Fission in Empire-II version 2.19 betal, Lodi;

M.Sin

Fission in EMPIRE-II
version 2.19 beta1, Lodi

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This is a description of the fission model implemented presently in EMPIRE-II in collaboration with M.Herman, A. Ventura and R. Capote.

In the compound nucleus statistical model the the fission cross section is calculated with the well-known formula:

$$\sigma_{a,f}(E) = \sum_{J\Pi} \sigma_a^{CN}(EJ\Pi) P_f(EJ\Pi). \qquad (1)$$

EMPIRE-II offers two ways to calculate the fission probability $P_f(EJ\Pi)$ selected by the parameter SUBBAR in the optional input.

- SUBBAR=0 (default option). The fission probability is calculated in the conventional way with the relation (26), where the fission coefficients are given by one of the formulae (9), (10) or (11). It is compulsory for the single barriers and for the multi-humped barriers for which no information about the well(s) is available. It is recommended for multi-humped barrier at over-barrier excitation energies or for odd-odd fissioning nuclei.

- SUBBAR=1. The fission probability is calculated with a general expression deduced in the optical model for fission which may be applied for the multi-humped barriers at any excitation energy but it requires more input parameters than SUBBAR=0. It can not be used for single barriers and it is recommended for multi-humped barriers at excitation energies under or around their heights, especially for even-even fissioning nuclei.

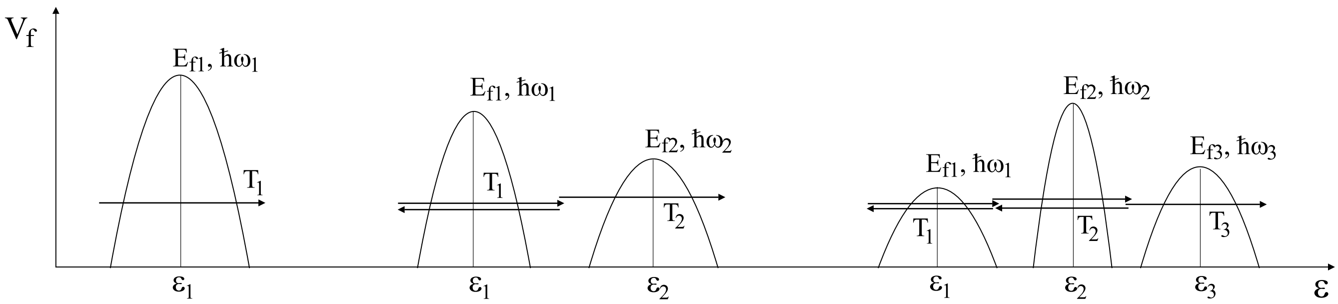

Figure 1: Transmission through two-humped fission barrier

1 Fission barriers

SUBBAR=0
The fissioning nuclides may have single-, double- or triple-humped fission barriers. The humps are considered independent (decoupled) and are usually aproximated by parabolas (Figure.1).

The fundamental fission barrier represents the lowest nuclear deformation energy as a function of an adimensional deformation parameter ε and is described by the relation:

$$V_{fi}(\varepsilon) = E_{fi} - \frac{1}{2}\mu\hbar^2\omega_i^2(\varepsilon - \varepsilon_i)^2 \tag{2}$$

where $i = 1$ for a single barrier, runs from 1 to 2 for a two-humped barrier and from 1 to 3 for a three-humped one. The energies E_{fi} represent maxima of V_i, ε_i are the corresponding abscissae, the harmonic oscillator frequencies ω_i define the curvature of each parabola and μ is the inertial mass parameter, assumed independent of ε and approximated by the semi-empirical expression:

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

where A is the mass number.
The heights E_{fi} (in MeV) and curvatures $\hbar\omega_i$ (in MeV) of the fundamental barrier are input parameters.

