	0.000000+0	0	0	1578	2637925	2151	5
-3.380000+1	2.000000+0	2.562000-1	1.562000-1	1.000000-1	0.000000+07925	2151	6
4.906000+0	2.000000+0	1.377000-1	1.520000-2	1.225000-1	0.000000+07925	2151	7
4.645000+1	1.000000+0	1.241300-1	1.300000-4	1.240000-1	0.000000+07925	2151	8
5.810000+1	1.000000+0	1.164000-1	4.400000-3	1.120000-1	0.000000+07925	2151	9

# Neutron Capture Gamma-Ray Detection



- **Activation**

- cross sections integrated over known neutron spectrum
- applicable to some nuclei only
- no time of flight

- **Level population spectroscopy**

- applicable to some nuclei only
- feasible with HPGe detectors,

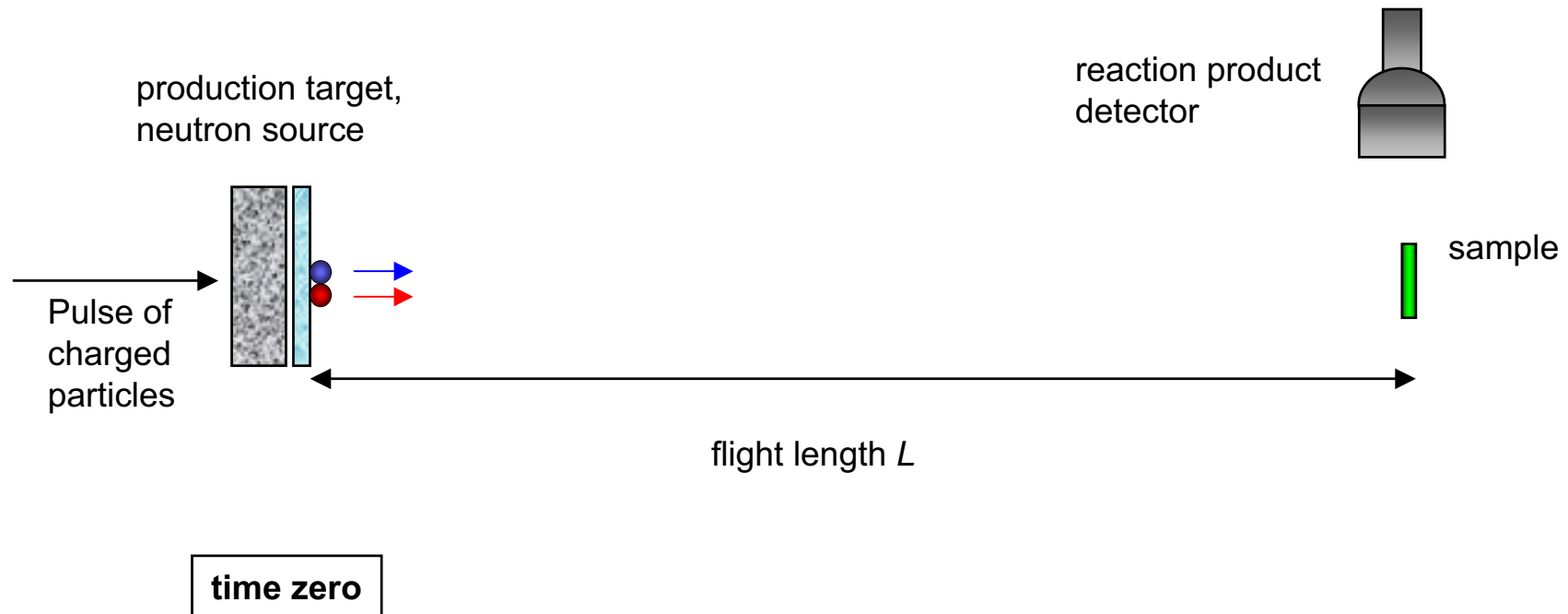
- **Total energy detection**

- $\varepsilon_c \sim E_x$ , requires weighting function
- neutron insensitive detector
- example:  $C_6D_6$  liquid scintillator

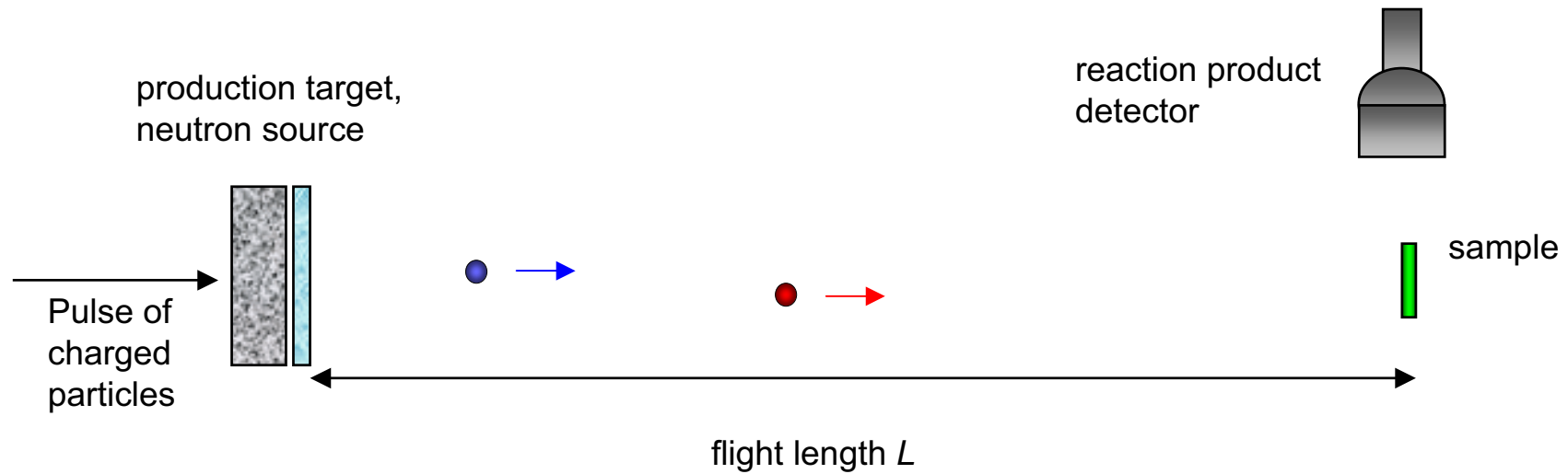
- **Total absorption detection**

- requires  $\Omega = 4\pi$ , efficiency 100%
- capture/fission discrimination in possible, example  $BaF_2$  total absorption calorimeter

