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Advances in Nuclear Model Evaluation of Fission Cross Section

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Advances in Nuclear Model Evaluation of Fission Cross Section

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Main topics

- Overview of the fission process
- Fission nuclear data
- Nuclear models used for fission cross section calculations

History

http://www.aip.org/history/mod/fission/fission1/01.html

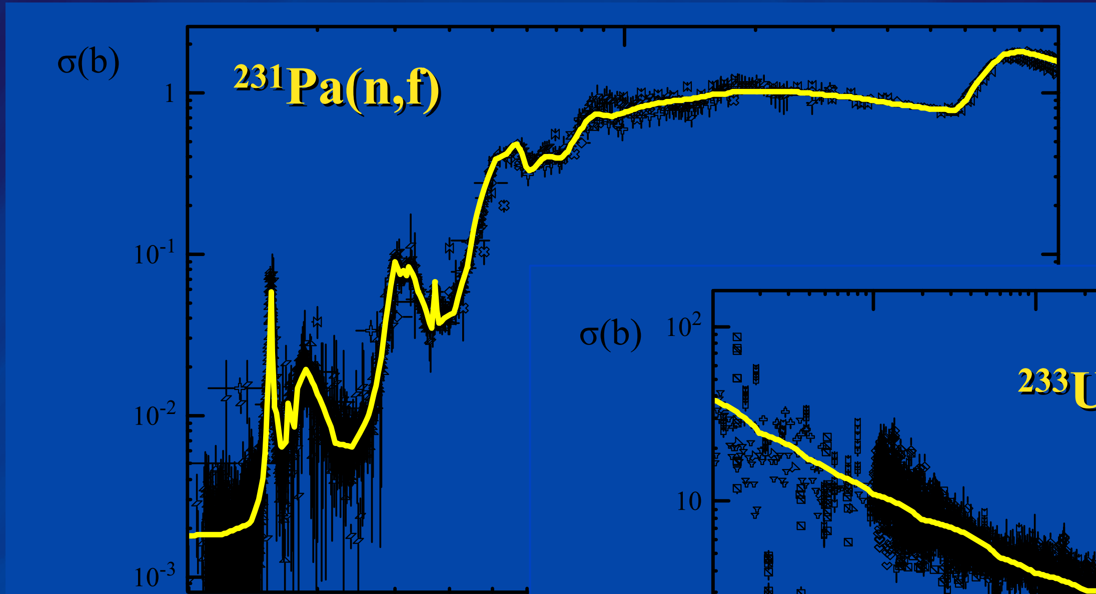
Why fission is still a hot topic?

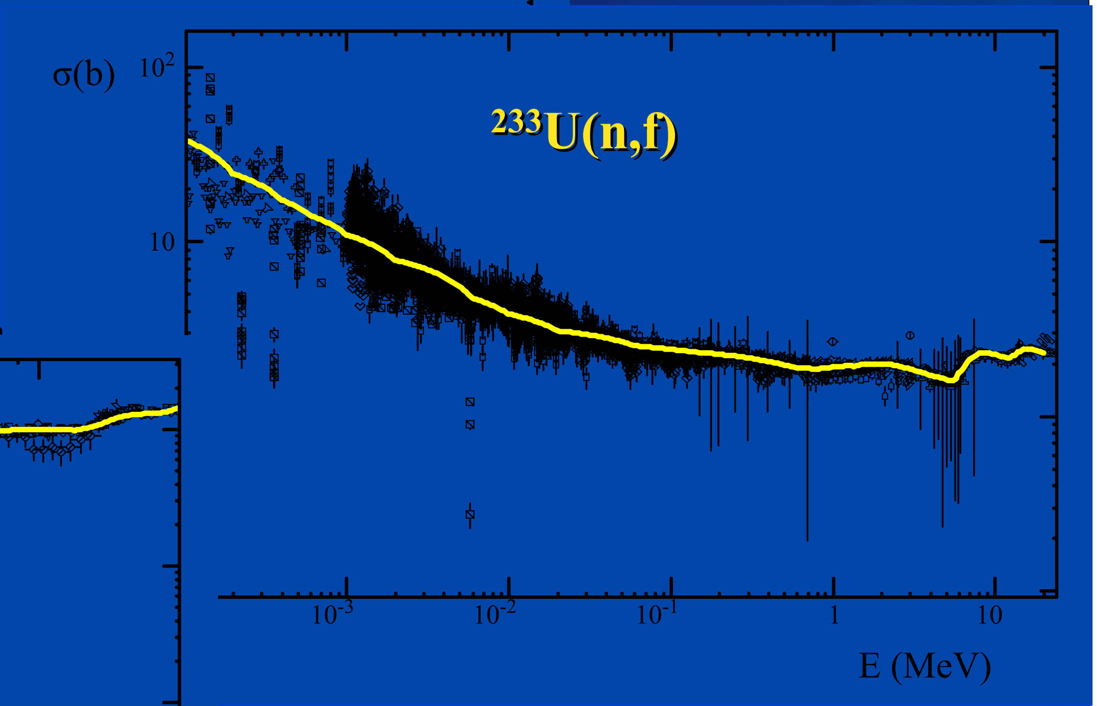
No theory or model is able yet to predict all fission observables (fission cross section, post-scission neutron multiplicities and spectra, fission fragments' properties like mass, charge, total kinetic energy and angular distributions) in a consistent way for all possible fissioning systems in a wide energy range.

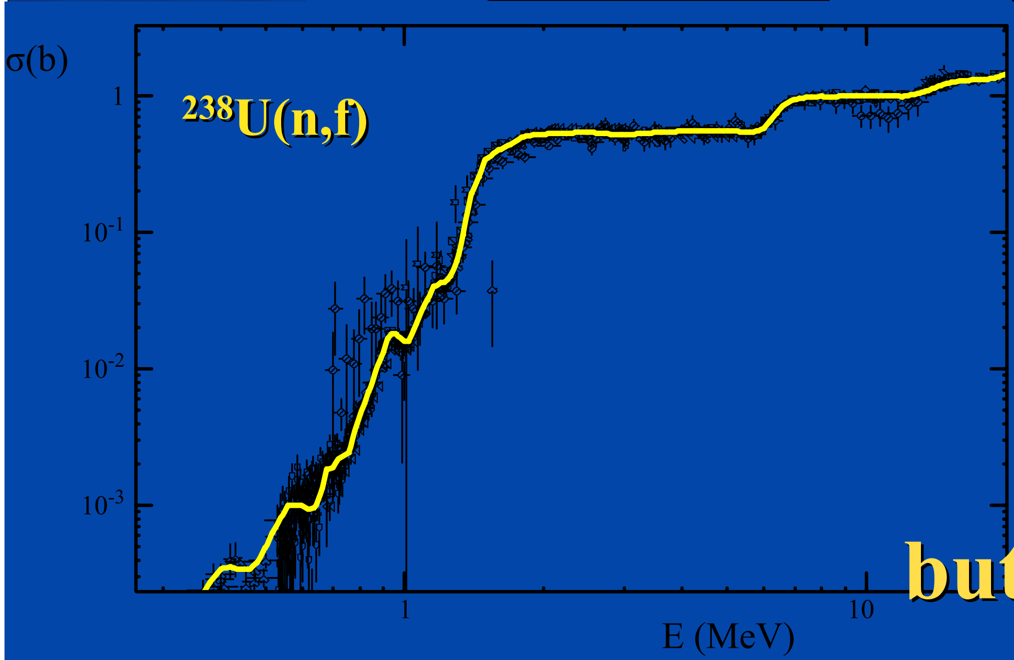
New nuclear technologies design requires increased accuracy of the fission data refinements of the fission models and better predictive power.

To reach the target accuracies more structural and dynamic features of the fission process must be included in the theoretical models.

Very good descriptive power





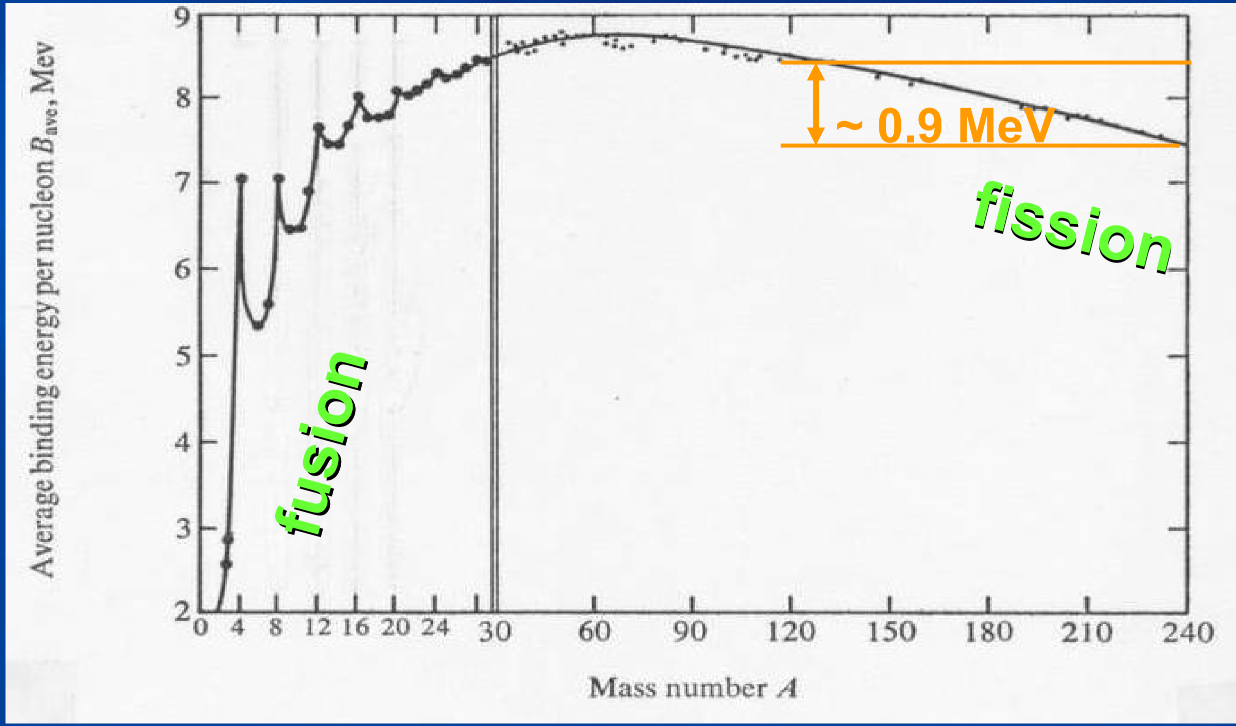


but the predictive power …

The origin of nuclear energy

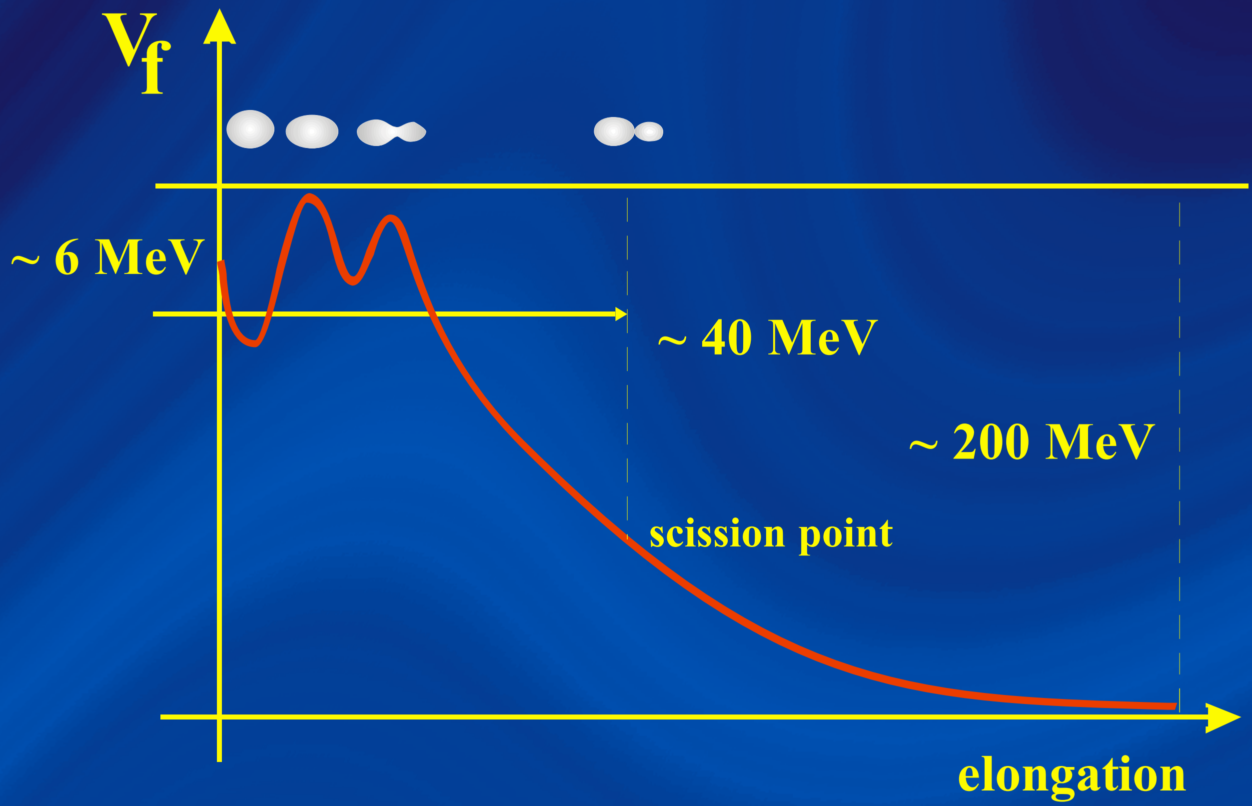
Nuclear fission is a very complex collective phenomenon in which a heavy nucleus undergoes a series of large vibrations until it becomes so strongly deformed that it breaks into two fragments of comparable masses. More than two fragments may be formed at scission but such mass divisions are very infrequent.

difference of binding energy



The total energy liberated by the process is about 200 MeV, the difference in mass (rest energy) between the original nucleus and the two newly formed fragments.