Above the barrier (2), which coresponds to the fundamental (ground) state, there are the transition states (fission channels) characterized by a given set of quantum numbers (energy, angular momentum J, parity π and angular momentum projection on the nuclear symmetry axis K). The excited transition states are rotational states built on vibrational or non-collective band-heads, according to the pattern:

$$E_i(J,K,\Pi) = E_{fi} + \epsilon_i(K,\Pi) + \frac{\hbar^2}{2I_i}[J(J+1) - K(K+1)] \qquad (4)$$

where: $\epsilon_i(K,\Pi)$ are the excitation energies of the band-heads, and $\hbar^2/2I$ are inertial parameters (the coupling term for $K = 1/2$ is neglected for now). To each transition state is associated a parabolic barrier with the height $E_i(J,K,\Pi)$ and the curvature $\hbar\omega_i$, equal to that of the fundamental barrier (for now).

The quantities $\epsilon_i(K,\Pi)$ and $\hbar^2/2I_i$ are input parameters.

The transition state spectra has a discrete part up to a certain energy E_{ci} above which is continous and described by level density functions $\rho_i(EJ\Pi)$.

SUBBAR=1

In this case the humps in the multi-humped fission barrier are no longer considered decoupled and the barrier is described by a set of parabolas smoothly joined (Fig.2):

$$V_i(\varepsilon) = E_{fi} + (-1)^i \frac{1}{2}\mu\hbar^2\omega_i^2(\varepsilon - \varepsilon_i)^2 \qquad (5)$$

where i runs from 1 to 3 for a two-humped barrier and from 1 to 5 for a three-humped one. In this case, the energies E_{fi} represent maxima of V_i in odd regions (humps) and minima in even regions (wells). The same is true for the barriers associated to the other discrete transition states.

In order to describe the absorption of the probability flux in the isomeric well (the well corresponding to the deformation region i=2) a complex potential $V_f(\varepsilon) = V(\varepsilon) + iW(\varepsilon)$ is usd to describe the fission process. For both double-humped and triple-humped barrier the imaginary potential is introduced in the deformation range corresponding to the isomeric well $i = 2$. A common assumption on W is that it depends quadratically on deformation, like the real part, and increases with the excitation energy:

$$W(\varepsilon) = -\alpha[E - V(\varepsilon)] \qquad (6)$$

The strength of the imaginary part of the fission potential is controlled by the input parameter α. It should be chosen to fit the width of the resonances in sub-barrier fission cross section and to be consistent with physical values for the transmission coeefficients at higher energies.