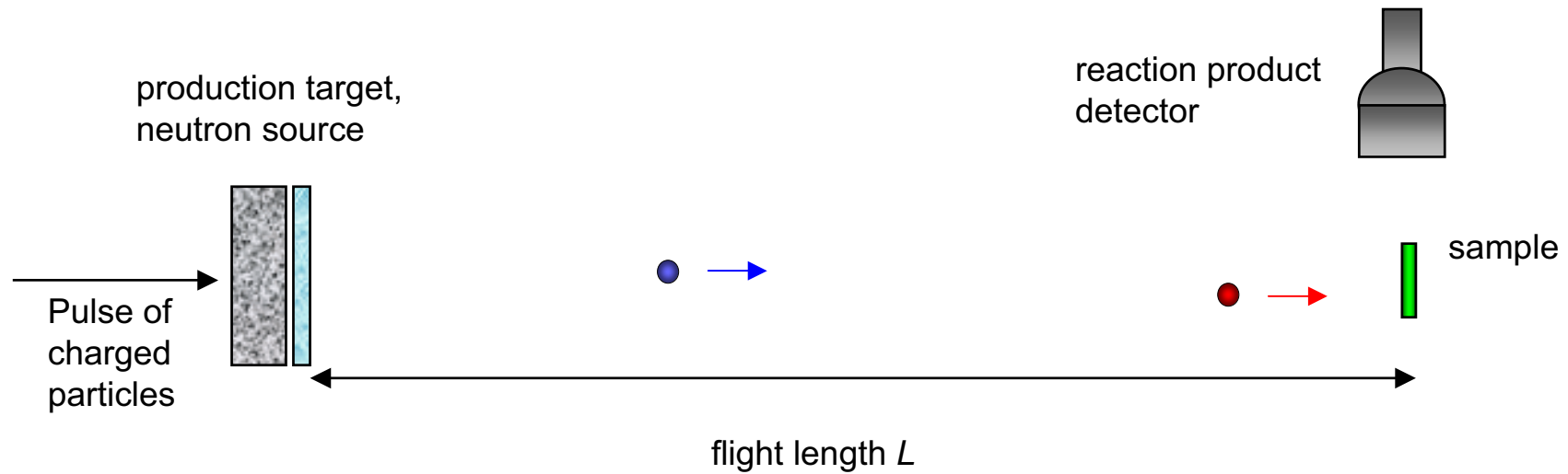
# Measuring a reaction yield using the time-of-flight technique



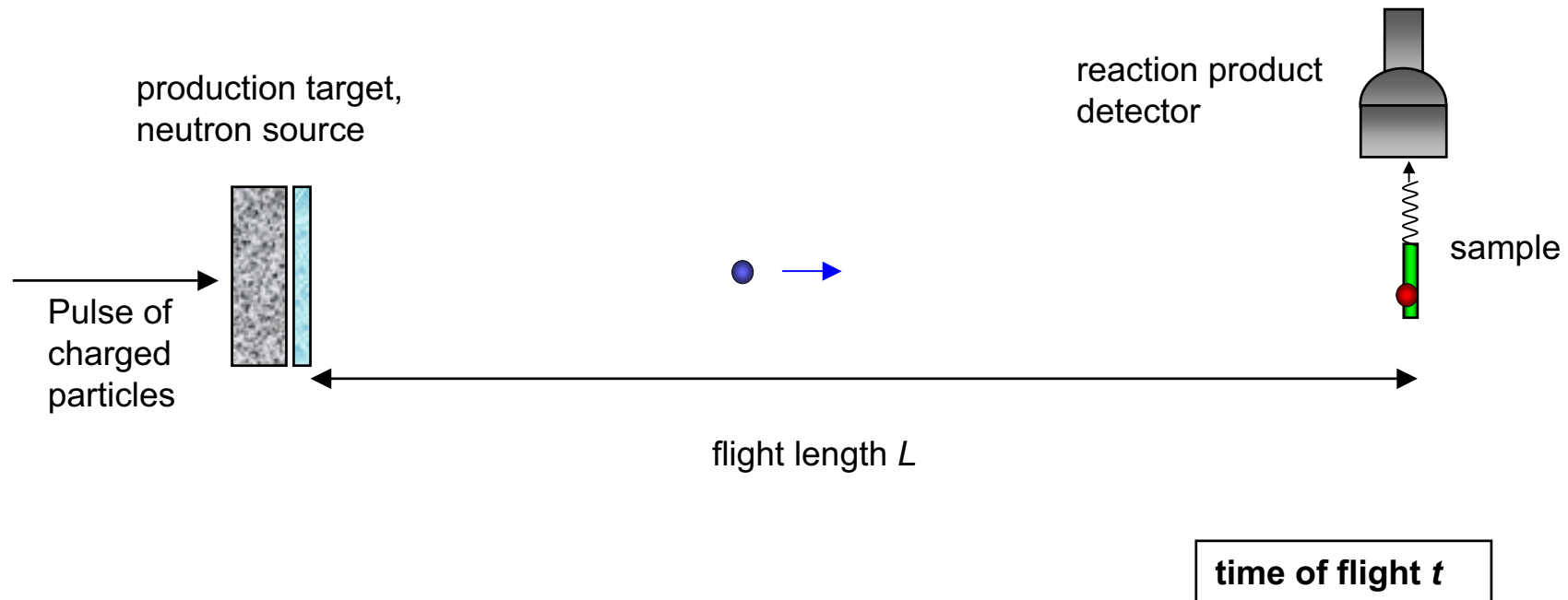
## Measuring a reaction yield using the time-of-flight technique



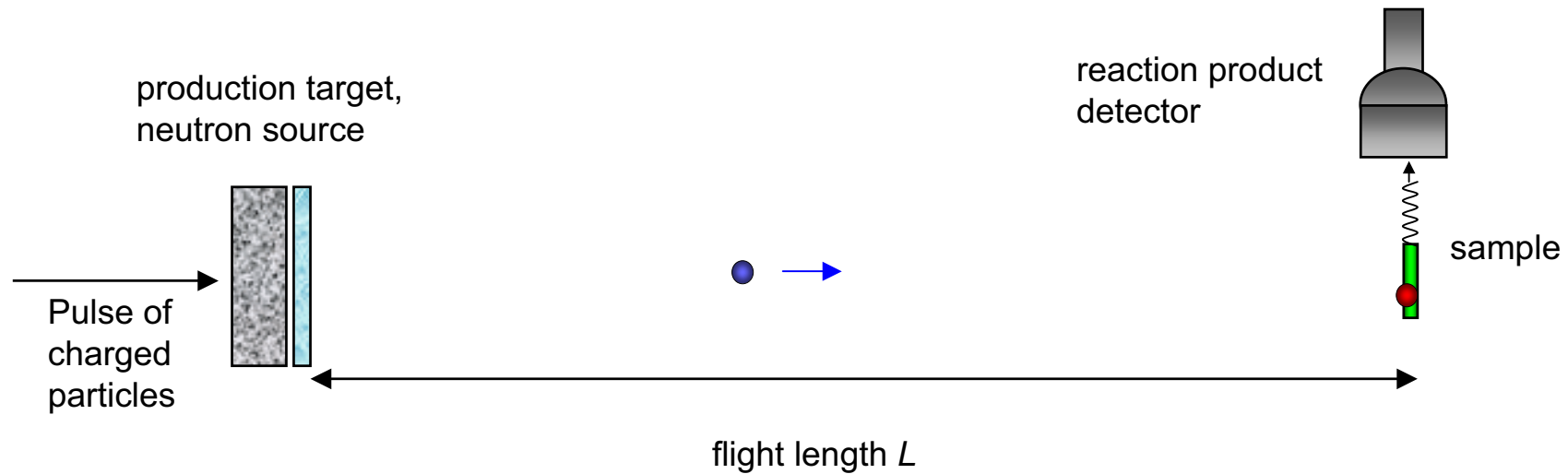
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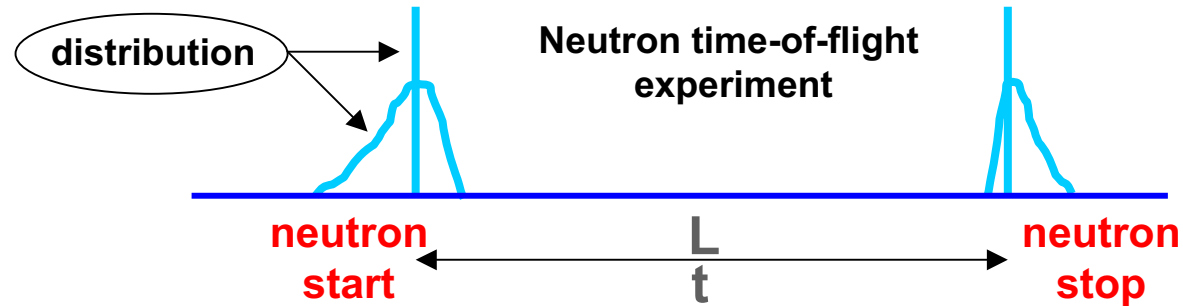