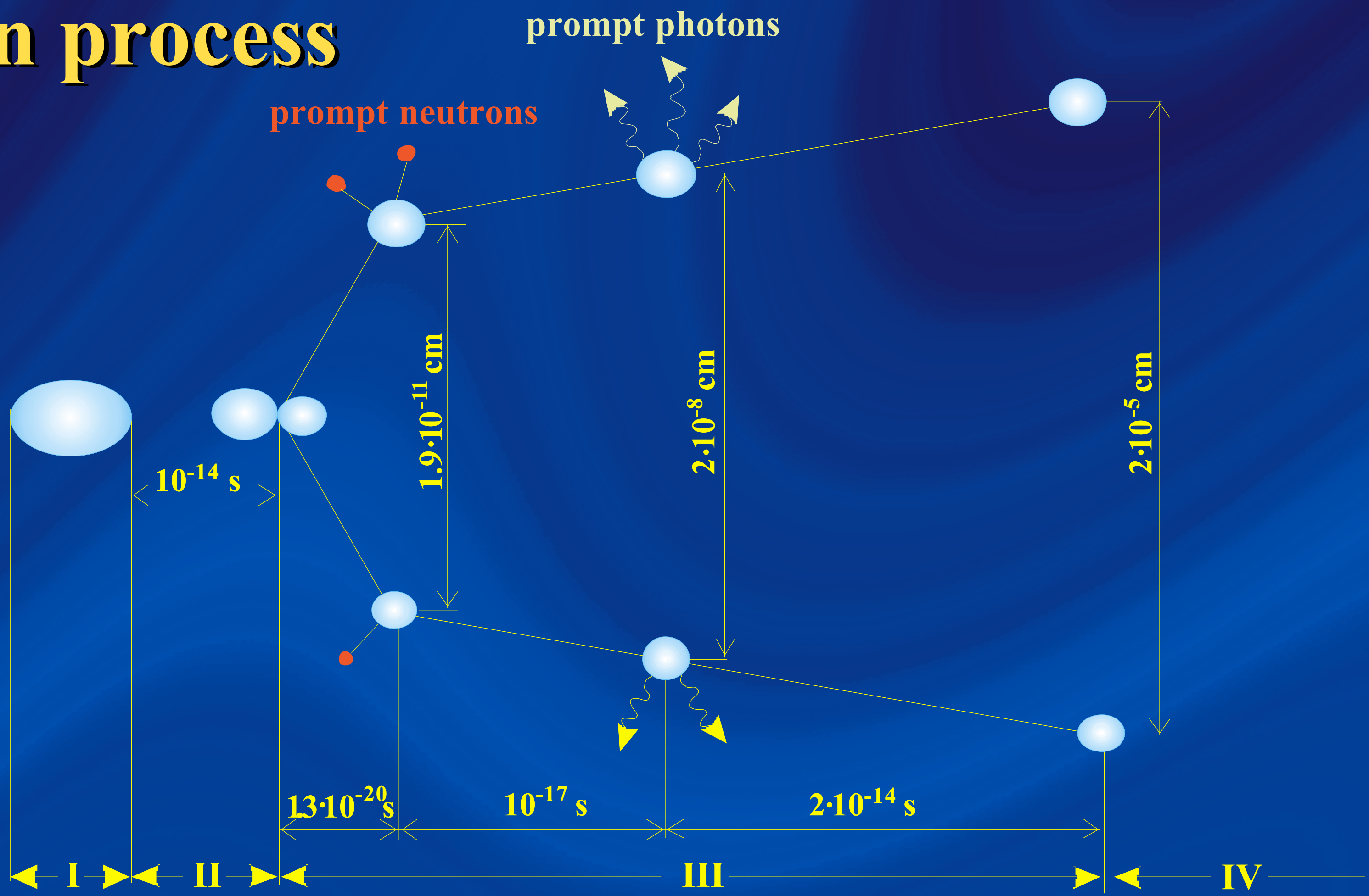
Fission process



Liquid Drop Model

- only the Coulomb (E_C) and surface term (E_S) depend on deformation
- near g.s. E_S increases more rapidly than E_C decreases – V rises
- at larger deformation the situation is reversed – V drops

Fission process



I formation of the initial state of the fissioning nucleus

II from the initial state to scission

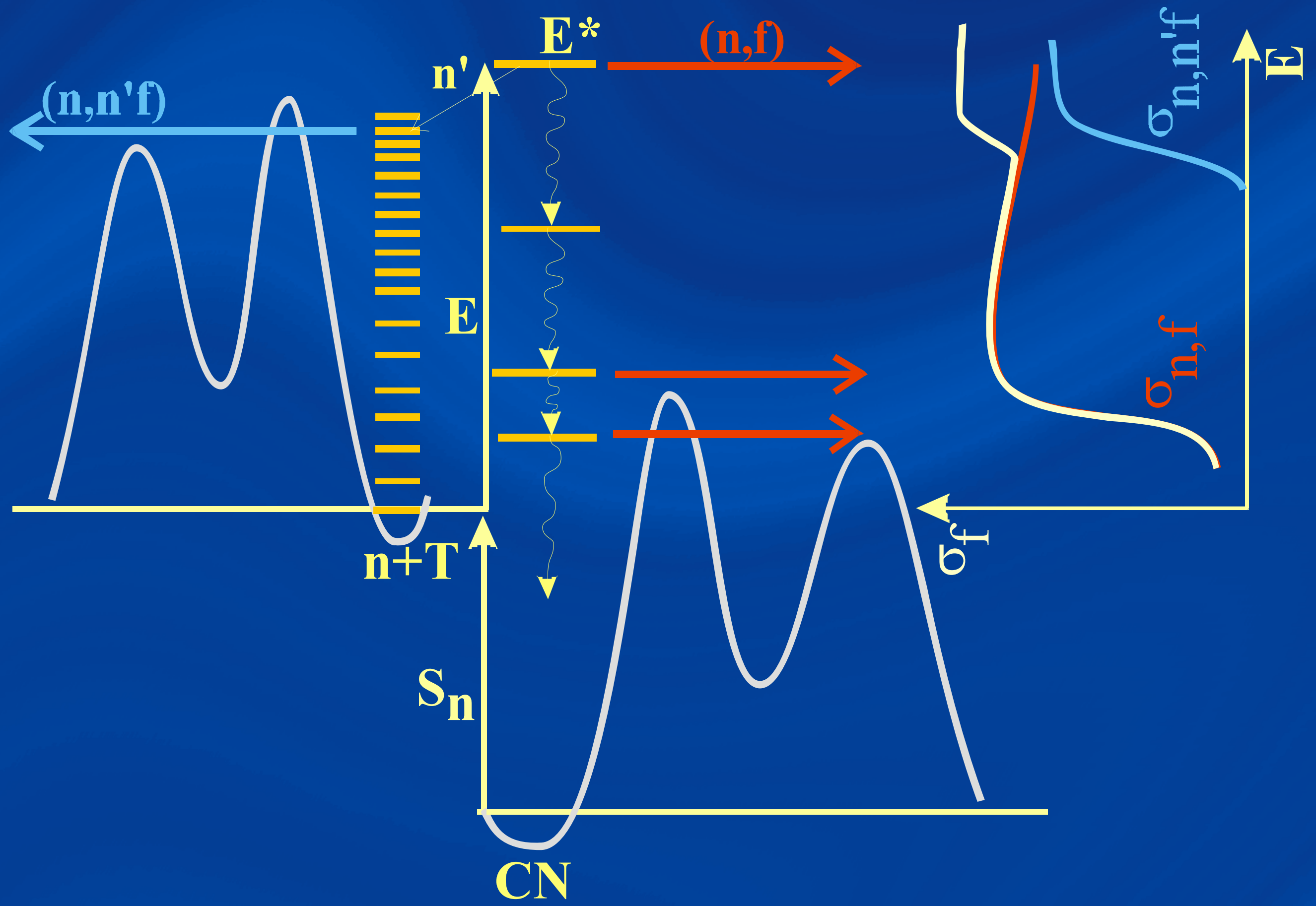
III from scission to the fission products formation by prompt processes

IV de-excitation of the fission products by delayed processes

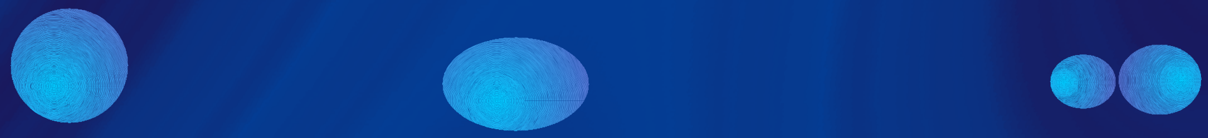
Initial state

- spontaneous fission (nuclei in g.s.) , …, heavy ion induced reactions (complex nuclei in very excited states with high angular momenta)

- neutron (γ, p, α…) induced fission:
  - CN states populated directly or after gamma-decay - (n,f)
  - states in residual nuclei - (n,n'f), (n,2nf), (n,3nf)



From the initial state to scission



- Parameterization of the nuclear shape;
- Calculation of the potential energy surface as function of deformation;
- Determination of the fission path(s), fission barrier, transition states.

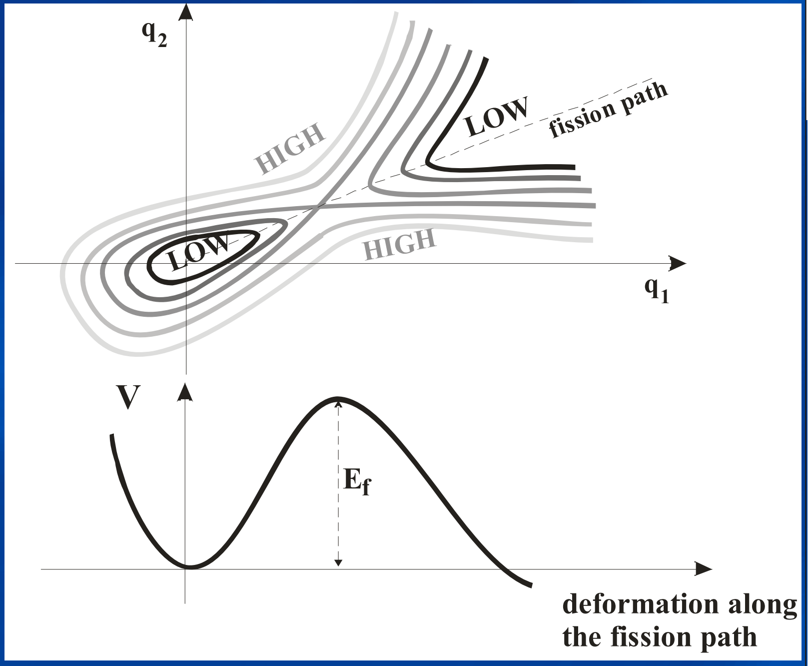
From the initial state to scission

The fissioning system shape modifies continuously during the motion from the formation of the initial state (characterized by a small deformation) to the elongated asymmetric pre-scission shape and even scission (where the nuclear system is composed of two touching fragments). Several types of parameterization and sets of deformation (shape) parameters {q} may be required to describe completely the fissionning nucleus in its various stages.

potential energy surface – potential energy as function of deformation V({q})

fission path – corresponds to the lowest potential energy when increasing deformation

fission barrier – one-dimensional representation of V; V as function of one deformation coordinate (ex. elongation)



From the initial state to scission

Statics and dynamics

-the motion along the fission path up to the outer saddle point is relatively a slow process governed mainly by the statics of the process

-the irreversible transition from the outer saddle point to scission is fast and dominated by the dynamics of the process

-inertia – the mass tensor appears when expressing the kinetic energy at certain deformations; it exhibits strong variations with deformation as an effect of shell correction variation with deformation.
– it is customary to assume it is diagonal in the deformation space coord. system and all diagonal elements are equal to a constant which is very important for the fission barrier parameterization and for the transmission coefficient calculation.

-viscosity – due to the coupling of the collective degrees of freedom to the intrinsic ones. It governs the sharing of the available energy in the fission mode and excitation energy.

From scission to the fission products formation by prompt processes

This phase is dominated by the Coulomb repulsion of the two fragments and by their prompt de-excitation by neutron and gamma-ray emission.

The primary fragments are strongly elongated because just before scission they were still submitted to a mutual nuclear attraction.

Just after scission the fragments are no longer subject to any nuclear force between them and they repel each other as an effect of the Coulomb force.

Rapidly the primary fragments take a more spherical shape, close to that of their g.s. and the deformation energy which is liberated appears in the form of excitation energy which adds to the excitation energy that existed already at scission. If this excitation energy is greater than the neutron separation energy in a primary fragment, then this fragment de-excites in flight by the evaporation of one or several neutrons until the residual nucleus is left with an excitation energy below the neutron emission threshold.

