FIESTA 2014
Fission School Lectures

FISSION CROSS SECTION THEORY

J. Eric Lynn

***** ADAPTED FOR PRINTING *****

Pages marked (NOTES) are from supplemental document. *Slide numbers referenced in notes have not been changed to account for merging of notes with slides.* If there is confusion, please see original (unmerged) version of slides and notes.

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:

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

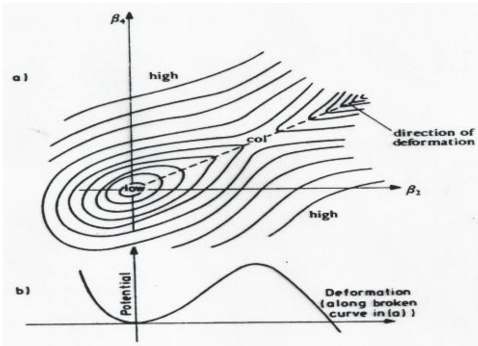
- ↓ ↓ ↓ ↓ ↓
- volume surface Coulomb isospin pairing
- (energy of classical charged liquid drop)
- For liquid drop model of fission the surface and Coulomb terms are given their classical dependence on drop shape (deformation)

(Notes)

References to mass formula:

Weizsacker, C.F., Z.Physik, 96, 431 (1935)
Bethe, H.A. and Bacher, R.F., 8,193 (1936)

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

(Notes)

- Fissility parameter. When the Coulomb energy of a sphere equals twice its surface energy the sphere becomes critically unstable towards spheroidal deformation followed by splitting into two parts:

$$x = \frac{E_c}{2E_s} = \frac{c_3}{2c_2}\left(\frac{Z^2}{A}\right)$$

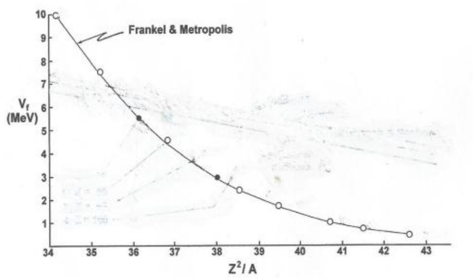
X = 1 when

$$\left(\frac{Z^2}{A}\right)_{crit} = \frac{2c_2}{c_3} \approx 50$$

For actinides $x \approx 0.7$ to 0.8, Z^2 /***A*** is known as the **Fissility parameter**

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



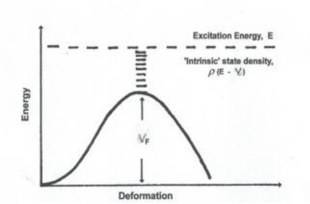
Note: experimental data on barrier heights for Z^2/A from 35-39 are in range 6.5 to 5.5 MeV

(Notes)

Reference: Frankel, S. and Metropolis, N., Phys.Rev. 72, 914 (1947)

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

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

(Notes)

- In the classical model fission will certainly occur if the excitation of the system is higher than the fission barrier energy V_F , but not if it is lower. Hence the transmission coefficient $T_F = 1$ if $E > V_F$, otherwise zero.
- When we translate the model to the nucleus, we must recognize that there are many different possible states of intrinsic excitation in which the nucleus may pass over the barrier. In their 1939 paper Bohr and Wheeler used this concept of the 'transition state' from chemical reaction theory as shown in the slide. The transmission coefficient is identified with the **Fission Strength Function** (ratio of fission width to level spacing) of nuclear cross-section theory.
- N. Bohr and J.A. Wheeler, *Phys.Rev.* **56,** 1939

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:

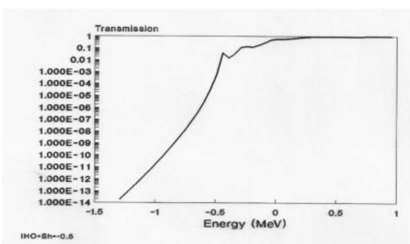
$$\sigma_F = \pi ƛ^2 \sum_{J,\pi} \frac{T_n^{J\pi} T_F^{J\pi}}{T_{tot}^{J\pi}}$$

- **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:

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

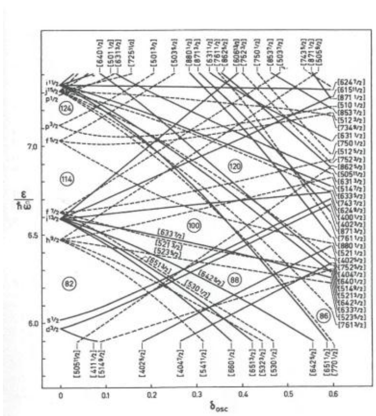
(Notes)

This expression for transmission coefficient with tunnelling is for a single transition state of energy *E'* (including barrier height).
Hill, D.L. and Wheeler, J.A., Phys.Rev.**89**, 1102
Note that other shapes of barrier can give weak maxima and minima in the penetrability factor.
For example, an inverted H.O. barrier with a constant "shelf" beyond the peak andlittle lower in energy
gives a transmission coefficient showing weak maxima and minima:

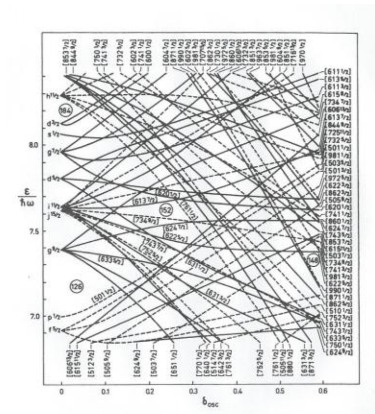


Effects of angular momentum and parity on Barrier:
Nilsson single particle level energies as function of deformation

Protons



Neutrons



(Notes)

These are eigenvalues of a nucleon in a spheroidal harmonic oscillator potential with parameters matching as far as possible those of a nucleus potential field. If $\omega_1 = \omega_2$ are the circular frequencies of the minor axes and ω_3 that of the major axis, the deformation parameter is defined as

$$\delta_{osc} = 3\frac{\omega_{1,2} - \omega_3}{2\omega_{1,2} + \omega_3}$$

The mean oscillator frequency is defined as

$$\varpi = \frac{1}{3}(\omega_1 + \omega_2 + \omega_3)$$

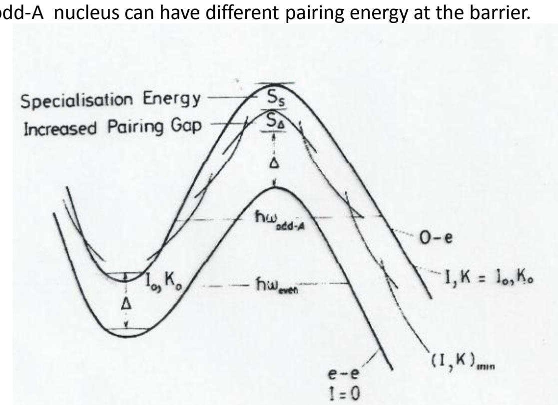
The asymptotic quantum numbers $\left|Nn_3\Lambda\Omega\right\rangle$ labelling each nucleon orbital are the total oscillator number *N*, the number of quanta perpendicular to the symmetry axis, n_3, the orbital angular momentum along the symmetry, Λ, and the component of total angular momentum along the symmetry axis Ω. A low-lying state of an odd-A nucleus can be a single quasi-particle, in which case the quantum number Ω is the projection of the total angular momentum on the symmetry axis, *K*.

Note the areas of sparsity of levels near zero deformation for magic number of nucleons 82, 126 etc and similar, less conspicuous, areas at different nucleon numbers at higher deformations.

Ref.: Gustafson, C., Lamm, I.L., Nilsson, B., Nilsson, S.G., *Arkiv.Fysik*,.**36,** 613 (1967)

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
- .´. 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.



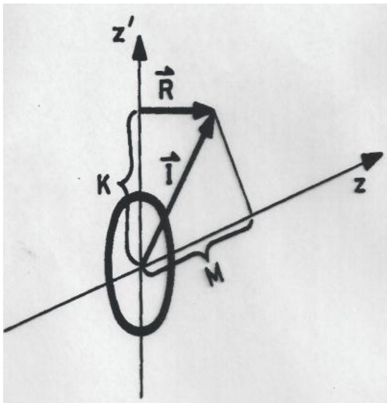
(Notes)

- With other quantum numbers (I^{π}, K) characterizing the system, as in an odd-A nucleus, specialization energy occurs at the barrier. This diagram shows, first, the potential energy for an e-e nucleus in its ground state (fully condensed at all deformations).
- The next higher odd-A nucleus has a quasi-particle excited above the condensed e-e state. Its potential energy has additional excitation energy for its ground state I^{π} , K at normal deformation. As deformation increases the excitation energy crosses that for other states of different $I^{\pi'}$, K' (see Nilsson diagrams) and will have different energy at the barrier owing to the specialization of its quantum numbers.
- Likewise, if pairing forces are dependent on deformation an odd-A nucleus can have different pairing energy at the barrier from that at the ground state and this affects the quasi-particle energy that is added to the e-e condensate:

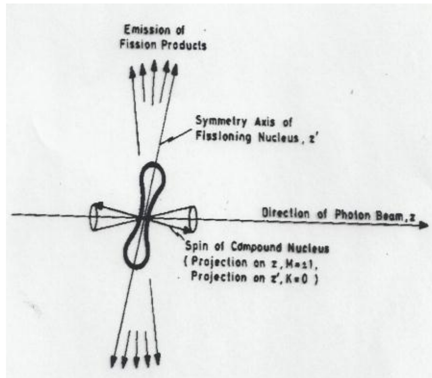
$$e_{i,qp} = \sqrt{(\varepsilon_i - \varepsilon_F)^2 + \Delta^2}$$

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



(Notes)

Concept of Individual Transition States

- Bohr and Wheeler had already used the idea that the nucleus could be in one of many different states of internal excitation as it passed over the barrier and used the density of these for estimating the fission transmission coefficient.
- Aage Bohr pointed out that an individual intrinsic state (now generally known as a transition state or fission channel) could have an influence on detailed fission properties.
- He observed that in low energy photofission of an e-e nucleus the fission products have a sideways angular distribution with respect to beam direction; this altered at higher energy, becoming more isotropic. He attributed this to the influence of the *K* quantum number in the lowest transition states. The ground state of the nucleus has $J^{\pi}= 0^{+}$, K=0. The E1 photon, which has spin projection on the beam direction $M = \pm1$, puts the nucleus in a $J^{\pi}= 1^{-}$ state which passes over the barrier in a rotational state of the $K^{\pi} = 0^{-}$ band. This changes at higher energy as a fission channel with $K^{\pi} = 1^{-}$ opens up.
- Thus it appears that the K quantum number of the transition state is frozen into the fissioning nucleus beyond the saddle. (See further discussion of this point by Barabanov and Furman)
- It follows that the individual transition states could affect other properties of the fission products, such as their dependence of overall yield on resonances in the excitation cross-section (see below).

Bohr, A., *Proc.Int.Conf.peaceful uses atom.en., Geneva,1955,* **2,** 220 (United Nations, New York, 1956)

Barabanov, A.I. and Furman, W.I., *Zeit. Phys.*A**357,** 411 (1997)

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	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
1·0 MeV →	~0·9	1^-	1^- 2^- 3^-, etc.	1 quantum of bending vibration

- 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) →				

(Notes)

This table is from a compilation given in J.E.Lynn, *Theory of Neutron Resonance Reactions*,p.396 (Oxford University Press, 1968)

Analysis is based on a single-hump fission barrier. Much of the information in the Table comes from a discussion given by

Wheeler, J. A., in *Fast Neutron Physics* (eds. J.L.Fowler and J.B.Marion), v.2, p.2051 (Interscience, New York, 1963).

Some estimates of Transition state energies come from experimental work referenced in Table 8.1 of Lynn (1968)

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):

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

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

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

(Notes)

Wigner, E.P. and Breit, G., *Phys.Rev.* **49,** 519 (1936)

- Low energy neutron cross-sections are dominated by resonances that are the manifestation of the virtual states of the excited compound nucleus, through which it decays. Although the resonances cannot generally be observed at higher energies, because of lack of resolution, they remain the essential feature and the basis of the theory of nuclear cross-sections up to several MeV of excitation energy.

- The average entrance channel width $\Gamma_{\lambda a}$ increases with increasing energy of particle *a* because of increasing penetration factor.

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:

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

- 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.

(Notes)

The reduced width amplitude $\gamma_{\lambda n}$ is the projection of the CN wave function amplitude on the channel wave function at the channel entrance and is expected to have zero-mean gaussian distribution owing to the highly complicated wave function expected when the compound nucleus is at high excitation. This transforms into the Porter-Thomas distribution for the reduced widths.

Porter, C.E. and Thomas R.G.,*Phys.Rev.***104,** 483(1956)

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:

$$\left\langle \sigma_{ab} \right\rangle = \pi ƛ^2 T_a T_b / T$$

where the transmission factors *are*:

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

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

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

(Notes)

Hauser, W. and Feshbach, H., *Phys.Rev.***87,** 366 (1952)

The Hauser-Feshbach theory is the formal application of Bohr's theory of the Compound Nucleus and its principle of independence of formation and decay applied to the calculation of reaction cross-sections. The transmission coefficient is the probability that the CN wave-function will (i) find itself in the configuration of channel wave function *c* at the channel entrance, and (ii) will overcome mis-matching wave-number factors and potential barriers in the channel. This corresponds to the factorization of a partial width into a reduced width and penetration factor (slide 13).

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*:

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

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

k (= $1/\lambda\!\!\!^{-}$) 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

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

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 <u>collision matrix</u> element

$$U_{cc'}$$

(Notes)

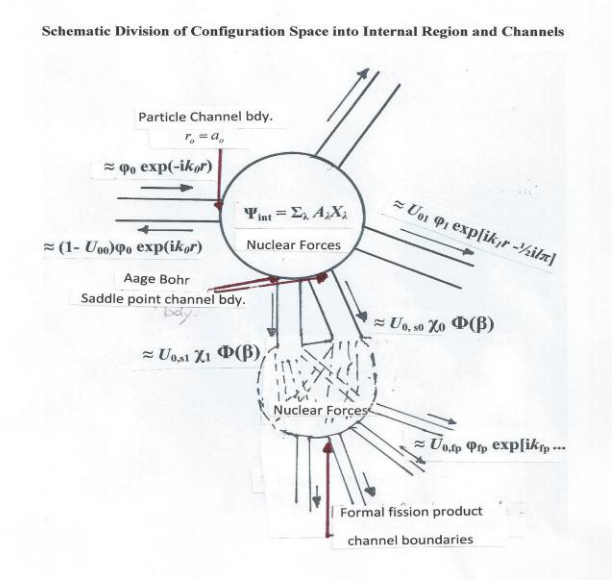
Refs.: Wigner, E.O. and Eisenbud, L., *Phys. Rev.***71,** 29 (1947)

Lane, A.M. and Thomas, R.G., *Rev.Mod.Phys.***30,** 257 (1958)

- Cross-section for a beam of neutrons to produce reaction *r* is σ_r = no.of events of type *r* per unit time per nucleus /neutron flux
- Wave function for unit flux plane wave travelling with velocity *v* and incorporating state of excitation of Target nucleus (and possibly projectile) α and channel spin $\bar{s} = \bar{I} + \bar{i}$ with projection *v* on *z*-axis:

$$(1/v^{1/2})\exp(ikz)\psi_{\alpha s v} = (\pi^{1/2}/krv_\alpha^{1/2})\sum_{\ell=0}^{\infty}(2\ell+1)^{1/2} i^{\ell}[I_\ell(kr) - O_\ell(kr)]Y_{\ell 0}(\theta,\varphi)\psi_{\alpha s v}$$

Internal region and channels in nuclear configuration space



(Notes)

This schematic diagram attempts to explain the concept of channels in formal R-matrix theory and the modifications required to take into account the Aage Bohr concept of transition states when fission has to be treated. The essential feature of R-matrix theory is that there is an internal region of configuration space where nuclear forces operate; there are no significant nuclear forces outside this internal region except those which can be characterized as a potential field acting on a single particle. This internal region corresponds to the Compound Nucleus. Outside the internal region, configuration space is broken up into channels in which the system consists of a particle (a nucleon or composite particle such as an α-particle) and a residual nucleus. The latter is in a discrete state, which may be its ground or an excited state. (If the particle is composite it too may be in an excited state). The particle and residual nucleus carry their own angular momentum and parity and have a relative orbital angular momentum ℓ. All these characteristics are wrapped up into a single function φ_c while the relative radial motion of an outgoing wave at very large separation is given in the factor $\exp[ik_cr_c - ½il_c\pi]$. Thus the channel wave-functions are in the form $\approx U_{0c}\varphi_c \exp[ik_c - i\ell\pi/2]$.

Real energy independent boundary conditions are set at channel entrances from the internal region. The discrete eigenfunctions X_λ with eigenvalues E_λ denote the solutions of the nuclear hamiltonian within the internal region.

The lower part of the diagram shows the features of configuration space required to describe fission. The main degree of freedom here is the elongation, β, of the compound nucleus towards the scission point. The first stage of this comprises the Aage Bohr transition states at the saddle-point. The "channel" wave functions are composed of the wave-function Φ(β) for the deformation β and the state of intrinsic excitation χ_μ. Beyond these saddle-point channels the nucleus enters a region where greatly increased internal excitation energy becomes available to produce highly complicated intrinsic state mixing. At the extreme deformation of this part of the internal region - the scission point - the entrances of the formal fission product channels are found. These are described in a similar way to the particle channels.

