FIESTA 2014
Fission School Lectures

FISSION CROSS SECTION THEORY

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Lecture 1 Topics

- Liquid drop Model
- Quantum and nuclear structure modifications
- Cross-sections and neutron resonances
- Formal cross-section theory
- Difficulties in liquid drop based model
- Nuclear shell effects in deformation energy landscape

Discovery of Fission and Theory

- Hahn and Strassmann established barium as one of the elements produced in absorption of slow neutrons by uranium (*Naturwissenschaften,* **27** (1939)
- Meitner and Frisch interpreted this as the splitting of the compound nucleus into 2 almost equal parts and deduced that this was due to the heavy nucleus behaving like an electrically charged liquid drop (*Nature,* **143** 1939)
- Essential theory of Liquid Drop model developed by N. Bohr and J.A. Wheeler (*Phys.Rev.* **56** 1939)

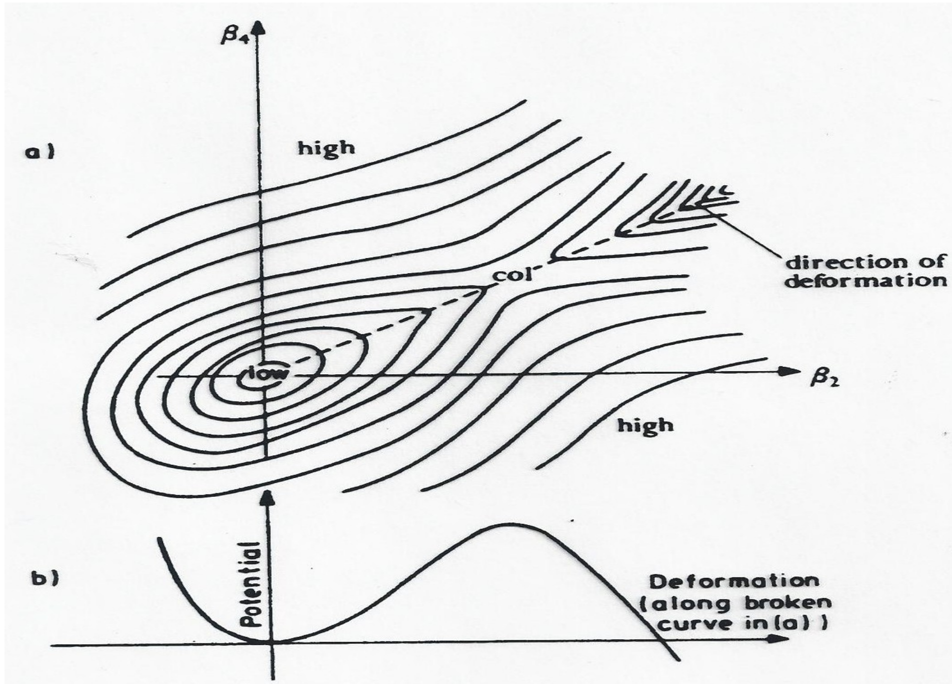
Binding energy *v.* Mass Number

- Bethe- Weizsacker semi-empirical mass formula:

$$E = -c_1 A + c_2 A^{2/3} + c_3 Z^2 / A^{1/3} + c_4 (N - Z)^2 / A \pm \delta$$

- $\downarrow$ $\downarrow$ $\downarrow$ $\downarrow$ $\downarrow$
- volume surface Coulomb isospin pairing
- (energy of classical charged liquid drop)
- For liquid drop model of fission the surface and Coulomb terms are given their classical dependence on drop shape (deformation)

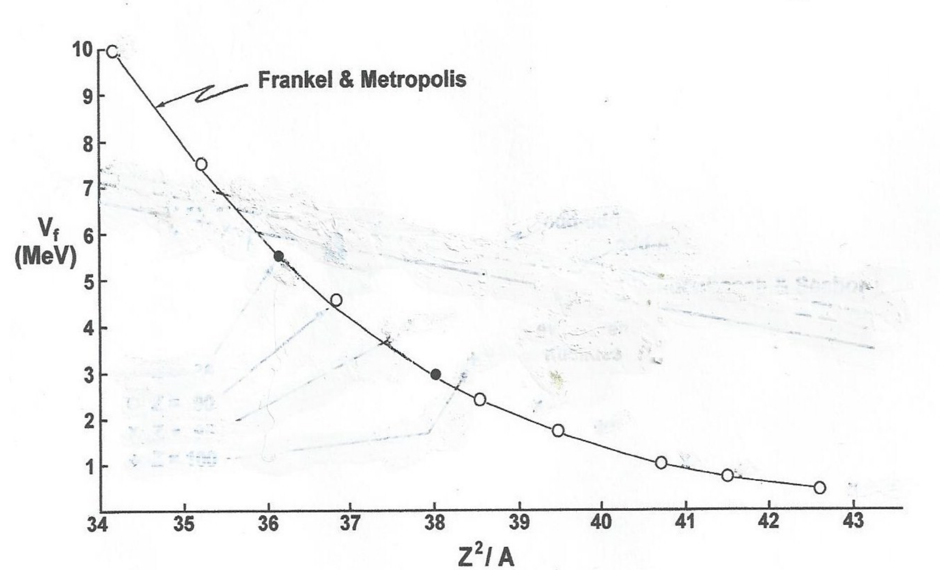
Energy of charged liquid drop as function of deformation



- Schematic diagram of contours of p**otential energy of a charged liquid drop** as a function of its two principal deformation parameters (above).
- The broken line is the path of minimum energy as the drop elongates.
- The potential energy along this path towards rupture into two equal parts (scission) is shown below the contour chart.
- Key parameter deciding barrier height is the fissility parameter Z^2 / A

Fission barriers in the Liquid Drop model

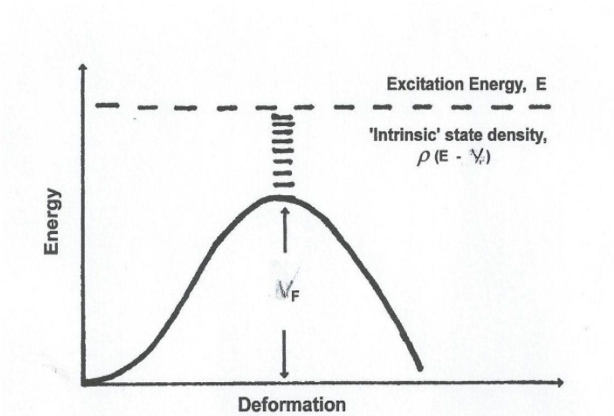
Frankel and Metropolis (1947) made calculations of barrier heights as a function of the fissility parameter Z^2/A



Note: experimental data on barrier heights for Z^2/A from 35-39 are in range 6.5 to 5.5 MeV

Fission reaction rate theory in Liquid Drop model

- Classical model :
  Transmission coefficient $T_F = 1$ if $E > V_F$, otherwise zero.
- Nuclear model:
- Bohr and Wheeler (1939) - many different possible states of intrinsic excitation as nucleus passes over barrier.



The transmission coefficient is

$$T_F = N = \int_{V_F}^{E} dE' \rho(E' - V_F) = \frac{2\pi\Gamma_F}{D}$$

Fission reaction rate theory contd.

- **The transmission coefficient** T_f can be used directly in Hauser-Feshbach theory in conjunction with the transmission coefficients for all the other channels for decay of the excited compound nucleus:

$$\sigma_F = \pi \mathrm{D}^2 \sum_{J,\pi} \frac{T_n^{J\pi} T_F^{J\pi}}{T_{tot}^{J\pi}}$$

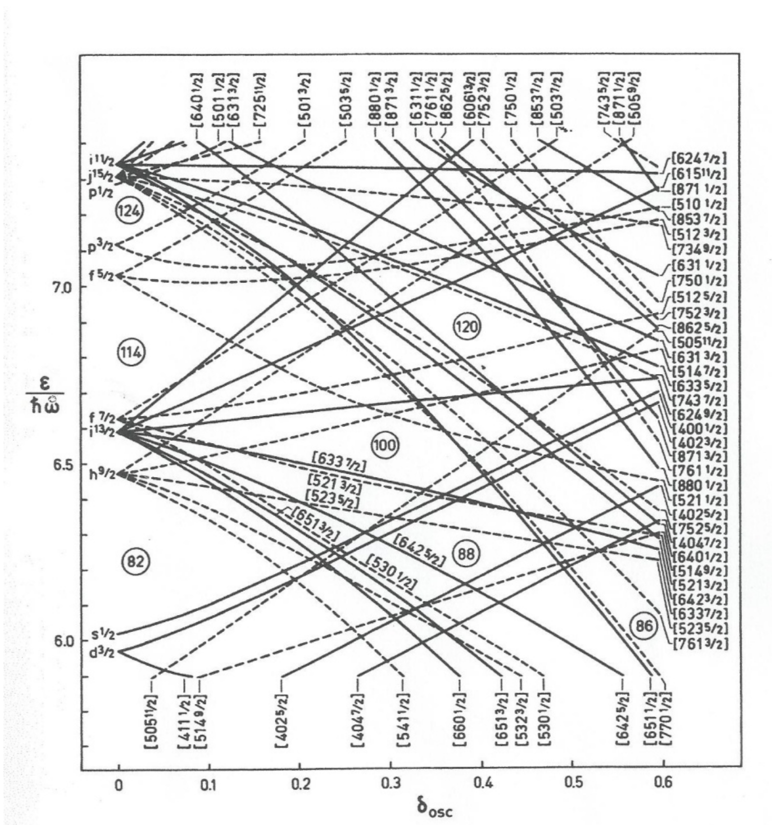
- **Quantal tunnelling of the barrier.** The classical step function form is replaced by a penetration factor. This depends on the potential energy variation with deformation and the inertial tensor (which can also be deformation dependent). **Hill-Wheeler formula** (1953) for barrier with inverted harmonic oscillator form and constant inertial tensor:

$$T = \frac{1}{1 + \exp[-2\pi(E - E') / \mathrm{h}\omega]}$$

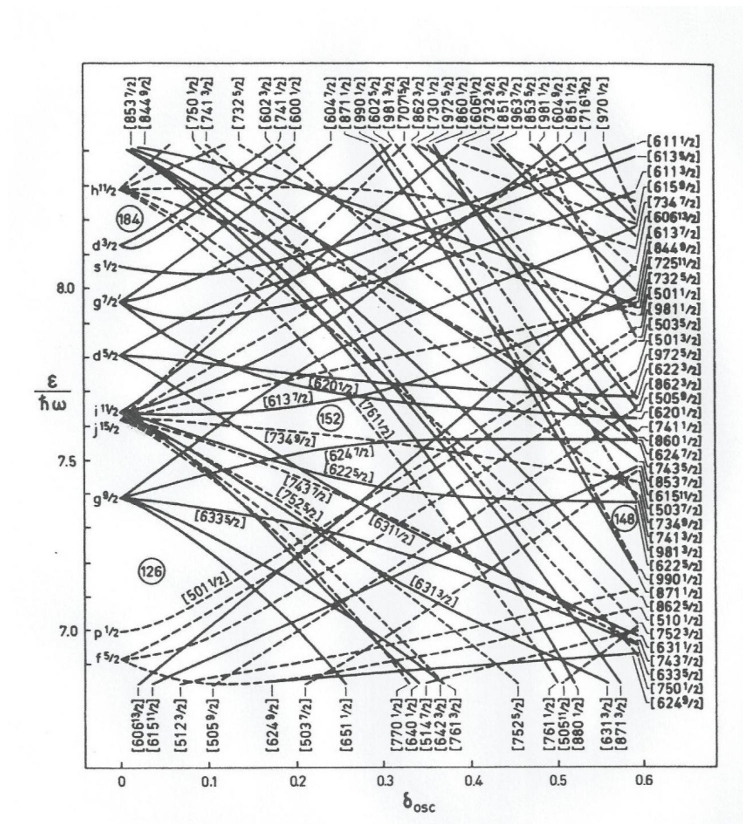
Effects of angular momentum and parity on Barrier:

Nilsson single particle level energies as function of deformation

Protons

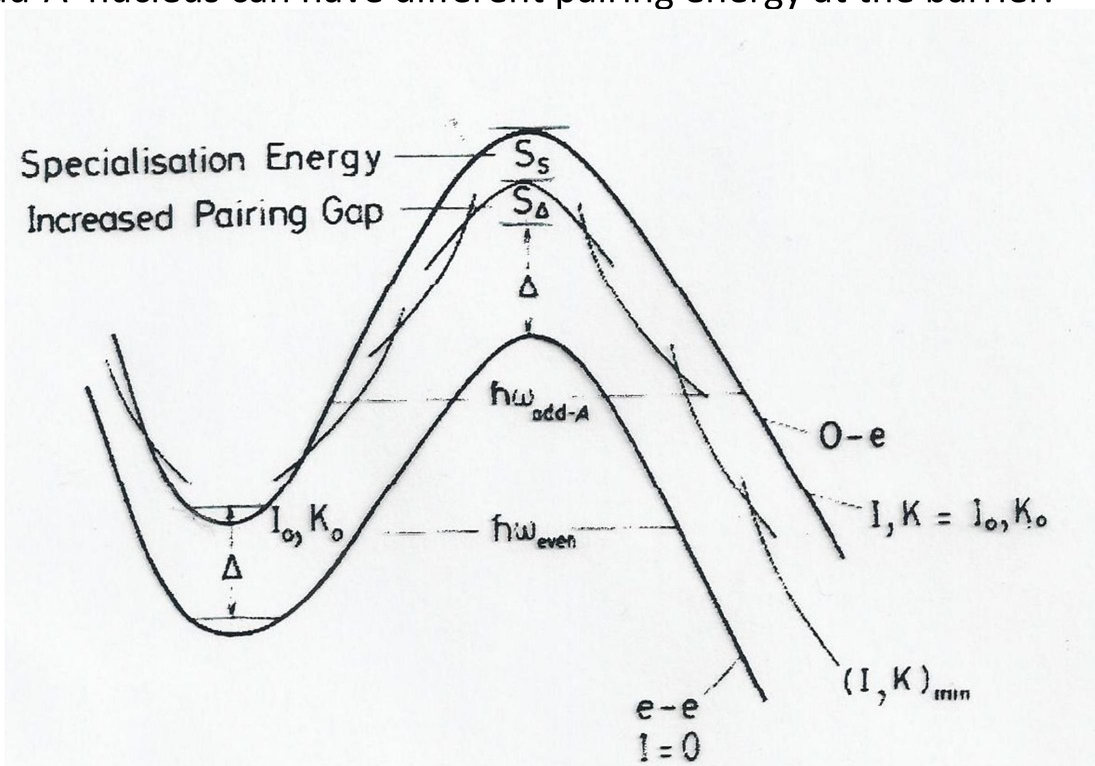


Neutrons



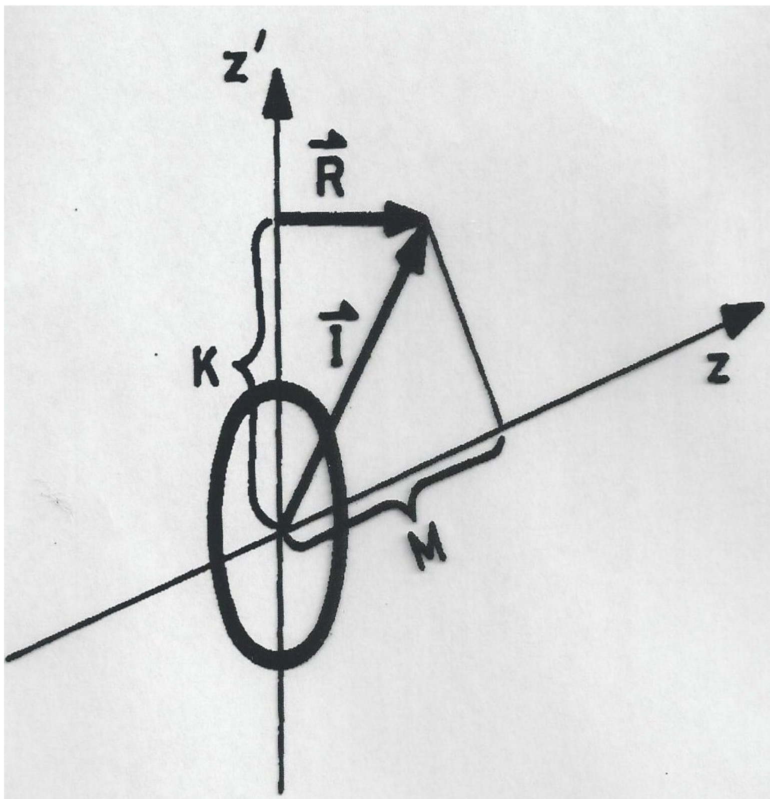
Effects of angular momentum & parity; specialization energy and deformation dependent pairing energy

- Ground state (I^{π} , K) has e-e energy plus $e(i,qp)$
- Lowest q-p state at greater deformation has different q-p quantum numbers
- $\therefore$ State with same (I^{π} , K) as ground rises above minimum energy envelope .
- This increase in energy is known as specialization energy
- Likewise, an odd-A nucleus can have different pairing energy at the barrier.