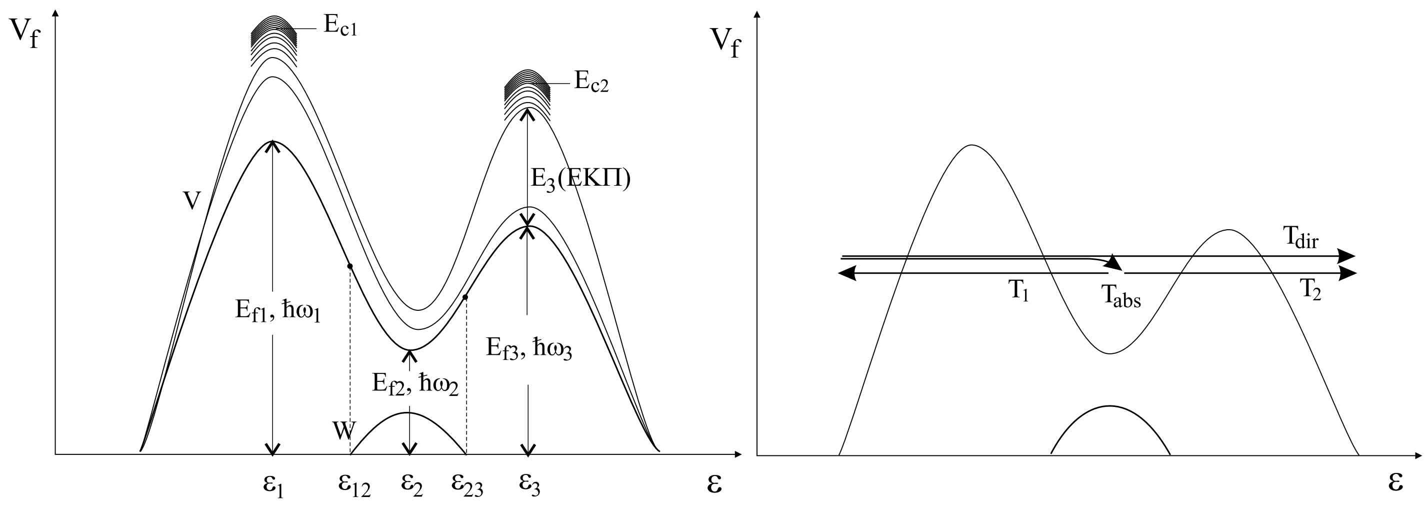

Figure 2: Transmission through two-humped fission barrier

2 Fission transmission coefficients

SUBBAR=0

The transmission coefficients through the parabolic barriers associated to the discrete transition states are calculated using Hill-Wheeler formula:

$$T_j(EKJ\Pi) = \frac{1}{1+\exp\left[-\frac{2\pi}{\hbar\omega_j}(E-E_j(EKJ\Pi))\right]}. \tag{7}$$

The total transmission coefficient is the sum of two contributions corresponding to the discrete and the continous part of the transition state spectrum:

$$T_j(EJ\Pi) = \sum_{K\leq J} T_j(EKJ\Pi) + \int_{E_{cj}}^{\infty} \frac{\rho_j(\varepsilon J\Pi)d\varepsilon}{1+\exp\left[-\frac{2\pi}{\hbar\omega_j}(E-V_j-\varepsilon)\right]} \tag{8}$$

where $j=1$ for a single barrier, runs from 1 to 2 for a two-humped barrier and from 1 to 3 for a three-humped one.

The fission coefficients for different types of barrier have the following expressions:

- single barrier:

$$T_f(EJ\Pi) = T_1(EJ\Pi) \tag{9}$$

- double barrier:

$$T_f(EJ\Pi) = \frac{T_1(EJ\Pi)T_2(EJ\Pi)}{T_1(EJ\Pi) + T_2(EJ\Pi)} \quad (10)$$

- triple barrier:

$$T_f(EJ\Pi) = \frac{T_1(EJ\Pi)T_2(EJ\Pi)T_3(EJ\Pi)}{T_1(EJ\Pi) + T_2(EJ\Pi)T_3(EJ\Pi)} \quad (11)$$

SUBBAR=1

In this case the multi-humped fission barrier is seen as a whole (the humps are not decoupled so that is no independent transmission through each of them), and the transmission can occure in two ways: directly and by reemission of the flux absorbed in the isomeric well.

The expressions for the direct transmission coefficient T_{dir} and for the coefficient of absorption in the isomeric well T_{abs} have been derived in WKB approximation for complex potential (sometimes called optical model for fission).

Fission coefficient for a two-humped barrier

$$T_{dir}(EKJ\Pi) = \frac{T_1T_2}{e^{2\delta} + 2[(1-T_1)^{1/2}(1-T_2)^{1/2}\cos(2\nu) + (1-T_1)(1-T_2)e^{-2\delta}]} \quad (12)$$

$$T_{abs}(EKJ\Pi) = T_{dir}\frac{e^{2\delta} - (1-T_2)e^{-2\delta} - T_2}{T_2} \quad (13)$$

$$T_1 = T_1(EKJ\Pi), \qquad T_2 = T_2(EKJ\Pi)$$

where ν is the momentum integral across the intermediate well for the real potential V and δ is the momentum integral for the imaginary negative potential W which causes the absorption of probability flux in the intermediate well:

$$\nu = \int_{\varepsilon_{12}}^{\varepsilon_{23}} K(\varepsilon)d\varepsilon, \qquad K(\varepsilon) = (2\mu[E - V(\varepsilon)]/\hbar^2)^{1/2} \quad (14)$$

$$\delta = -\left(\frac{\mu}{2}\right)^{1/2}\int_{\varepsilon_{12}}^{\varepsilon_{23}} \frac{W(\varepsilon)}{[E-W(\varepsilon)]^{1/2}}d\varepsilon = \alpha\left(\frac{\mu}{2}\right)^{1/2}\int_{\varepsilon_{12}}^{\varepsilon_{23}}[E-W(\varepsilon)]^{1/2}d\varepsilon \quad (15)$$