Wavefunctions in regions of configuration space

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

- External region wavefunction :

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

$\mathscr{I}$ and $\mathscr{O}$ are incoming and outgoing wave functions generalized to specific channels by incorporating intrinsic excitation and angular momentum couplings

- The cross-section is

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

(Notes)

- Nuclear forces in Internal Region affects outgoing waves. New outgoing waves appear in other channels c'. Their amplitudes are denoted by collision matrix elements $U_{cc'}$, c denoting the entrance channel with angular momentum coupling, parity and target state of excitation. In the external region the wavefunction is

$$\Psi_{ext} = \sum_c (\pi^{1/2}/k_c)(2\ell_c+1)^{1/2} \sum_{J=|\ell_c - s_c|}^{J+s_c} \langle \ell_c 0 s_c \nu_c \,|\, JM(=\nu_c)\rangle \left[\mathscr{I}_{c(s_c \ell_c JM)} - \sum_{c'} U_{cc'} \mathscr{O}_{cc'(s_{c'}' \ell_{c'}' JM)} \right]$$

$\mathscr{I}$ and $\mathscr{O}$ are incoming and outgoing wave functions generalized to specific channels by incorporating intrinsic excitation and angular momentum couplings

- The cross-section is

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

- The cross-section integrated over angle is

$$\sigma_{cc'} = \left(\frac{\pi}{k^2}\right) \sum_J \frac{2J+1}{(2i+1)(2I+1)} \sum_{s=|I-i|}^{I+i} \sum_{s'=|I'-i'|}^{I'+i'} \sum_{\ell=|J-s|}^{J+s} \sum_{\ell'=|J-s'|}^{J+s'} \left| \delta_{c(l,s),c'(\ell' s')} - U_{c,c'} \right|^2$$

Internal region wavefunction

- Wave function for Internal Region

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

- 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

$$\mathbf{U} \square \Omega\mathbf{P}^{1/2}\{\mathbf{1} - \mathrm{i}\mathbf{PR}\}^{-1}\{\mathbf{1} + \mathrm{i}\mathbf{PR}\}\mathbf{P}^{-1/2}\Omega$$

- The R-matrix is the central quantity here:

(Notes)

- A complete set of discrete eigenstates is set up for the internal region by placing real boundary conditions at the channel entrances and solving the full nuclear hamiltonian. These are denoted by E_{λ} and their wavefunctions by X_{λ}. The internal wavefunction is expanded accordingly

$$\Psi_{\text{int}} = \sum_{\lambda} \mathrm{X}_{\lambda}$$

- Evaluation of the collision matrix is made by matching logarithmic derivatives of wavefunction of internal region to those of outgoing wavefunctions in channels (latter denoted by $L_c = S_c + iP_c$; the real part S_c is the shift factor, P_c is the penetration factor containing the effects of potential barriers in channels).
- The expression for the collision matrix is
-

$$\mathbf{U} = \Omega\mathbf{P}^{1/2}\{\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B}\}^{-1}\{\mathbf{1} - \mathbf{R}(\mathbf{L}^{*} - \mathbf{B})\}\mathbf{P}^{-1/2}\Omega$$

- The R-matrix is the central quantity here. **It contains values (projected on to spin and excited state of the channel function) of internal eigenstates at channel entrances a_c ; these are denoted $\gamma_{\lambda c}$.** They are the **reduced width amplitudes**. **B a**nd **Ω** are diagonal matrices containing the boundary conditions and phase factors at the channel entrances.
- The R-matrix element for entrance channel *c*, exit channel c' is

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

(Notes - continued)

Single-level formula: If only one level λ is retained in the sum, the inversion of (**1-RL**) can be done exactly and the Breit-Wigner formula is obtained

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

with level shift

$$\Delta_\lambda = \sum_c (S_c - B_c) \gamma_{\lambda c}^2$$

partial widths $\Gamma_{\lambda c''} = 2P_{c''} \gamma_{\lambda c''}^2$ and total width $\Gamma_\lambda = \sum_{c''} \Gamma_{\lambda c''}$. The effect of spins (target and projectile spins *I, i* and orbital angular momentum ℓ) coupling to total angular momentum *J* is contained in the spin-weighting factor *g(J).*

Note the 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.

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

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

- $\Delta_{\lambda} = \sum_{c"} (S_{c"} - B_{c"})\gamma_{\lambda c"}^2$ 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 <u>nuclear component</u> $\gamma_{\lambda c"}^2$ and a channel component, the <u>penetration factor</u>, which contains the effect of potential variations in the channel region e.g., for fission, the Hill-Wheeler factor.

(Notes)

The more general form, when the boundary conditions are not set equal to the shift factors, is:

$$\mathcal{R}_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_{\lambda} - \Delta_{\lambda}^{e} - E - \Gamma_{\lambda}^{e}/2}$$

Δ_{λ}^{e} being the contribution to the level shift from the eliminated channels.

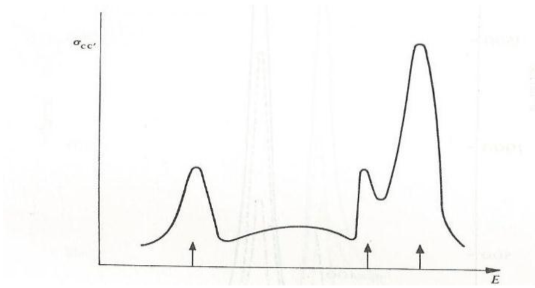
Note: the level shift, both here and in the single-level approximation above, can be made zero at a specific energy by equating the boundary conditions B_c to the shift factors S_c. Since the energy variation of *S* is usually very small over the range of a level spacing *D* the resonance is thus identified with the eigenstate, giving physical content to the formal theory.

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 $\mathfrak{R}$-matrix:

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

- 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.



(Notes)

Ref. Reich, C.W. and Moore, M.S., *Phys.Rev.* **111**, 929 (1958)

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

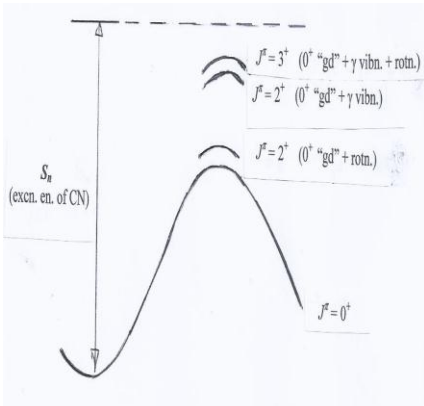
$$\left\langle \gamma_{\lambda n}^2 \right\rangle = \left(\hbar^2 / Ma^2\right)\left((D / D_{sp}\right) = \left(D / \pi K a_0\right)$$

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

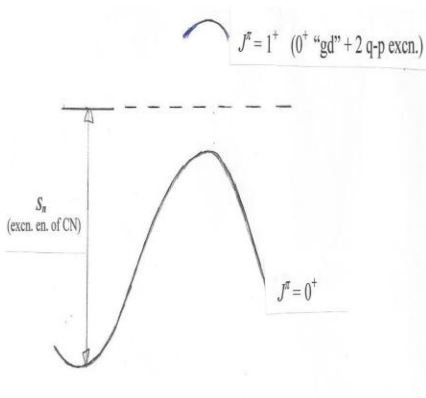
$$\Gamma_n^0 / D = 2P(1eV)\gamma_n^2 / D = 2k(1eV)a_0\gamma_n^2 / D$$

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

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



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



(Notes)

In the case of odd-A target nuclei the target nucleus spin can have an important effect on the average fission width of the slow neutron resonances. For example, the target nucleus ^{233}U (I^{π} = 5/2^{+}) has resonances with spin J^{π} = 2^{+}, 3^{+} in its neutron cross-section. The lowest transition states at the barrier are;

a) for J = 2

2+ - a member of the "ground" state rotational band,

2+ - the gamma vibrational state lying at several 100 keV, but still well below the neutron separation energy

b) for J = 3

3+ - a member of the rotational band built on the gamma vibration (still below the neutron separation energy)

.

By contrast, the target nuclei ^{239}Pu (I^{π} = 1/2^{+}) and ^{237}U have resonances with spin J^{π} = 0^{+}, 1^{+} in their neutron cross-section. The lowest transition states at the barrier are;

a) for J = 0

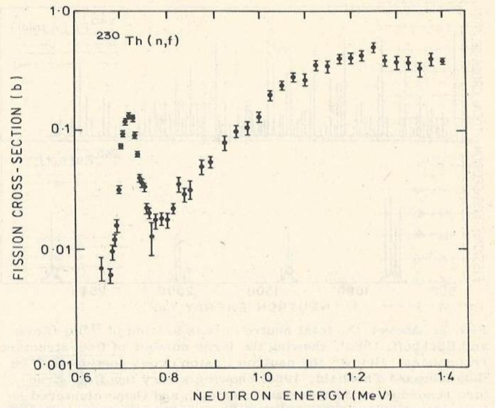
0+ - the "ground" state rotational band (these resonances are expected to have large fission widths),

b) for J = 1

1+ - Either a combination of the bending vibration and the mass-asymmetry vibration or a 2-quasi-particle state. Both are expected to be above the neutron separation energy, giving these resonances unusually small fission widths for a fissile nucleus.

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)



(Notes)

- For a quarter century or so fission theory depended on a qualitative version of the liquid drop model, with quantal and nuclear physics concepts incorporated.
- The difficulties so far met with in the liquid drop theory tended to be glossed over. These were of course the systematics of barrier heights and also the long-standing problem of highly asymmetric mass yields leading to questions about the pathway through the potential landscape from saddle to scission. In the 1950's Fong had developed a theory which seemed to offer a way to explain this, relying on shell effects in the level densities of the incipient fission products but could not quite be made to work. This was probably one of the first attempts to put shell effects into fission theory.