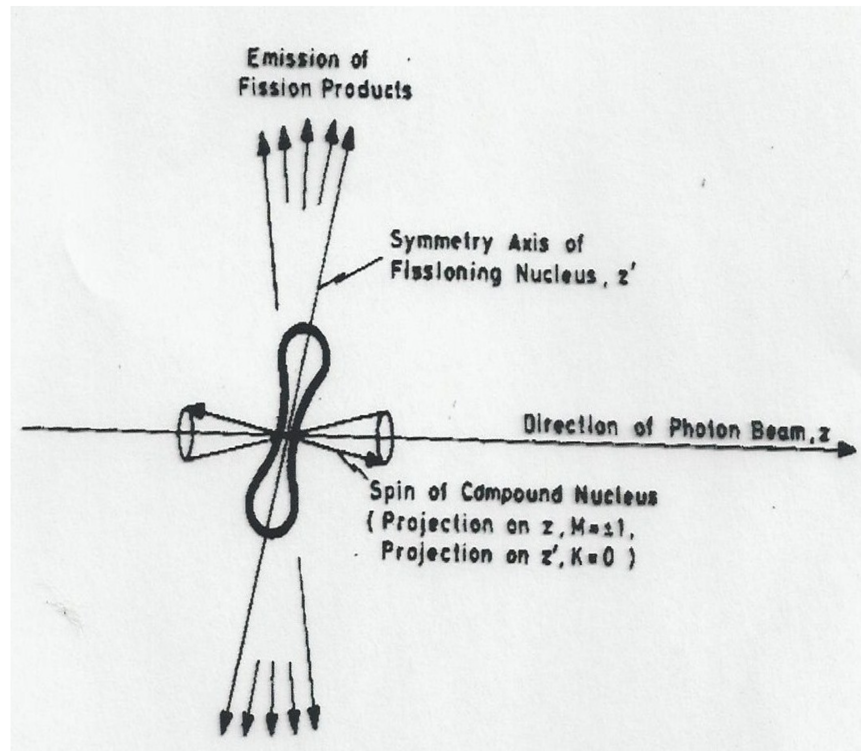


Concept of Individual Transition States & Effect on Fission Product Characteristics

- The *K* quantum number at the barrier*:* Projection of spin on axis of cylindrically symmetric nucleus couples with rotation *R* to give *I*



- How angular relations of *K,R,I* and *M* may determine angular distribution of fission products. Example is for *K*=0 e-e nucleus and *E*1 photofission



Aage Bohr Transition States

- Extended from Wheeler; largely speculative

Approximate features on the energy scale (origin is the fission threshold)	Approximate energy of transition state (in MeV)	Transition state quantum numbers K^{π}	Transition state quantum numbers I^{π}	Description of transition state
0·0 MeV (fission threshold) →	0·0	0^+	0^+ 2^+ 4^+, etc.	'Ground'
	~0·5	0^-	1^- 3^- 5^-, etc.	1 quantum of mass asymmetry vibration
$\approx E_{th,n}$ for ^{242}Pu →	~0·7	2^+	2^+ 3^+ 4^+ etc.,	1 quantum of gamma vibration
	~0·9	1^-	1^- 2^- 3^-, etc.	1 quantum of bending vibration
1·0 MeV →				

- Transition states above 1 MeV

$\approx E_{th,n}$ for ^{236}U →	~1·2	2^-	2^- 3^- 4^-, etc.	1 quantum of mass asymmetry vibration combined with 1 quantum of gamma vibration
$\approx E_{th,n}$ for ^{234}U → $\approx E_{th,n}$ for ^{240}Pu →	~1·4	1^+	1^+ 2^+ 3^+, etc.	1 quantum of mass asymmetry vibration combined with 1 quantum of bending vibration
→ (Top of energy gap according to Strutinsky 1965)	~1·6	0^+ 4^+	0^+ 2^+, etc. 4^+ 5^+, etc.	2 quanta of gamma vibration
	~1·7	1^- 3^-	1^- 2^-, etc. 3^- 4^-, etc.	1 quantum of gamma vibration combined with 1 quantum of bending vibration
2·0 MeV → (Top of energy gap at saddle point according to Griffin 1963) →				

Features of Neutron Resonances

- Resonances in low energy neutron cross-sections are the manifestation of the virtual states of the excited compound nucleus, through which it decays.
- Resonances not generally observed at higher energies (lack of resolution).
- Are essential feature and basis of theory of nuclear cross-sections up to several MeV excitation energy.
- Form of isolated resonance at energy E_λ (Breit-Wigner formula):

$$\sigma_{ab} = \frac{\pi \mathrm{D}^2 \Gamma_{\lambda a} \Gamma_{\lambda b}}{(E - E_\lambda)^2 + \Gamma_\lambda{}^2 / 4}$$

- A channel width can be factorized into a reduced width and penetration factor: $\Gamma_{\lambda c} = 2P_c \gamma_{\lambda c}^2$
- The integrated cross-section across the resonance is

$$\left\langle \sigma_{ab} \right\rangle D = \pi \mathrm{D}^2 (2\pi \Gamma_{\lambda a} \Gamma_{\lambda b} / \Gamma_\lambda)$$

Features of resonances contd.

- For capture cross-sections the exit channel width $\Gamma_{\lambda b}$ is replaced by the total radiation width $\Gamma_{\lambda\gamma}$
- Neutron widths $\Gamma_{\lambda n}$ fluctuate greatly from resonance to resonance. The fluctuation is in the reduced width component.
- The distribution of the reduced widths has the Porter-Thomas form:

$$P(\gamma_n{}^2)d\gamma_n^2 = \frac{1}{\sqrt{2\pi\left\langle\gamma_n^2\right\rangle\gamma_n^2}}\exp\left(-\frac{\gamma_n{}^2}{2\left\langle\gamma_n^2\right\rangle}\right)d\gamma_n^2$$

- Total radiation widths are the sum of the partial radiation widths for very many primary transitions. If these are mostly uncorrelated (as expected) the total radiation width should fluctuate very little from resonance to resonance.
- The fission width is also the sum of very many partial widths for different fission product pairs in many different states of excitation and angular momentum combinations . It is therefore expected to be constant from resonance to resonance.
- This is at variance with the wide fluctuation observed experimentally. This is explained by the A. Bohr concept of transition state or barrier channel; the many fission pair channel widths are correlated to the few open barrier channel widths.

Average cross-sections: Hauser-Feshbach theory

- The integrated cross-section over a Breit-Wigner resonance is divided by the level spacing *D* to obtain the local average cross-section:

$$\langle \sigma_{ab} \rangle = \pi \mathrm{D}^2 T_a T_b / T$$

where the transmission factors *are*:

$$T_c = 2\pi \langle \Gamma_c \rangle / \langle D \rangle$$

and $T = \sum_c T_c$. With full account of target spin *I,* projectile spin *s,* orbital angular momentum, l , coupled to total angular momentum *J,* the full Hauser-Feshbach expression is

$$\sigma_{ab} = \pi \mathrm{D}^2 \sum_J \frac{(2J+1)}{(2i+1)(2I+1)} \sum_{s,s'=|I-i|}^{I+i} \sum_{\mathrm{l}=|J-s|}^{J+s} \sum_{\mathrm{l}'=|J-s'|}^{J+s'} \frac{T_{a(\mathrm{l}s)}{}^J T_{b(\mathrm{l}'s')}{}^J}{T^J}$$

Formal cross-section theory; R-matrix theory

- To understand properly the effect of CN levels on the cross-sections we need a formal microscopic theory of nuclear reactions. There are several approaches to this. Here, we adopt the R-matrix theory (Wigner and Eisenbud).
- OUTLINE
- Wave function for plane wave travelling with velocity *v*:

$$\exp(ikz) : \sum_{l=0}^{\infty} (2l+1)^{1/2} i^{l} [I_{l}(kr) - O_{l}(kr)] Y_{l0}(\theta, \varphi)$$

plane wave in *z* dirn. expansion in polar co-or. system

k (= $1/D$) is wave no. of neutron-target system, Y_{lm} are spherical harmonics.

For neutrons, asymptotic forms of incoming, outgoing waves at large distances r are

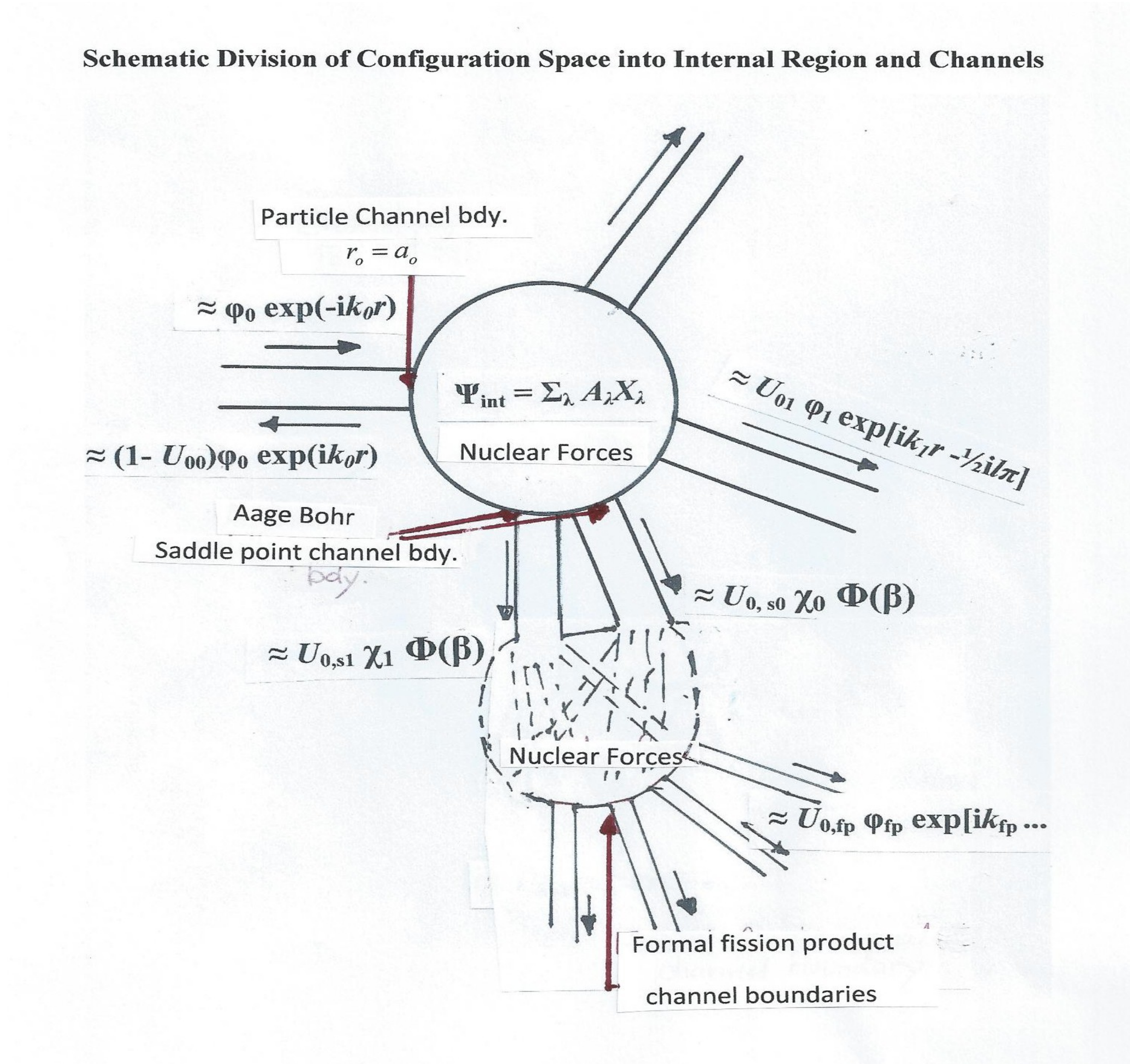
$$I_{l} = \exp[-ikr + (1/2) i l \pi] \qquad O_{l} \approx \exp[ikr - (1/2) i^{l} l \pi]$$

Nuclear forces in compound system of target +neutron change amplitudes of outgoing waves and produce outgoing waves of different kinds.

Amplitudes of outgoing waves in this system are denoted by collision matrix element

$$U_{cc'}$$

Internal region and channels in nuclear configuration space



Wavefunctions in regions of configuration space

- Nuclear forces in Internal Region cause outgoing waves in other channels *c′.* <u>Amplitudes</u> denoted by collision matrix elements $U_{cc'}$, (*c* for entrance).

- External region wavefunction :

$$\Psi_{ext} : \mathscr{I}_c - \sum_{c'} U_{cc'} \mathscr{O}_{c'}$$

  I and **O** are incoming and outgoing wave functions generalized to specific channels by incorporating intrinsic excitation and angular momentum couplings

- The cross-section is

$$\sigma_{cc'} = \left| \left\langle \Psi_{ext} - \Psi_{plane} \,|\, c' \right\rangle \right|^2$$

Internal region wavefunction

- Wave function for Internal Region

$$\Psi_{\mathrm{int}} = \sum_{\lambda} A_{\lambda} X_{\lambda}$$

- Evaluation of the collision matrix is made by matching logarithmic derivatives of wavefunction of internal region to those of outgoing wavefunctions in channels
- Collision matrix is

$$\mathbf{U} : \ \boldsymbol{\Omega}\mathbf{P}^{1/2}\{\mathbf{1} - \mathbf{iPR}\}^{-1}\{\mathbf{1} + \mathbf{iPR}\}\mathbf{P}^{-1/2}\boldsymbol{\Omega}$$

- The R-matrix is the central quantity here:

Form of the R-matrix and the single-level approximation

- The R-matrix element for entrance channel *c*, exit channel c' is

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

Single-level Breit-Wigner formula:

One level λ retained in the sum: inversion of $(\mathbf{1\text{-}RL})^{-1}$ is exact

$$\sigma_{cc'} = \pi \text{Ɖ}^2 g(J) \frac{\sum_{sl} \Gamma_{\lambda c(sl)} \sum_{s'l'} \Gamma_{\lambda c'(s'l')}}{(E_{\lambda} - \Delta_{\lambda} - E)^2 + (1/4)\Gamma_{\lambda}^2}$$

- $\Delta_{\lambda} = \sum_{c''} (S_{c''} - B_{c''})\gamma_{\lambda c''}^2$ is the level shift

$\Gamma_{\lambda c''} = 2P_{c''}\gamma_{\lambda c''}^2$ are the partial widths and the total width is $\Gamma_{\lambda} = \sum_{c''} \Gamma_{\lambda c''}$

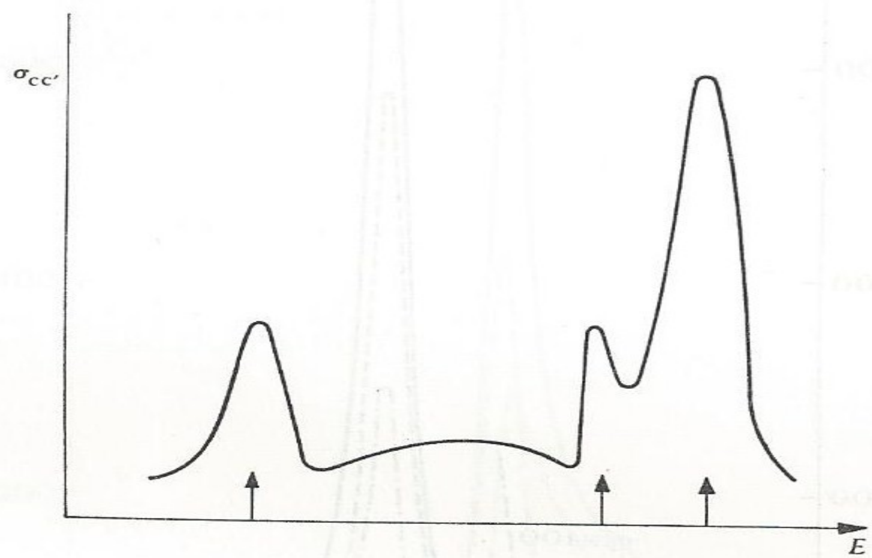
Note factorization of partial widths into nuclear component $\gamma_{\lambda c''}^2$ and a channel component, the penetration factor, which contains the effect of potential variations in the channel region e.g., for fission, the Hill-Wheeler factor.

Reduced R-matrix approx.: Reich-Moore application

- Useful for limited number of explicit channels. Eliminated channels must have small partial widths and be uncorrelated. Reduced R-matrix:

$$\mathscr{R}_{cc'} \;;\; \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_{\lambda} - E - \frac{1}{2} i\Gamma^{e}_{\lambda}}$$

- Reich and Moore : radiation channels are all eliminated, thus identifying Γ^{e}_{λ} as the total radiation width $\Gamma_{\lambda\gamma}$: viable for treatment of fission using Aage Bohr saddle-point channel concept.
- Example of 2-channel reaction with 3 levels included. Note some asymmetry in resonance shapes and marked interference between the individual level terms.



Reduced neutron widths

- **Possible expansion of Internal Eigenstates**

$$\mathbf{X}_\lambda = \Sigma_{cp}\, C_{\lambda,cp}\, \varphi_c\, u_p(r_c)$$

where ϕ_c is state of internal excitation and u_p is state of single neutron motion in field of residual nucleus (with wave number *K*).