Prompt fission neutron properties: ν_p ,N(E)

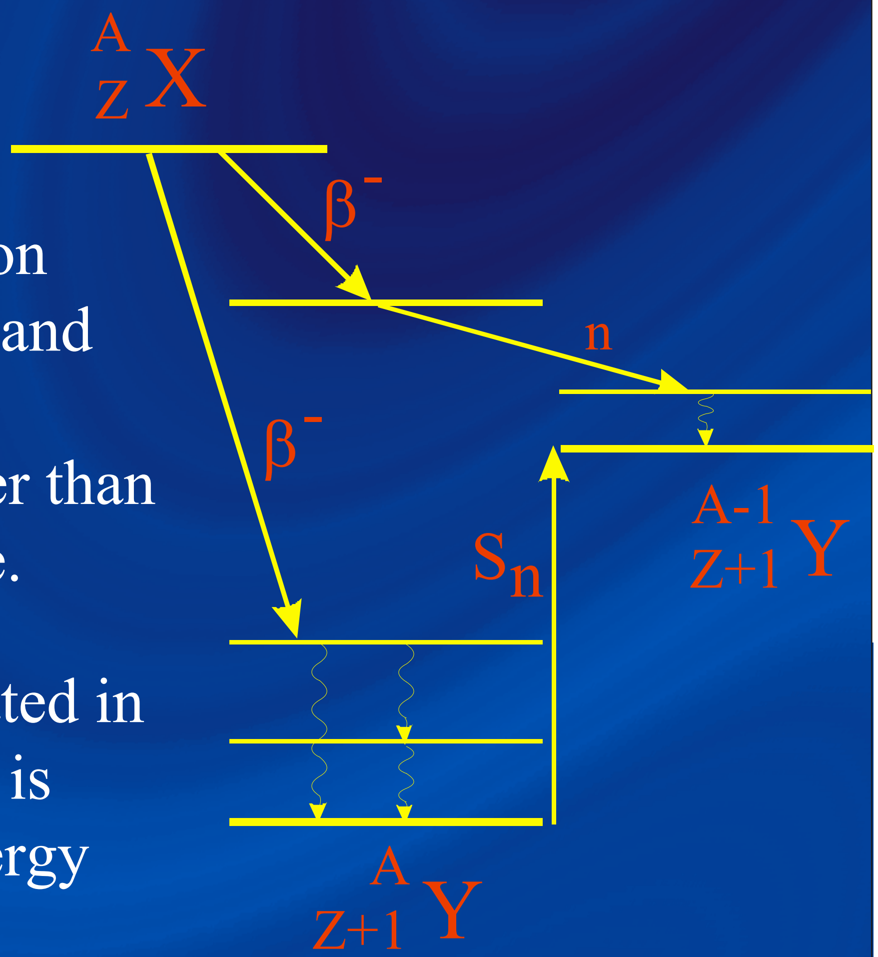
- **Early representations** (Maxwellian and Watt spectrum and a simple polynomial, in the incident neutron energy representation for nubar) are simple, contain a small number of parameters adjusted to reproduce the experimental data, but have no predictive power.

- **Modern representations** (Los Alamos, Dresden, Hauser-Feshbach models) are based upon standard nuclear theory and treat simultaneously prompt neutron spectra and average prompt neutron multiplicities. They account for physical aspects like distribution of fission-fragment excitation energy, the motion of the fission fragments emitting neutrons, multiple-chance fission at high incident neutron energy etc. They have a better predictive power.

Delayed processes

Despite neutron evaporation, the fission products are usually still neutron-rich and therefore decay beta. The beta-decay, governed by weak interaction is slower than the prompt processes described before.

The residual nuclei are usually populated in excited states; if the excitation energy is higher than the neutron separation energy they may decay by neutron emission, otherwise they emit only gamma-rays to reach the ground state. Such neutrons and gamma-rays are called *delayed* though they are emitted promptly after beta-decay which is in fact the delayed process.



Fission data in ENDF-6

Fission neutron properties

- **multiplicities** MF=1: MT=452 (ν_t), MT=455 (ν_d), MT=456 (ν_p)
  The values may be tabulated as a function of energy or coefficients provided for a polynomial expansion.
- **angular distributions** MF=4, MT=18
- **spectra** MF=5:prompt neutrons MT=18-21,38; delayed neutrons MT=455
  The energy distribution may be decomposed into partial distributions described by different analytic representations named energy distributions laws. Simple fission spectrum (Maxwellian), energy dependent Watt spectrum and energy dependent fission neutron spectrum (Madland and Nix), arbitrary tabulated function.

Fission cross section

- resonance parameters MF=2 MT=18
- tabular representation MF=3 MT=18 -21,38

Fission data in ENDF-6

Components of energy release in fission MF=1 MT=458

The energy released in fission (ET) is carried by fission fragments (EFR), neutrons (ENP,END), gammas (EGP, EGD), betas (EB) and anti-neutrinos (ENU). The term fragments includes all charged particles that are emitted promptly, since for energy deposition calculations all such particles have short ranges and are usually considered to lose their energy locally. Neutrons and gammas transport their energy elsewhere and need to be considered separately. In addition, some gammas and neutrons are delayed and in a shut-down assembly, one needs to know the amount of energy tied up in these particles and the rate at which it is released from the metastable nuclides or precursors. The neutrino energy is lost completely in most applications.

Fission product yield data MF=8

The fission products are specified by giving an excited state designation and a charge-mass identifier.

- **-independent yields** (MT=454) - the direct yields per fission prior to delayed neutron-, beta-, etc. decay
- **-cumulative yields** (MT=459) - account for all decay branches, including delayed neutrons.

Covariance data MF=30, MF=31-35

Fission barrier

- macroscopic models: LDM
  - give only a qualitative account of the phenomenon

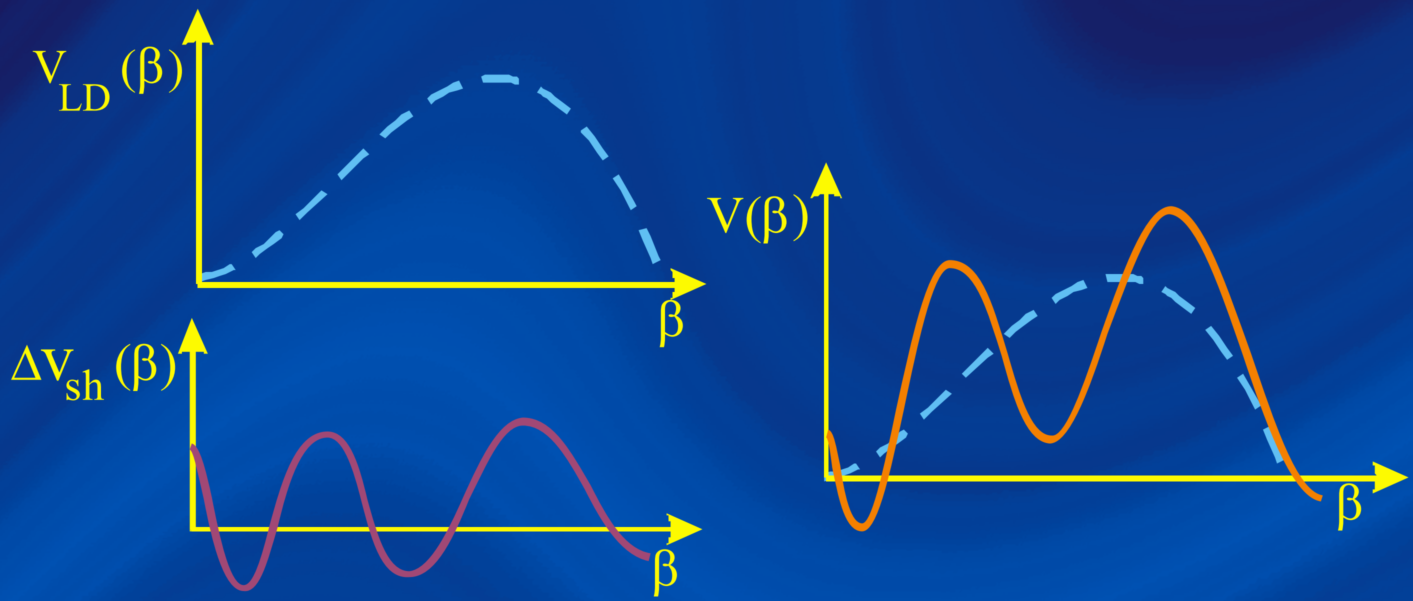
- microscopic-macroscopic model: LDM + shell correction
  - explained a significant number of experimental data

- microscopic models: HFB
  - can not provide accurate results for V_f yet, but provide the trend and are improving

Fission barrier

Strutinsky's procedure

$$V(\beta) = V_{LD}(\beta) + \Delta V_{sh}(\beta)$$



The value of the shell correction is +, - depending on whether the density of single-particle states at Fermi surface is great or small.

Negative corrections for actinides

- **g.s. - permanent deformation**
- **vicinity of macroscopic saddle point – second well** ⟹ **double-humped fission barrier**

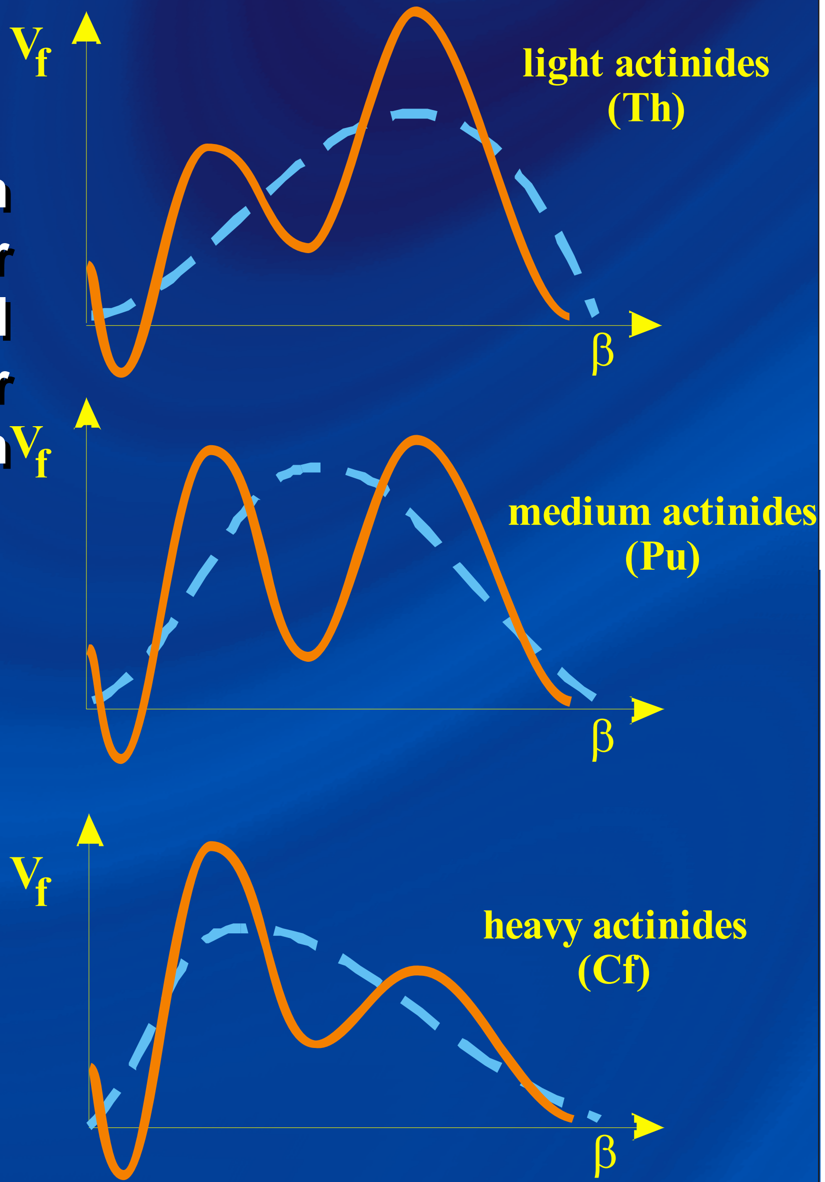
Fission barrier

Variation of the shell correction amplitude with changing Z,N together with the variation of the LD potential barrier with changing fissility parameter ($E_C/2E_S$) lead to a variation of the fission barrier from nucleus to nucleus:

- inner barriers almost constant 5-6 MeV for the main range of actinides; fall rapidly in Th region;

- secondary well's depth around 2 MeV;

- outer barriers fall quite strongly from the lighter actinides (6-7 MeV for Th) to the heavier actinides (2-3 MeV for Fm).

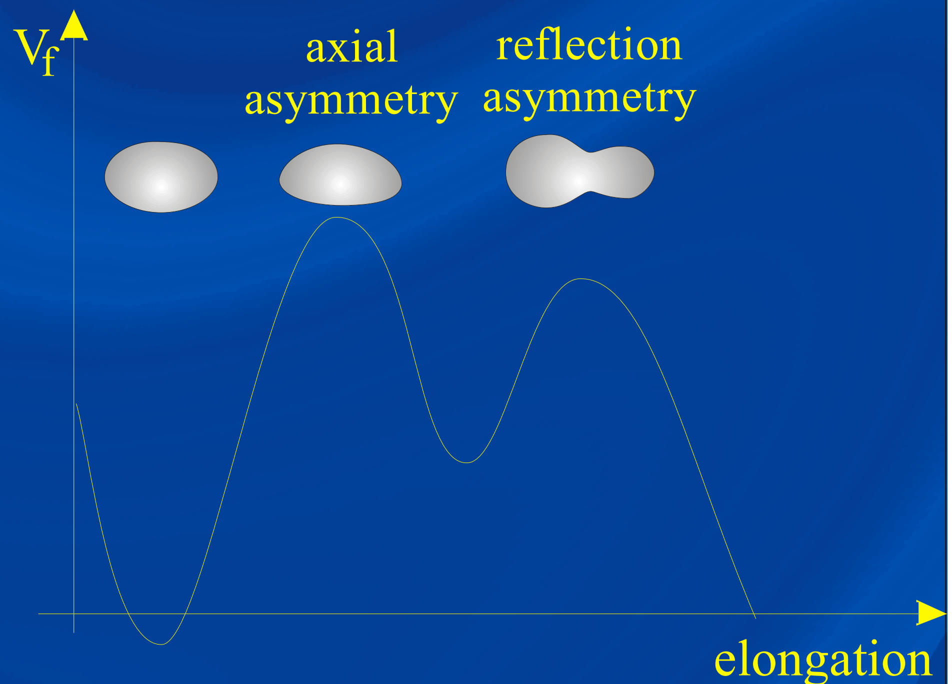


Fission barrier

Early calculations assumed a maximum degree of symmetry of the nuclear shape along the fission path and the theoretical predictions were not in agreement with the experimental barrier heights and the asymmetric mass distribution of the fission fragments.

