R-matrix Theory in the Analysis of Fission Cross Sections

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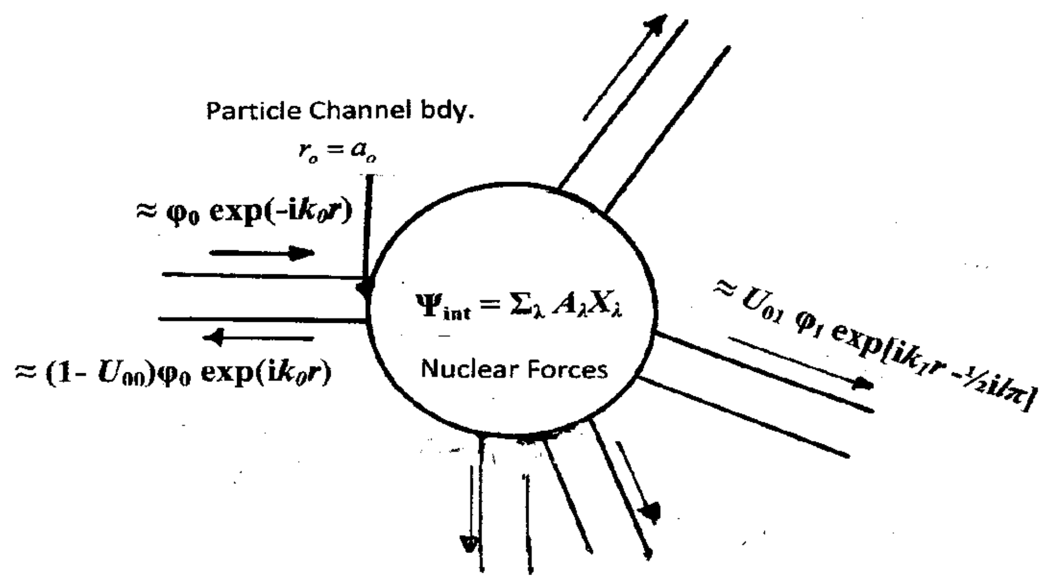
This work is part of a collaboration with Patrick Talou (LANL) and Olivier Bouland (CEA, Cadarache)

Topics

- Introduction
- Fundamentals of fission in R-matrix theory
- a) Simple barrier
- b) Double hump barrier
- Intermediate resonance formulation
- Averaging over fine & intermediate structure
- a)R-matrix to S-matrix pole conversion
- b) Fluctuations
- Conclusions

Internal region and channels in nuclear configuration space

Schematic Division of Configuration Space into Internal Region and Channels



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

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

- where $\mathbf{L} = \mathbf{S} + \mathbf{iP}$
- The R-matrix is the central quantity here:

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

- The EM radiation channels can be included on the same basis by perturbation theory (Lane and Thomas)

Fission reaction rate theory in Liquid Drop model

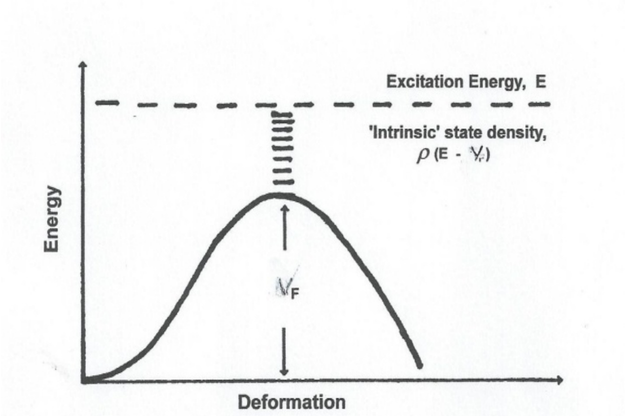
Classical model :

Transmission coefficient $T_F = 1$ if $E > V_F$, otherwise zero.

Hill and Wheeler (1953) gave quantal tunnelling version

Nuclear model:

Bohr and Wheeler (1939) - many different possible states of intrinsic excitation as nucleus passes over barrier.