Incident neutron channel is

$$\varphi_0 u_q(r_0)$$

Value at channel radius $r_0 = a_0$ is the reduced neutron width amplitude:

$$\gamma_{\lambda,0q} \sim C_{\lambda,0q}\, u_q(a_0)$$

- For high density of states (CN states) expectation value of $C_{\lambda,0q}^2 \sim D_\lambda / D_{sp}$

- Reduced neutron width of single particle state is $\hbar^2 / Ma^2$. Hence for strong mixing

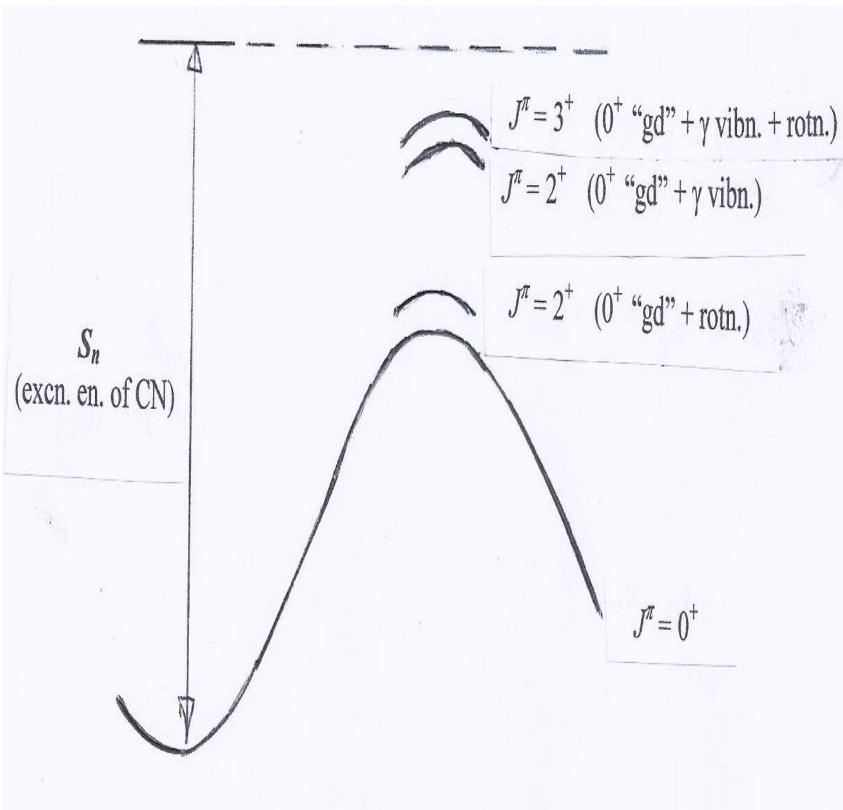
$$\left\langle \gamma_{\lambda n}^2 \right\rangle = \left(\hbar^2 / Ma^2 \right)\left((D / D_{sp} \right) = \left(D / \pi K a_0 \right)$$

Ratio $< \gamma_{\lambda n}^2 > / D_\lambda$ is <u>neutron strength function,</u> usually given in form (for s-waves)

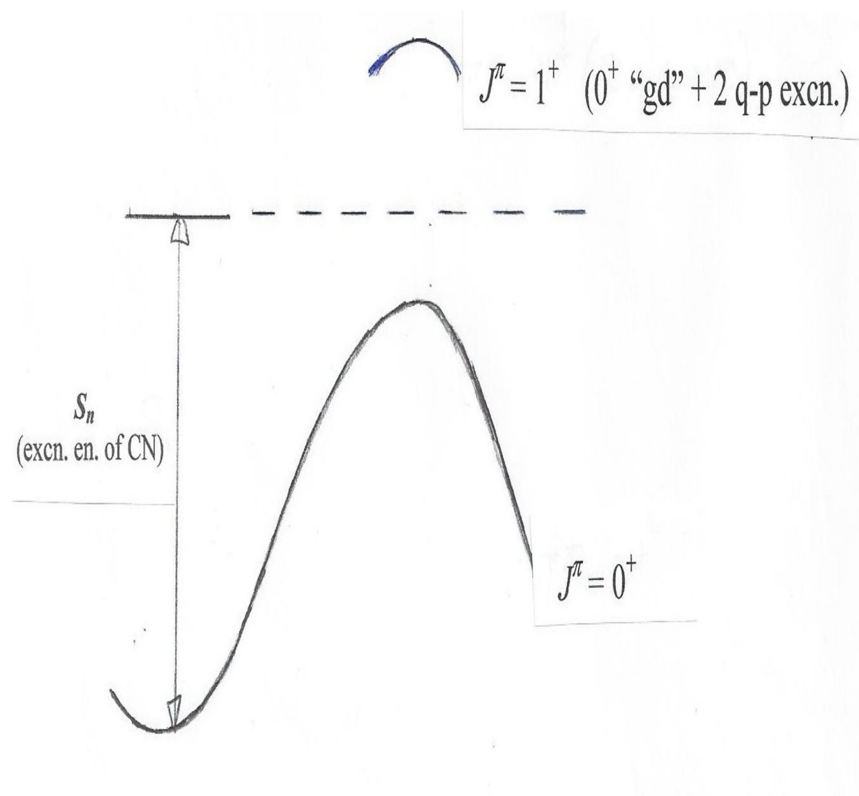
$$\Gamma_n^0 / D = 2P(1eV)\gamma_n^2 / D = 2k(1eV)a_0\gamma_n^2 / D$$

Fission widths and strength functions: Effect of target spin on fission strength

^{233}U : $I^{\pi} = 5/2^{+}$ CN : $J^{\pi} = 2^{+}$ and 3^{+}

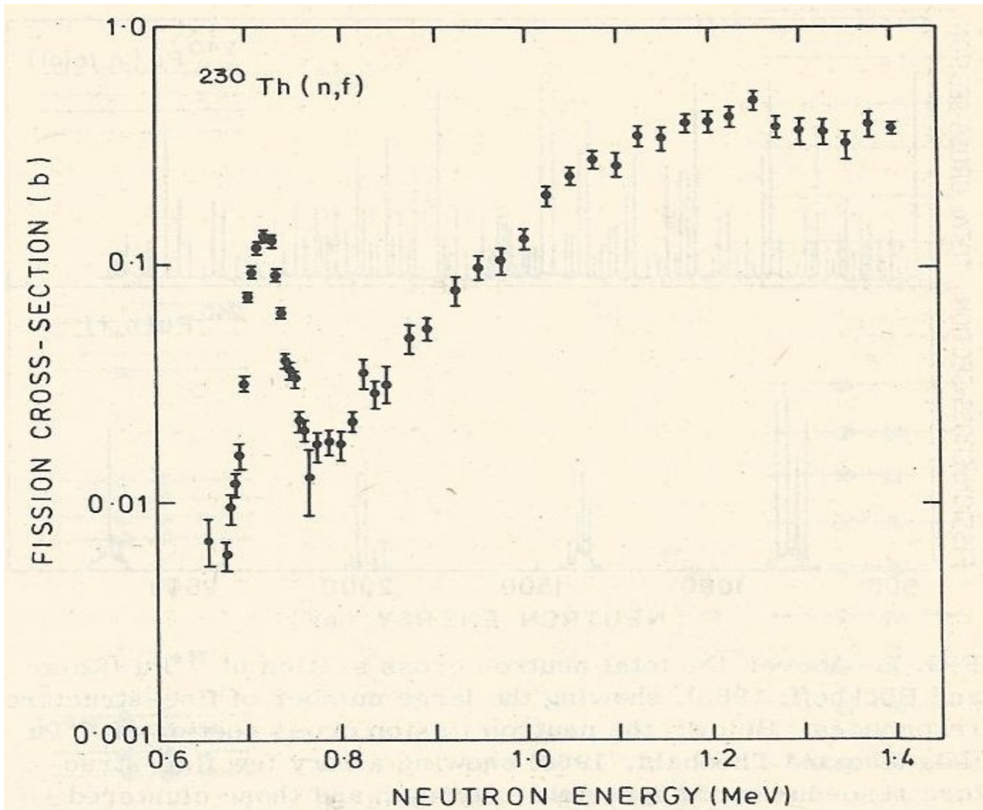


^{237}U : $I^{\pi} = 1/2^{+}$ CN : $J^{\pi} = 0^{+}$ and 1^{+}



Difficulties in Liquid Drop based model

- Systematics of barrier heights .
- Highly asymmetric mass yields.
- Structure in fission cr.secn. of non-fissionable nuclei: e.g. James *et al* (1972)

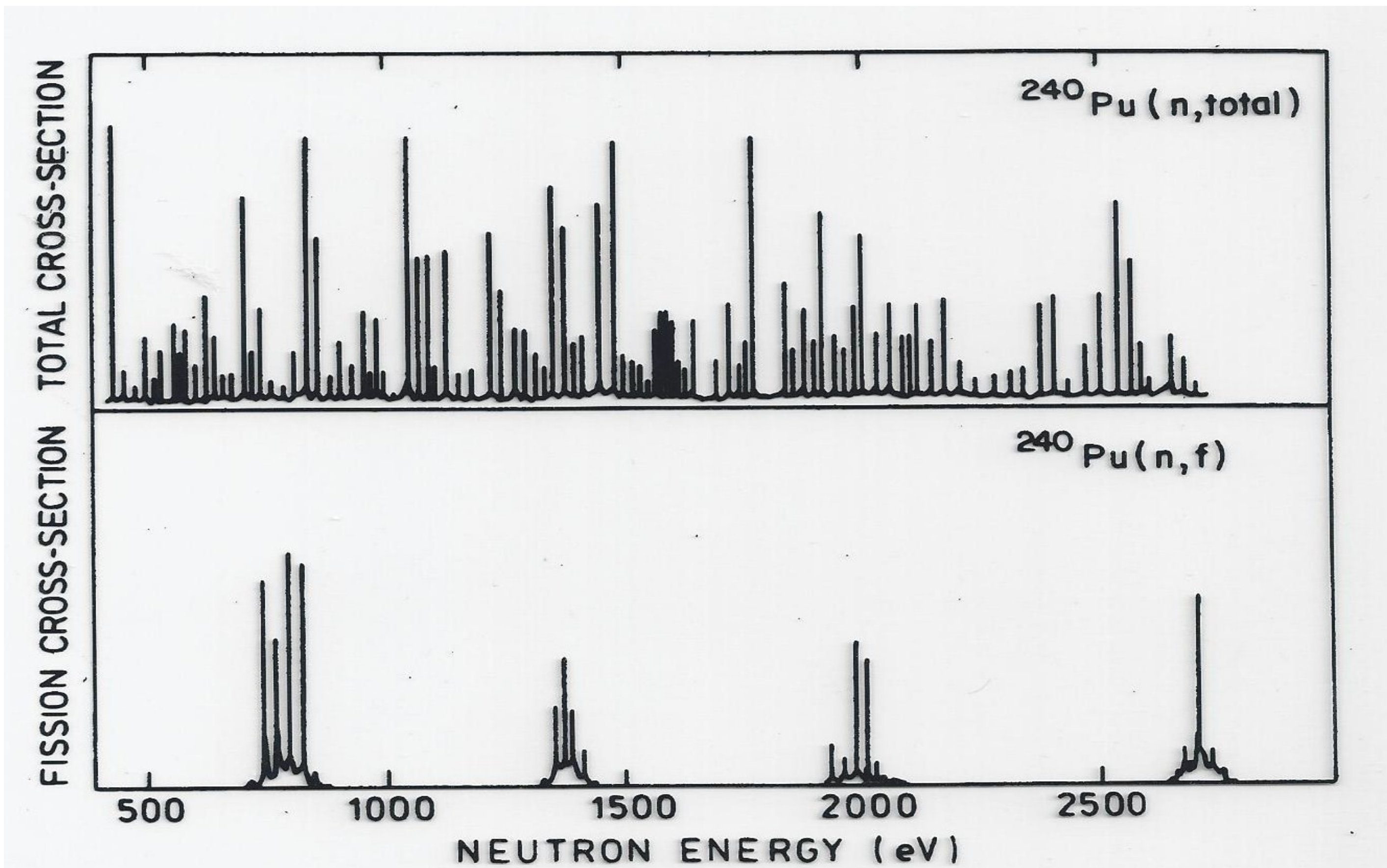


Spontaneously Fissioning Isomers (Flerov and Polikanov)

- Search for new elements – activity attributed to Am-242
- Properties (very unlike normal isomers, which have low E, high I)
- --- ½-life $\approx 14\text{ms}$
- Low spin
- High excitation energy $\approx 3\text{ MeV}$

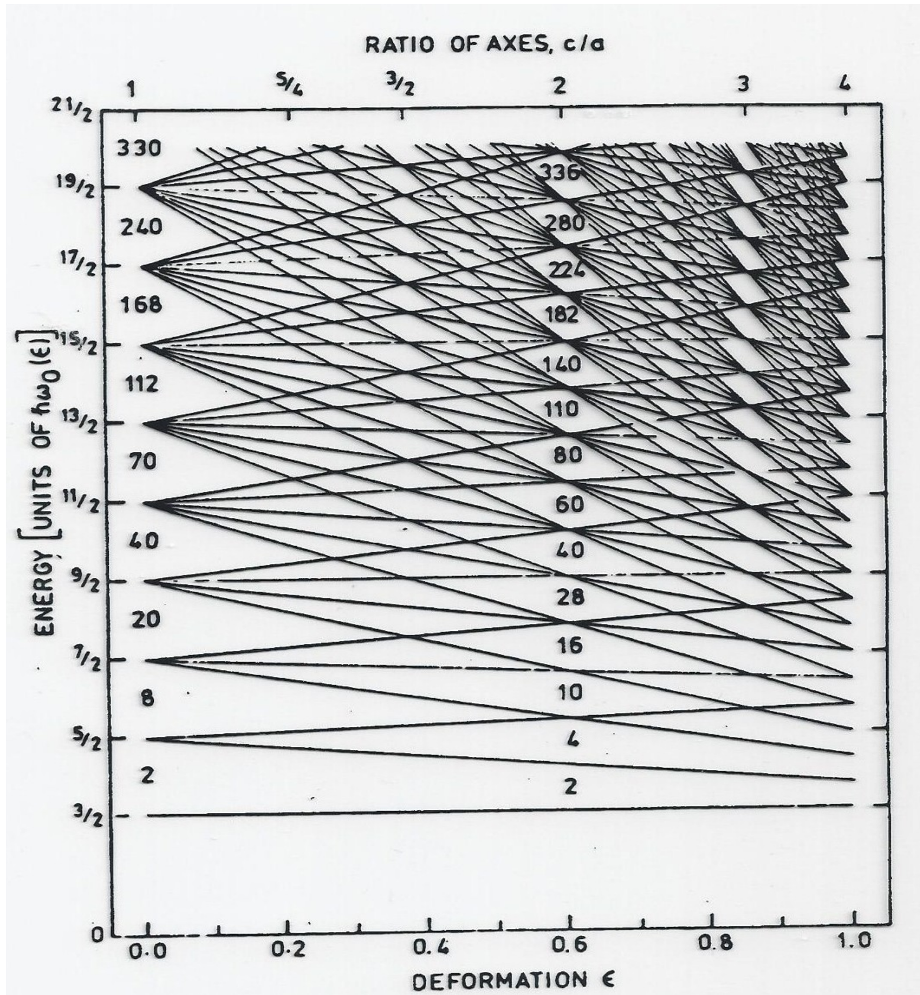
Narrow Intermediate Structure in Fission cross-sections

- Discovered in resonance region by Migneco & Theobald and Paya *et al* (1968)



Shell effects in deformed nuclei – Strutinsky theory

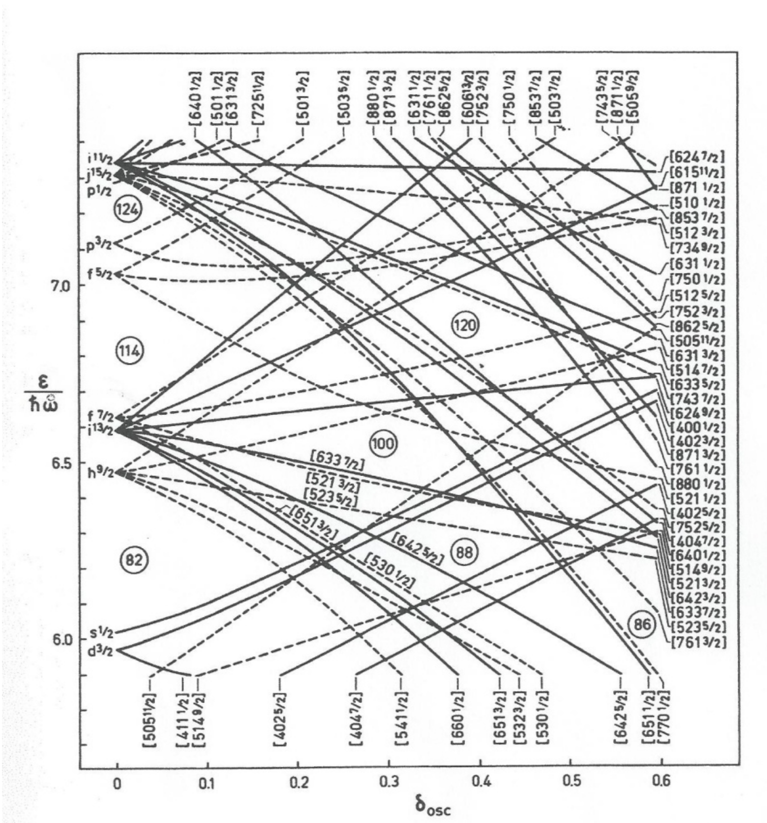
- Levels of a spheroidally deformed harmonic potential (no spin-orbit coupling)



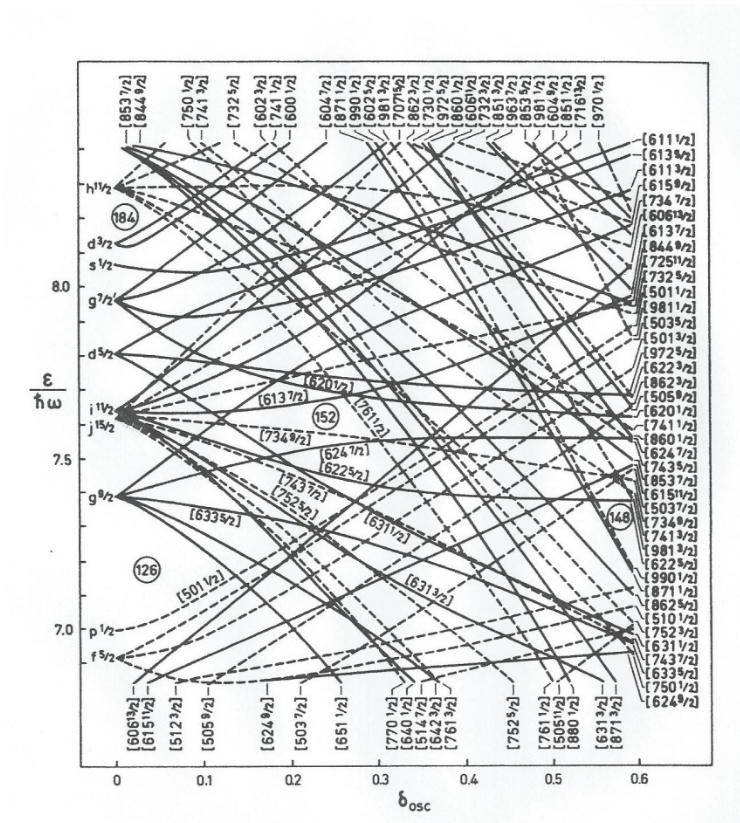
(from Nix (1972))

