Workshop on
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Physics, Design and Safety

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Models for Nuclear Fission

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These are preliminary lecture notes, intended only for distribution to participants
MODELS FOR NUCLEAR FISSION
USED IN EVALUATION

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Main topics:

- Overview of the fission process
- Fission nuclear data
- Nuclear models used for fission cross section calculations (implemented in EMPIRE)
1934 - Fermi bombarded uranium with neutrons
1938 – official discovery of nuclear fission:
- the experiments of Hahn and Strassman
- the interpretation of Meitner and Frisch
1942 - first chain fission reaction

Almost since the time of its discovery, it has been an academic and applied interest for nuclear fission. It has economical, social, political and ecological implications.
Despite all of the progress in the understanding of the fission process, after more than 60 years of research, still no theory or model is able to predict all the 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.

The increased accuracy of the fission data requested by the designers of the new nuclear technologies requires 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.
Fission process (1)

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.

The total energy liberated by the process is about 200 MeV, the difference in mass between the original nucleus and the two newly formed fragments.
Fission process (2)

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

\[ V \approx 6 \text{ MeV} \] \[ \approx 40 \text{ MeV} \] \[ \approx 200 \text{ MeV} \]

scission point
Fission process (3)

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
Formation of the initial state

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

- neutron 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 (1)

This phase plays an essential role for the determination of the fission properties

- 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.
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 fissioning 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 (3)

- **saddle point** – a point on the potential energy surface where the energy is stationary as a function \( \{q\} \); it has a maximum as a function of the main deformation parameter, but a minimum as a function of the others; corresponds to the maximum of the fission barrier.
Potential landscape

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

- microscopic models: HFB
  – can not provide accurate results for $V_f$ yet

- microscopic-macroscopic models: LDM+shell correction
  – explains a significant number of experimental data
  – the most used procedure to calculate fission barriers
From the initial state to scission (5)

Strutinsky’s procedure

\[ V(q) = V_{LD}(q) + \Delta V_{sh}(q) \]

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
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; fall rapidly in Th region
- secondary well’s depth around 2-3 MeV
- outer barriers fall quite strongly from the lighter actinides (6-7 MeV for Th) to the heavier actinides (2-3 MeV for Fm).
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. After extensive studies was concluded that axial asymmetry is indicated for the inner and reflection asymmetry for the outer barrier. These results have large implications for the barrier heights but also for the level densities at the saddle points.

The double-humped fission barrier can explain the existence of spontaneously fissioning (shape) isomers and the extent of shape isomerism (the U-Bk island).
From the initial state to scission

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).

Each mode has its own contribution to the observables of the fission process.

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.
- transition states – excited states at saddle points
- class I (II) states – states of the nucleus with deformation corresponding to first (second) well
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.
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 the initial state to scission

Potential energy - conclusions

- The calculation of the potential energy is difficult and still a challenge to the theorists.

- Basic calculations from first principles are possible but do not give very accurate results yet.

- Phenomenological procedures are more precise but still need to be justified.

- At present the Strutinsky’s hybrid model is considered the best method of calculating fission barriers. It explains most of the experimental data (fission barrier heights, shape isomerism, resonant structure of the fission c.s. at sub-barrier energies, fission fragments’ properties).

- The nuclei can exhibit one- two- or triple-humped fission barrier; they can be represented by parabolas defined by heights and widths.
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. Very 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.

The neutrons emitted in this phase are called prompt neutrons. The knowledge of prompt fission neutron spectrum and of the average prompt neutron multiplicity is extremely important for reactor calculations.
Prompt fission neutron properties: $\gamma_p, N(E)$

- **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 good predictive power.

D.G. Madland, Theory of neutron emission in fission, Workshop on nuclear data… Trieste 1998
De-excitation of the fission products by 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 ($\nu_t$), MT=455 ($\nu_d$), MT=456 ($\nu_p$)
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 (2)**

**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 cross section in statistical models (1)

The fission cross section:

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

- $\sigma_{\alpha}(EJ\pi)$ - cross section of the initial state formation
- $P_f(EJ\pi)$ - fission probability

- $a$ - entrance channel
- $E$ - energy of the incident particle inducing fission
- $Jp$ - spin, parity of the CN state
Fission cross section in statistical models (2)

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

- \( H_\beta \) 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 the other degrees of freedom.