But with great improvements in experimental techniques further cracks began to appear in the LD edifice.

1960's higher energy resolution measurements of fission cross sections of non-fissionable nuclei showed signs of structure, dips following rising cross-sections. Wheeler explained these asdue to inelastic scattering competition as successive levels in the residual nucleus became energetically available. This explanation failed when new measurements by Jones (1965) at Harwell showed peak with a 4:1 ratio to the following dip.

High resolution measurements by James *et al* showed this ratio to be about 10:1

Fong, P., *Phys.Rev.***102**, 434 (1956)
Wheeler, J. A., in *Fast Neutron Physics* (eds. J.L.Fowler and J.B.Marion), v.2, p.2051 (Interscience, New York, 1963).

James, G.D., Lynn, J.E. and Earwaker, L. *Nucl.Phys.*, A**189,** 225 (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 $\approx$ 14ms
- Low spin
- High excitation energy ≈ 3 MeV

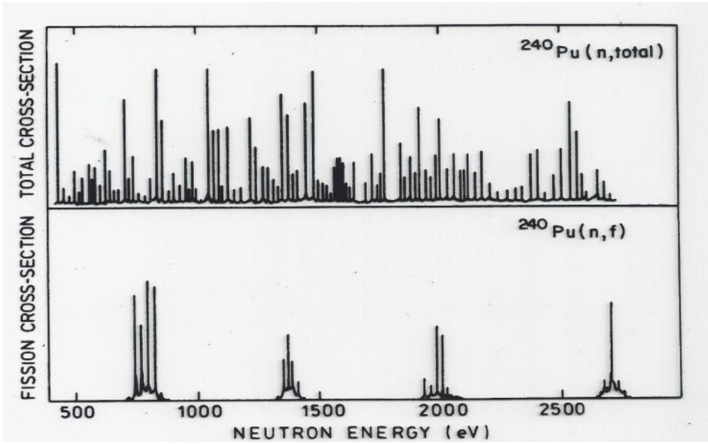
(Notes)

Flerov, G.N. and Polikanov, S.M., *Compt. Rend.Cong.Int.Phys.Nucl.*,**1, 407** (Paris, 1964).

Many other spontaneously fissioning isomers were subsequently discovered, mainly in isotopes of plutonium, americium and curium.

Narrow Intermediate Structure in Fission cross-sections

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



(Notes)

Unlike slide 24, which is for a neutron energy region covering several 100keV and totally washes out the underlying resonance fine structure, the cross-sections of ^{240}Pu shown here covers a few 100eV and shows the strengths of all the individual resonances comparing total (proportional to the neutron width) above with fission strength (depending on both neutron and fission width) (below). The scatter in the strengths of the total cross-section resonances is due to the Porter-Thomas distribution. The tight clustering of fission strength, the clusters being separated by several hundred eV, cannot be attributed to a stochastic process.

Migneco, E. and Theobald, J.P., *Nucl.Phys.* A**112,** 603 (1968)

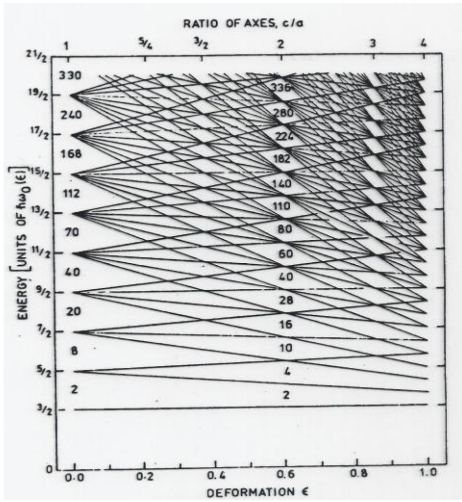
Weigmann, H., *Z.Phys.* **214, 7** (1968)

A similar striking situation was discovered for ^{237}Np about the same time.

Paya, D., Blons, J., Derrien, H., Fubini, Michaudon, A. and Ribon, P., *J. Phys.*(Paris) **29**, 159 (1968)

Shell effects in deformed nuclei – Strutinsky theory

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



(from Nix (1972))

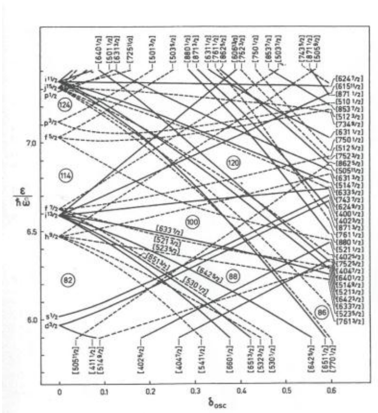
(Notes)

Note the significant "shell" gaps esp. at major to minor axis ratios 3:2, 2:1 and 3:1

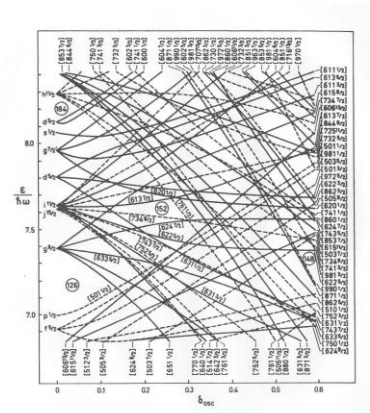
Nix, J.R. *Ann.Rev.Nucl.Sc.*.**22**, 65 (1972)

Nilsson diagrams: deformed HO + spin-orbit coupling

Protons



Neutrons

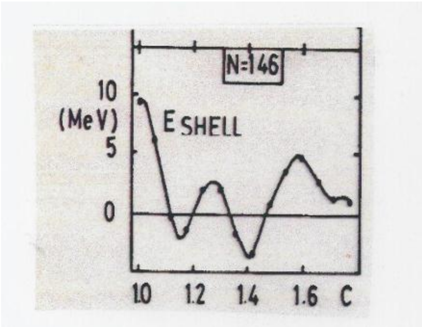


(Notes)

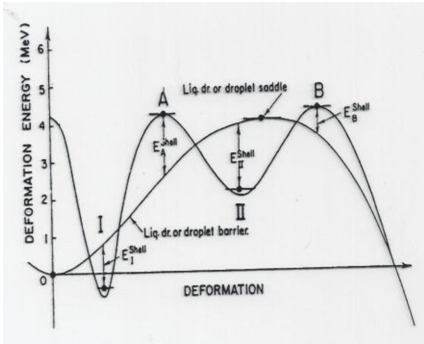
This is the same as slide 9. However, now note regions of sparse single-particle level density at deformations of about 0.25 and 0.4.

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

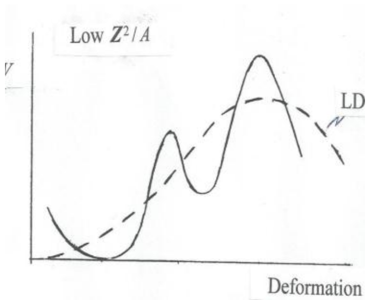


(Notes)

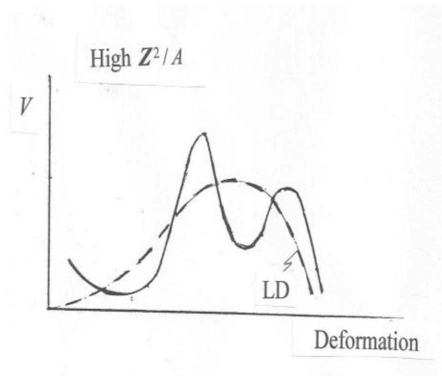
Strutinsky, V.M., *Nucl.Phys.* A**95.** 420 (1967)

Barrier height dependence on Z^2/A

Low Z^2/A



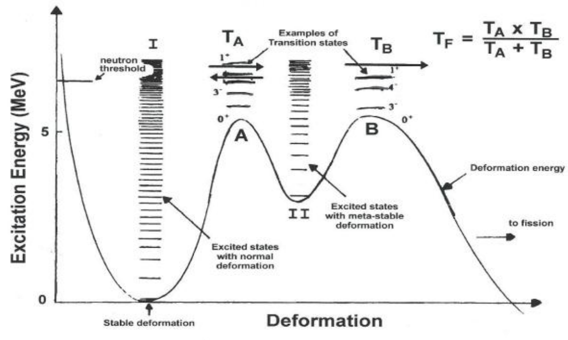
High Z^2/A



(Notes)

The variation of the shell correction on deformation is not expected to change much with significant changes in Z and N, whereas the liquid drop energy varies strongly both in the height of the barrier and its position with changing 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:

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

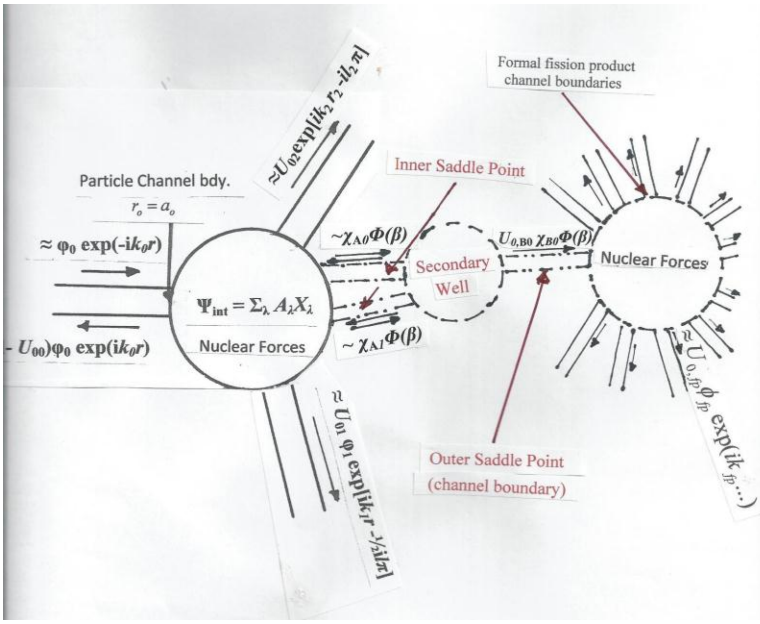
(Notes)

Bjornholm, S. and Strutinsky, V.M., *Nucl.Phys.*A**136** 1 (1969)

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

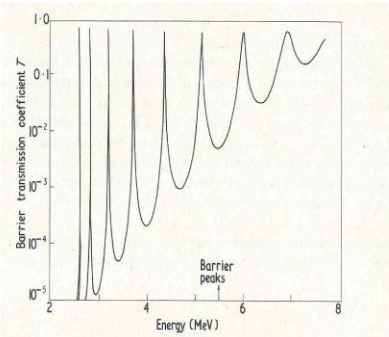


(Notes)

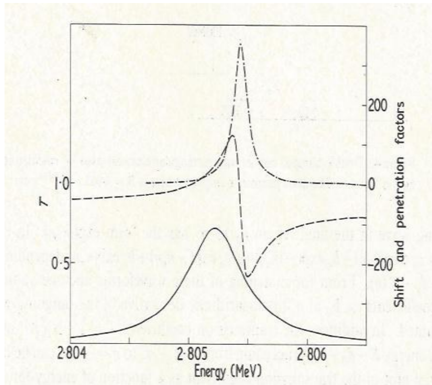
The region associated with increasing elongation is now elaborated to include a secondary well and an outer barrier with Aage Bohr transition states; at the outer barrier these are taken as the class-II fission channel boundaries with which the formal fission product channel amplitudes are correlated. The transition states at the inner barrier govern the coupling of the class-II states in the secondary well to the class-I states in the main part of the internal region, the primary well of the elongation variable.

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

- Transmission coefficient



- Shift and penetration factors

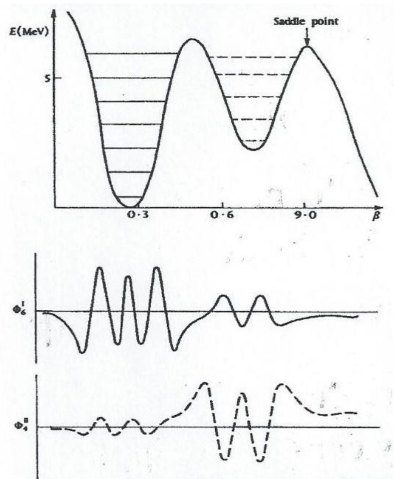


(Notes)

Residual nuclear forces remain after the potential of the secondary well and beyond is subtracted. If these were negligible, we could place the channel boundary at the inner barrier. The barrier now consists of the outer barrier, the secondary well and inner barrier. The transmission coefficient through this now shows resonance features that are undamped at the peaks but have widths that depend strongly on the excitation energy available. The logarithmic derivative of the elongation channel wave-function, giving the shift and penetration factors of R-matrix theory, has a dispersive character as it traverses the transmission resonance peaks. An example is shown for one "resonance" in the r.h. diagram. This logarithmic derivative provides the intermediate structure for the fission widths of the fine structure resonances from the main central part of the internal region.

Lynn, J.E., *J.Phys.* A**6**, 542

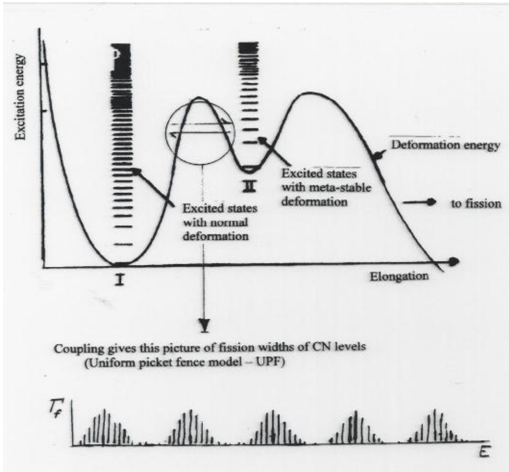
Vibrational wave functions for Double well; discrete states with real bdy.condn.at outer barrier



(Notes)

Real boundary conditions are imposed at the outer peak. The discrete eigenstates of the vibrational hamiltonian that have eigenvalues lower than the inner peak have either large amplitude in the primary well and small amplitude in the secondary well or vice versa (unless there is an accidental degeneracy). The former states are designated class-I vibrational states, the latter class-II. Eigenstates with higher energy should all have significant amplitude in the secondary well and therefore be included with the class-II set.

CN states in double well



(Notes)

Compound nucleus states can be considered as combinations of vibrational states and states of internal excitation. The main contribution to the density of the CN states comes from the internal excitations. Most excitation energy is available for these when the vibrational component is one of the lowest class-I vibrational states. Hence these, the fine structure resonance levels in first approximation, are considered to be localized in the primary well and are known as class-I CN states. States that have class-II states as their major vibrational component are much less dense, because of the much lower internal excitation available are are known as class-II CN states.

If the inner barrier were infinite these classes would be exact. In fact there is mixing of the two sets across the inner barrier. This causes the mixing of the class-II CN states into the class-I fine structure CN states as shown in the lower part of the slide.

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:

$\boldsymbol{\Phi_v(\beta)}$ (eigenvalues ε)

- Eigensolutions of *H* are expanded:

$$\boldsymbol{X_\lambda = \Sigma_\lambda C_{\lambda,\mu v}\chi_\mu\Phi_v}$$

(Notes)

The hamiltonian of the internal region is written schematically in three components

$$H = H_{\text{int}}(\beta_0,\xi) + H_{def}(\beta) + H_{coup}(\beta,\xi)$$

The solutions of the intrinsic part (at a fixed deformation β_0) are denoted by $\chi_\mu(\xi)$. where ξ denotes the set of internal degrees of freedom and eigenvalues are denoted by E_μ

The solutions of the deformation part are vibrational-type functions $\Phi_v(\beta)$ in the deformation variable β and eigenvalues ε_v

(These are defined as discrete states with suitable real boundary conditions applied). The eigensolutions of the full hamiltonian are expanded:

$$\boldsymbol{X_\lambda = \Sigma_\lambda C_{\lambda,\mu v}\chi_\mu\Phi_v}$$

(A full exposition may be found in Bjornholm, S. and Lynn, J.E., *Rev.Mod.Phys.*, **52,** no.4 (1952) p.754)

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

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

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

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

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

(Notes)

- The characteristics of the vibrational functions (see Slide 36) suggest that the basis states can be separated into two classes:

- Class I: with negligible amplitude in 2y well: $\mu'\nu_I'$
- Class II: with main component of amplitude in 2y well: $\mu''\nu_{II}''$

- We can now solve the Scrodinger eqn. for the Hamiltonian with the limited bases provided by these two classes of vibrational wave functions. The Hamiltonian matrix elements for the first basis are

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

This Hamiltonian can be diagonalized (conceptually) to give the class-I eigenstates with wave function expansions

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

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.

(Notes)

- Class-I states contain the zero-phonon vibrational state Φ_0 in their eigenfunctions (as well as the lowest few phonon states above this). Hence, the ground state and lowest excited states of the Compound Nucleus are included in the class-I set.
- This element of a configuration also allows maximum available excitation energy to be used for constructing intrinsic states (particle degrees of freedom, other collective modes). Hence, class I states have high density.
- Φ_0 is essential for CN component for reduced neutron width amplitude (for neutron emission leaving residual nucleus in its ground state). Also for inelastic scattering.
- The class-I states have 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.

(Notes)

- Lowest class-II vibration in secondary well is some 2 - 3 MeV higher than the ground state in the primary well. Hence the available energy for intrinsic excitation is much lower, giving a much lower density of class-II states.
- Having no Φ_0 component the class-II states have no reduced neutron width and hence, in their pure form cannot be excited by neutron bombardment.
- On the other hand they have, from the higher class-II vibration components, significant amplitude at the outer barrier and hence have fission widths.
- The lowest state in their spectrum is the spontaneously fissioning isomer. Hence, radiation from higher class-II states terminates at the isomer. Negligible overlap with class-I states prevents "cross-over" radiation to class-I states

Final Diagonalization of Hamiltonian

- Full Hamiltonian:

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

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

(Notes)

- We have now effectively partitioned the full Hamiltonian matrix thus:

$$
\begin{array}{cc}
\mathbf{H}_{\mathrm{I,I}} & \mathbf{H}_{\mathrm{I,II}} \\
\mathbf{H}_{\mathrm{II,I}} & \mathbf{H}_{\mathrm{II,II}}
\end{array}
$$

with the sub-matrices $\mathbf{H}_{\mathrm{I,I}}$, $\mathbf{H}_{\mathrm{II,II}}$ already diagonalized.