Nilsson diagrams: deformed HO + spin-orbit coupling

Protons

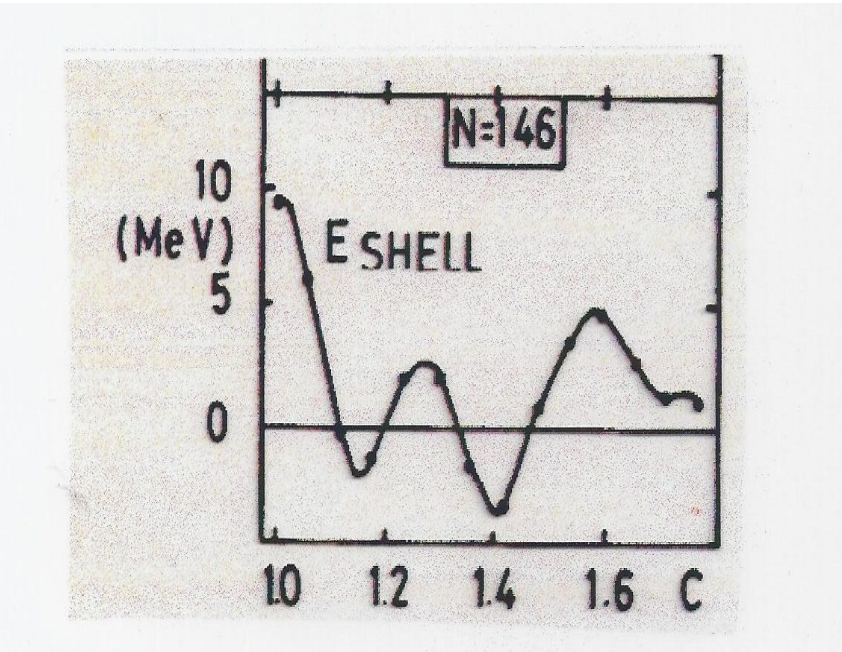


Neutrons



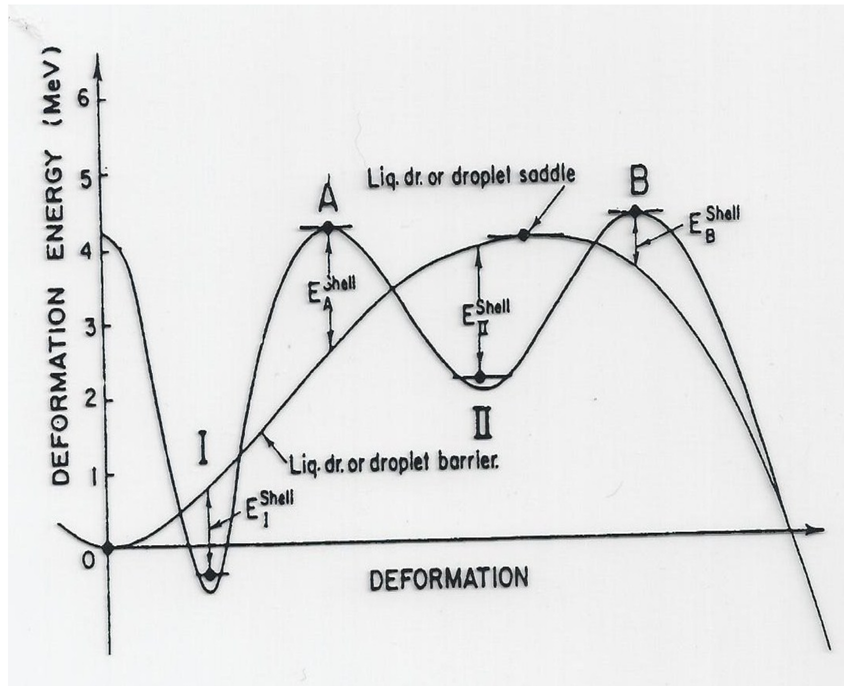
Strutinsky Theory: Liquid drop + shell correction

Shell correction term



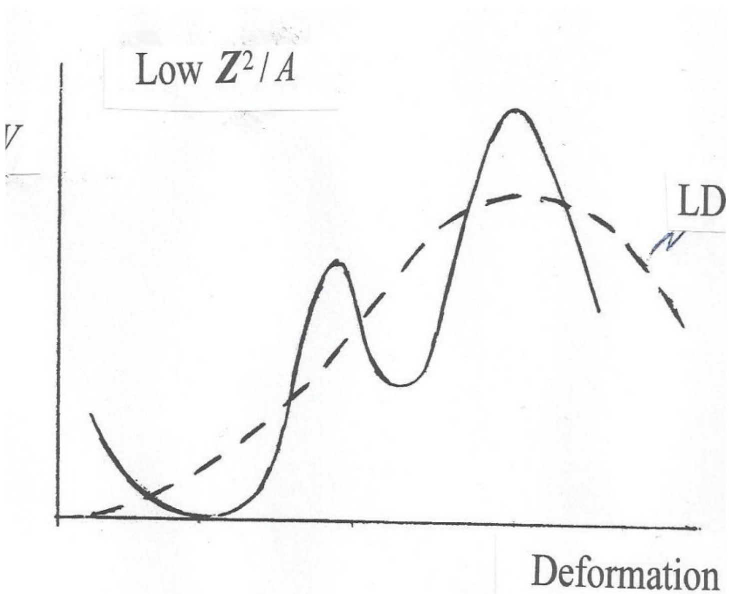
Shell corrn. added to liquid drop energy

The minimum marked II offers an explanation for spontaneously fissioning isomers

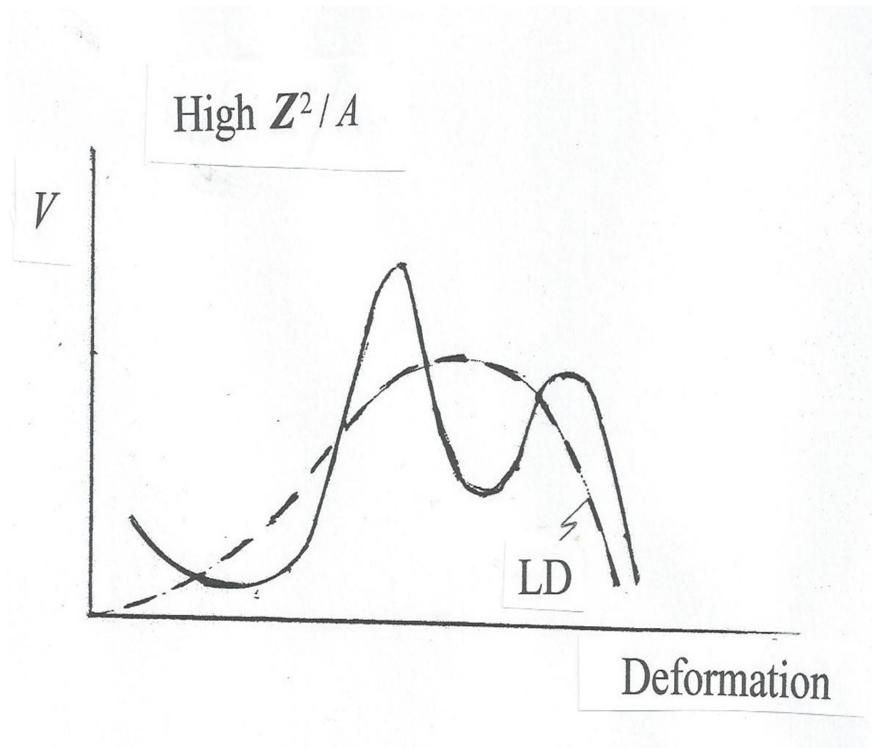


Barrier height dependence on Z^2/A

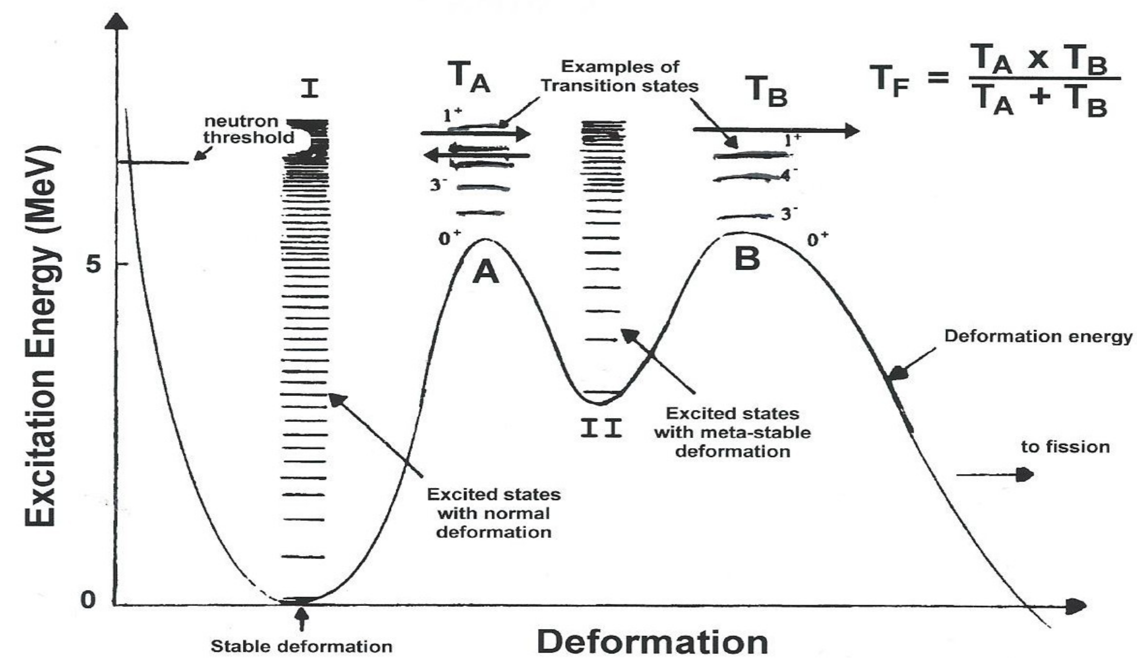
Low Z^2/A



High Z^2/A



Effect on Fission transmission coefficient



T_A , T_B are transmission coefficients of inner and outer barriers separately

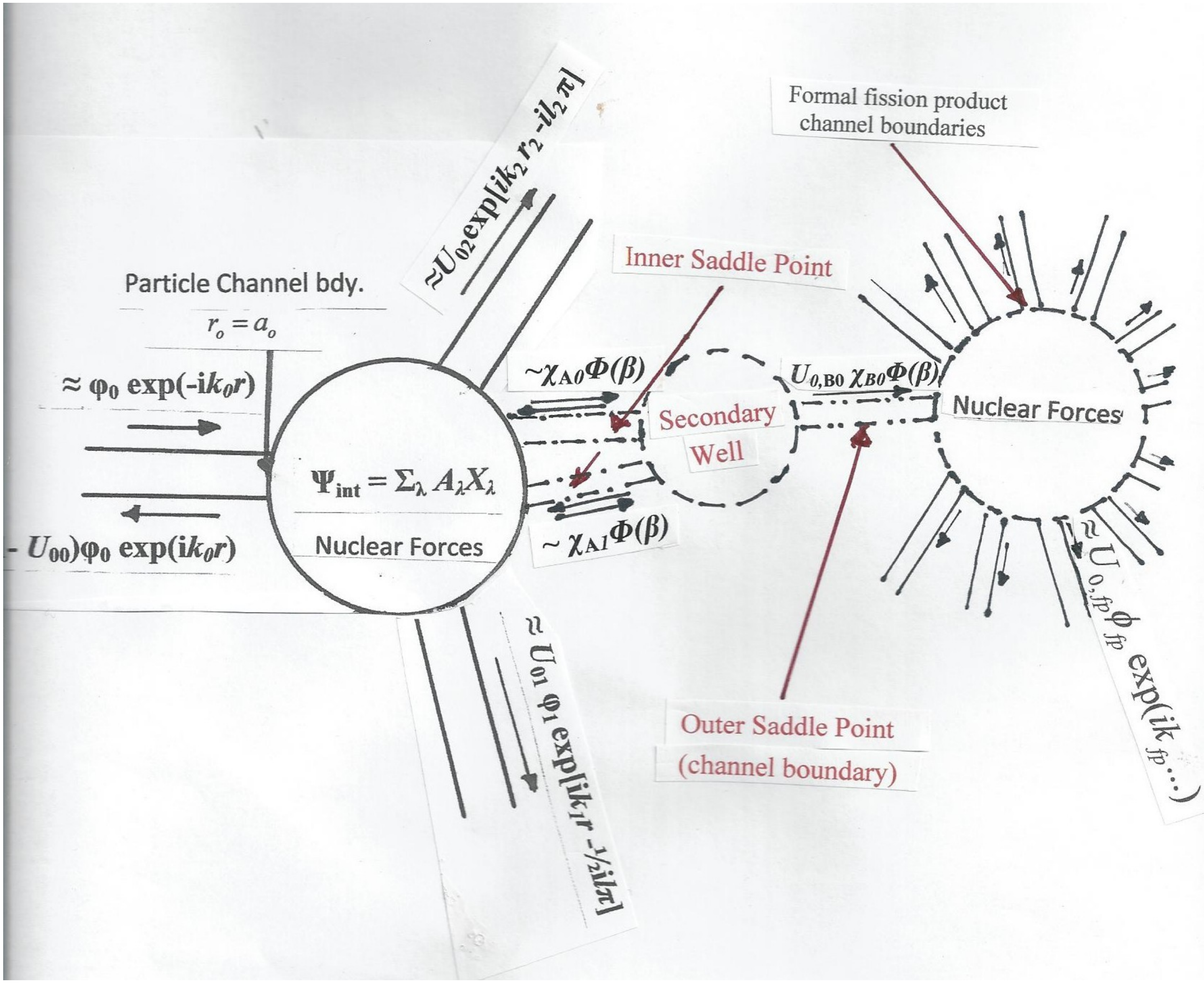
- This is the fission transmission coefficient of the Statistical Model:

$$T_F = T_A T_B / (T_A + T_B)$$

Lecture 2 Topics

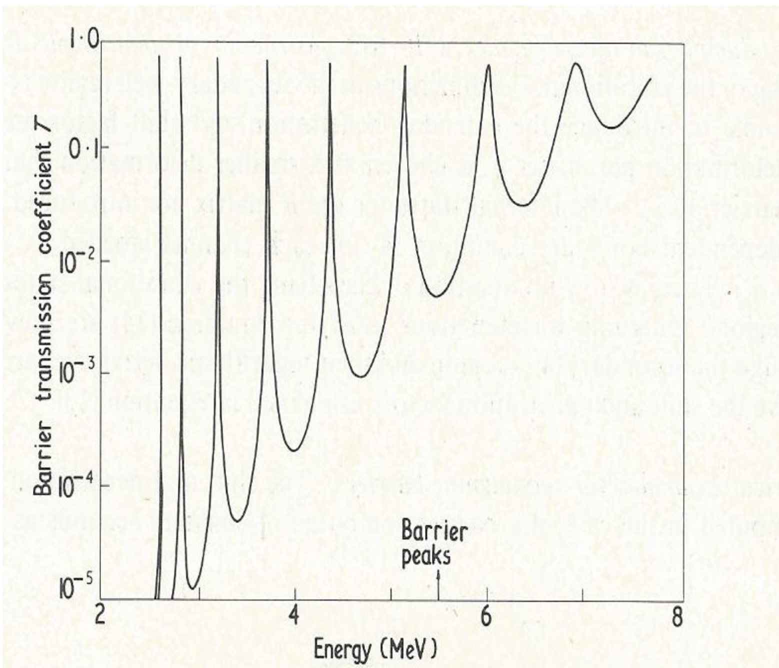
- Configuration space for R-matrix theory incorporating fission
- Wave functions in deformation space
- Formal exposition of intermediate structure
- Fine structure properties within intermediate structure
- Statistical fluctuations and average cross-sections
- Transition states at inner and outer barriers
- Examples of cross-section calculations for Pu isotopes

Configuration Space: choice of channel boundary

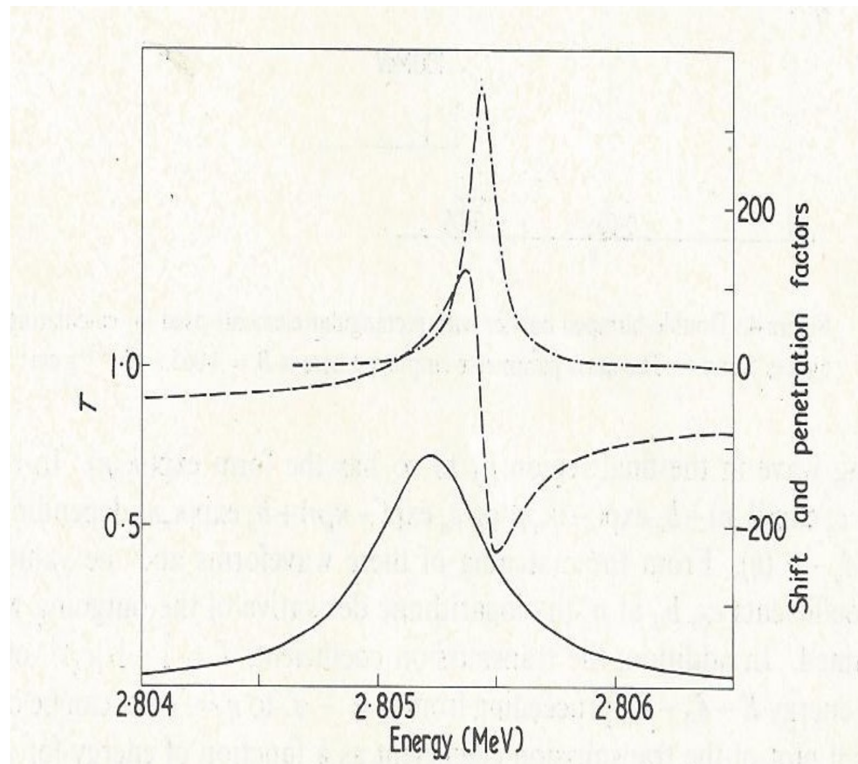


No nuclear interactions in Secondary Well; channel boundary at inner saddle point