Kinetic energy of the neutron by time-of-flight

$$E_n = E_{tot} - mc^2 = c^2 p^2 + m^2 c^4 - mc^2 = mc^2(\gamma - 1) \quad \gamma = (1 - v^2/c^2)^{-1/2}$$

$$E_n = \frac{1}{2}mv^2 = \alpha^2 \cdot \frac{L^2}{t^2}$$

## Resolution



time-energy relation

$$\sqrt{E} = \alpha \frac{L}{t}$$

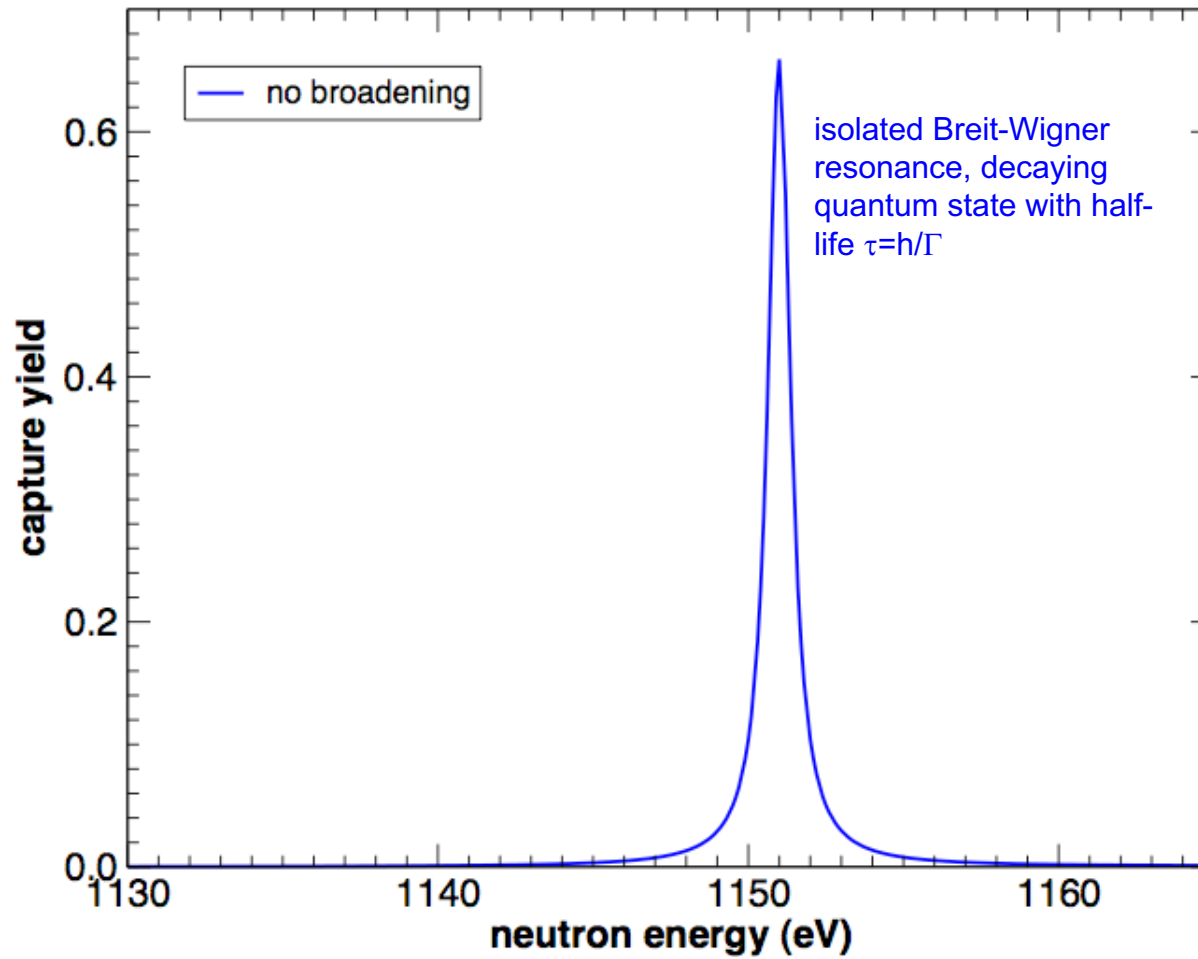
- neutron time-of-flight:  $t + \delta t$
- flight length:  $L + \delta L$
- neutron kinetic energy:  $E + \delta E$

The resolution can be expressed equivalently in time, distance and energy:

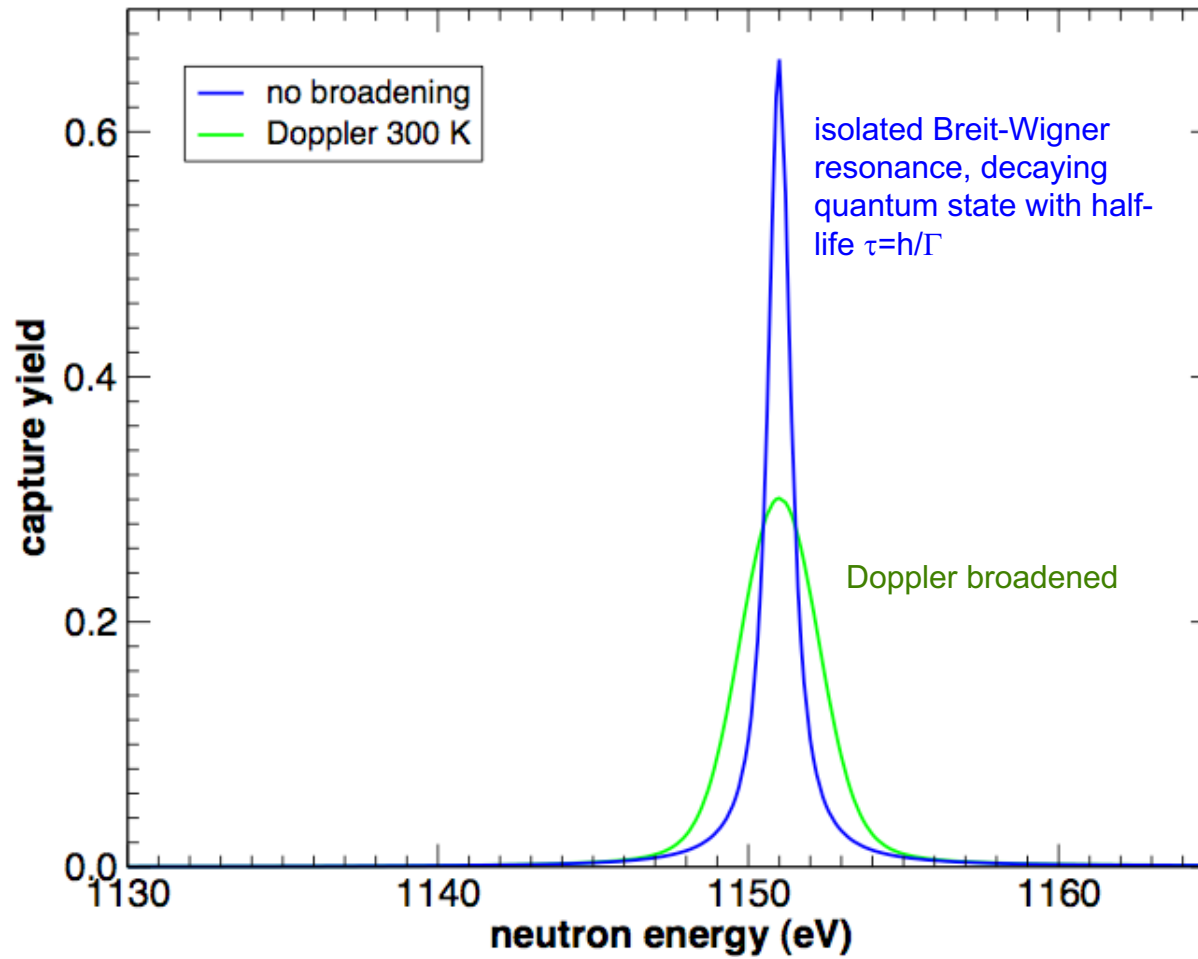
$$R_t(\delta t)d\delta t = R_L(\delta L)d\delta L = R_E(\delta E)d\delta E$$