The 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 cross section in statistical models (3)

Models for fission probability calculation
- conventional approach – complete damping of vibrational class I and II
- doorway-state model – the elements of the coupling matrix are calculated
- optical model for fission – the absorption out from fission channel is described by an imaginary potential
CONVENTIONAL APPROACH (1)

- two independent inverted parabolas

\[ V_{fi} = E_{fi} - \frac{1}{2} \mu \hbar^2 \omega_i^2 (\beta - \beta_i)^2 \quad i=1,2 \]

- discrete

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

- continuum

\[ \rho_i(E \ast J\pi) \]

\[ \mu \approx 0.054 A^{5/3} \text{MeV}^{-1} \]
CONVENTIONAL APPROACH (2)

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

\[
T_{fi} = \frac{1}{1 + \exp \left( \frac{2p}{\hbar} (E_{fi} - E^*) \right)}
\]

\[
T_i(E^* J\pi) = \sum_{K \leq J} T_i(E^* K J\pi) + \int_{E_{ci}}^{\infty} \frac{\rho_i(\varepsilon J\pi) d\varepsilon}{1 + \exp \left[ \frac{2\pi}{\hbar \omega_i} (E_{fi} + \varepsilon - E^*) \right]}
\]
Total fission coefficient:

\[ T_f (E^* J\pi) = T_1 (E^* J\pi) \cdot \frac{T_2 (E^* J\pi)}{T_1 (E^* J\pi) + T_2 (E^* J\pi)} \]

Fission probability:

\[ P_f (EJ\pi) = \frac{T_f (E^* J\pi)}{T_f (E^* J\pi) + \sum_{\alpha'} T_{\alpha'} (EJ\pi)} \]
CONVENTIONAL APPROACH (4)

- is simple, requires a relatively small number of input parameters:
  - fundamental barrier $E_{fi}$, $h\omega_i$
  - discrete transition barriers $\varepsilon_i(K\Pi)$, $\mathcal{Z}_i$
  - level densities

- can be applied at over-barrier energies, where fission cross section has a smooth dependence on energy.

**Example:** Fissile nuclei odd-N targets (e.g. $^{235}$U)
CONVENTIONAL APPROACH (5)

... but not at sub-barrier energies (neutron induced fission of fertile target, photo-fission, fission induced in direct transfer reactions (e.g. (d,pf)))

Example: Fertile nuclei even-N targets (e.g. $^{238}$U)

The parameters of the discrete barriers and the level densities at saddle points are deduced simultaneously from the fit of the experimental fission cross section. If a combination discrete+continuum describes the data does not necessarily mean that taken separately are still appropriate.
OPTICAL MODEL FOR FISSION (1)

- Low damping
- Medium damping
- Complete damping

Class II vibrational states

Energy $E$ vs. Fermi energy $V_f$
OPTICAL MODEL FOR FISSION (2)

Complex potential
- real part: 3 parabolas smoothly joined

\[ V_{fi} = E_{fi} + (-1)^i \frac{1}{2} \mu \hbar^2 \omega^2 (\beta - \beta_i)^2 \quad i=1,3 \]

- imaginary part:

\[ W = -\alpha [ E^* - V_f ] \]
OPTICAL MODEL FOR FISSION (3)

Transmission through the complex double-humped barrier

- direct
- reemission after absorption in the isomeric well

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

\[ T_f = T_1 \frac{T_2}{T_1 + T_2} \]

Diagram showing transmission through the complex double-humped barrier with labels for direct transmission ($T_{dir}$), absorption ($T_{abs}$), and reflection ($T_{\gamma II}$).
OPTICAL MODEL FOR FISSION (4)

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

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

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

\[
\nu = \int_{\beta_{12}}^{\beta_{23}} K(\beta) \, d\beta
\]

\[
K(\beta) = \left(2\mu [E^* - V(\beta)]/\hbar^2 \right)^{1/2}
\]

\[
\delta = -\left(\frac{\mu}{2}\right)^{1/2} \int_{\beta_{12}}^{\beta_{23}} \frac{W(\beta)}{[E^* - V(\beta)]^{1/2}} \, d\beta = \alpha \left(\frac{\mu}{2}\right)^{1/2} \int_{\beta_{12}}^{\beta_{23}} [E^* - V(\beta)]^{1/2} \, d\beta
\]
OPTICAL MODEL FOR FISSION (5)

\[ T_{dir}(E^* J\pi) = \sum_{K \leq J} T_{dir}(E^* K J\pi) \]

Full K-mixing:

\[ T_{abs}(E^* J\Pi) = \sum_{K \leq J} T_{abs}(E^* K J\pi) + \int_{E_{c1}}^{\infty} \frac{\rho_1(\epsilon J\pi) d\epsilon}{1 + \exp \left[ \frac{2\pi}{\hbar \omega_1} (E_{f1} + \epsilon - E^*) \right]} \]
OPTICAL MODEL FOR FISSION (6)

Decay probabilities

- considering an infinite number of shape transitions
- averaging over one resonance