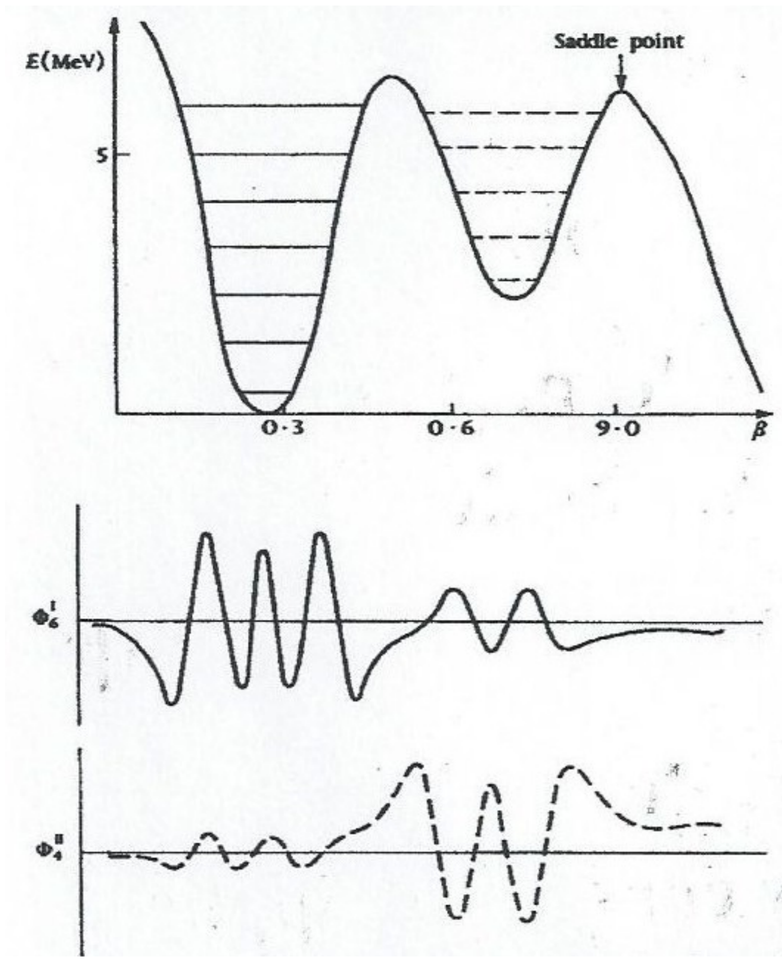
- Transmission coefficient



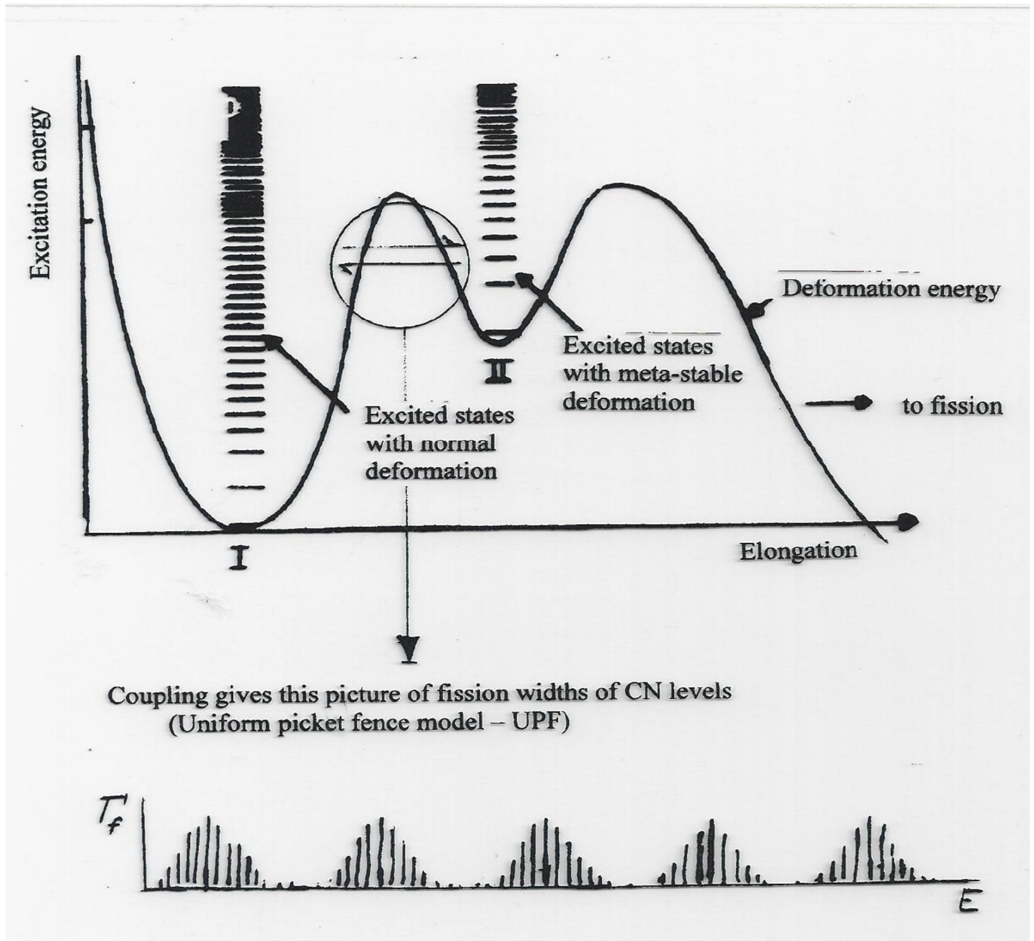
- Shift and penetration factors



Vibrational wave functions for Double well;
discrete states with real bdy.condn.at outer barrier



CN states in double well



Formal exposition of Intermediate Structure

-
- **Hamiltonian**

$$\boldsymbol{H = H_{\text{intrinsic}} + H_{\text{def}} + H_{\text{coup}}}$$

- Solutions of intrinsic part for fixed deformation β_0 denoted by χ_μ
-
- Solutions of deformation part are vibrational-type functions in the deformation variable β:

$$\boldsymbol{\Phi_\nu(\beta)} \qquad \text{(eigenvalues } \varepsilon\text{)}$$

- Eigensolutions of *H* are expanded:

$$\boldsymbol{X_\lambda = \Sigma_\lambda\, C_{\lambda,\mu\nu}\chi_\mu\Phi_\nu}$$

Intermediate structure continued

- Two classes of basis states:
- Class I: with negligible vibrational amplitude in 2y well: $\mu'\nu_I$‘
- Class II: main component of vibrational amplitude in 2y well: $\mu''\nu_{II}''$

- Solve Scrodinger eqn. for the Hamiltonian with the limited bases of the two classes.
- The Hamiltonian matrix elements for the first basis are

$$<\nu_I\mu \mid H_{coup} \mid \nu_I'\mu'> = (\varepsilon_{\nu(I)} + E_\mu)\delta_{\nu(I)\mu,\nu'(I)\mu'} + <\mu\nu_I \mid H_{coup} \mid \mu'\nu_I'>$$

This Hamiltonian can be diagonalized to give class-I eigenstates with wave function expansions

$$X_{\lambda(I)} = \Sigma_{\mu\nu(I)} < \lambda_I \mid \mu\nu_I>\chi_\mu\Phi_{\nu(I)}$$

- and eigenvalues $E_{\lambda(I)}$

Intermediate structure continued

- Similarly, for the class-II basis set:

  The Hamiltonian matrix elements are

$$<\nu_{II}\mu \mid H_{coup} \mid \nu_{II}'\mu'> = (\varepsilon_{\nu(II)}+E_\mu)\delta_{\nu(II)\mu,\nu'(II)\mu'} + <\mu\nu_{II} \mid H_{coup} \mid \mu'\nu_{II}'>$$

and we diagonalize it to give the class-II eigenstates with wave function expansions

$$X_{\lambda(II)} = \Sigma_{\mu\nu(II)} < \lambda_{II} \mid \mu\nu_{II}>\chi_\mu \Phi_{\nu(II)}$$

and eigenvalues $E_{\lambda(II)}$

Properties of Class-I eigenstates.

- These contain the zero-phonon vibrational state Φ_0 in their eigenfunctions. Hence, the ground state and lowest excited states of the Compound Nucleus are included in the class-I set.
- Maximum available excitation energy for constructing intrinsic states. Hence, large level density.
- Φ_0 essential for CN component for reduced neutron width amplitude(for neutron emission leaving residual nucleus in ground state). Also for inelastic scattering.
- Primary radiative transitions to low-lying states.
- In fact, the class-I states have most of the characteristics of the CN states we see as neutron resonances, except that they have no reduced fission width.

Properties of Class-II eigenstates

- Class-II level density is much lower.

- No reduced neutron width ; cannot be excited by neutron bombardment.

- From the higher class-II vibration components, significant amplitude at the outer barrier and hence fission widths.

- Lowest state in spectrum is spontaneously fissioning isomer. Radiation from higher class-II states terminates here. No "cross-over" radiation.

Final Diagonalization of Hamiltonian

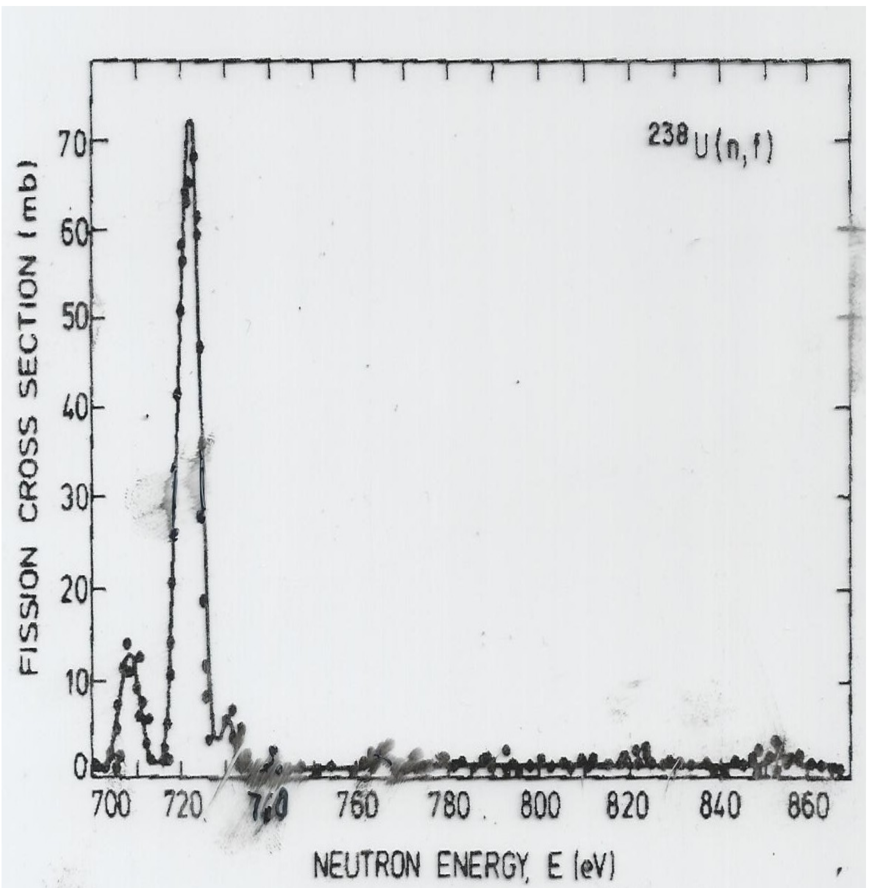
- Full Hamiltonian:

$$
\left.\begin{array}{cccc|ccc}
E(\lambda \mathrm{I}) & 0 & 0 & \ldots\ldots & \langle\lambda \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle & \langle\lambda \mathrm{I}|\, H\mathrm{c}\, |\lambda' \mathrm{II}\rangle & \ldots\ldots\ldots \\
0 & E(\lambda' \mathrm{I}) & 0 & \ldots\ldots & \langle\lambda' \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle & \langle\lambda' \mathrm{I}|\, H\mathrm{c}\, |\lambda' \mathrm{II}\rangle & \ldots\ldots\ldots \\
0 & 0 & E(\lambda'' \mathrm{I}) & \ldots & \langle\lambda'' \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle & \langle\lambda'' \mathrm{I}|\, H\mathrm{c}\, |\lambda' \mathrm{II}\rangle & \ldots\ldots \\
0 & 0 & 0 & \ldots\ldots & & & \\
: & & & & & & \\
0 & 0 & 0 & & \langle\lambda'''' \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle\ \ldots\ldots & & \\
\hline
\langle\lambda \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle & \langle\lambda' \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle & \langle\lambda'' \mathrm{I}|\, H\mathrm{c}\, |\lambda \mathrm{II}\rangle & .. & E(\lambda \mathrm{II}) & 0 & 0 \\
\langle\lambda \mathrm{I}|\, H\mathrm{c}\, |\lambda' \mathrm{II}\rangle & \langle\lambda' \mathrm{I}|\, H\mathrm{c}\, |\lambda' \mathrm{II}\rangle & \langle\lambda'' \mathrm{I}|\, H\mathrm{c}\, |\lambda'' \mathrm{II}\rangle & & 0 & E(\lambda' \mathrm{II}) & 0 \\
\ldots\ldots\ldots & \ldots\ldots\ldots & \ldots\ldots\ldots & \ldots & 0 & 0 & E(\lambda'' \mathrm{II}) \\
: & : & : & & & &
\end{array}\right.
$$

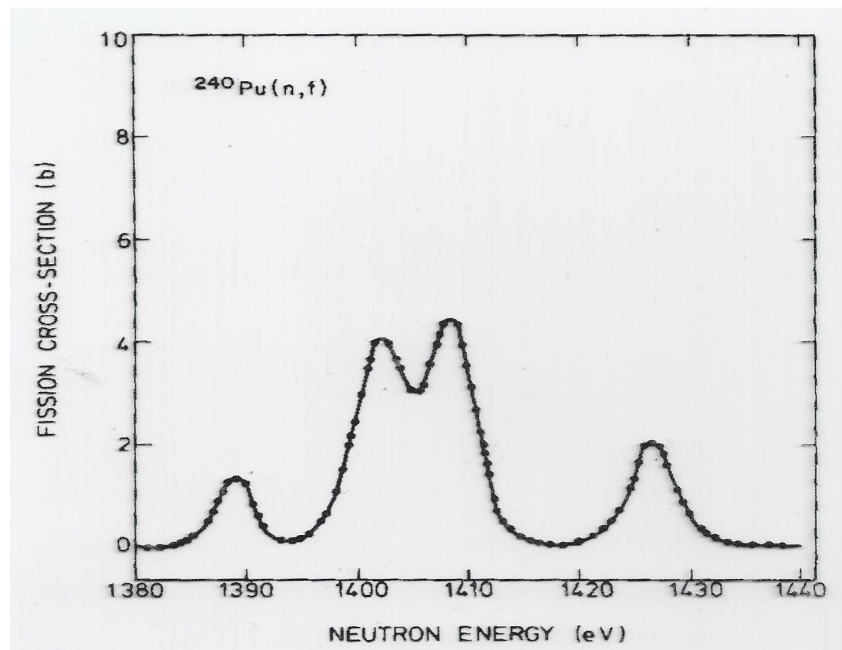
Matrix element core $\langle \nu \mathrm{I}\ |H\mathrm{c}|\ \nu \mathrm{II}\rangle$ is very small

Very weak mixing: perturbative treatment

- **^{238}U (n,f):**
- **very small neutron width; $\Gamma_\gamma \approx 7$meV (average radiation width ≈ 22meV)**



- **^{240}Pu (n,f):**
- **2 strong fission resonances (total fission width $\approx$ 3.5 eV**
- **Accidental degeneracy of class-II state with very close class-I**



Moderately weak coupling:

- The mixing of a single class-II state with many class-I level can be solved exactly.

$$2\pi\gamma^2_{\lambda,\mathrm{F}}/D_\mathrm{I} = \frac{\Gamma_{\lambda(\mathrm{II}),\,\mathrm{C}}\ \gamma^2_{\lambda(\mathrm{II}),\,\mathrm{F}}}{(E_{\lambda(\mathrm{II})} - E_\lambda)^2 + (\tfrac{1}{2}\Gamma_{\lambda(\mathrm{II}),\,\mathrm{C}})^2}$$

The "coupling width" across the inner barrier A:

which we have identified with the transmission coefficient across the inner barrier T_A.

Coupling to the fission continuum

- Lorentzian eqn. above is for R-matrix reduced widths. Fission widths of resonances can be different owing to coupling to the continuum.