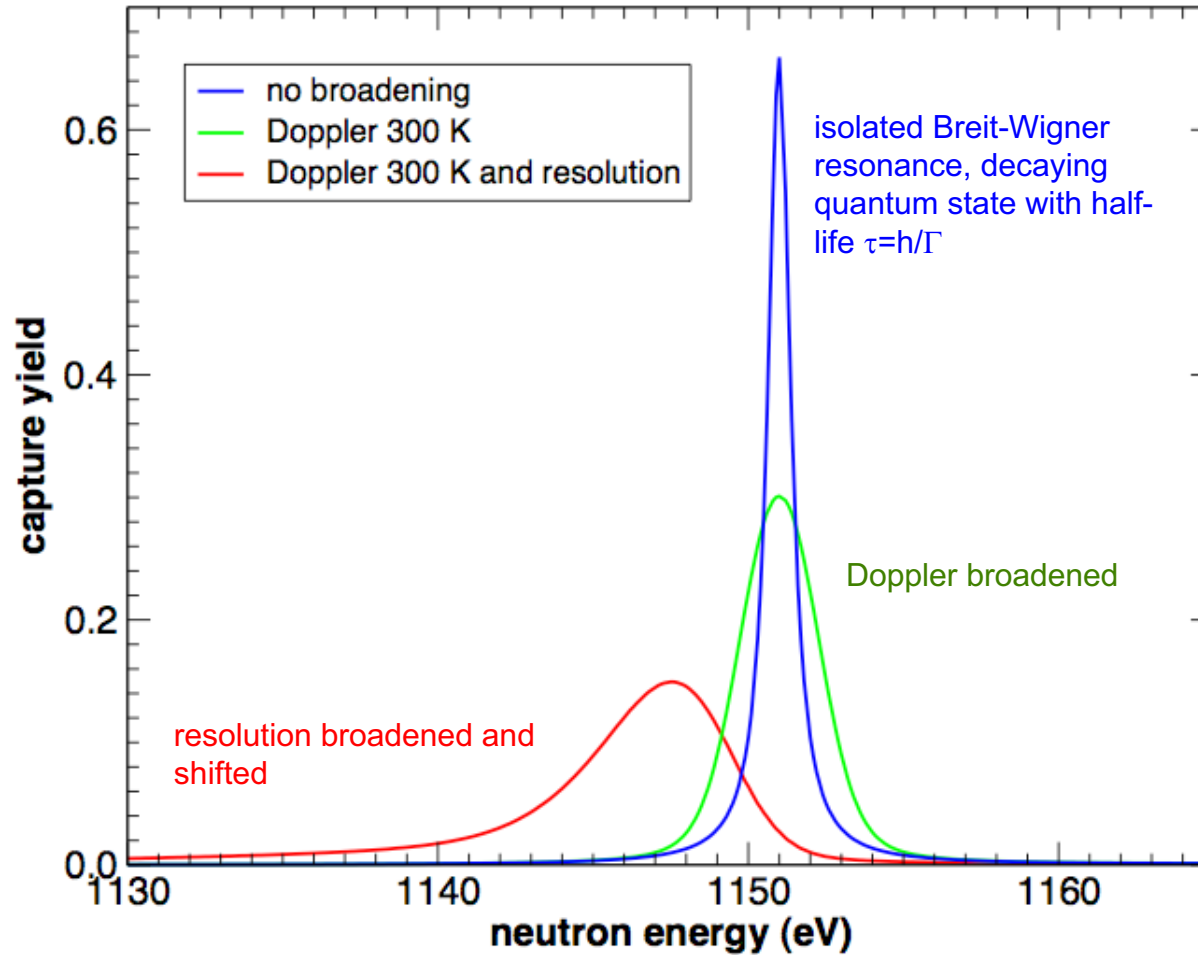
## Measured reaction yield



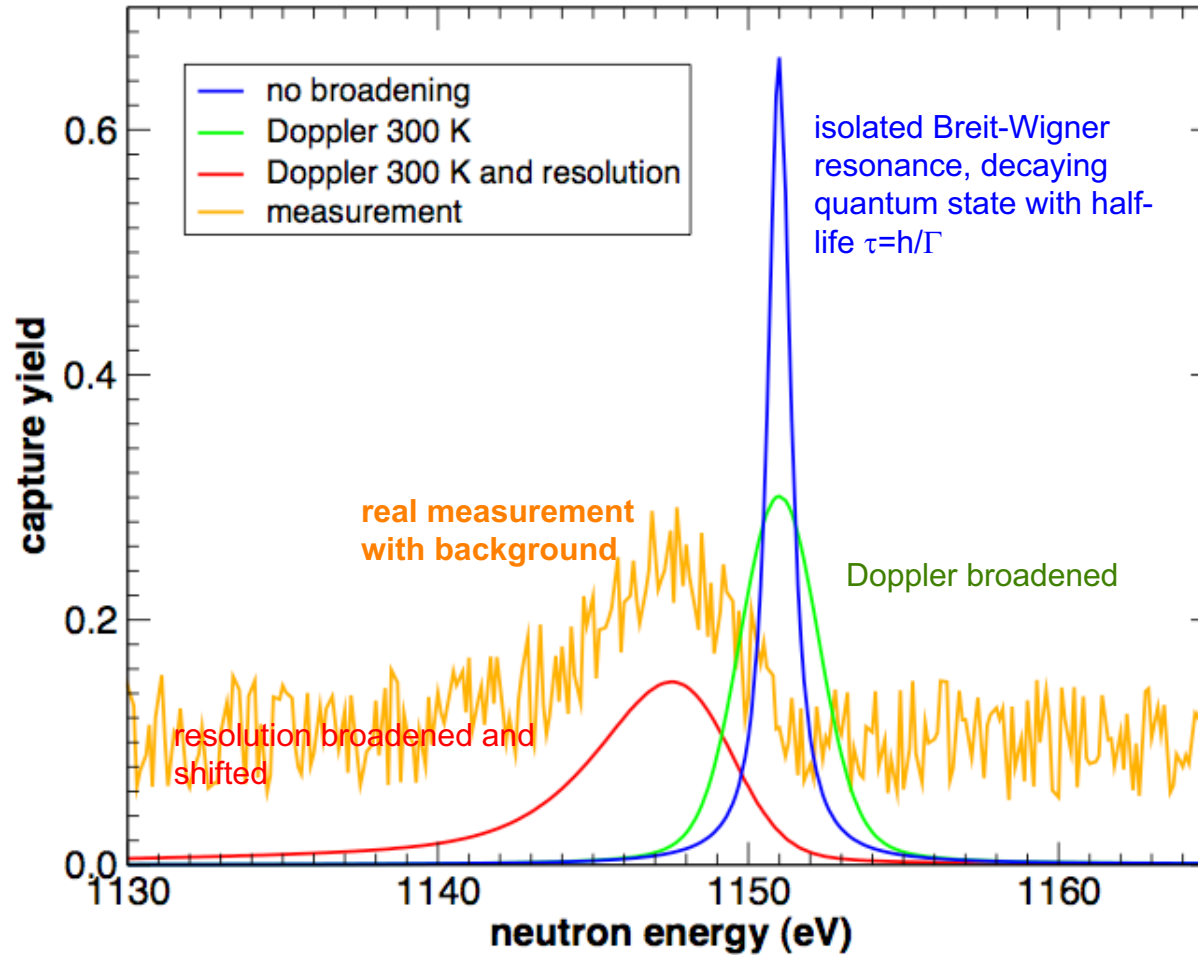
## Measured reaction yield



## Measured reaction yield



## Measured reaction yield



## Further Reading

### Books/Papers

- K. S. Krane, *Introductory Nuclear Physics*, Wiley & Sons, (1988).
- G. F. Knoll, *Radiation Detection and Measurement*, Wiley & Sons, (2000).
- P. Reus, *Précis de neutronique*, EDP Sciences, (2003).
- J. E. Lynn, *The Theory of Neutron Resonance Reactions*, Clarendon Press, Oxford, (1968).
- F. Fröhner, *Evaluation and analysis of nuclear resonance data*, JEFF Report 18, OECD/NEA (2000).
- C. Wagemans, *The Nuclear Fission Process*, CRC, (1991).
- A. M. Lane, R. G. Thomas, “R-matrix theory of nuclear reactions”, *Rev. Mod. Phys.* **30** (1958) 257.
- G. Wallerstein, et al., “Synthesis of the elements in stars: forty years of progress”, *Rev. Mod. Phys.* **69** (1997) 995.

### Web sites

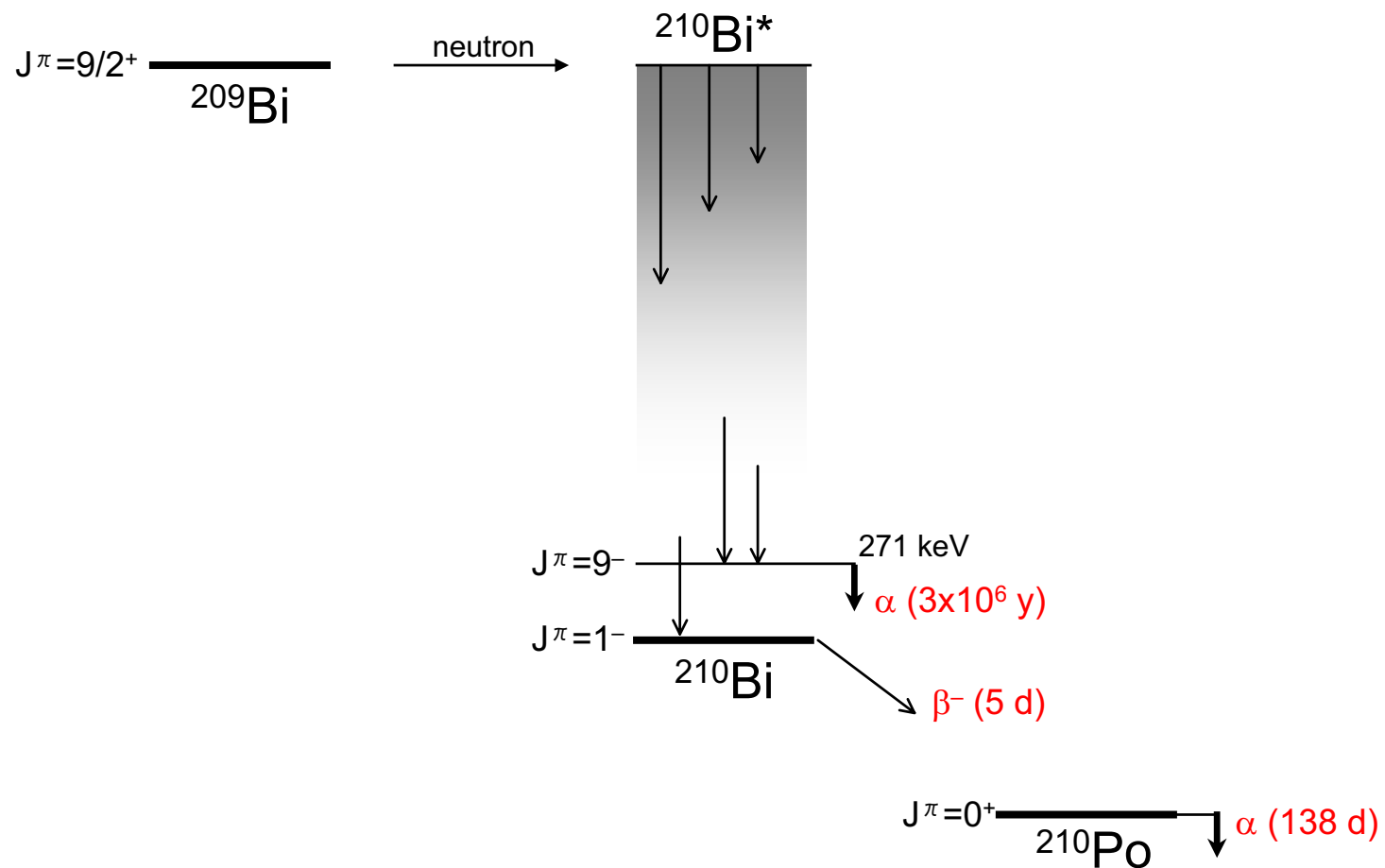
[www.nea.fr](http://www.nea.fr)  
[www.nndc.bnl.gov](http://www.nndc.bnl.gov)  
[www.iaea.org](http://www.iaea.org)  
[www.cern.ch/ntof](http://www.cern.ch/ntof)  
[www.irmm.jrc.be](http://www.irmm.jrc.be)