Extensive studies concluded that neutron rich nuclei have axial asymmetry at the inner saddle point and reflection (mass) asymmetry at the outer saddle point.

These results have large implications for the barrier heights and for the level densities at the saddle points and explain the mass asymmetry of the fission fragments.

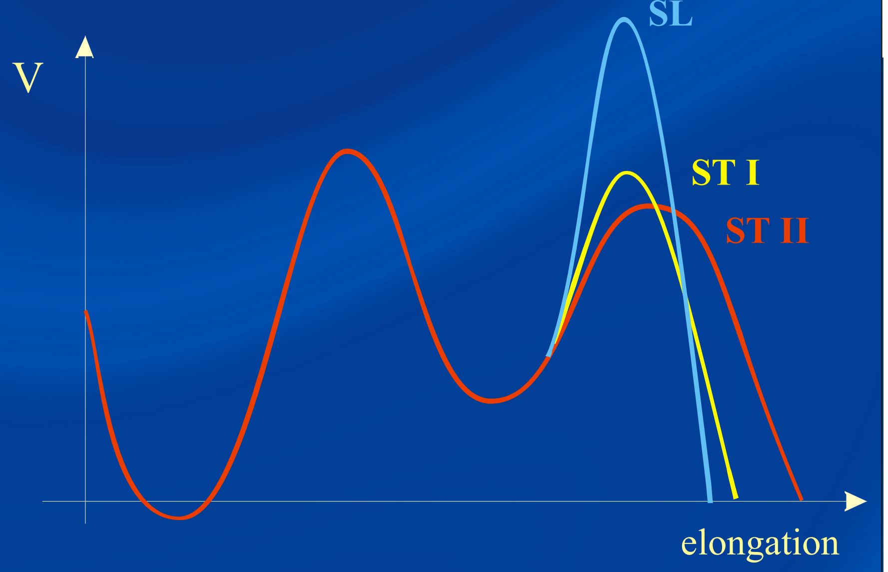


Fission barrier

The multi-modal fission

In Brosa model the mass distribution of the fission fragments can be described considering minimum 3 pre-scission shapes, 3 fission paths which branch from the standard fission path at certain bifurcation points on the potential energy surface. To each of them corresponds a fission mode: symmetric super-long (SL) and asymmetric standard 1 (ST I) and II (ST II).

The different barrier characteristics give rise to a separate fission probability along the various fission paths. The corresponding fission probabilities should add up to the total fission probability.



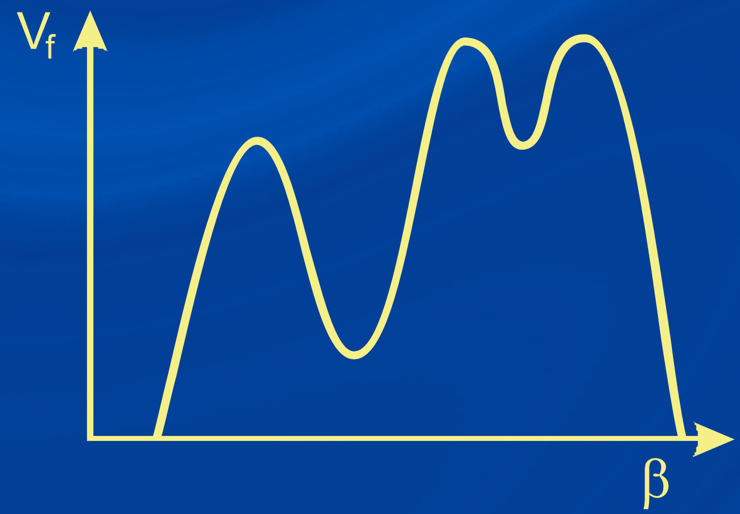
The final distributions of the fission fragment properties (mass, charge and TKE) are a superposition of the different distributions stemming from the various fission modes.

Fission barrier

The triple-humped fission barrier (Th anomaly)

In the thorium region, the second hump appears just under the maximum predicted by the liquid drop model, therefore its exact shape is very sensible to the shell effects. It was demonstrated that a shell effect of second-order would split the outer barrier giving rise to a third very shallow well.

A triple-humped barrier for the actinides in thorium region, allowing the existence of hyper-deformed undamped class III vibrational states could explain the disagreement between the calculated and experimental inner barrier height and also the structure in the fission cross section of non-fissile Th, Pa and light U isotopes.



Fission barrier - description

- parabolic barriers

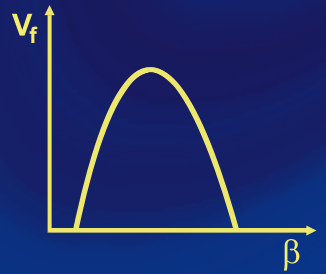
- numerical barriers

  Static fission barriers extracted from full 3-dimensional HFB energy surfaces as function of quadrupole deformation

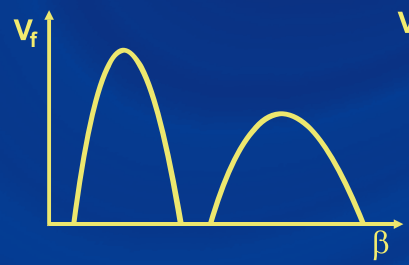
Fission barrier - description

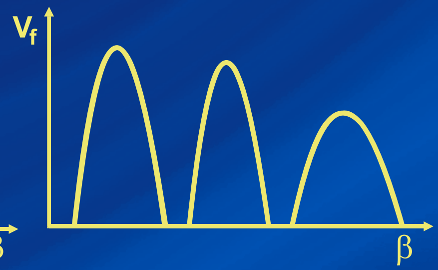
- parabolic barriers

humps only described by decoupled parabolas



$$V_{fi} = E_{fi} - \frac{1}{2}\mu\hbar^2\omega_i^2(\beta - \beta_i)^2$$

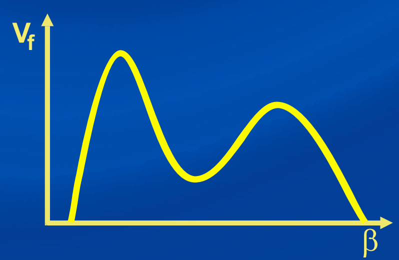


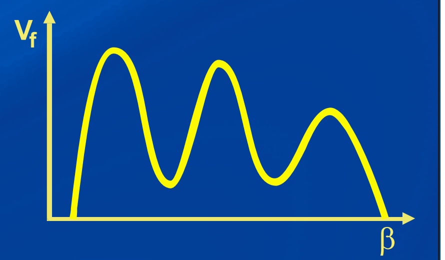


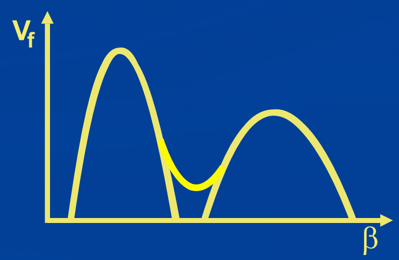
entire fission path described by smoothly joined parabolas

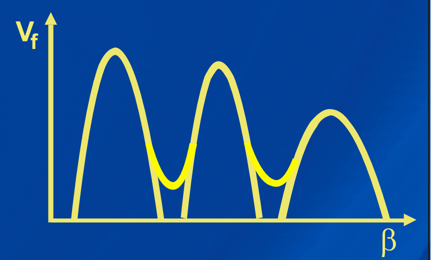
$$V_{fi} = E_{fi} \mp \frac{1}{2}\mu\hbar^2\omega_i^2(\beta - \beta_i)^2$$

$$\mu \approx 0.054\, A^{5/3}\mathrm{MeV}^{-1}$$





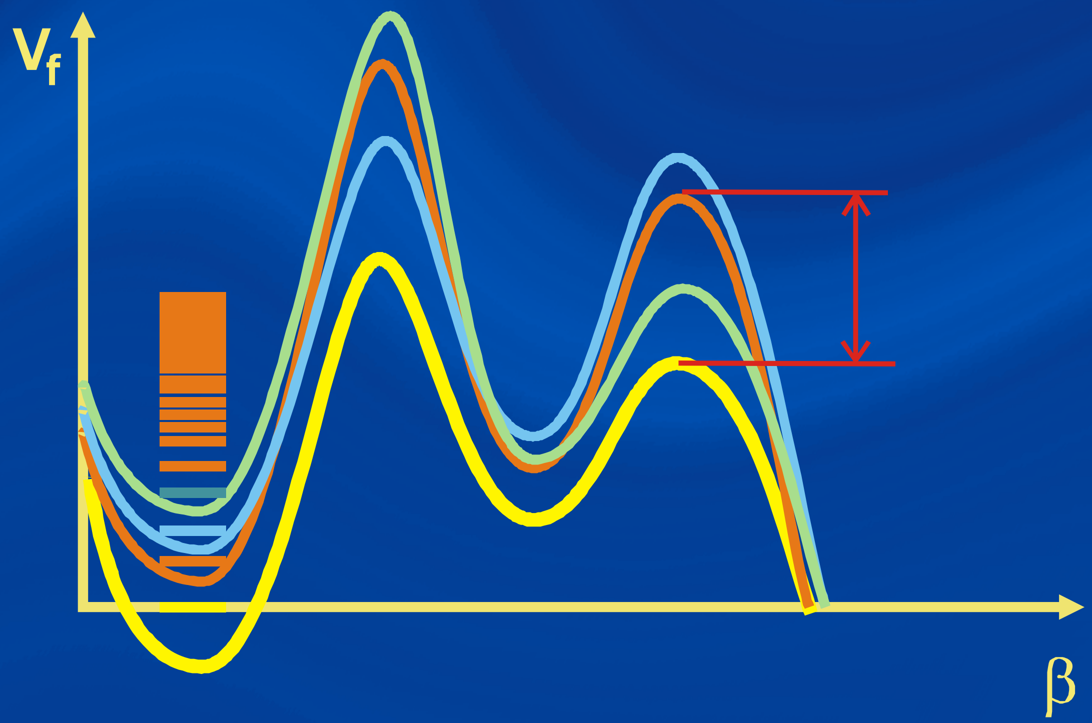




Fission barriers

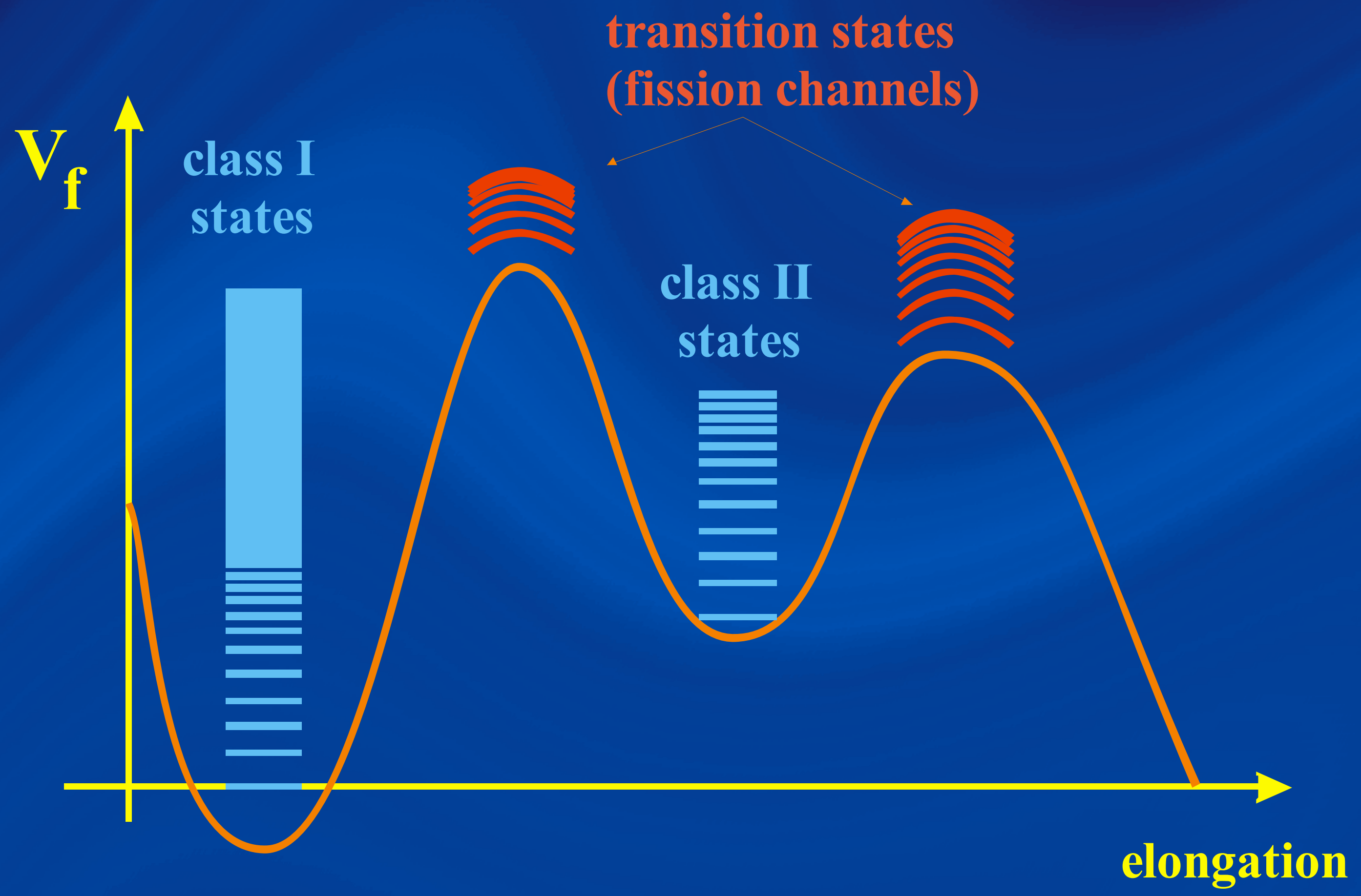
Transition states, class I, II, …states

- transition states – excited states at saddle points
- class I (II,III) states – states of the nucleus with deformation corresponding to first (second, third) well