- The off-diagonal sub-matrices have matrix elements (for $\mathbf{H}_{\mathrm{I,II}}$)

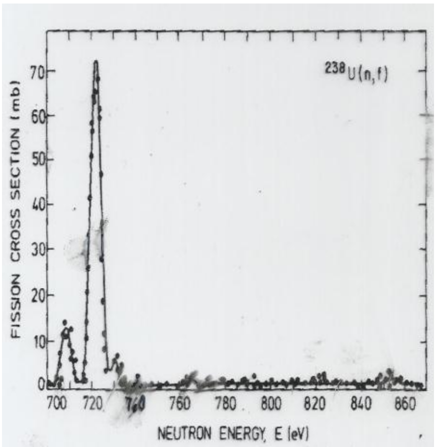
$$\langle\lambda_{\mathrm{I}} \,|\, H_{coup} \,|\, \lambda_{\mathrm{II}}'\rangle = \Sigma_{\mu\nu(\mathrm{I}),\, \mu'\nu'(\mathrm{II})} \langle \lambda_{\mathrm{I}} \,|\, \mu\nu_{\mathrm{I}}\rangle\langle\mu\nu_{\mathrm{I}} \,|\, H_{coup} \,|\, \mu'\nu_{\mathrm{II}}'\rangle\langle \mu'\nu_{\mathrm{II}}' \,|\, \lambda_{\mathrm{II}}'\rangle$$

(and similarly for $\mathbf{H}_{\mathrm{II,I}}$)

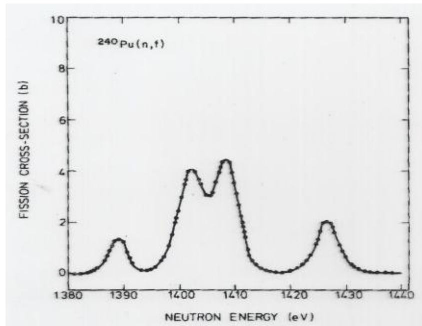
- Because of the weak spatial overlap between the vibration modes these mixing elements between Class I and II CN states are small in the excitation region near and below the fission barrier. Perturbation and similar techniques can be used to elucidate the properties of the final states of the full Hamiltonian.

Very weak mixing: perturbative treatment

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



(Notes)

Reference for ^{238}U: DiFillipo, F.C., Perez, R.B., de Saussure, G., Olsen, D.K. and Ingle, R.W., *Nucl.Sci.Eng.*,**63**, 153 (1977)

Reference for ^{240}Pu: Auchampaugh, G.F. and Weston, L.W.,*Phys.Rev.*, **C12,** , 1350 (1975)

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.

(Notes)

Specialization of the exact solution for uniform coupling matrix element we obtain
Lorentzian profile of R-matrix state reduced fission widths:

$$\gamma^2_{\lambda F} = \frac{H_c^2 \gamma^2_{\lambda_{II} f}}{(E_{\lambda_{II}} - E_\lambda)^2 + \pi^2 H_c^2 / D_I^2 + H_c^2}$$

The half-width W is known as the coupling width:

$$\Gamma_{\lambda(\mathrm{II}),\,\mathrm{C}} = 2W = (2\pi H^2 / D_\mathrm{I})\sqrt{(1 + D_\mathrm{I}^2 / \pi^2 H^2)} \quad (\approx 2\pi H^2 / D_1 \text{ for } D_\mathrm{I} / \pi H >> 1)$$

which lets us write

$$2\pi\gamma^2_{\lambda f} / D_I = \frac{\Gamma_{\lambda_{II} c}\gamma^2_{\lambda f}}{(E_{\lambda_{II}} - E_\lambda)^2 + (\Gamma_{\lambda_{II} c} / 2)^2}$$

- The formula for eigenvalues is:

$$E_{\lambda_{II}} - E_\lambda = -\frac{\pi H_c^2}{D_I}\cot\left(\frac{\pi E_\lambda}{D_I}\right)$$

The spacing of eigenvalues becomes closer as they approach the class-II eigenvalue. Therefore. The strength function, the locally averaged reduced fission width to spacing ratio turns out to have a Lorentzian with half-width exactly $\pi H_c^2 / D_I$

Thus we have for the “coupling width” across the inner barrier A:

$$\Gamma_{II,c} = \frac{2\pi H_c^2}{D_I} = \frac{D_{II}}{2\pi} T_A$$

which we have related to the transmission coefficient across the inner barrier T_A.

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

$$\Gamma_{\lambda_{II}F} \ll \Gamma_{\lambda_{II}C}$$

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

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

Example:

(Notes)

- The intermediate resonance profile for the reduced fission widths of the R-matrix eigenstates, as shown above, is not yet the profile for the fission widths of the fine structure resonances. The coupling with the fission continuum has now to be included, through the calculation of the collision matrix.
- If the class-II state fission width is much smaller than its coupling width, $\Gamma_{\lambda_{II}f} \ll \Gamma_{\lambda_{II}c}$,

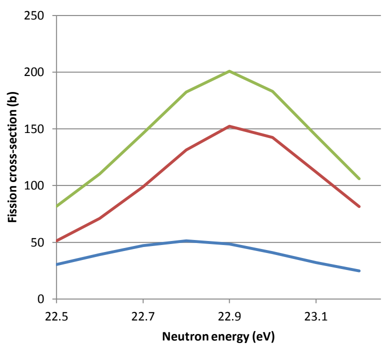
that profile does indeed approximate to the intermediate resonance profile, but if the R-matrix fission widths $\Gamma_{\lambda f} = 2P_f\gamma_{\lambda f}^2$ in a single saddle-point channel appreciably overlap, the solution of the R-matrix equations can give surprising results.

Ref.: Lynn, J.E., *Phys.Rev.Lett.*, **13**, 417 (1964)

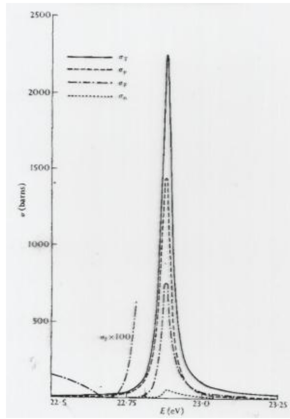
,, , *Proc. Int. Conf. Nuclear Reactions with Neutrons*, Antwerp, 1965 (ed. M. de Nevergnies *et al*), p.125 (North Holland, Amsterdam, 1966)

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.

(Notes)

- Mainly developed by Humblet and Rosenfeld in the 1960s, this formalism expands the collision matrix ($U_{cc'} = S_{cc'} + \delta_{cc'}$) about its poles in the complex energy field:

$$S_{cc'} = \mathcal{P}_c \mathcal{P}_{c'} \left[\mathcal{Q}_{cc'} - i \sum_{\ell} \frac{G_{\ell c} G_{\ell c'} \exp[i(\xi_{\ell c} + \xi_{\ell c'})]}{|\mathcal{P}_{\ell c}||\mathcal{P}_{\ell c'}|(\mathcal{E} - E_\ell^H + i\Gamma_\ell^H)} \right]$$

The *P* factors describe threshold behaviour in the channels and the ξ terms are pole phase factors. 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

$$\mathcal{E}_\ell^H = E_\ell^H - i\Gamma_\ell^H / 2$$

Ref.: Humblet, J. and Rosenfeld, L., *Nucl.Phys.* **26**, 529 (1961)

- Advantages: parameters of poles (e.g. pole width, partial width amplitudes) directly reflect characteristics of resonances in cross- section
- Disadvantages: unlike R-matrix theory, 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: $\Gamma_{\lambda(II)F} \gg D_I$ and $\Gamma_{\lambda(II)F} \gg \Gamma_{\lambda(II)C}$

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.

(Notes)

- 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.
- For a “broad” class –II R-matrix state ($\Gamma_{\lambda_{II} f} \gg D_I$ and $\Gamma_{\lambda_{II} f} \gg \Gamma_{\lambda_{II} c}$

  the fission widths of fine structure resonances (from poles):

-

$$\Gamma_{\lambda_{II} f} = \frac{D_I}{2\pi} \frac{\Gamma_{\lambda_{II} c}\Gamma_{\lambda_{II} f}}{(E_\lambda - E_{\lambda_{II}})^2 + \Gamma^2_{\lambda_{II} f}/4}$$

Ref.: Lynn, J.E., *J.Phys.* A**6**, 542

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

- Remaining class-II fission strength is

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

- This is 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.
-
- This suggests a hypothesis for a general formula:
-

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

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

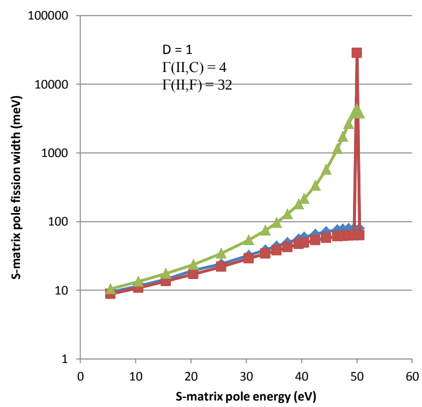
  $[1 - \Gamma_{\lambda(II),\, \mu'\nu(II)} / (\Gamma_{\lambda(II),\, \mu'\nu(II} + \Gamma_{\lambda(II),\, c})]\, \Gamma_{\lambda(II),\, \mu'\nu(II)}$

  (this is component for transition state **$\mu'\nu_{II}$**)
- This formula is approximate.
- General prescription:

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

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

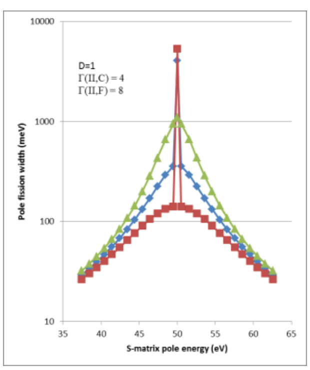
- Blue : S-matrix pole fission widths;
  Red : from hypothesis formula;
  Green: R-matrix fission widths.