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## Conclusion

- Neutron induced reactions are important nuclear data necessary for a wide range of fields ranging from nuclear structure and astrophysics to advanced nuclear technology applications.
- The R-matrix formalism is adapted to describe compound nucleus reactions at low energy ( $E_n < 10$  MeV, resonance region).
- Resolved resonances need to be measured accurately, they cannot be predicted by nuclear models.

## Rapport de branchement $^{209}\text{Bi} + n$

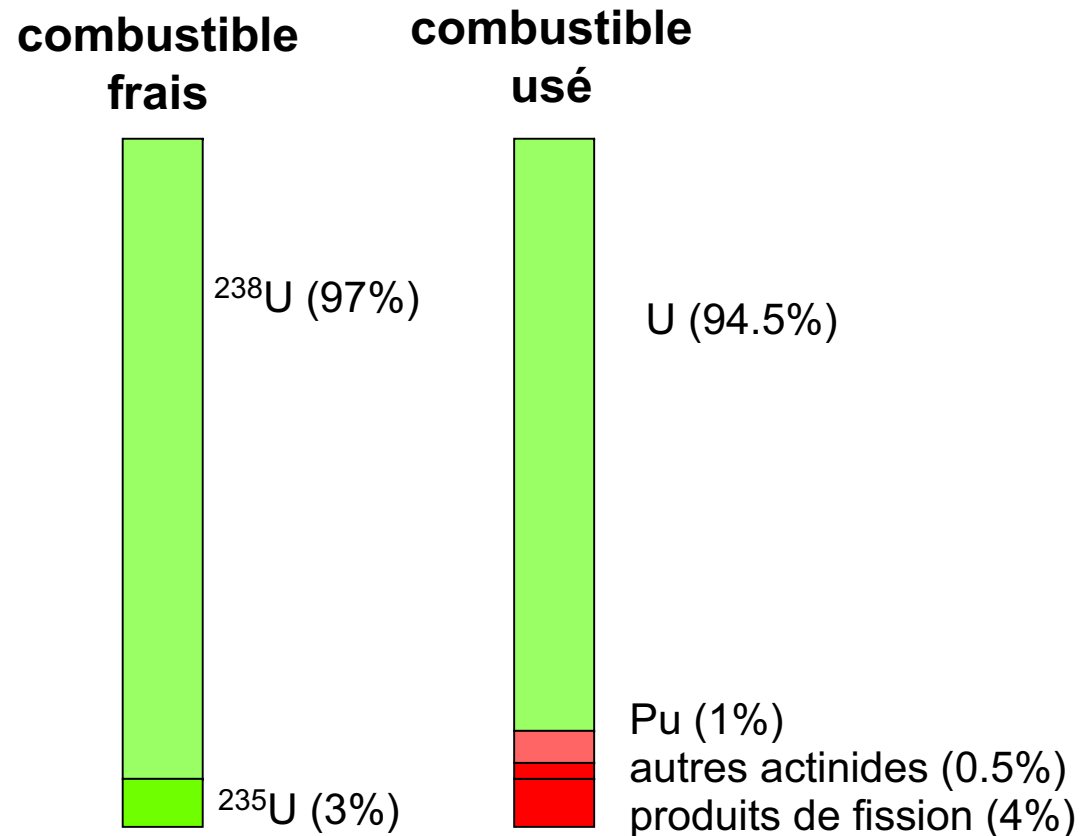


## L'origine des déchets nucléaires

Quantité des déchets en France:  
2500 kg/an par habitant  
dont 1 kg radioactif  
dont **20 g** hautement radioactif

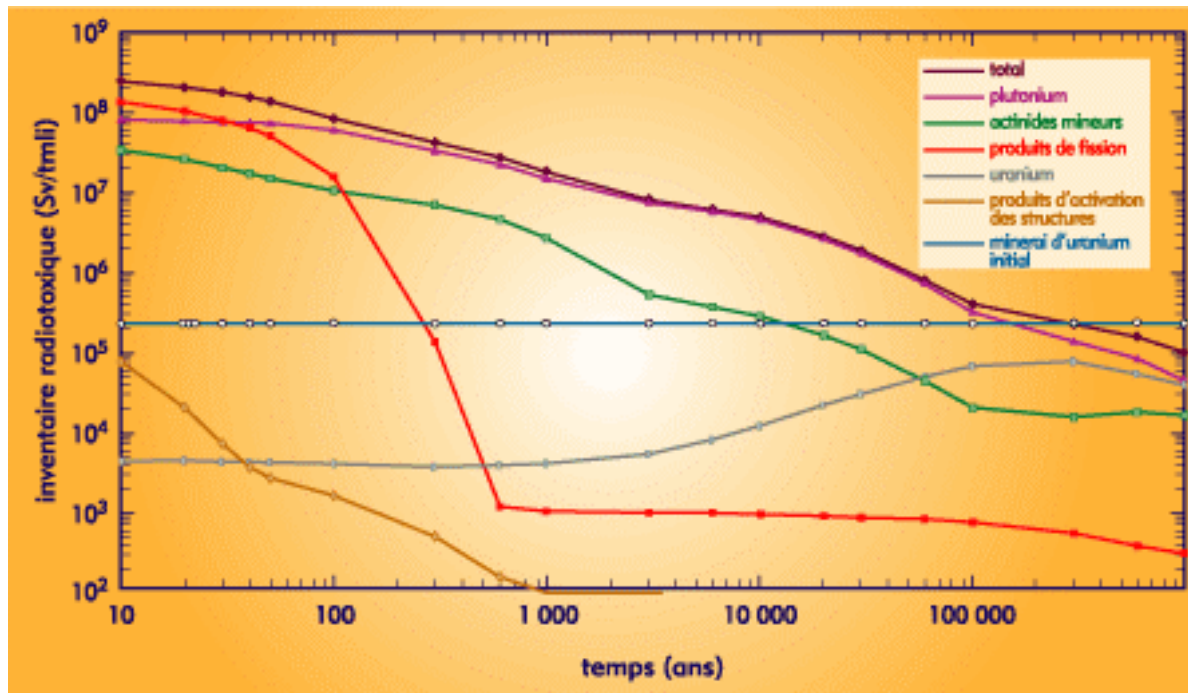
Loi Bataille:  
recherche 1991 - 2006

- séparation et transmutation
- stockage profonde
- conditionnement et entreposage