We notice the presence of the periodical function 'cos(ν)' in (12) and (13) which introduces the resonant character of these coefficients. When the strength of the imaginary potential increases, the momentum integral δ increseas also and from (12)-(13) results $T_{dir} \to 0$, $T_{abs} \to T_1$. Consequently, the direct fission appears only for sub-barrier excitation energies and occures only through discrete channels:

$$T_{dir}(EJ\Pi) = \sum_{K \leq J} T_{dir}(EKJ\Pi) \tag{16}$$

while the absorption in the isomeric well occurs through all fission channels. In full K-mixing approximation all the discrete channels with the same $J\Pi$ contribute irrespective to their K value to the total absorption coefficient. The continuum fission channels contribute at higher energies where the class II states are completely damped, the direct fission disappeares and the entire flux transmitted through the inner barrier is absorbed in the isomeric well:

$$T_{abs}(EJ\Pi) = \sum_{K \leq J} T_{abs}(EKJ\Pi) + \int_{E_{cj}}^{\infty} \frac{\rho_j(\varepsilon J\Pi) d\varepsilon}{1 + \exp\left[-\frac{2\pi}{\hbar\omega_1}(E - V_1 - \varepsilon)\right]}. \tag{17}$$

The total fission coefficient for a two-humped barrier is:

$$T_f(EJ\Pi) = T_{dir}(EJ\Pi) + T_{abs}(EJ\Pi) \frac{T_2(EJ\Pi)}{T_1(EJ\Pi) + T_2(EJ\Pi)} \tag{18}$$

Fission coefficient for a triple-humped barrier

The fission coefficient for the triple-humped barrier is derived considering the particular features of the barriers exhibited by Thorium isotopes: a shallow second (or third if the first corresponds to equilibrium deformation) well in which there is no damping of the vibrational states, no absorption, no imaginary potential (see Fig.3).

The relations for the transmission coefficients derived in WKB approximation are :

$$T_{dir}(EKJ\Pi) = \frac{T_1 T_2 T_3}{A_T + B_T \cos(2(\nu_1 - \nu_2)) + C_T \cos(2(\nu_1 + \nu_2)) + D_T \cos(2\nu_1) + E_T \cos(2\nu_2)}$$

where:

$$\begin{aligned}
A_T &= e^{-2\delta_1}(1 - T_1)(1 - T_2) + e^{2\delta_1}(1 - T_2)(1 - T_3) + e^{-2\delta_1}(1 - T_1)(1 - T_3) + e^{2\delta_1} \\
B_T &= 2(1 - T_1)^{1/2}(1 - T_2)(1 - T_3)^{1/2} \\
C_T &= 2(1 - T_1)^{1/2}(1 - T_3)^{1/2} \\
D_T &= 2(1 - T_1)^{1/2}(1 - T_2)^{1/2}(2 - T_3) \\
E_T &= 2(1 - T_2)^{1/2}(1 - T_3)^{1/2}\left[e^{-2\delta_1}(1 - T_1) + e^{2\delta_1}\right]
\end{aligned} \tag{20}$$