Coupling to the fission continuum

- Lorentz profile with width $\Gamma_{\lambda_{II}c}$ is for reduced fission widths of R-matrix states.
- The coupling with the fission continuum has now to be included to obtain profile for the fission widths of the fine structure resonances.
- If
$$\Gamma_{\lambda_{II}F} = \Gamma_{\lambda_{II}C}$$

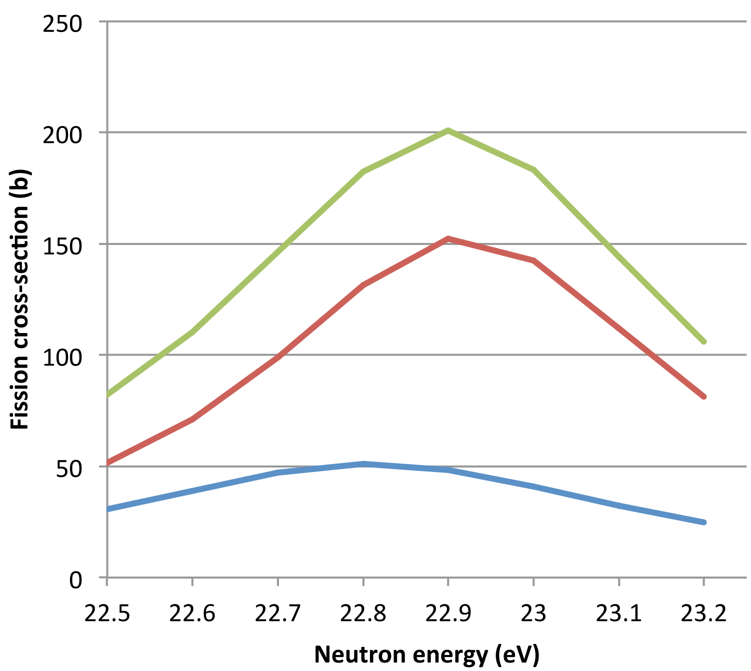
  R-matrix fission width profile approximates to intermediate resonance profile.

  If R-matrix fission widths $\Gamma_{\lambda f} = 2P_f\gamma^2_{\lambda f}$ appreciably overlap, solution of R-matrix equations not obvious.

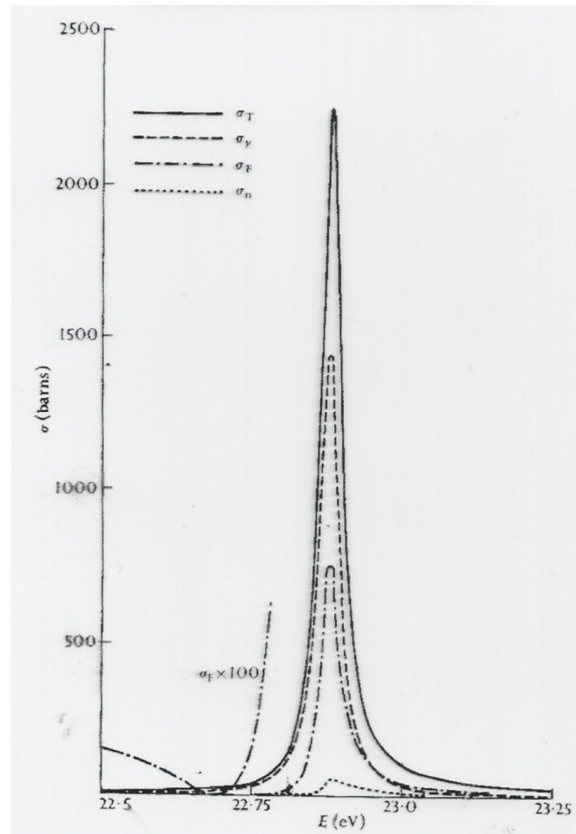
  Example:

2-level, 2-channel cross-section
(neutron entrance channel, single fission channel)

2 Breit-Wigner terms added (red and blue; total shown in green)



R-matrix calculation: note energy scale is same, cross-section scale increased x10



S-matrix theory

- S-matrix formalism expands the collision matrix about its poles in the complex energy field:

$$S_{cc'} = U_{cc'} - \delta_{cc'} \approx \sum_m \frac{G_{mc} G_{mc'}}{\mathcal{E} - \mathcal{E}_m^H}$$

- The quantities *G* are effectively partial width amplitudes of the poles.
- $\mathcal{E}$ is the complex energy and the poles are at the complex energies

$$\mathcal{E}_m^H = E_m^H - i\Gamma_m^H / 2$$

- Advantages: parameters of poles (e.g. pole width, partial width amplitudes) directly reflect characteristics of resonances in cross- section

- Disadvantages: S-matrix theory is not unitary.

  Statistical distributions of partial widths change with strength function.

Transforming R-matrix parameters to S-matrix parameters

- U and R matrices are extended into the complex energy field. S-matrix poles can be found analytically in certain cases or generally by numerical methods.
- 2-level case: analytic – as R-matrix levels become closer, poles repel each other in imaginary direction. Two broad R levels become a narrow resonance and a broad resonance.

- "Broad" class –II R-matrix state:
  $\Gamma_{\lambda(II)F} \ ? \ D_I$ and $\Gamma_{\lambda(II)F} \ ? \ \Gamma_{\lambda(II)C}$

Fine structure resonance fission widths

$$\Gamma_{mF} = \frac{D_I}{2\pi} \frac{\Gamma_{\lambda(II)C}\Gamma_{\lambda(II)F}}{(E_{\lambda(II)} - E_m)^2 + \Gamma_{\lambda(II)F}{}^2 / 4}$$

Neutron widths & resonance energies are close to class-I values.

- Remaining class-II fission strength is

  $[1 - \Gamma_{\lambda(II),C} / \Gamma_{\lambda(II),F}]\ \Gamma_{\lambda(II),F}$

  contained in one broad pole (width ~ $\Gamma_{\lambda(II)F}$) with weak neutron width ($\Gamma_{\lambda(II),C} < \Gamma_{\lambda(I),n} > / \ \Gamma_{\lambda(II),F}$) underlying the Lorentzian group.

General formula for fission widths of resonances

- Fine structure fission widths

$$\Gamma_{\lambda F} = \frac{D_I}{2\pi} \frac{\Gamma_{\lambda(II)C}\Gamma_{\lambda(II)F}}{(E_{\lambda(II)} - E_{\lambda_I})^2 + (\Gamma_{\lambda(II)C} + \Gamma_{\lambda(II)F})^2 / 4}$$

with remaining class-II fission width

$[1 - \Gamma_{\lambda(II),\, \mu'\nu(II)} / (\Gamma_{\lambda(II),\, \mu'\nu(II} + \Gamma_{\lambda(II),\, C})]\ \Gamma_{\lambda(II),\, \mu'\nu(II)}$

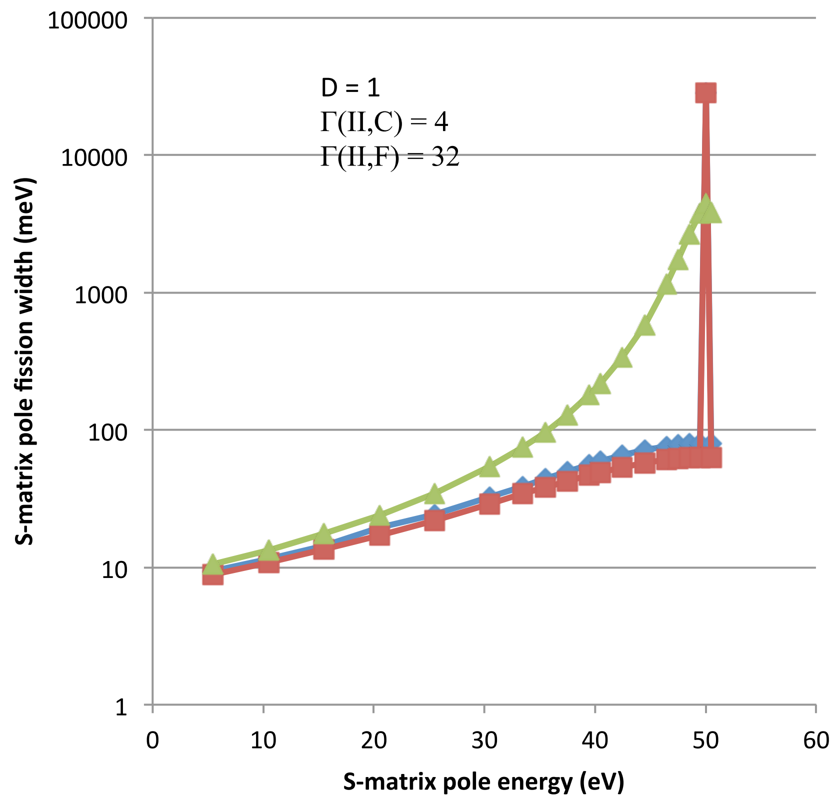
(this is component for transition state **$\mu'\nu_{II}$**)

- This formula is approximate.
- General prescription:

  Use R-matrix parameters for $\Gamma_{\lambda_{II} f} \le \Gamma_{\lambda_{II} c}$

  Use General formula for $\Gamma_{\lambda_{II} f} \ge \Gamma_{\lambda_{II} c}$

- Blue : S-matrix pole fission widths;
  Red : from hypothesis formula;
  Green: R-matrix fission widths.



Statistical fluctuations of widths: effect on average cross-sections

- **Possible expansion of Internal Eigenstates**

$$\mathbf{X}_\lambda = \Sigma_{cp}\, C_{\lambda,cp}\, \varphi_c\, u_p(r_c)$$

where ϕ_c is state of internal excitation and u_p is state of single neutron motion in field of residual nucleus

Incident neutron channel is

$$\sim \varphi_0 u_q(r_0)$$

Value of $\mathbf{X}_\lambda$ at channel radius $r_0 = a_0$ is the reduced neutron width amplitude:

$$\gamma_{\lambda,0q} \sim C_{\lambda,0q}\, u_q(a_0)$$

- For high density of states (CN states) expectation value of $C_{\lambda,0q}^2 \sim D_\lambda/D_{sp}$

Distribution of $C_{\lambda,0q} \rightarrow$ gaussian with zero mean.

- Hence, distribution of reduced widths $x \equiv \gamma_{\lambda,0q}^{\ 2}$ is the Porter-Thomas form

$$p(x)dx = \frac{1}{\sqrt{2\pi x\bar{x}}}\exp\left(-\frac{x}{2\bar{x}}\right)dx$$

The non-uniform distribution affects averaging of cross-sections over resonances.

Statistical fluctuations of widths: effect on average cross-sections contd.

- Porter-Thomas distribution applies to every individual channel.
- Distribution of the sum $y = \Sigma_n x_n$ is

$$p(y) = \frac{1}{\Gamma(n/2)}\left(\frac{n}{2\overline{y}}\right)^{n/2} y^{(n-2)/2} \exp\left(-\frac{ny}{2\overline{y}}\right) dy$$

This is the χ^2 distribution with *n* degrees of freedom. (P-T is the member with *n* =1)

Variance is

$$\mathrm{var}(y) = 2\overline{y}^2 / n$$

- Total capture width comprises large number of 1ry transitions. Variance small.
- Fission widths through a single channel has Porter-Thomas distribution.
- The Hauser-Feshbach expression for average cross-sections has to be modified to take account of these width distributions.

Statistical fluctuations of widths: effect on average cross-sections (contd. 2)

- This is usually denoted by multiplying the core Hauser-Feshbach term by a fluctuation factor S_{ab} thus:

$$\sigma_{ab} : \frac{T_a T_b}{T} \mathscr{S}_{ab}$$

  $\boldsymbol{T_a}$ etc. being the usual transmission coefficients expressed in terms of average width $T_c = 2\pi\bar{\Gamma}_c / D$.

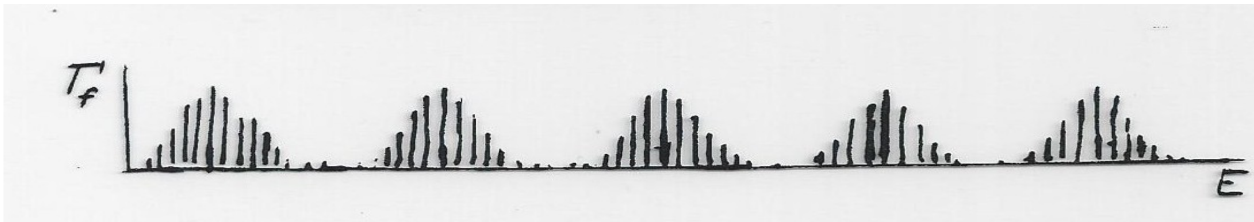
- For some cases of few channels and (constant) capture width, S can be calculated analytically. In general, however it is reduced to an integral in one variable, which can be calculated numerically.

  In reactions that are dominated by a very few channels the fluctuation factors can be as low as ~ 0.7.

  For elastic scattering with many competing reactions S_{nn} can approach 3.

Averaging over Intermediate Structure

- Uniform picket fence model.



With no width fluctuations the average fission cross-section is:

$$\sigma_{nf} = \pi \lambda\!\!\!^{-2} g_J \frac{T_n}{\{1 + (T_{\mathrm{I}}/T_F)^2 + (2T_{\mathrm{I}}/T_F)\coth[\tfrac{1}{2}(T_A + T_B)]\}^{1/2}}$$

T_{I} is total class-I transmission coefficients ;

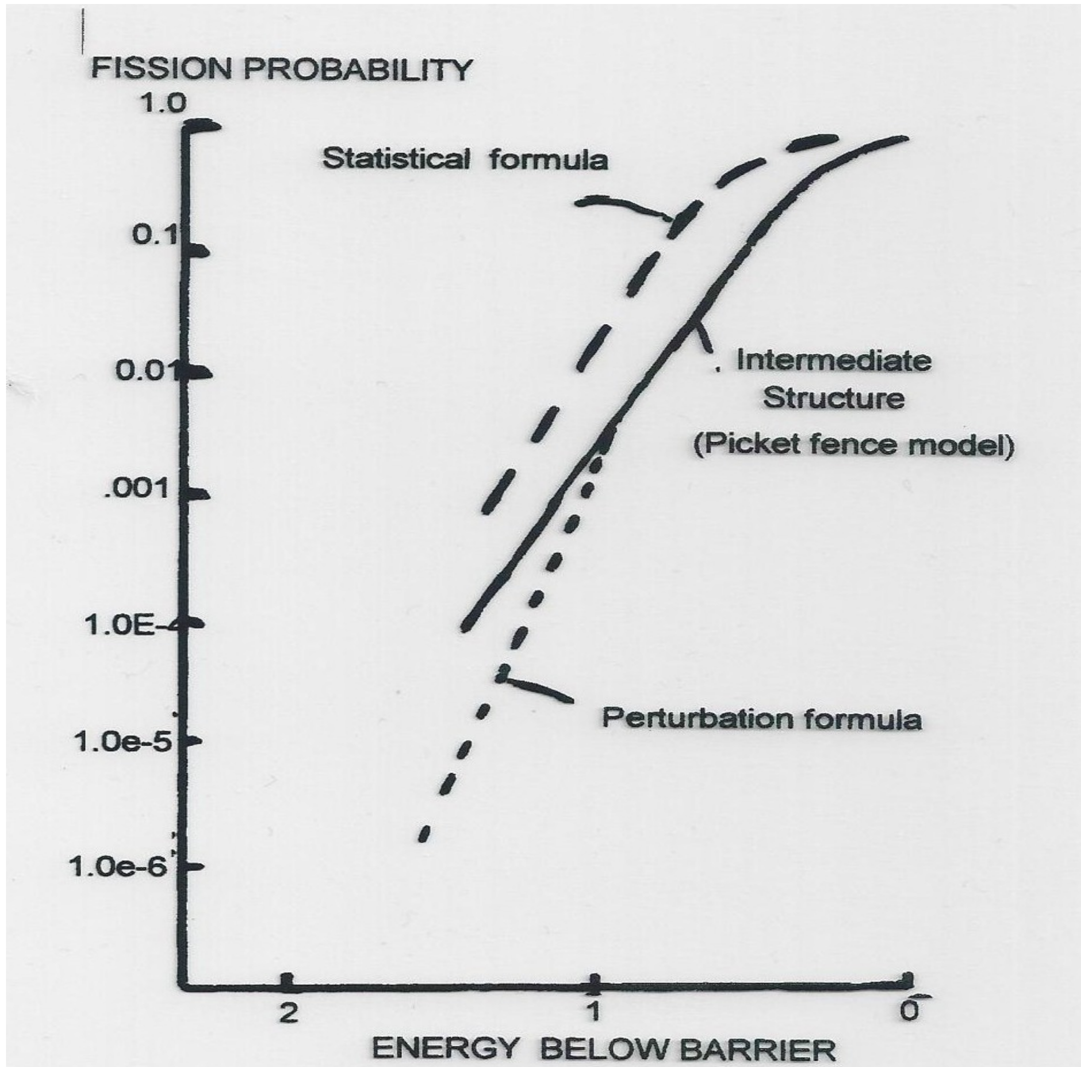
T_A , T_B are inner and outer barrier transmission coefficients,

$T_F = T_A\, T_B\, /\, (T_A + T_B\,)$ is the statistical fission transmission coefficient.