## Réduire la radiotoxicité: la transmutation en complément de stockage



Clefs CEA 46 (2002)

### Composition des déchets

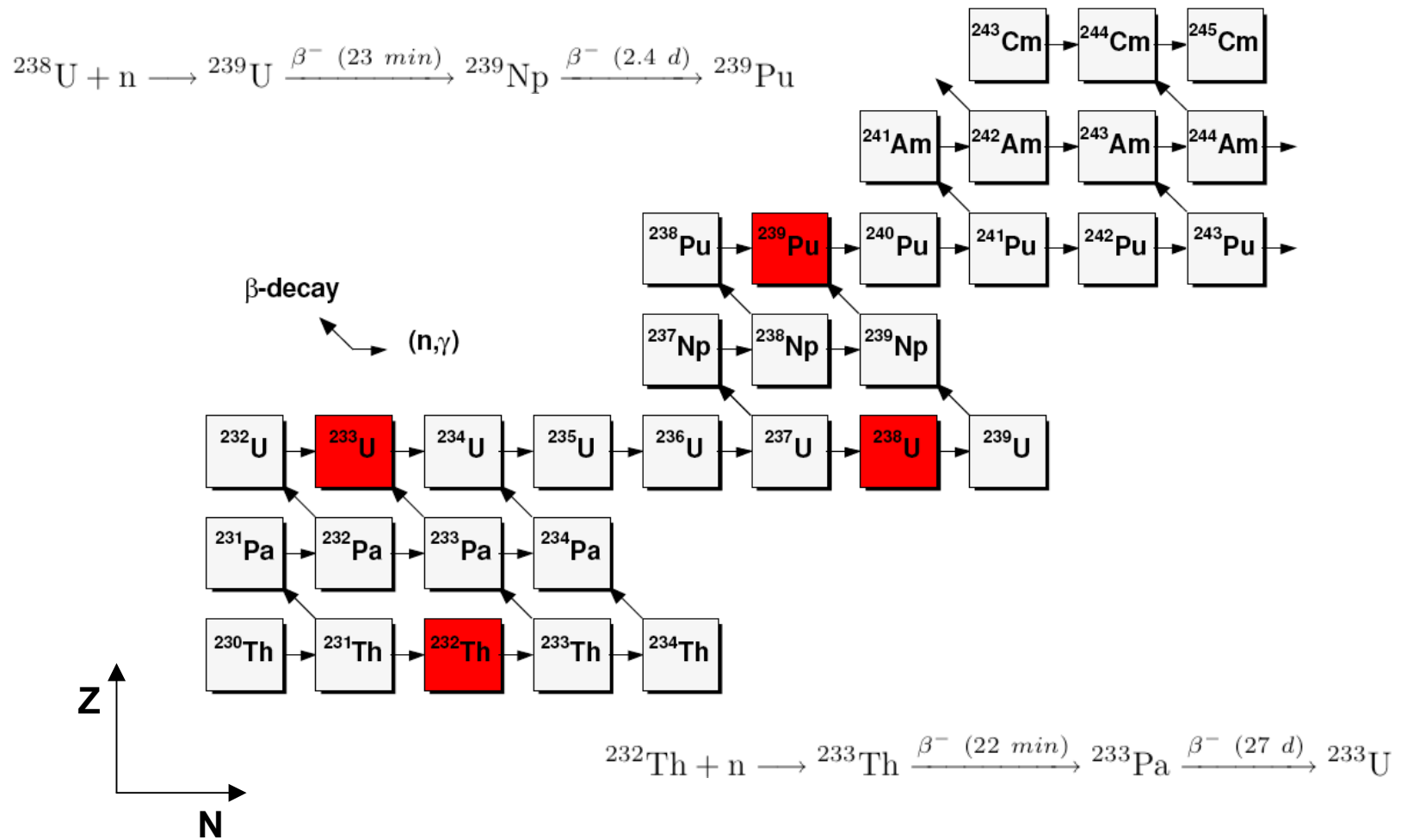
- **produits de fission**

transmutation par capture de neutrons  
dans flux de neutrons thermique

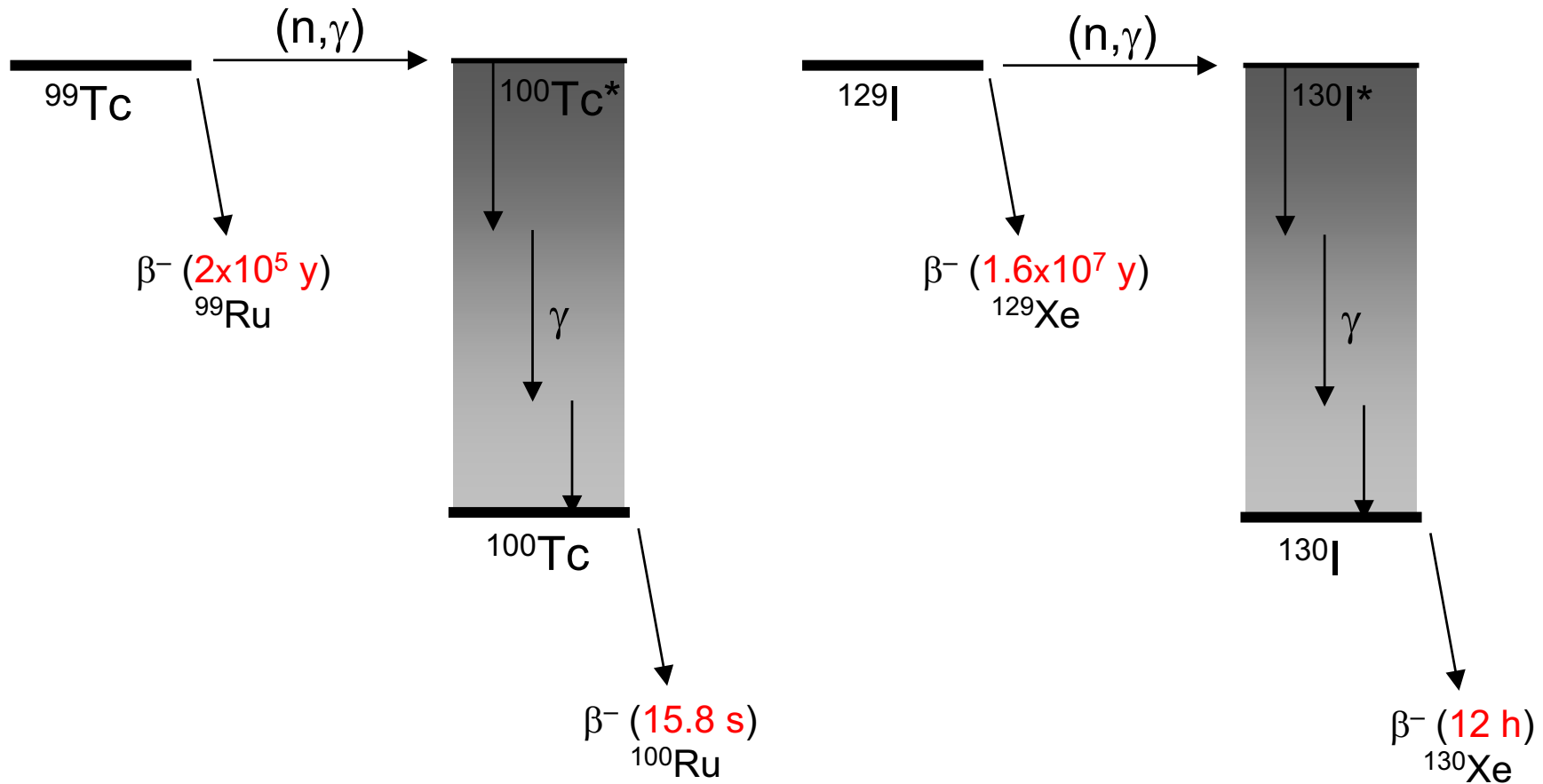
- **actinides mineurs**

transmutation par fission induite par  