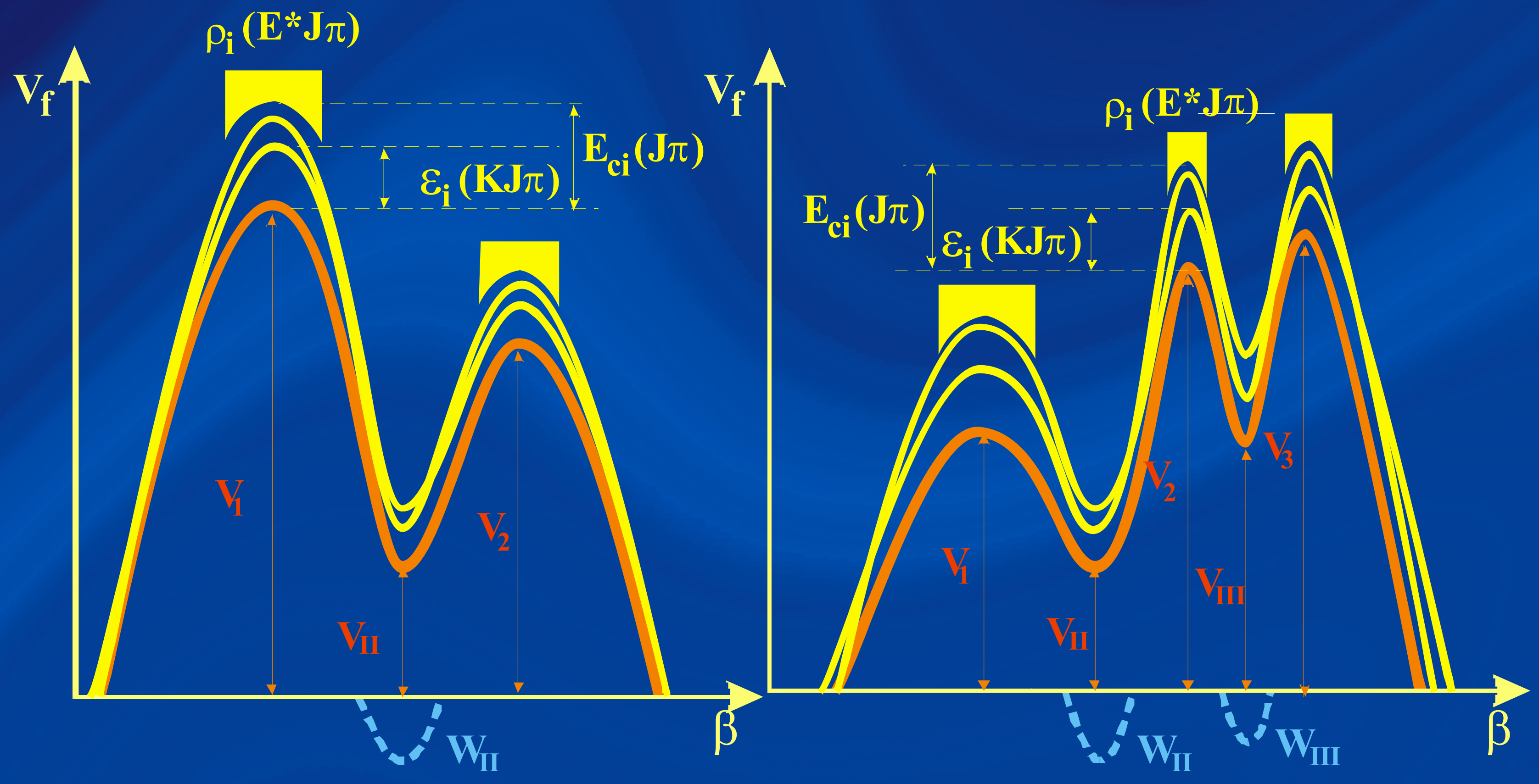
Fission barriers

Transition states, class I, II, …states



Fission barriers

Transition states, class I, II, …states



Fission barriers   Transition states

- discrete
$$E_i(JK\pi) = E_{fi} + \varepsilon_i(K\pi) + \frac{\hbar^2}{2\Im_i}[J(J+1) - K(K+1)]$$

Quantum structure of the fission channels is important for accurate descriptions of fission cross sections at the sub-barrier and near-barrier energies; it depends on the nuclear shape asymmetry and the odd-even nucleus type.

Mirror-asymmetric even-even nuclei have ground-state rotational band levels with

$K\pi$ = 0+, J = 0, 2, 4... - that unify with the octupole band levels $K\pi$ = 0−, J = 1, 3, 5...

in the common rotational band. Additional unification arises for axial asymmetric shapes and levels of the γ-vibrational band with $K\pi$ = 2+, J = 2, 4...

The quantum number of the corresponding rotational bands for odd and odd-odd nuclei are estimated in accordance with the angular momentum addition rules for unpaired particles and the corresponding rotational bands.

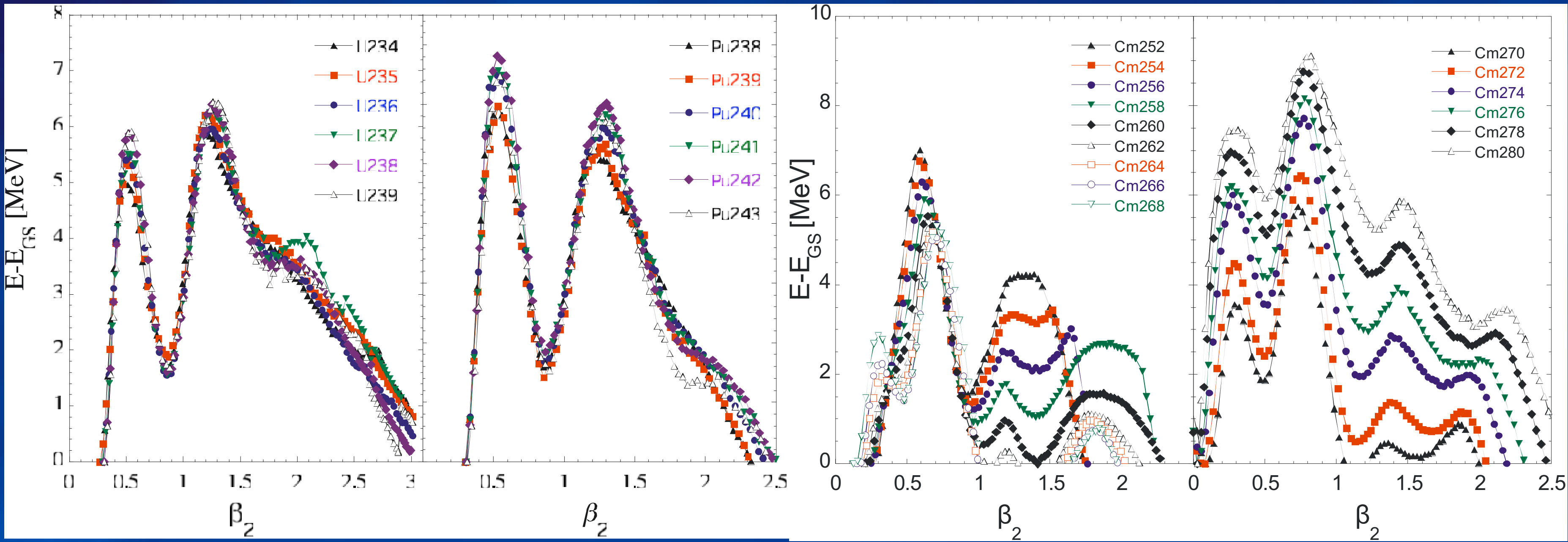
- continuum $\rho_i(E^* J\pi)$

Consistent treatment of all reaction channels would require for the transition state densities the same formulation used for the normal states, adapted to consider the deformation and collective enhancement specific for each saddle point.

Fission barrier - description

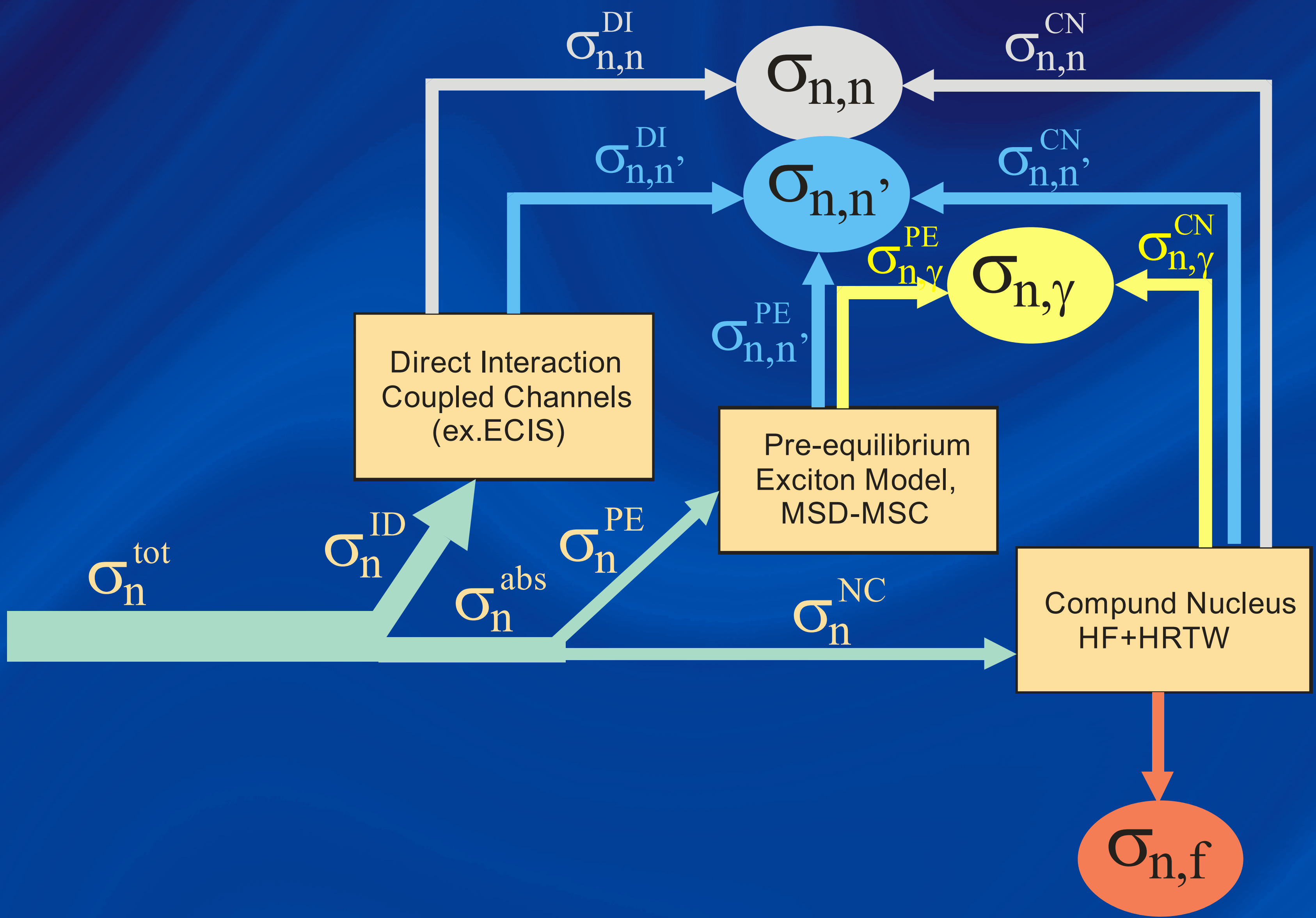
- numerical barriers

  - Static fission barriers extracted from full 3-dimensional HFB energy surfaces as function of quadrupole deformation



  - Global microscopic nuclear level densities within the HFB plus combinatorial method.