Averaging for different intermediate structure models

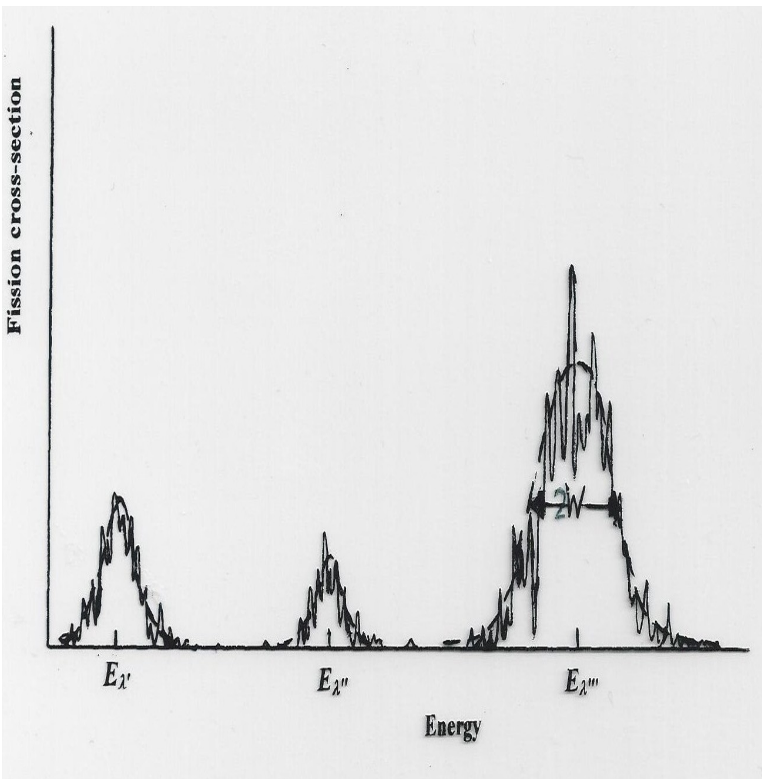
- Fission probability in different models. (σ_{CN} is compound nucleus formation cross-section).

$$P_F = \sigma_F / \sigma_{CN}$$



Intermediate structure averaging

Width fluctuations to be considered



Width of intermediate resonance:

$$2W_{\lambda\mathrm{II}} \approx \Gamma_{\lambda\mathrm{II(F)}} + \Gamma_{\lambda\mathrm{II(C)}}$$

Strength of intermediate resonance:

$$\propto \Gamma_{\lambda\mathrm{II(C)}}\,\Gamma_{\lambda\mathrm{II(F)}} / W_{\lambda\mathrm{II}}$$

Relations for the coupling width:

$$<\Gamma_{\lambda\mathrm{II(C)}}> = D_{\mathrm{II}} T_A / 2\pi\,, \qquad \Gamma_{\lambda\mathrm{II(C)}} = 2\pi <H(\lambda_{\mathrm{II}}, \lambda_{\mathrm{I}})^2>_{\lambda\mathrm{I}} / D_{\mathrm{I}}$$

Fission width of fine structure resonance:

$$\Gamma_{\lambda\mathrm{(F)}} \propto H(\lambda_{\mathrm{II}}, \lambda_{\mathrm{I}})^2\, \Gamma_{\lambda\mathrm{II(F)}} / [(E_{\lambda\mathrm{II}} - E_{\lambda})^2 + W_{\lambda\mathrm{II}}^2]$$

Strength of fine structure resonance:

$$\propto \Gamma_{\lambda\mathrm{(n)}}\, \Gamma_{\lambda\mathrm{(F)}} / \Gamma_{\lambda}^2$$

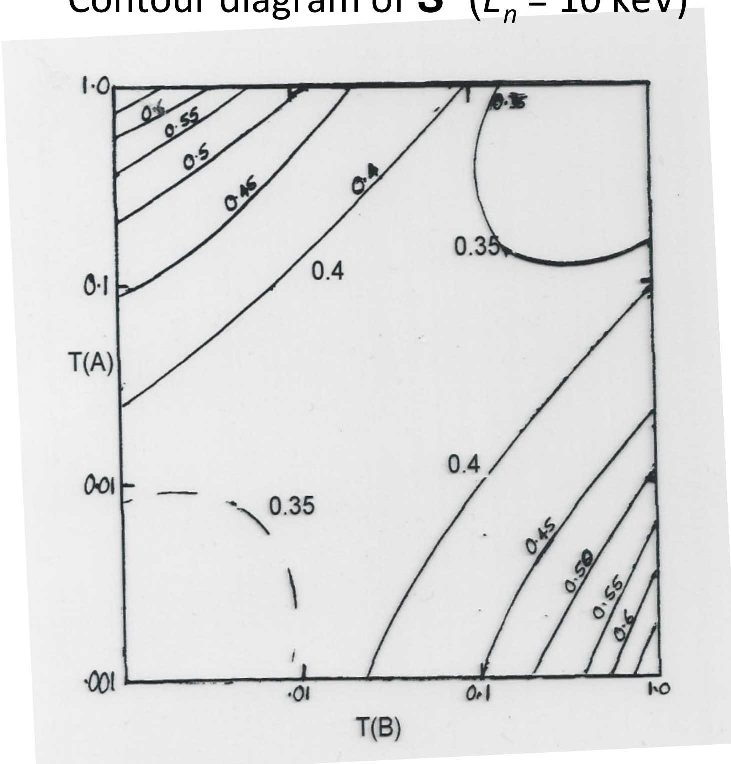
Magnitude of width fluctuation effect

Single channel both barriers.

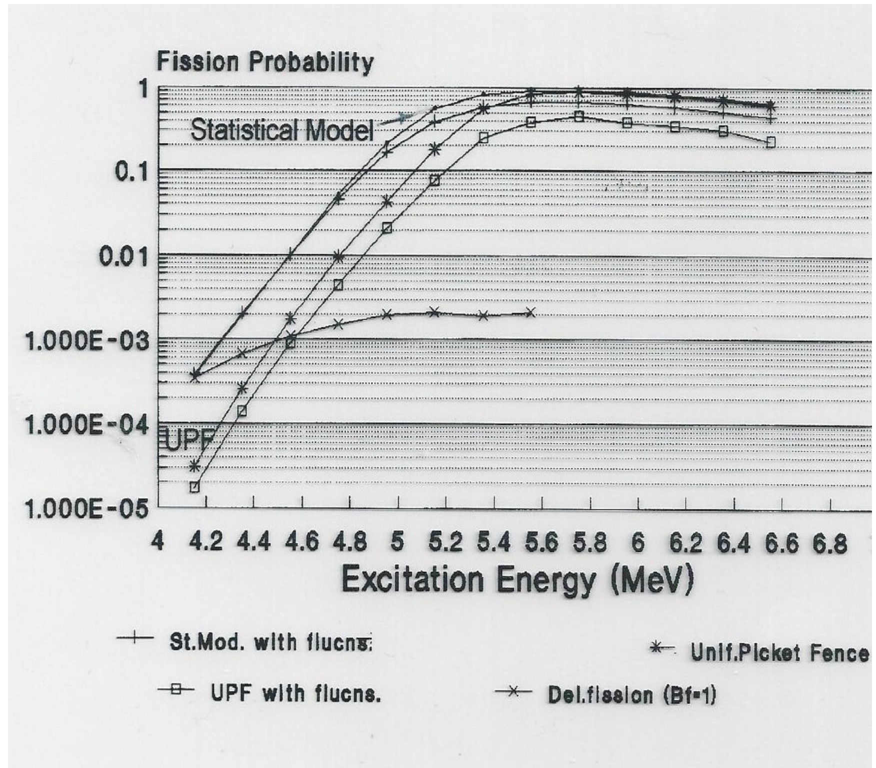
Use convention of fluctuation factor $\boldsymbol{S}$ with UPF model:

$$\left\langle \sigma_{nf} \right\rangle = \sigma_{nf,UPF} \mathscr{S}_{nf}$$

Contour diagram of $\boldsymbol{S}$ (E_n = 10 keV)



Different model calculations for *(t,pf)* reaction



Model for $J^{\pi} = 4^{+}$ states populated in (t,pf):

Barriers at 5.5 MeV (for 0^{+}), 4^{+} transition state 0.07 MeV above barriers

$h\omega_A$ = 1.0 MeV, $h\omega_B$ = 0.6 MeV

Summary of fission cross-section theory for single (or few) specified transition states

- Statistical model – only useful if channel nearly fully open. Should be used with fluctuation factor $\boldsymbol{S_{II}}$ for distribution of inner and outer barrier class-II widths applied to $\boldsymbol{T_F}$ **.**

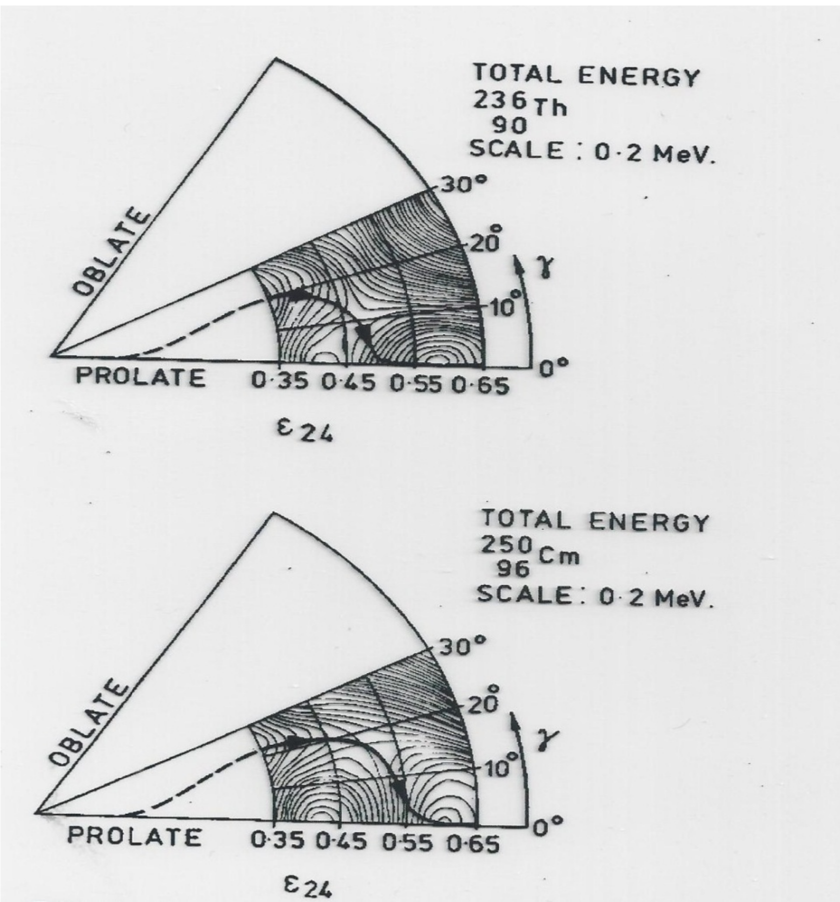
- Unified picket fence model – first approximation when energy is near or below barrier. As above, $\boldsymbol{S_{II}}$ should be included in $\boldsymbol{T_F}$ **.**

- UPF model with fine structure fluctuation factors $\boldsymbol{S_I}$ applied. This is in principle a rather crude approximation but is fairly good in practice.

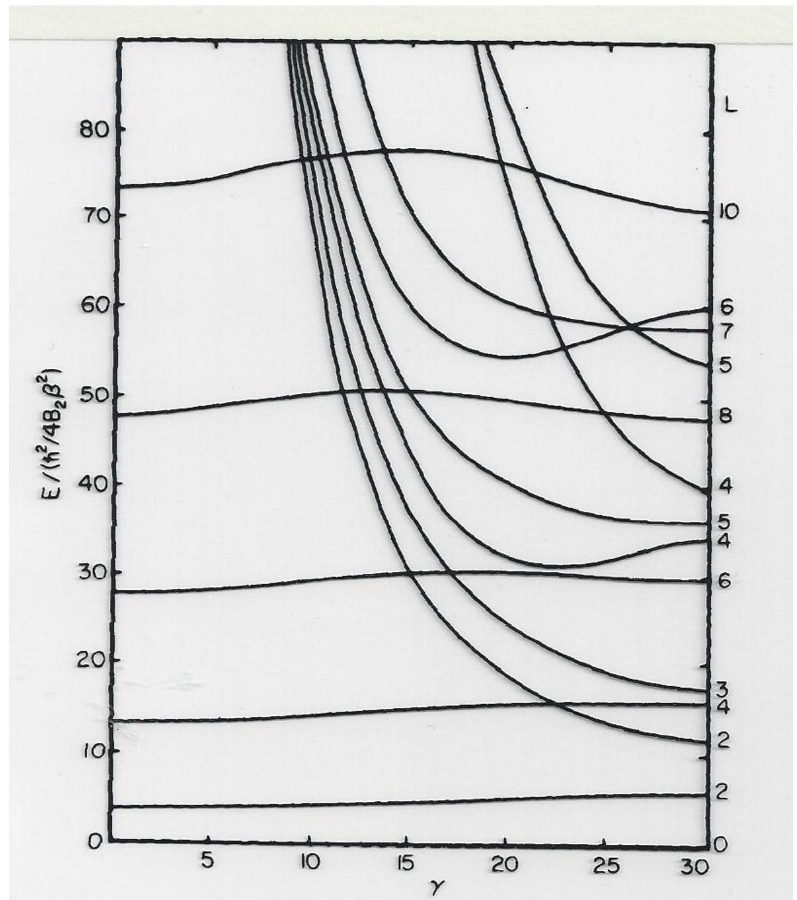
- Full modeling of intermediate structure with class-II and class-I width and coupling matrix element fluctuations, class-II fission width spreading for fine structure poles; Monte Carlo averaging.

Deformation energy & transition states at inner barrier

- Inner barrier: nuclear structure effects in deformation from cylindrical asymmetry.

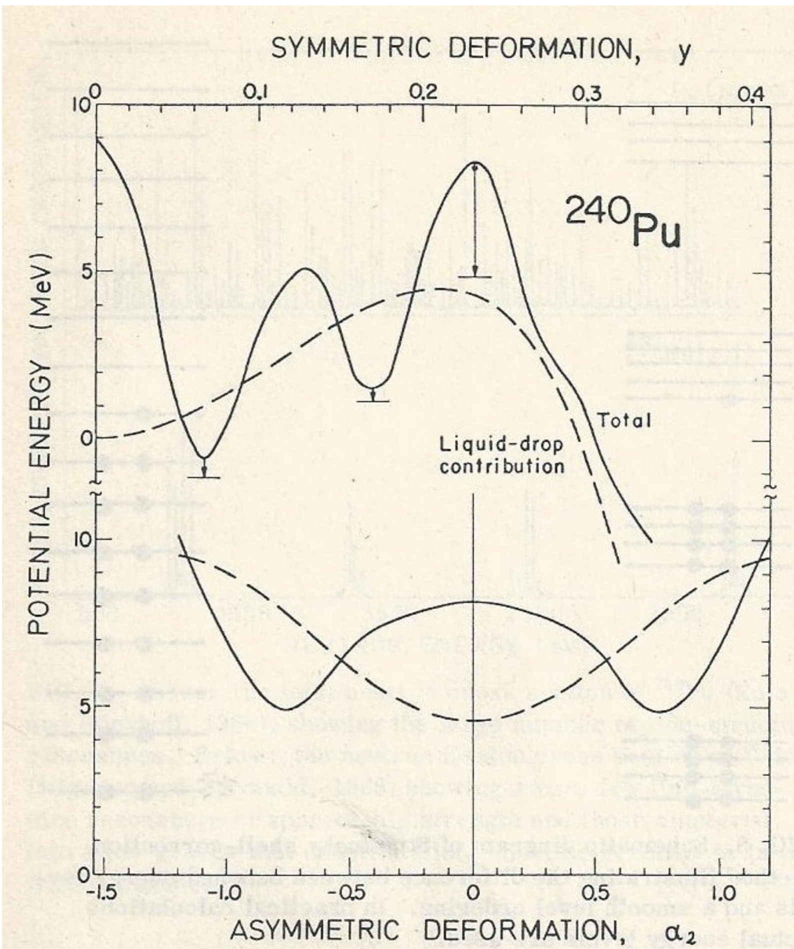


- Eigenvalues of deformed, asymmetric rotator as function of asymmetry parameter **γ.**



Deformation energy & transition states at outer barrier

- Outer barrier: deformation around octupole symmetry.



- Effect of octupole asymmetry on vibrational eigenstates

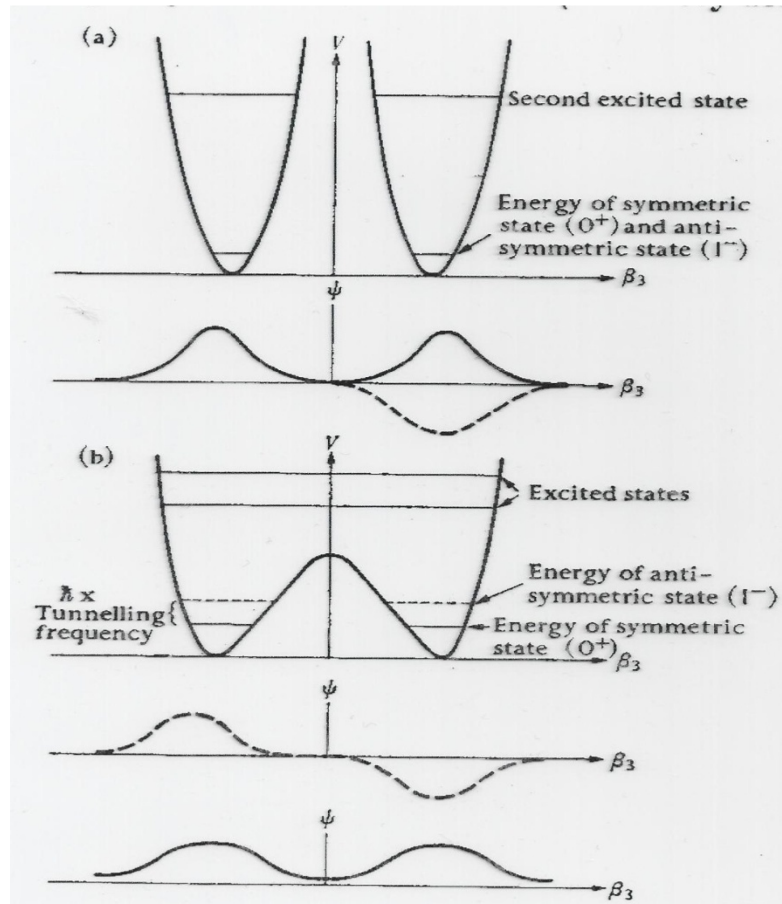


FIG. 8.3. Wave-functions in the β_3-potential.