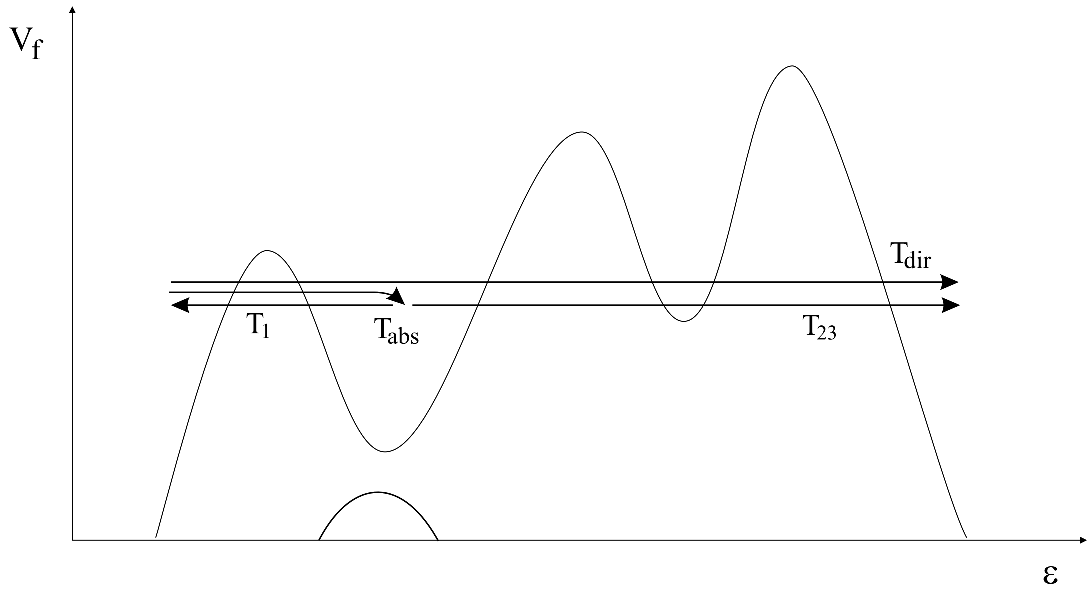

Figure 3: Transmission through three-humped fission barrier

$$T_1 = T_1(EKJ\Pi), \quad T_2 = T_2(EKJ\Pi), \quad T_3 = T_3(EKJ\Pi).$$

and ν_1, ν_2 are the momentum integrals for the two wells of the real potential, while δ_1 the momentum integral for the imaginary potential introduced in the deformation range corresponding to the first well.

$$T_{abs} = 1- \tag{21}$$

$$\frac{T_1T_2T_3 + A_R + B_R\cos(2(\nu_1-\nu_2)) + C_R\cos(2(\nu_1+\nu_2)) + D_R\cos(2\nu_1) + E_R\cos(2\nu_2)}{A_T + B_T\cos(2(\nu_1-\nu_2)) + C_T\cos(2(\nu_1+\nu_2)) + D_T\cos(2\nu_1) + E_T\cos(2\nu_2)}$$

where:

$$\begin{aligned} A_R &= e^{-2\delta_1}(2-T_2-T_3) + e^{2\delta_1}(1-T_1)[(1-T_2)(1-T_3)+1] \\ B_R &= 2(1-T_1)^{1/2}(1-T_2)(1-T_3)^{1/2} \\ C_R &= 2(1-T_1)^{1/2}(1-T_3)^{1/2} \\ D_R &= 2(1-T_1)^{1/2}(1-T_2)^{1/2}(2-T_3) \\ E_R &= 2(1-T_2)^{1/2}(1-T_3)^{1/2}\left[e^{-2\delta_1} + e^{2\delta_1}(1-T_1)\right] \end{aligned} \tag{22}$$

The total fission coefficient is:

$$T_f(EJ\Pi) = T_{dir}(EJ\Pi) + T_{abs}(EJ\Pi)\frac{T_{23}(EJ\Pi)}{T_1 + T_{23}(EJ\Pi)} \tag{23}$$