Nuclear reaction mechanisms and models



Fission in CN statistical model

The fission cross section:

$$\sigma_{\alpha f}(E) = \sum_{J\pi} \sigma_{\alpha}(E, J\pi) P_f(E, J\pi)$$

$\sigma_{\alpha}(E, J\pi)$ - cross section of the initial state formation

$$P_f(E, J\pi) = \frac{T_f(E, J\pi)}{T_f(E, J\pi) + \sum_{\alpha'} T_{\alpha'}(E, J\pi)}$$

- fission probability

α - entrance channel

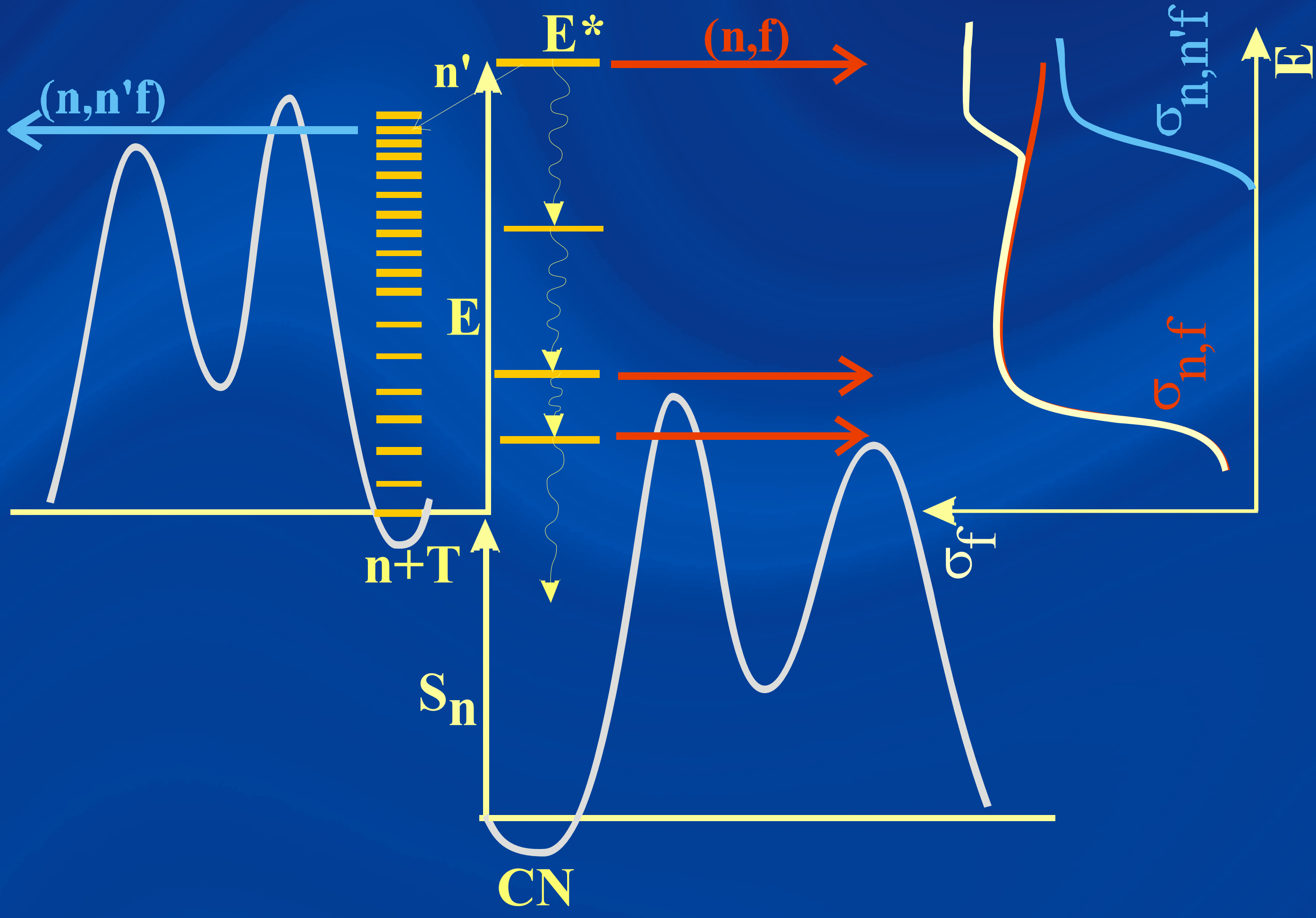
α' - outgoing competing channels

E - energy of the incident particle inducing fission

Jπ - spin, parity of the CN state

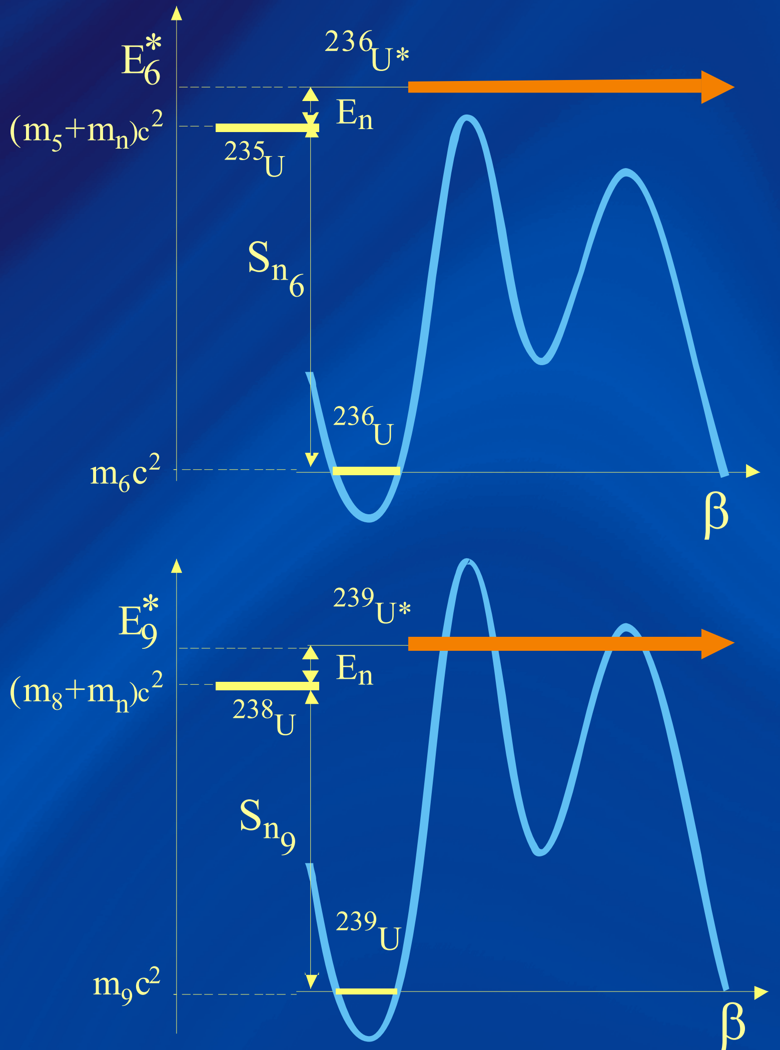
Initial state

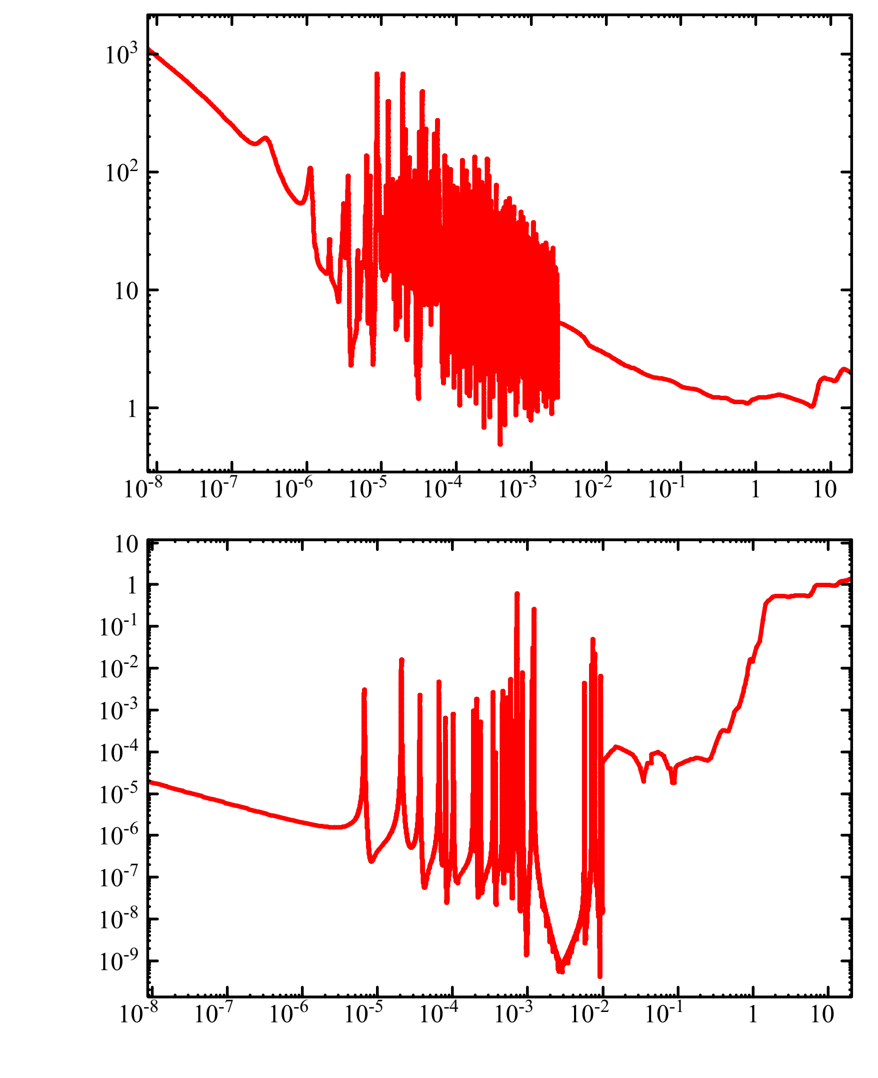
- neutron (γ, p, α…) induced fission:
  - CN states populated directly or after gamma-decay - (n,f)
  - states in residual nuclei - (n,n'f), (n,2nf), (n,3nf)



Initial state

- neutron induced fission: fertile and fissile nuclei



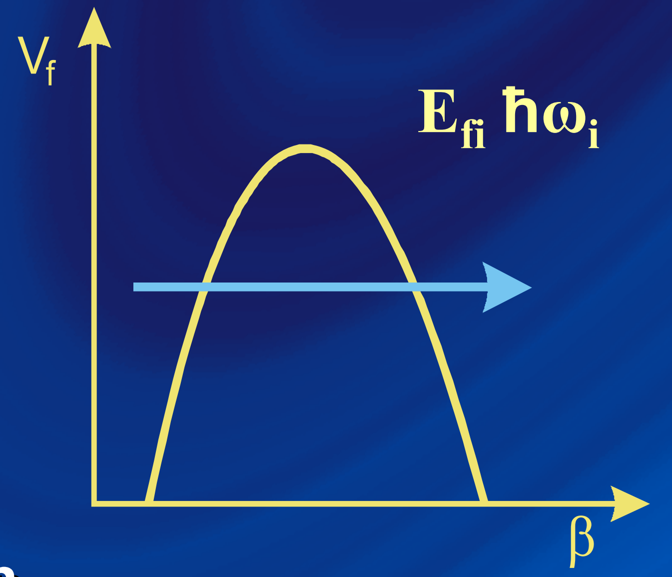


Fission probability

$$P_f(E,J\pi)=\frac{T_f(E,J\pi)}{T_f(E,J\pi)+\sum_{\alpha'}T_{\alpha'}(E,J\pi)}$$

Transmission coefficients

- parabolic barrier

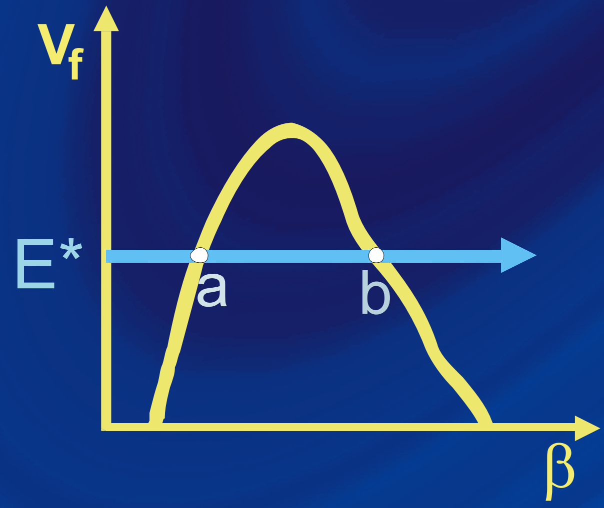


Hill-Wheeler formula for the transmission coefficient through a parabolic barrier:

$$T_i = \frac{1}{1 + \exp\left(\frac{2\pi}{\hbar\omega_i}(E_{fi} - E^*)\right)}$$

Transmission coefficients

- **non-parabolic barrier**

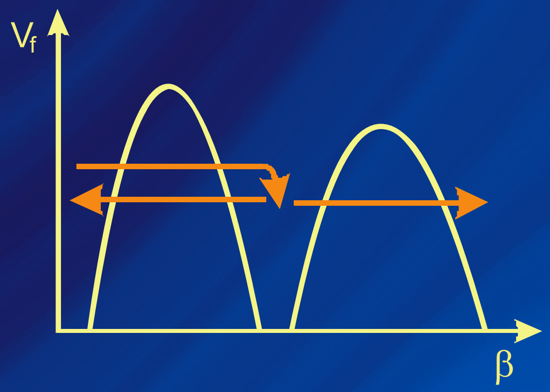


The coefficients T_i are expressed in the first-order WKB approximation in terms of the momentum integrals for the humps:

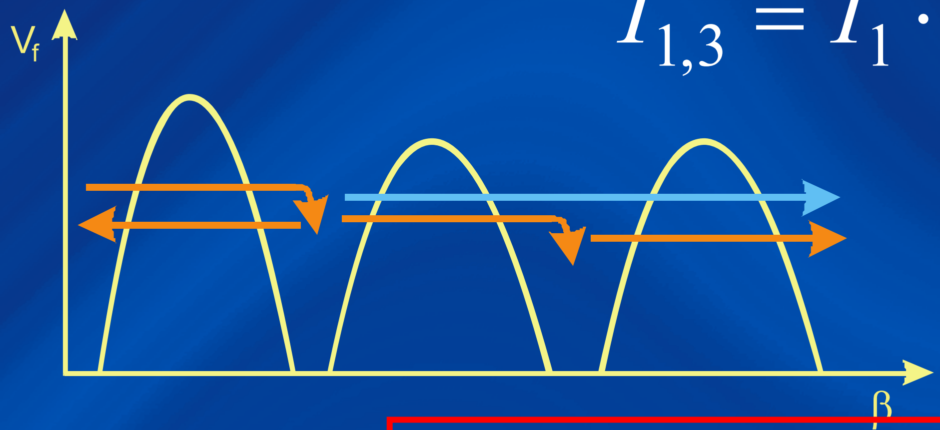
$$M_i = \pm \left| \int_{a_i}^{b_i} [2\mu(E^* - V_i(\beta))/\hbar^2]^{1/2} d\beta \right|$$

$$T_i = \frac{1}{1+\exp(2M_i)} \xrightarrow{\text{parabola}} \text{Hill} - \text{Wheeler}$$