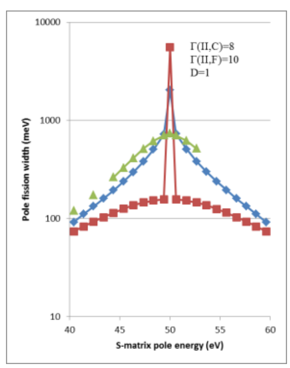


(Notes)

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

- This formula is too simplified, however. Some calculations of S-matrix pole fission widths from R-matrix fission width Lorentzians (width comprising only coupling) are shown below.





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

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

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

Variance is

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

- 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.

(Notes)

- Porter-Thomas distribution applies to every individual channel.
- For the sum of group of n uncorrelated channels of equal mean reduced width, the distribution of the sum $y = \Sigma_n x_n$ is
-

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

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

Its variance is

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

- The capture width for all but the lightest nuclei is composed of a large number primary transitions. It is therefore found and expected that it will fluctuate very little from resonance to resonance.
- Fission widths through a single saddle point transition state (channel) will have a 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 $\mathbb{S}_{ab}$ thus:

$$\sigma_{ab} \approx \frac{T_a T_b}{T} \mathbb{S}_{ab}$$

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

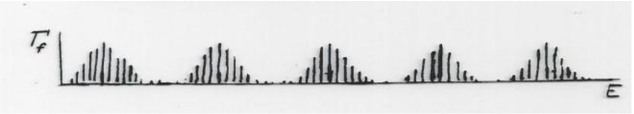
- For some cases of few channels and (constant) capture width, $\mathbb{S}$ can be calculated analytically. In general, however it is reduced to an integral in one variable, which can be calculated numerically.

  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 $\mathbb{S}_{nn}$ can approach 3.

Averaging over Intermediate Structure

- Uniform picket fence model.



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

$$\sigma_{nf} = \pi ƛ^2 g_J \frac{T_n}{\{1 + (T_I/T_F)^2 + (2T_I/T_F)\coth[\tfrac{1}{2}(T_A + T_B)]\}^{1/2}}$$

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.

(Notes)

- Uniform picket fence model.

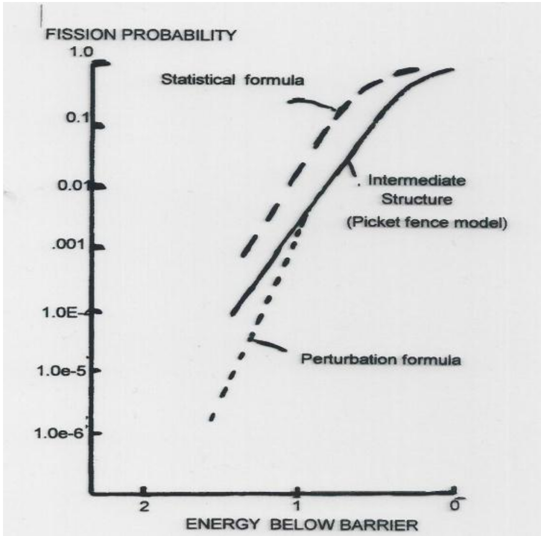
Even in the case when there are no width fluctuations the intermediate resonances lower the average fission cross-section below the Hauser-Feshbach value. In the exact expression for the cross-section in this model, T_I is the sum of all class-I transmission coefficients ; T_A , T_B are inner and outer barrier transmission coefficients, $T_F = T_A T_B / (T_A + T_B)$ is the statistical transmission coefficient. This expression is radically different from Hauser-Feshbach for low T_A and T_B but asymptotically approaches it as the barrier coefficients tend to unity.

Ref.: Lynn, J.E. and Back, B.B.,, *J.Phys.* A**7**, 395 (1974)

Averaging for different intermediate structure models

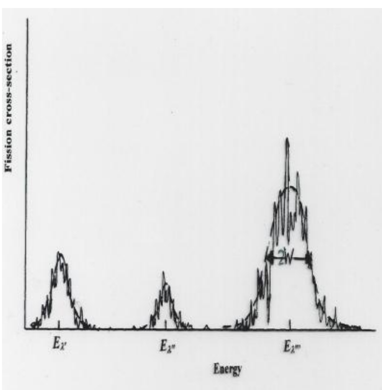
- Fission probability in different models. (σ_{CN} is compound nucleus formation cross-section).

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



Intermediate structure averaging

Width fluctuations to be considered



Width of intermediate resonance:

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

Strength of intermediate resonance:

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

Relations for the coupling width:

$$\langle \Gamma_{\lambda II(C)} \rangle = D_{II} T_A / 2\pi , \qquad \Gamma_{\lambda II(C)} = 2\pi \langle H(\lambda_{II}, \lambda_I)^2 \rangle_{\lambda I} / D_I$$

Fission width of fine structure resonance:

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

Strength of fine structure resonance:

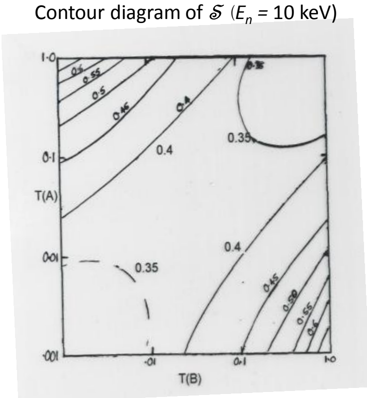
$$\propto \Gamma_{\lambda(n)} \Gamma_{\lambda(F)} / \Gamma_\lambda^2$$

Magnitude of width fluctuation effect

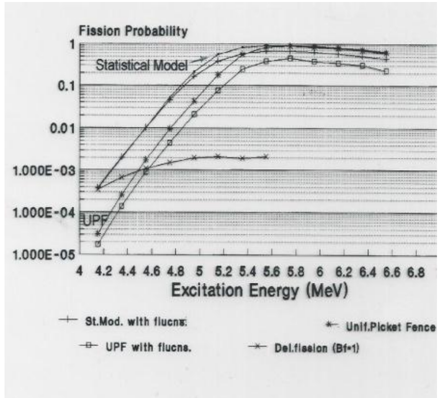
Single channel both barriers.
Use convention of fluctuation factor $\mathcal{S}$ with UPF model:

$$\langle \sigma_{nf} \rangle = \sigma_{nf,UPF} \mathcal{S}_{nf}$$

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



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



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

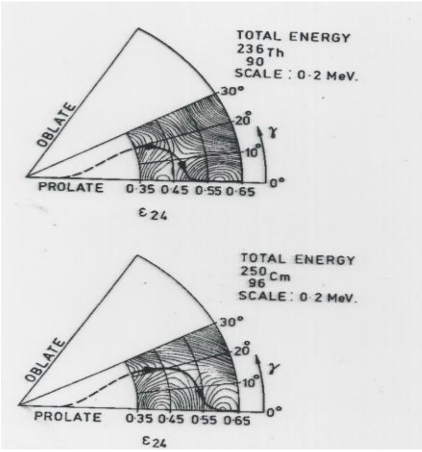
Barriers at 5.5 MeV (for 0^+), 4^+ transition state 0.07 MeV above barriers
$\hbar\omega_A$ = 1.0 MeV, $\hbar\omega_B$ = 0.6 MeV

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

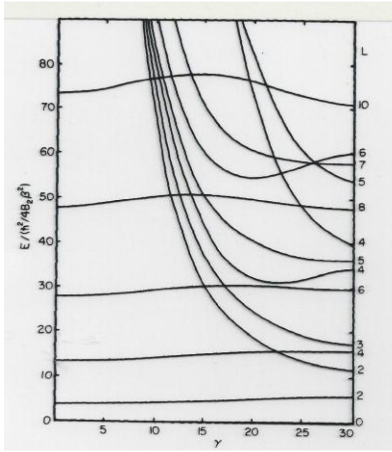
- Statistical model – only useful if channel nearly fully open. Should be used with fluctuation factor $\mathcal{S}_{II}$ for distribution of inner and outer barrier class-II widths applied to T_F .
- Unified picket fence model – first approximation when energy is near or below barrier. As above, $\mathcal{S}_{II}$ should be included in T_F .
- UPF model with fine structure fluctuation factors $\mathcal{S}_I$ 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.