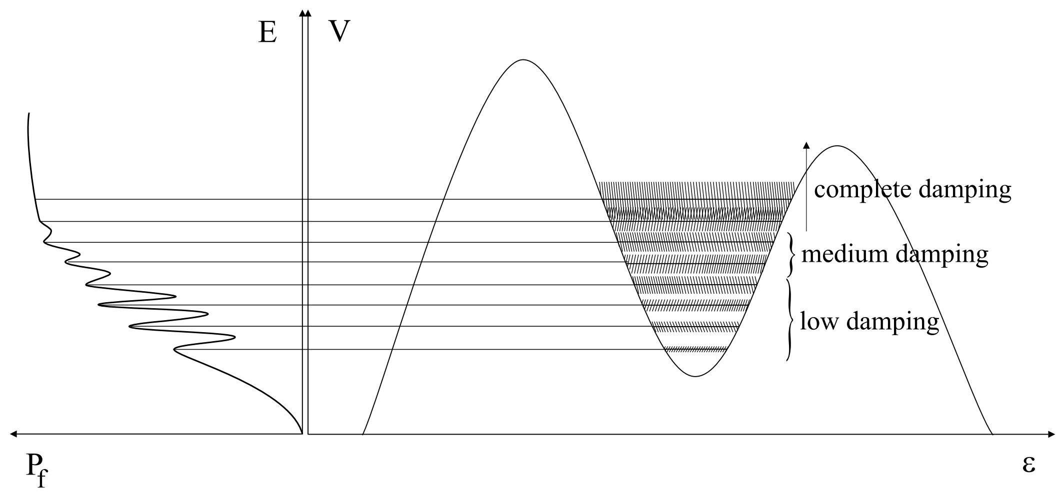

Figure 4: The effect of the vibrational damping

where $T_{dir}(EJ\Pi)$ and $T_{abs}(EJ\Pi)$ are calculated according to (16) and (17) and $T_{23}(EJ\Pi)$ reffers to the direct transmission through the second and third humps:

$$T_{23}(EKJ\Pi) = \frac{T_2 T_3}{1 + 2[(1-T_2)^{1/2}(1-T_3)^{1/2}\cos(2\nu_2) + (1-T_2)(1-T_3)]} \quad (24)$$

$$T_{23}(EJ\Pi) = \sum_{K \le J} T_{23}(EKJ\Pi). \quad (25)$$

The fission coefficients are calculated in SUB FISfis in 'HF-comp.f'.

3 Fission cross section

SUBBAR=0 The fission probability is calculated as the branching ratio:

$$P_f(EJ\Pi) = \frac{T_f(EJ\Pi)}{T_{part}(EJ\Pi) + T_\gamma(EJ\Pi) + T_f(EJ\Pi)} \quad (26)$$

SUBBAR=1 The fission probability is calculated in this case with a general expression deduced in the optical model for fission, which may be applied from deep sub-barrier up to over-barrier excitation energies. This general expression becomes simpler when the excitation energy increases and the vibrational states in the isomeric well get more damped (see Fig.4).

The relations specific to different degrees of damping are presented below. For the sake of simplicity the dependence of all quantities on $EJ\Pi$ will be not written explicitly.

- **Low damping**.

$$P_f = \frac{T_{dir}}{T_{dir} + T_{part} + T_\gamma} + \frac{T_{part} + T_\gamma}{T_{dir} + T_{part} + T_\gamma} \cdot \frac{1}{a} \tag{27}$$

where:

$$a = \left[1 + b^2 + 2b \coth\left(\frac{T_1 + T_{2(3)}}{2}\right)\right]^{1/2}, \tag{28}$$

$$b = \frac{(T_{dir} + T_{part} + T_\gamma)(T_1 + T_{2(3)})}{T_{abs} T_{2(3)}}. \tag{29}$$

$T_{2(3)}$ means T_2 for a two-humped barrier and T_{23} for a three-humped barrier.
The resonant character of T_{dir} and T_{abs} is reflected in the resonant character of the fission cross section specific for even-even fissioning nuclei at sub-barrier excitation energies.
The flux conservation ($P_f + \sum_j P_j = 1$) requires the following modification for the competitive decay probabilities:

$$P_j = \frac{T_j}{T_{dir} + T_{part} + T_\gamma}\left(1 - \frac{1}{a}\right) \qquad j = part,\ \gamma. \tag{30}$$

- **Medium damping** When the damping of the vibrational states in the isomeric well increases, the entire flux transmitted through the inner barrier is practically absorbed in the isomeric well and $T_{dir} \to 0$, $T_{abs} \to T_1$. The relations (27), (30) and (29) become:

$$P_f = \frac{1}{a} \tag{31}$$

$$P_j = \frac{T_j}{T_{part} + T_\gamma}\left(1 - \frac{1}{a}\right) \qquad j = part,\ \gamma \tag{32}$$

$$b = \frac{(T_{part} + T_\gamma)(T_1 + T_{2(3)})}{T_1 T_{2(3)}} = \frac{(T_{part} + T_\gamma)}{T_f} \tag{33}$$

The resonant structure of the fission cross section is lost.