Transmission coefficients - decoupled humps



$$T_{1,2} = T_1 \cdot \frac{T_2}{T_1 + T_2} = \frac{1}{\frac{1}{T_1} + \frac{1}{T_2}}$$



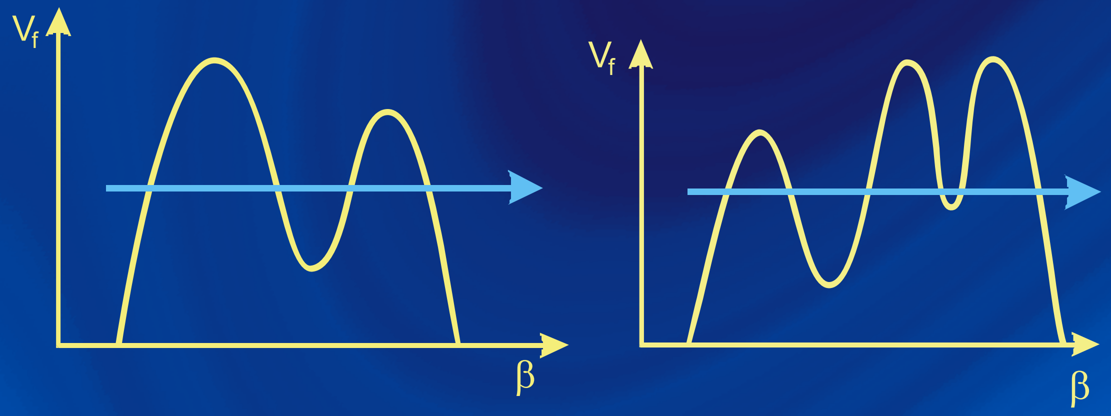
$$T_{1,3} = T_1 \cdot \frac{T_{2,3}}{T_1 + T_{2,3}} = \frac{1}{\frac{1}{T_1} + \frac{1}{T_2} + \frac{1}{T_3}}$$

N_h humps

$$\frac{1}{T_{1,N_h}} = \sum_i^{N_h} \frac{1}{T_i}$$

$$T_{1,N_h} \xrightarrow{E^* >> V_f} \frac{1}{N_h}$$

Transmission coefficients – entire barrier



WKB approximation

$$T_{dir12} = \frac{T_1 T_2}{1 + 2(1-T_1)^{1/2}(1-T_2)^{1/2}\cos(2\upsilon) + (1-T_1)\ (1-T_2)}$$

$$T_{dir13} = \frac{T_1 T_{dir_{23}}}{1 + 2(1-T_1)^{1/2}(1-T_{dir_{23}})^{1/2}\cos(2\upsilon) + (1-T_1)\ (1-T_{dir_{23}})}$$

$$\upsilon = \int_{\beta_{12}}^{\beta_{23}} M(\beta)d\beta \qquad M(\beta) = \left(2\mu[E^* - V(\beta)]/\hbar^2\right)^{1/2}$$

Fission mechanisms

Hamiltonian of a fissionable nucleus: $H = H_\beta + H_i + H_{i\beta}$

H_β **describes the fission degree of freedom**

H_i **describes the other collective and intrinsic degree of freedom**

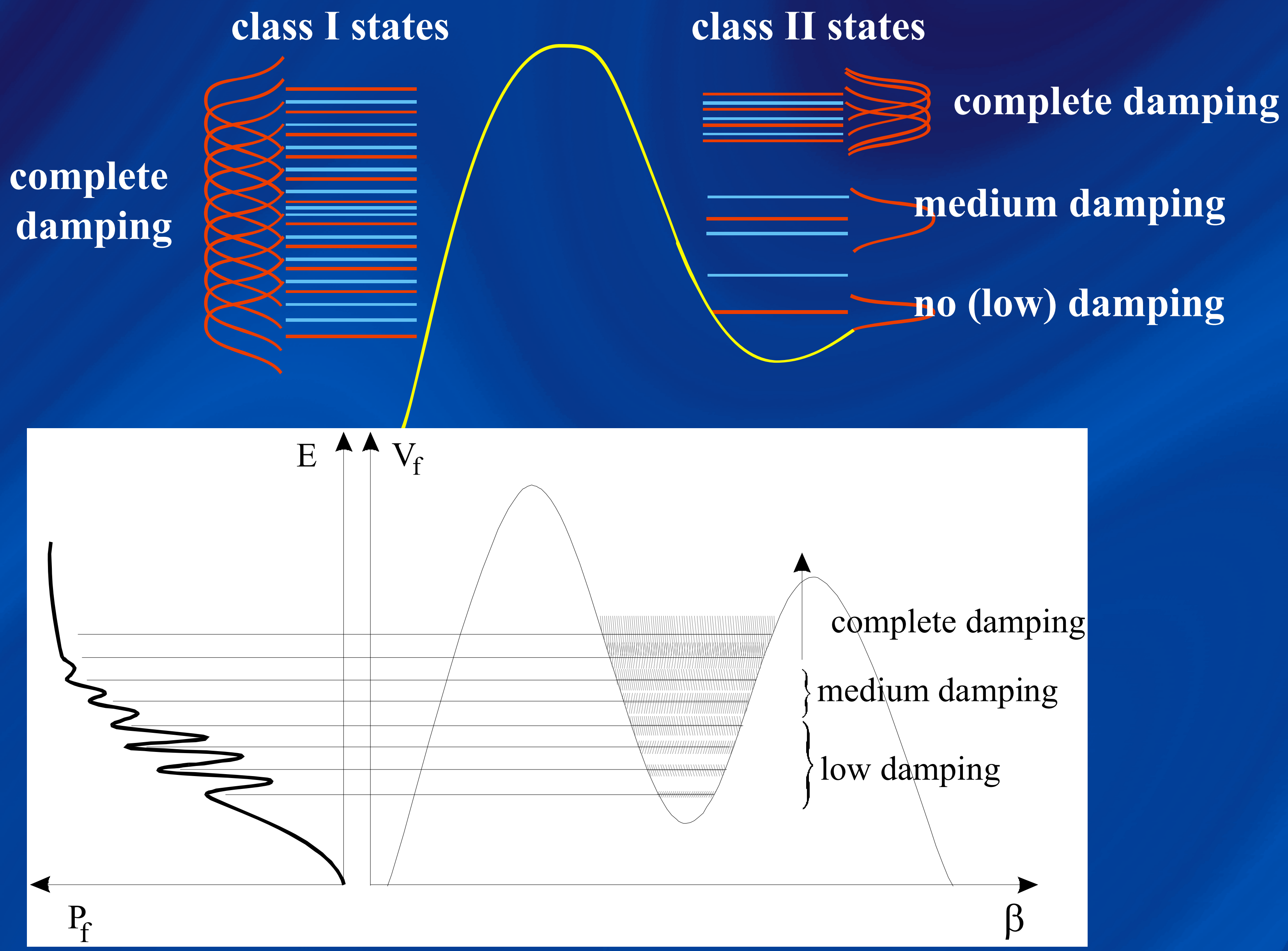
$H_{i\beta}$ **accounts for the coupling between the fission mode and other degrees of freedom.**

Wave functions of the total Hamiltonian: $|c> = \sum_{m,n} a_{mn} |\beta n>|im>$

Below the inner barrier the vibrational states $|\beta$ n> may be classified as class I and class II vibrations depending on whether the amplitude is greater in the ground state (I) or secondary minimum (II). The compound states |c> of the system may be classified as class I and class II, according to the type of vibrational states dominating in the expansion.

The interaction term $H_{i\beta}$ leads both to a coupling between the vibrational and intrinsic degrees of freedom (the vibrational damping) and between class I and class II states.

Fission mechanisms



Fission mechanisms

Models for fission coefficient calculation

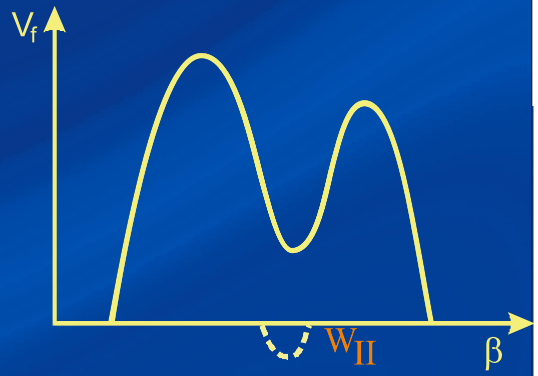
- conventional approach – complete damping of vibrational class I and II (III)

- doorway-state model – the elements of the coupling matrix are calculated

- optical model for fission – the absorption out of fission mode is described by an imaginary potential

Fission mechanisms – optical model for fission

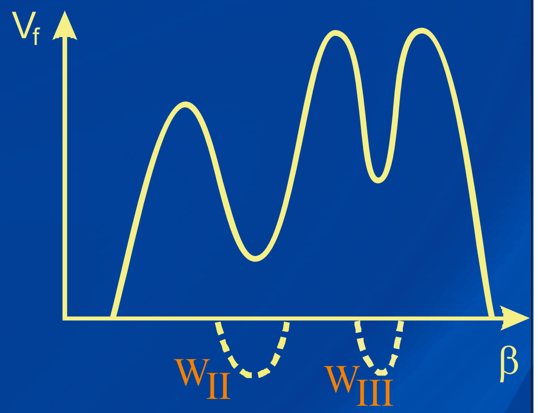
The coupling between the vibrational and non-vibrational class II (III) states makes possible for the nucleus to use the excitation energy to excite other degrees of freedom and this is interpreted as a loss, an absorption out from the flux initially destinated to fission. This absorption is described by an imaginary potential in the second well.



Complex potential

- real part: 3 (5) parabolas smoothly joined

$$V_{fi} = E_{fi} + (-1)^i \frac{1}{2} \mu\hbar^2 \omega_i^2 (\beta - \beta_i)^2$$



- imaginary part:

$$W_j = -\alpha_j(E)[E^* - V_{f_j}]$$

Fission mechanisms within optical model for fission

Transmission through the complex double-humped barrier

- direct - via the vibrational states
- indirect - reemission after absorption in the isomeric well

$$T_f = T_{dir} + T_{abs}\left(\frac{T_2}{T_1 + T_2 + T_{\gamma II}} + \frac{RT_{\gamma II}}{T_1 + T_2 + T_{\gamma II}}\right)$$