neutrons dans flux de neutrons rapide

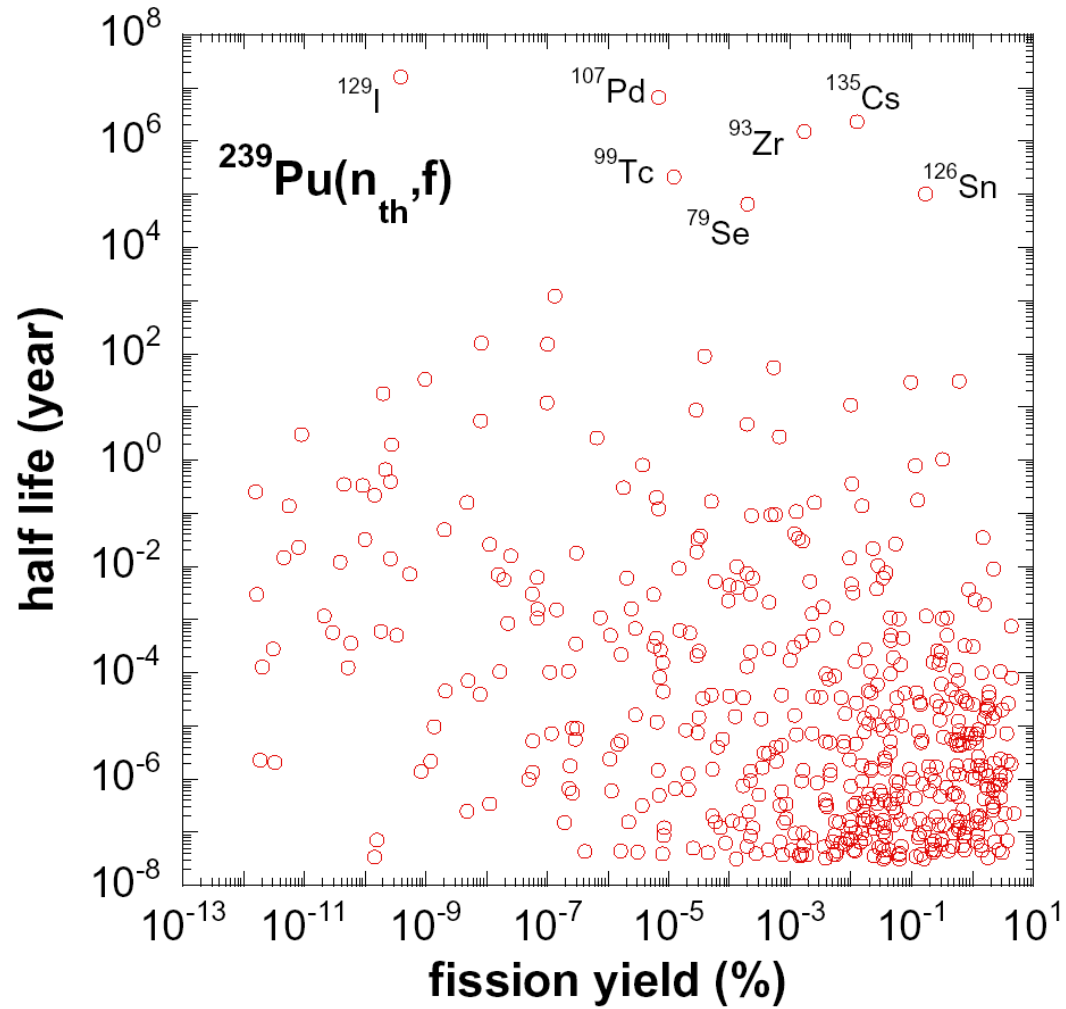
# Réduire la radiotoxicité des déchets: le cycle du thorium



## Réduire la radiotoxicité des déchets: la transmutation

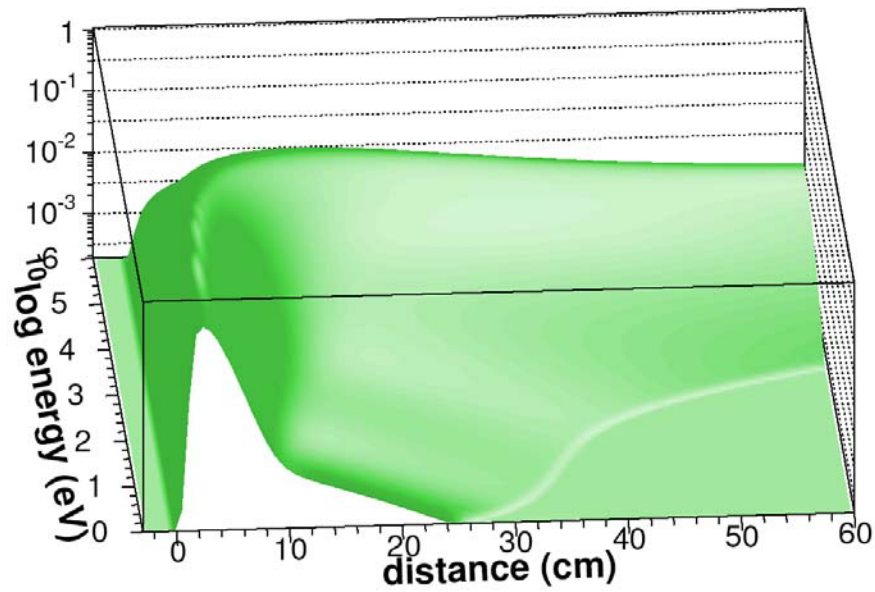


## Produits de fission: temps de vie versus rendement



# Resolution

n\_TOF



GELINA (0°)