- **Complete damping** When the vibrational states in the isomeric well are completely damped, their decay widths exceed significantly the distances between them. This means $\coth((T_1 + T_{2(3)})/2) \to 1$ and $a = 1 + b$. The previous relations for the decay probabilities become the well-known:

$$P_f = \frac{1}{a} = \frac{1}{1+b} = \frac{T_f}{T_f + T_{part} + T_\gamma} \tag{34}$$

$$P_j = \frac{T_j}{T_{part} + T_\gamma}\left(1 - \frac{1}{a}\right) = \frac{T_j}{T_f + T_{part} + T_\gamma} \qquad j = part,\ \gamma. \tag{35}$$

The fission cross sections are calculated together with the rest of compound nucleus cross section in 'main.f'.

4 Fission files

Beside SUBBAR there are other three parameters entering the optional input (FISBAR, FISDIS, FISDEN) whose values indicate the files the input data can be taken from.

Taking into acount the values of the parameters in the optional input, EMPIRE creates automatically (in SUB INPFIS in 'input.f') an input file FISSION.INP at the first run, which can be modified by the user editing it and used for the following runs if the command CLEAN is not used.

FISSION.INP contains data about all the fissioning nuclei involved in the studied reaction. Depending on SUBBAR, FISBAR, FISDIS, FISDEN values, these data are:

1. Fundamental fission barrier parameters:

    - SUBBAR=0
      - NRBAR=number of humps
      - heights E_{fi} $\leftrightarrow$ EFB(1,NRBAR)
      - curvatures $\hbar\omega_i$ $\leftrightarrow$ H(1,NRBAR)
      - inertial parameters $\hbar^2/2I_i$ $\leftrightarrow$ HJ(1,NRBAR)

- FISBAR=0 (default): NRBAR, EFB(1,NRBAR) are taken from Ripl-2, H(1,NRBAR) are provided by the code accordingly to Lynn's systematics.
- FISBAR=1: NRBAR, EFB(1,NRBAR), H(1,NRBAR) are read from the experimental data file in RIPL-1 (should we keep it?)
- FISBAR=2: NRBAR, EFB(1,NRBAR), H(1,NRBAR) are read from the internal fission barrier library 'barfis.fnd'.

- SUBBAR=1
  In this case NRBAR=number of parabolas and beside the parameters of the real potential the factor α must be provided. For the moment, it has a constant value and is included in 'barfis.fnd', but it should depend on energy, probably quadratically; default energy dependence coefficients should be provided by the code and introduced in FISSION.INP.
  - FISBAR=2 is the only choice.

In all cases the inertial parameters are provided by the code (for now).

2. Discrete transition states

   - NRFDIS(1,NRBAR)=number of discrete transition states

   - excitation energies ϵ_i $\leftrightarrow$ EFDIS(1,NRFDIS; 1,NRBAR)

   - spin projections K_i $\leftrightarrow$ SFDIS(1,NRFDIS; 1,NRBAR)

   - parities Π_i $\leftrightarrow$ IPFDIS(1,NRFDIS; 1,NRBAR).
   If SUBBAR=0, NRFDIS(1,NRBAR) can differ from one hump to the other, but if SUBBAR=1, it must be the same for all parabolas (humps or wells).

   - FISDIS=0 (default) - NRFDIS=1; EFDIS=0; $K\Pi$ are those of the ground state;
   - FISDIS=1 - NRFDIS>1 provided by the code only to help the user editing them, they have no physical values.

3. Level densities at the saddle points

- FISDEN=0 - (default) level densities at the saddle points taken from Ripl-2; a normalization factor, maybe energy dependent, should be added;
- FISDEN=1 - specific Empire level densities adapted for saddle points (not ready yet);
- FISDEN=2 - ”constant-temperature” (will be introduced very soon).
- FISDEN=3 - Maslov level density (will be introduced).

The input parameters and the main results are written in the output file FISSION.OUT.

Relevant references

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