$$R = \frac{T^{iso}_{\gamma 1/2}}{T^{iso}_{\gamma 1/2} + T^{iso}_{f 1/2}}$$

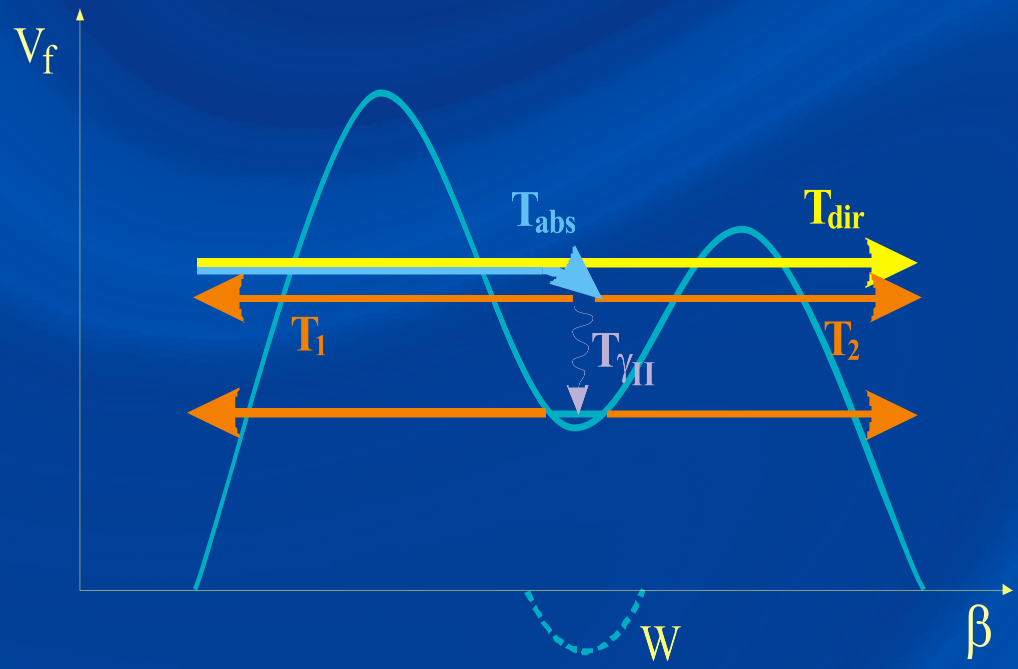
$$\xrightarrow{E^*}$$

$$T_{dir} \rightarrow 0$$

$$T_{abs} \rightarrow T_1$$

$$T_{\gamma II} \rightarrow 0$$

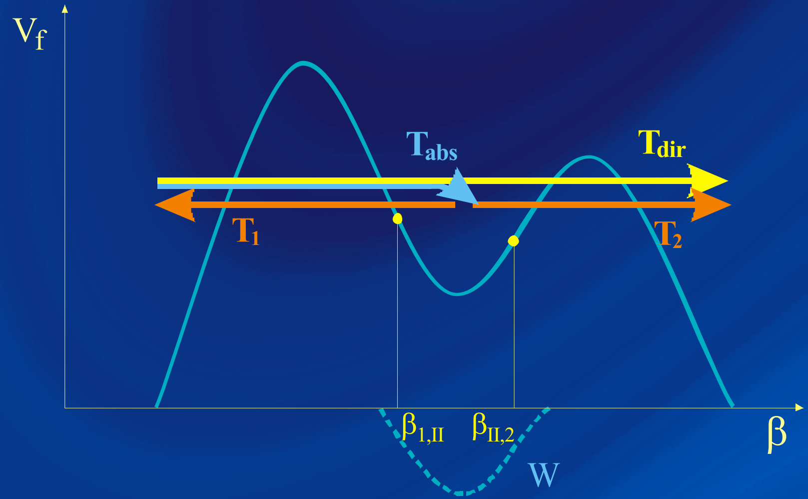
$$T_f = T_1 \frac{T_2}{T_1 + T_2}$$



Fission coefficients within optical model for fission

Double-humped barrier

T_{dir}, T_{abs} are derived in WKB approximation for complex potential



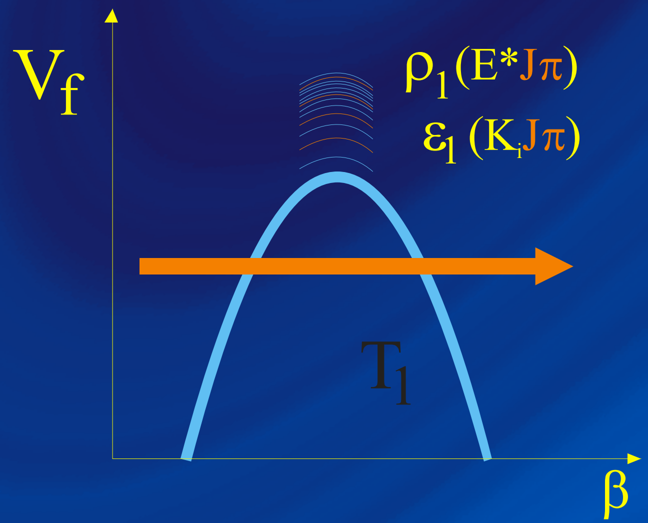
$$T_{dir} = \frac{T_1 T_2}{e^{2\delta} + 2[(1-T_1)^{1/2}(1-T_2)^{1/2}\cos(2\upsilon) + (1-T_1)(1-T_2)e^{-2\delta}]}$$

$$T_{abs} = T_{dir}\frac{e^{2\delta} - (1-T_2)e^{-2\delta} - T_2}{T_2}$$

$$\upsilon = \int_{\beta_{1,II}}^{\beta_{II,2}} M(\beta)d\beta \qquad M(\beta) = \left(2\mu[E^* - V(\beta)]/\hbar^2\right)^{1/2}$$

$$\delta = -\left(\frac{\mu}{2}\right)^{1/2}\int_{\beta_{1,II}}^{\beta_{II,2}} \frac{W(\beta)}{[E^* - V(\beta)]^{1/2}}d\beta = \alpha\left(\frac{\mu}{2}\right)^{1/2}\int_{\beta_{1,II}}^{\beta_{II,2}}[E^* - V(\beta)]^{1/2}d\beta$$

Transmission coefficients



$$T_i(EJ\pi) = T_i^{dis}(EJ\pi) + T_i^{cont}(EJ\pi)$$

$$T_i^{dis}(EJ\pi) = \sum_{K \le J} T_i(EKJ\pi)$$

$$T_i^{cont}(EJ\pi) = \int_{E_{ci}}^{\infty} \frac{\rho_i(\varepsilon J \pi)d\varepsilon}{1 + \exp\left[\frac{2\pi}{\hbar\omega_i}(E_{fi} + \varepsilon - E^*)\right]}$$

$$T_i^{cont}(E, J, \pi) = \int_{Ec_i}^{\infty} \frac{\rho_i(\varepsilon, J, \pi)d\varepsilon}{1 + \exp(2M_i)}.$$

Fission coefficients within optical model for fission

Double-humped barrier

$$T_f = T_{dir} + T_{abs}\left(\frac{T_2}{T_1 + T_2 + T_{\gamma II}} + \frac{RT_{\gamma II}}{T_1 + T_2 + T_{\gamma II}}\right)$$

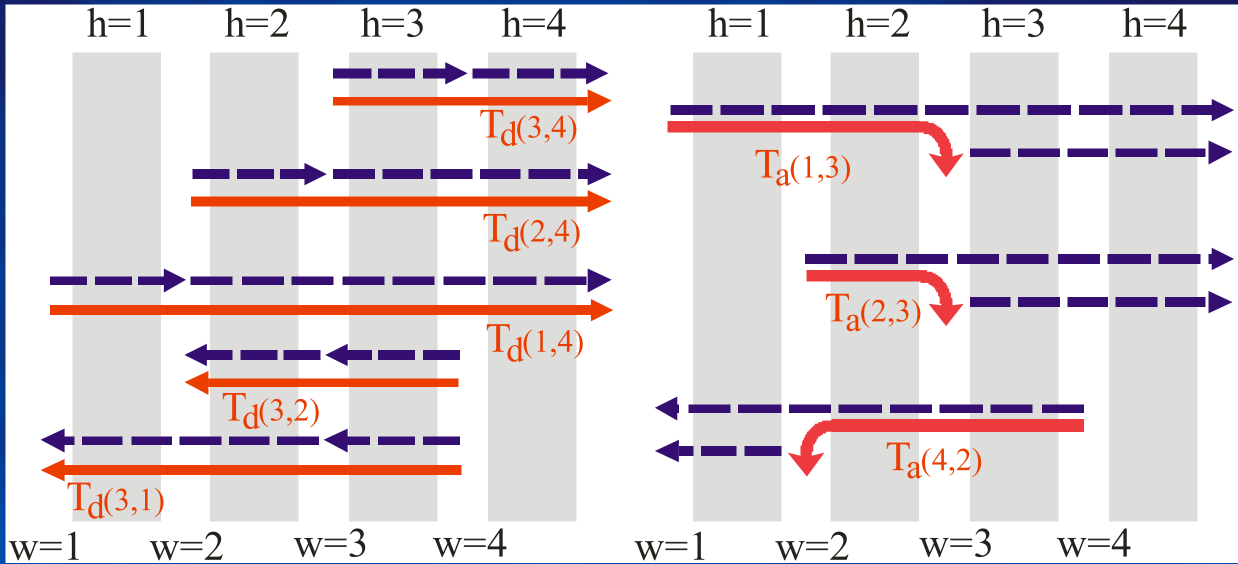
$$T_{dir}(E, J\pi) = \sum_{K \le J} T_{dir}(E, KJ\pi)$$

Full K-mixing:

$$T_{abs}(E^* J\Pi) = \sum_{K \le J} T_{abs}(E^* KJ\pi) + \int_{E_{c1}}^{\infty} \frac{\rho_1(\varepsilon J\pi)d\varepsilon}{1 + \exp\left[\frac{2\pi}{\hbar\omega_1}(E_{f1} + \varepsilon - E^*)\right]}$$

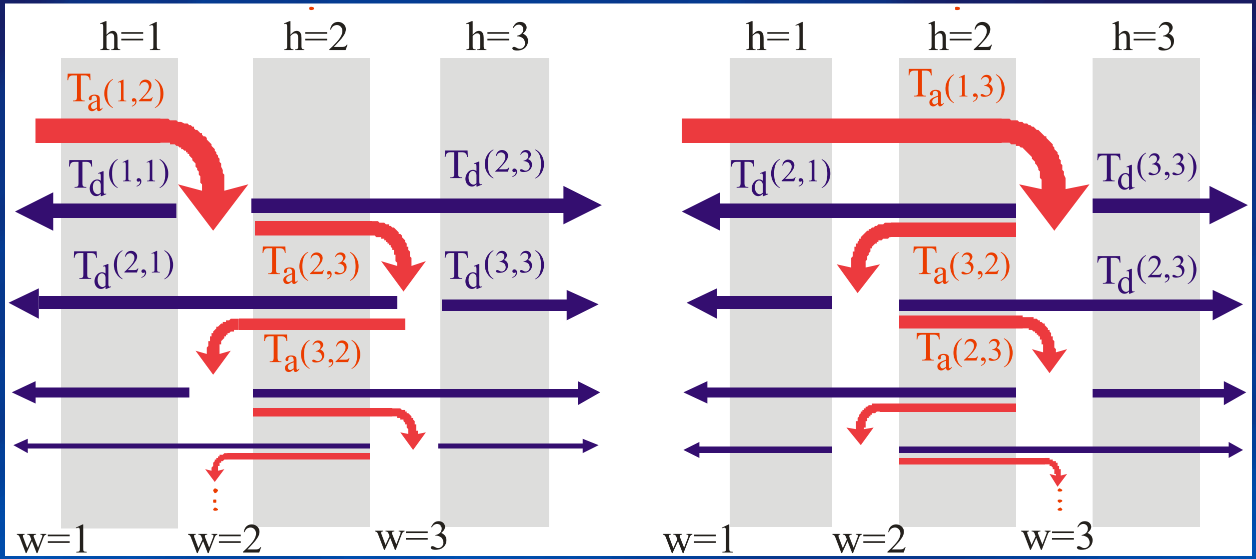
Based on these relations, a recursive method was developed to describe transmission through triple- and n-humped barriers.

Transmission through multi-humped barriers



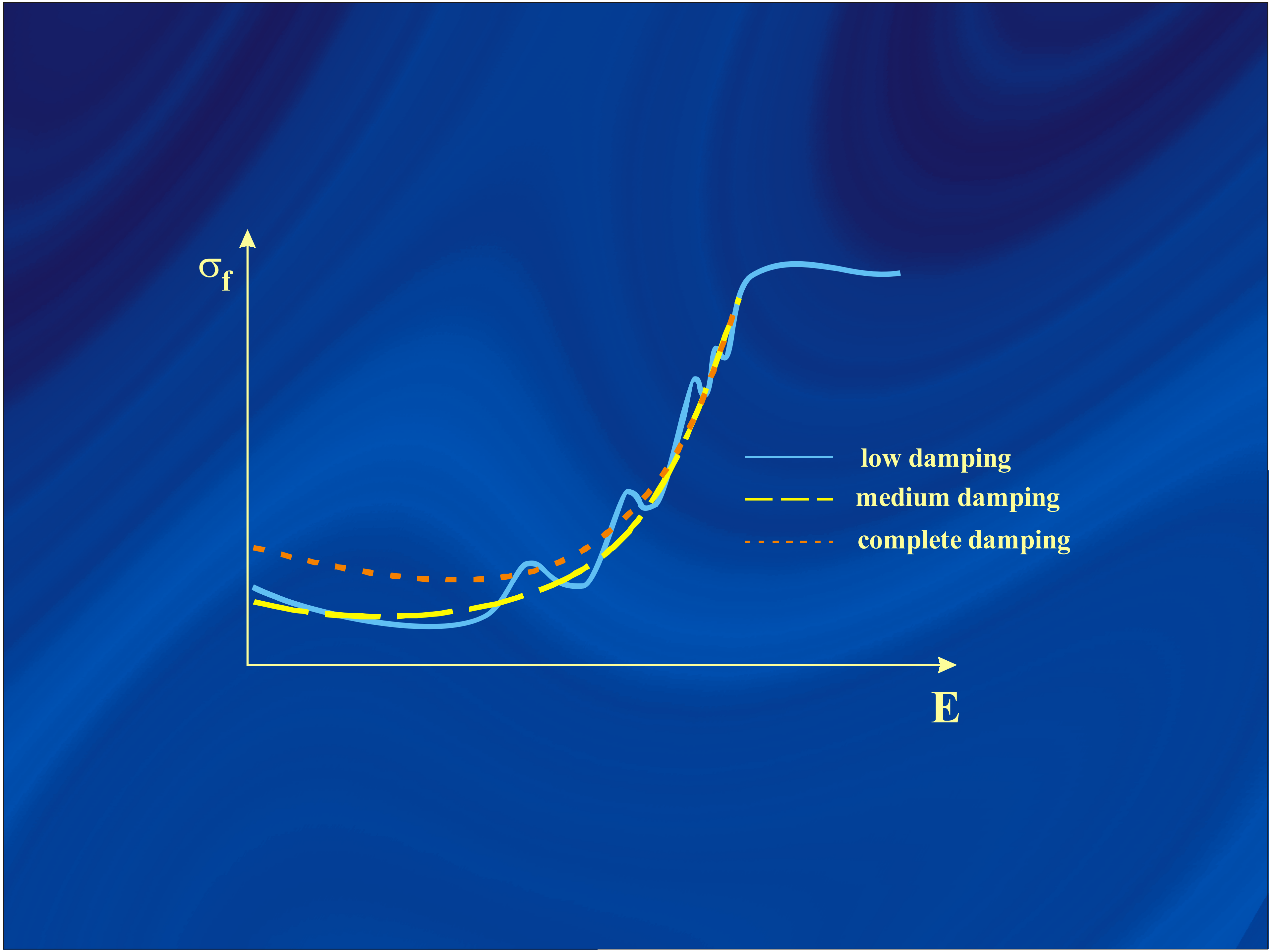
Graphic representation of the recursive method used to calculate some of the direct and absorption coefficients for a four-humps barrier. The transmission coefficients entering the calculations are represented by dashed arrows and the derived coefficients are represented by full arrows.

Transmission through multi-humped barriers



The evolution of the flux absorbed in the second and third wells.

Each time new contributions are accumulated to the flux undergoing fission and to the one absorbed in the first well. The shape changing between the second and third wells continues till the fractions initially absorbed in these wells are exhausted.



σf
low damping
medium damping
complete damping
E