Adopted barrier transition states for 2-hump barrier

- Inner barrier (even nucleus):
- $K^{\pi} = 0^{+}$ - "ground"

  + rotational band ($J^{\pi} = 2^{+}, 4^{+}$…)

  $$\hbar^2 / 2\Im \approx 3.5 keV$$
- Gamma vibration, $K^{\pi} = 2^{+}$ - ~ 200keV

  + rotational band ($3^{+}, 4^{+}$…)
- Gamma vibrations, $K^{\pi} = 0^{+}$, 4^{+} - ~ 400 to 500 keV

  + rotational band ($2^{+}, 4^{+}$…; $5^{+}, 6^{+}$ resp.)
- Mass asymmetry vibration, $K^{\pi} = 0^{-}$ - ~ 700keV

  + rotational band ($1^{-}, 3^{-}$…)
- Bending vibration, $K^{\pi} = 1^{-}$ - ~ 800keV

  + rotational band ($2^{-}, 3^{-}$…)
- Combinations of above

- Outer barrier:
- $K^{\pi} = 0^{+}$ - "ground"

  + rotational band ($J^{\pi} = 2^{+}, 4^{+}$…)

  $$\hbar^2 / 2\Im \approx 2.5\text{keV}$$
- Mass asymmetry vibration, $K^{\pi} = 0^{-}$ - ~ 100keV

  + rotational band ($1^{-}, 3^{-}$…)
- Gamma vibration, $K^{\pi} = 2^{+}$ - ~ 800keV

  + rotational band ($3^{+}, 4^{+}$…)
- Gamma vibrations, $K^{\pi} = 0^{+}$, 4^{+} - ~ 1.5MeV + rotational band ($2^{+}, 4^{+}$ …; $5^{+}, 6^{+}$ resp.)
- Bending vibration, $K^{\pi} = 1^{-}$ - ~ 800keV

  + rotational band ($2^{-}, 3^{-}$…)
- Combinations of above

Adopted transition states

- Even nuclei: above energy gap (1-1.5 MeV)
- 2 quasi-particle states

  These are calculated at appropriate deformation of inner or outer barrier (Nilsson diagrams for example)
- Above energy gap transition states are becoming numerous and discrete counting is replaced by level density; our work uses computed combinatorial model QPVR

  (multi -quasi-particles +vibration and rotation bands)

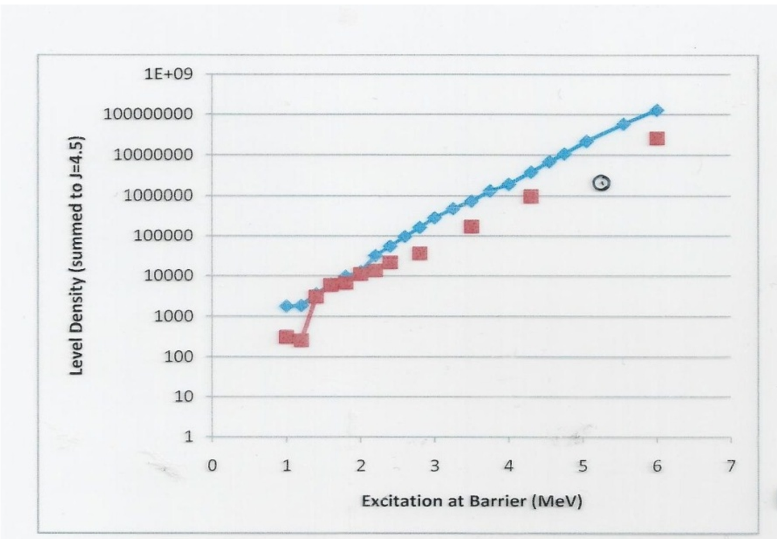
- Odd-A nuclei: from “ground”
- 1 quasi-particle states

  Calculated at appropriate deformation of inner or outer barrier
- Above energy gap discrete state counting is replaced by level density

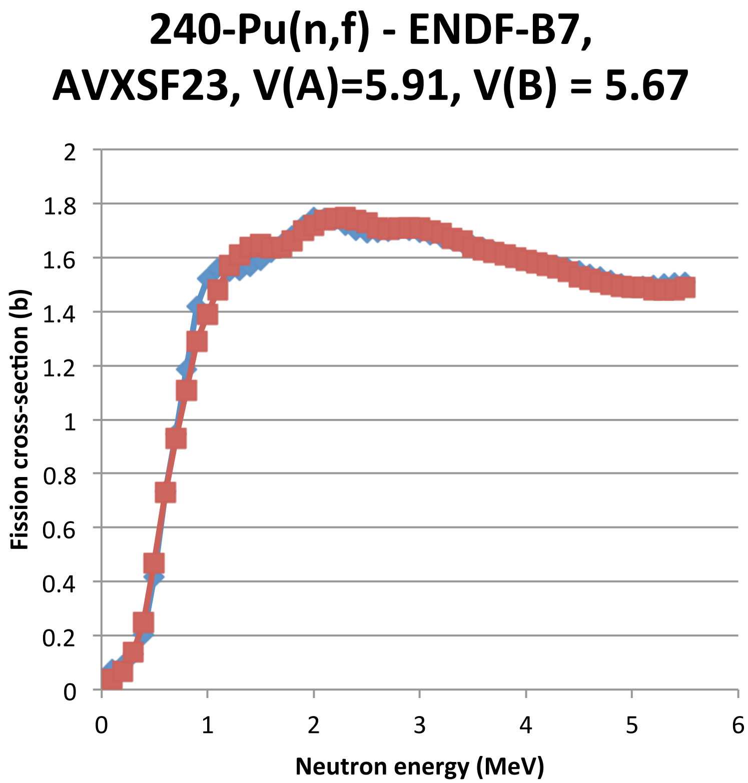
- Odd-odd nuclei; 2-quasi-particle states from “ground”

Example: Pu-240+n

- Fissionable nuclide
- Barrier level densities used:- Blue rhomboids - Inner barrier, calculated with Δ_p = 0.95 MeV, Δ_n = 0.75 MeV
- Red squares - Outer Barrier, fitted to cross-section; can be modeled approx. with Δ_p = 1 MeV, Δ_n = 0.85 MeV
- Black circle - LD from neutron resonance spacing of Pu-240+n: QPVR gives this with Δ_p = 0.71 MeV, Δ_n = 0.63 MeV



- Fit to cross-section

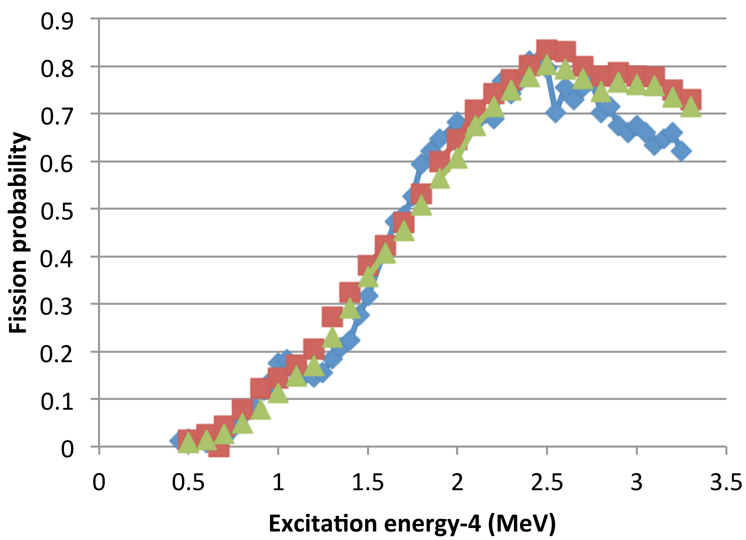


Blue rhomboids - ENDF-B7.

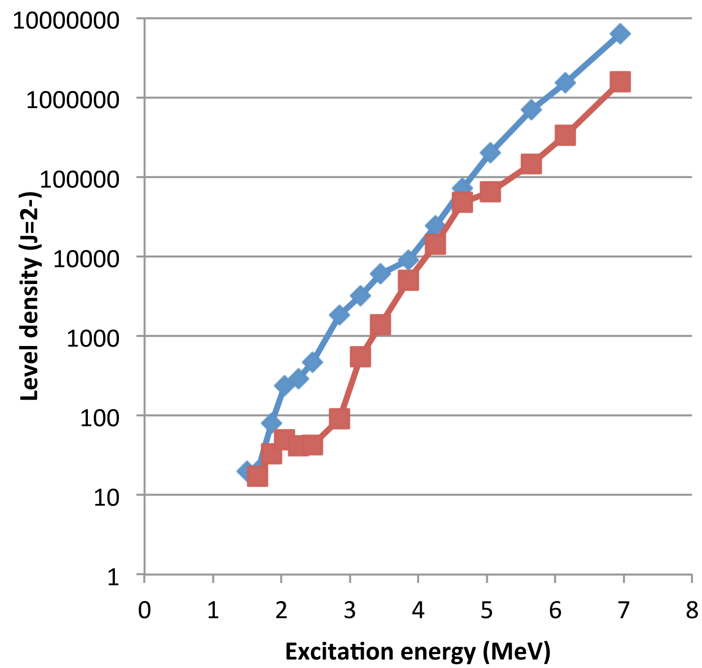
Example B): Pu-239+n.

- This is a fissile nucleus with barrier well below neutron separation energy. Therefore barrier heights are determined from Pu-238(*t,p*F)

Pu-238(t,pf):rn data;V=5.6,5.3: V=5.6,5.4



- Barrier level densities

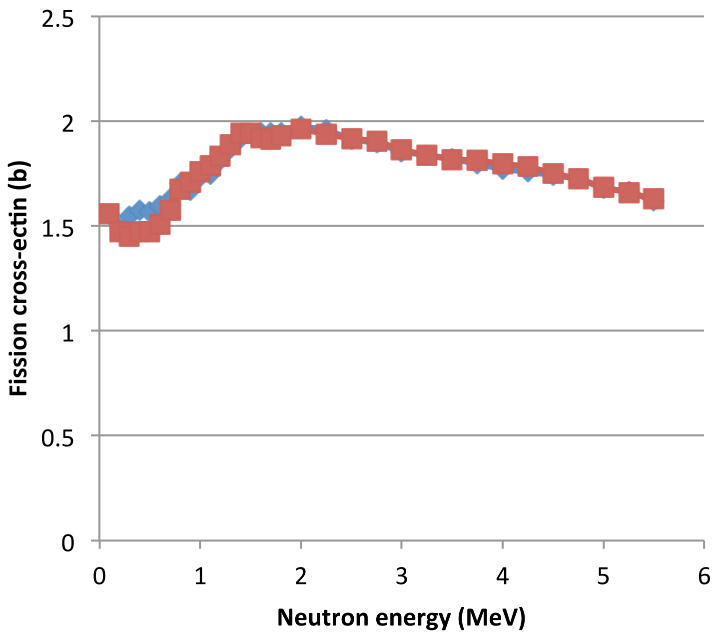


Inner barrier model; Δ_p = 1.0 MeV, Δ_n = 0.79 MeV

Outer barrier fitted to cross-section, LD can be approximated by model with Δ_p = 1.1 MeV, Δ_n = 0.9 MeV

Plutonium isotope summary

- Fit to $^{239}Pu(n,f)$ cross-section



- Blue rhomboids - ENDF-B7
- Red squares - AVXSF calculation

- Note: Pairing gap parameters increase with deformation.

- **Barrier heights of Pu series:**
- The Table below gives the best fit barrier heights to date for an extensive sequence of Pu isotopes

CN	237	238	239	240	241	242	243	244	245
V_A	5.6	5.8	6.05	5.65	5.91	5.4	5.88		5.59
V_B	4.95	5.65	5.55	5.23	5.67	5.3	5.43		5.08

- Note the overall trend of a maximum about A = 240, but especially the odd-even staggering, which can be explained by pairing gap increasing with deformation, in agreement with analysis of barrier level densities. This pairing energy dependence is in qualitative agreement with theory of Dave Madland .

Other Barrier Forms: Th-region nuclides

- Barrier topography:

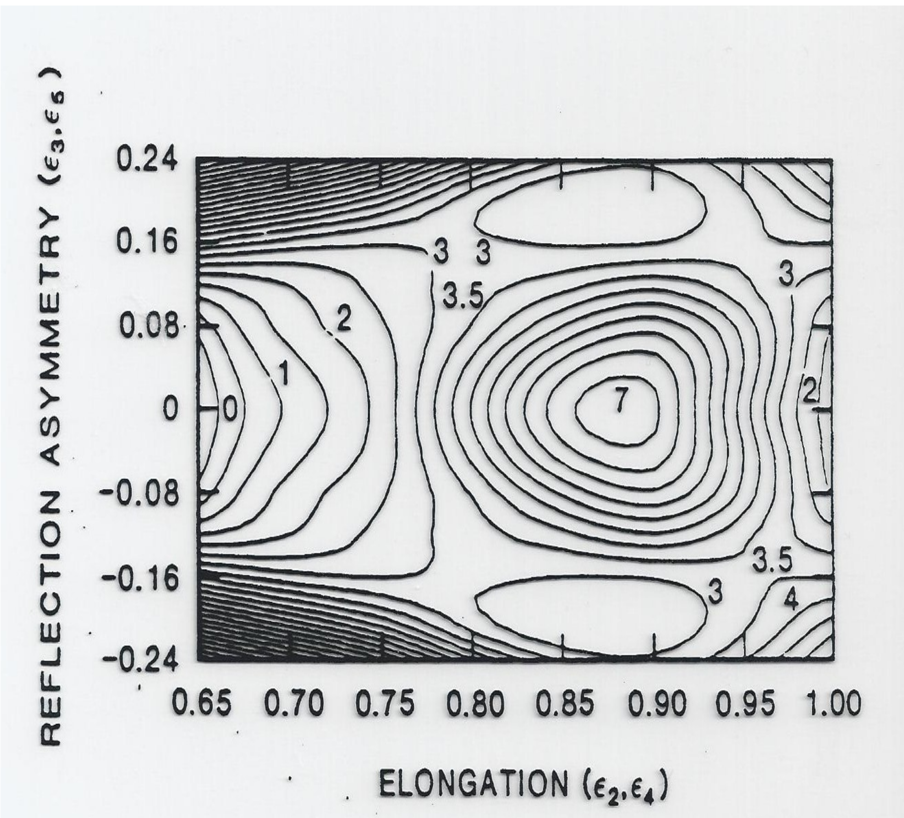
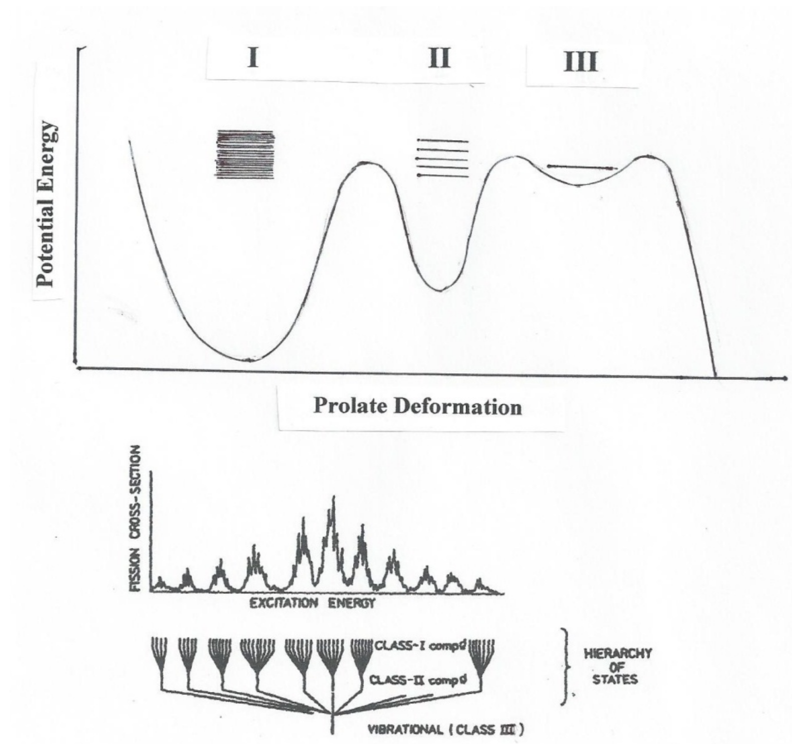


Figure 22. Potential energy contours calculated for ^{232}Th. After Åberg et al.(1980)

- Vibrational, intermediate and fine structure



Concluding Remarks

- Phase 1: Liquid Drop Model + quantum and nuclear modifications
  - barrier tunnelling
  - Barrier transition states
- Phase 2: Modification by shell effects in deformed nucleus
  - Double-humped barriers for transuranic nuclides
  - Triple-humped barriers for lighter actinides
  - intermediate resonance structure
- Incorporation of Intermediate structure into formal R-matrix theory
- Quantum chaos – averaging over resonance structure
- Above barrier cross-sections – level densities at barrier deformations

Status of present knowledge

Good for: analysis (elucidation of barrier properties)
interpolation, extrapolation of cross-sections (incg. capture, inelastic)
to new energy ranges and nuclides)

Future Requirements and Prospects

- Better knowledge of CN formation cross-sections
- Coupled channels in inelastic scattering

- Further development of microscopic and Möller-Nix theory of potential energy landscape in deformation space
- Sound models and calculations of inertial tensor:
  - improvements of barrier tunnelling and penetration factors
  - improved estimates of barrier transition states of collective type
- Improved calculations of quasi-particle states and level densities at barrier deformations
- Direct modelling of coupling matrix elements and fission width amplitudes in R-matrix formalism of intermediate resonances