**Low damping**

- prompt fission probability
- isomeric fission probability
- competitive process probability

\[ P_f = \frac{T_{dir} + \sum_{c'} T_{c'}}{T_{dir} + \sum_{c'} T_{c'}} \cdot \frac{1}{a} \]

\[ P_{iso} = \frac{RT_{\gamma II} \cdot 1}{T_2 + T_{\gamma II} \cdot a} \]

\[ P_c = \frac{T_c}{T_{dir} + \sum_{c'} T_{c'} \left( 1 - \frac{1}{a} \right)} \]

\[ a = \left[ 1 + b^2 + 2b \text{cosech} \left( \frac{T_{1} + T_{2(3)} + T_{\gamma II}}{2} \right) \right]^{1/2} \]

\[ b = \frac{T_{dir} + \sum_{c'} T_{c'} \left( T_{1} + T_{2(3)} + T_{\gamma II} \right)}{T_{abs} \left( T_{2(3)} + T_{\gamma II} \right)} \]

\( R \) – branching ratio for fission of the isomeric state

\[ R = \frac{T_{iso}^{\gamma 1/2}}{T_{iso}^{\gamma 1/2} + T_{f 1/2}^{iso}} \]
OPTICAL MODEL FOR FISSION (7)

Decay probabilities

Medium damping

\[
b = \frac{T_{\text{dir}} + \sum_{c'} T_{c'}}{T_{\text{abs}} (T_{2(3)} + T_{\gamma II})} \left( T_1 + T_{2(3)} + T_{\gamma II} \right)
\]

\[
P_f = \frac{T_{\text{dir}}}{T_{\text{dir}} + \sum_{c'} T_{c'}} + \frac{\sum_{c'} T_{c'}}{T_{\text{dir}} + \sum_{c'} T_{c'}} \cdot \frac{1}{a}
\]

Complete damping

\[
a = \left[ 1 + b^2 + 2b \text{cth} \left( \frac{T_1 + T_{2(3)}}{2} \right) \right]^{1/2}
\]

\[
T_{\text{dir}} \to 0
\]

\[
T_{\text{abs}} \to T_1
\]

\[
T_{\gamma II} \to 0
\]

\[
c = n, p, \alpha, \gamma, \ldots
\]

\[
b = \sum_{c'} T_{c'} \frac{T_1 + T_{2(3)}}{T_1 T_{2(3)}} = \sum_{c'} T_{c'}
\]

\[
P_f = \frac{1}{a}
\]

\[
a = 1 + b = \frac{T_f + \sum_{c'} T_{c'}}{T_f}
\]

\[
P_f = \frac{T_f}{T_f + \sum_{c'} T_{c'}}
\]

\[
P_e = \frac{T_e}{T_f + \sum_{c'} T_{c'}}
\]
OPTICAL MODEL FOR FISSION (8)

- fission cross section of $^{238}\text{U}$ (first chance)
**OPTICAL MODEL FOR FISSION (9)**

Thorium three-humped fission barrier

\[
T_f = T_{\text{dir}} + T_{\text{abs}} \frac{T_{\text{dir}23}}{T_1 + T_{\text{dir}23}}
\]

\(T_{\text{dir}}, T_{\text{abs}}\) are derived in WKB approximation for complex potential

Complete damping

\[
T_f = \frac{T_1 T_2 T_3}{T_1 + T_2 T_3}
\]
OPTICAL MODEL FOR FISSION (10)

Extension of the statistical model at sub-barrier energies

- general expressions for prompt and delayed fission probability
- general expressions for competitive processes’ decay probability

Rules to obtain the value of the parameters not explicitly available from direct measurements more strongly based on physical considerations:

- parameters of the discrete fission barriers deduced from the fit of the fission probability at sub-barrier energies where the continuum’s contribution is negligible;
- level densities at the saddle points deduced from the fit of the fission cross section at over-barrier energies considering the parameters of the discrete fission barriers deduced previously.
Fission in EMPIRE 2.19 beta 12

**SUBEFF**

= 0 sub-barrier effects are not considered
= 1 sub-barrier effects are considered; information about the well(s) and the imaginary potential are requested.

**FISBAR**

= 0 NRBAR, NRWEL, \((V_i, \hbar\omega_i, i=1, \text{NRBAR})\) read from the internal library fisbar.dat
= 1 \(V_i, \hbar\omega_i, i=1, 2\) exp. data file in RIPL-2
= 2 \(V_i, i=1,2\) theor. data file in RIPL-2 \(\hbar\omega_i\) provided by the code
Fission in EMPIRE 2.19 beta 12

**FISDIS** = 0  No discrete transitional states, beside the fundamental  
= 1  Up to 50 rotational band heads may be included

**FISDEN** = 0  EMPIRE specific level densities which take into account deformation dependent collective enhancement  
= 1  RIPL-2 HF-BCS level densities for the inner and the outer barrier