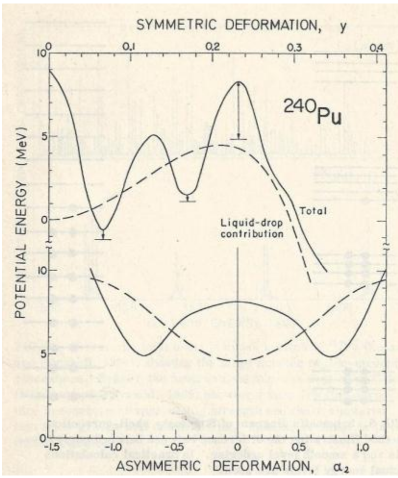


(Notes)

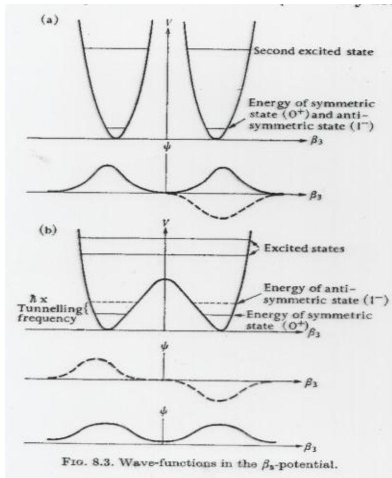
Ref.: Davidson, J.P., *Collective Models of the Nucleus* p.44 (academic, NY and London, 1968

Deformation energy & transition states at outer barrier

- Outer barrier: deformation around octupole symmetry.



- Effect of octupole asymmetry on vibrational eigenstates



(Notes)

Ref.: Moller, P. and Nix, J.R., *Physics and Chemistry of Fission*, Proc. Conf., Rochester, **1**, 103 (IAEA, Vienna, 1974)

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”

(Notes)

Barrier level densities

- Combinatorial model of Level Density, **QPVR**.

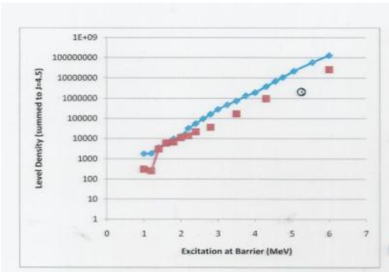
  Combination of multi-quasi-particle states coupled to vibrations and rotations.

  Calculated for a given nuclear deformation (primary well, inner barrier or outer barrier). Pairing gap parameters may depend on deformation.
- The density of the combination states thus computed for normally deformed nuclei, using pairing gap parameters that are determined from nuclear mass differences, agree with neutron resonance spacings at the neutron separation energy within a factor of ±3 over the whole range of actinides. A small adjustment of the pairing gap parameter for each individual nuclide can bring agreement between calculation and neutron resonance data.
- For barrier deformations, the pairing gap parameters are determined so that a reasonable fit to fission cross-sections over the higher energy ranges can be obtained. (In our present work we are modelling the inner barrier level density, and fitting the outer barrier density to the fission cross-section.

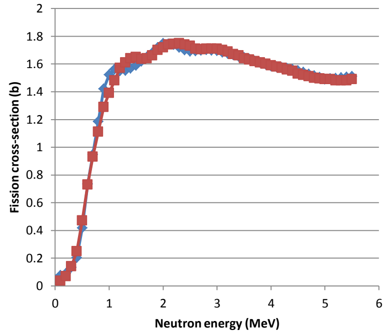
Ref.: Bouland, O., Lynn. J.E. and Talou, P. *Phys.Rev,* C**88**, 054612 (2013)

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



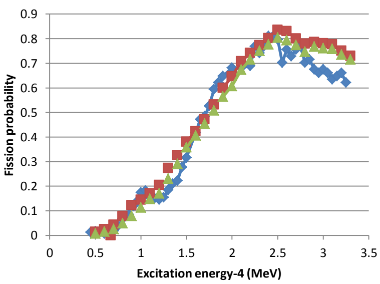
- Fit to cross-section



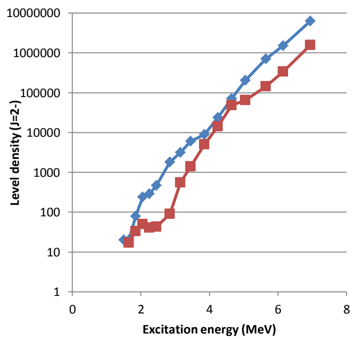
Blue rhomboids - ENDF-B7.

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)



- Barrier level densities

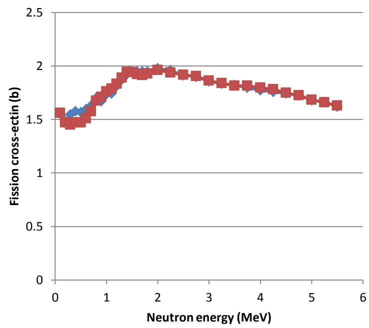


Inner barrier model; Δ_p = 1.0 MeV, Δ_n = 0.79 MeV

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:

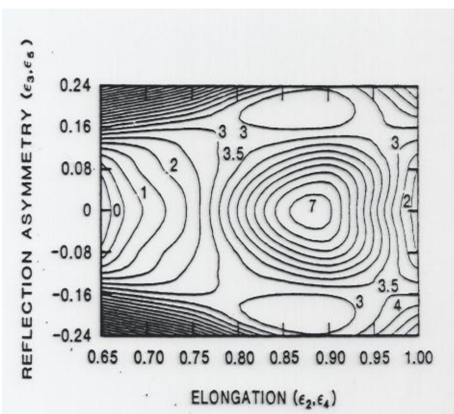
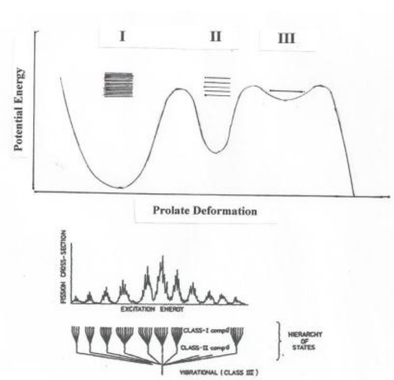


Figure 22. Potential energy contours calculated for ^{232}Th. After Åberg et al.(1980)

- 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

(Notes)

The present status of fission cross-section theory as described in these lectures is that it is a sound tool for analysis of fission cross-section and related data. As such it can be used for extracting important fission parameters with confidence, as shown by the work on the Pu isotopes. It can be used for interpolation and extrapolation of fission, capture and inelastic cross-sections, not only to other energy regions but to other nuclides. Examples include the 25 m isomer of U-235 and the fission cross-section of U-237.

However, predictive capacity is limited by several areas of uncertainty. First is the compound nucleus formation cross-section. This is largely determined by optical model fitting to total and elastic scattering cross-sections. These, of course, contain the shape elastic cross-section as a major component, contributing to the uncertainty of interpretation. Unambiguous experimental information is available at higher energies (above 2 MeV or so) in the form of measurements of non-elastic cross-sections (spherical shell transmission) but errors on these are not much better than 10-15%. We badly need much more accurate information the CN cross-section because the accuracy with which we know this directly affects everything else.

We also have a problem with the inelastic scattering to the lowest collective states of the residual nucleus. While we have some experimental knowledge in the nuclides of major technological importance, we are mainly dependent on coupled channel models. Enhanced inelastic scattering (above normal statistical model estimates) is usually termed direct inelastic scattering. However, some of this enhancement could also be described as a CN component correlated with elastic scattering. This could be elucidated by putting the coupled channel model into the R-matrix formalism. We need transmission coefficients from the coupled channel model with degree of correlation with the elastic scattering (this affects the averaging factor in Hauser-Feshbach formalism) and background direct inelastic terms to improve our calculations of fission and related cross-sections.

(Notes - continued)

Beyond this, there are several basic aspects of fission itself to be explored and improved. The potential energy landscape has been a subject of continuous study since the late 1960s and has shown impressive results both from the microscopic and Möller-Nix theory. So far the accuracy of barrier heights has not become sufficient for *ab initio* calculations of fission cross-sections. For practically useful results this would have to be of the order of 100-200 keV, and this must be the aim. The next important requirement is for sound models and calculations of the inertial tensor. Not only would this greatly help the calculation of sub-barrier cross-sections, especially when combined with improved barrier topography, through the estimation of more realistic barrier penetrability parameters, but could also lead to much better estimates of collective transition state energies, which are at present largely guesswork. This in turn would help improve the estimation of the density of transition states at higher excitation energies. We can here anticipate also that the full pairing equations including blocking would be solved for the quasi-particle states.
It may also be fruitful to discard our reliance on the statistical estimate of barrier transmission coefficient, and directly model the coupling matrix element in R-matrix theory. For this we would need to build the necessary vibrational states on improved potential energy landscapes and inertial tensors and would also require knowledge of the nucleon single-particle wavefunctions over a large region of deformation space.

Most, if not all of these advances , will, of course equire considerable computer facilities. There is much interesting work to be done.