The transmission coefficient is

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

Aage Bohr Transition States

- Extended from Wheeler; largely speculative

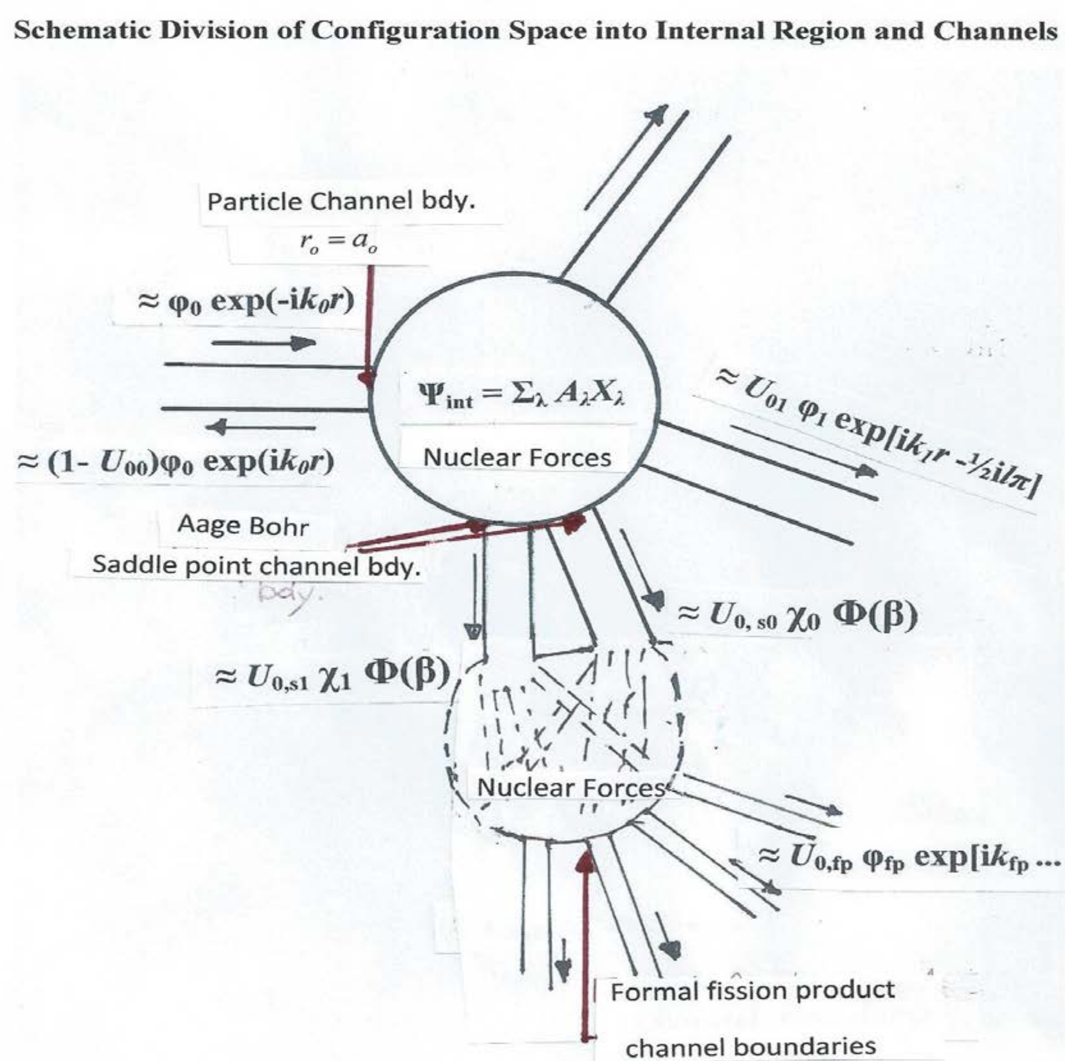
Approximate features on the energy scale (origin is the fission threshold)	Approximate energy of transition state (in MeV)	Transition state quantum numbers		Description of transition state
		K^{π}	I^{π}	
0·0 MeV (fission threshold) →	0·0	0^+	0^+, 2^+, 4^+, etc.	'Ground'
	∼0·5	0^-	1^-, 3^-, 5^-, etc.	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

- Bohr speculated that these widely spaced 'transition states' at the barrier could influence the state of the splitting nucleus at scission point

- Explained angular distributions of fission products (through *K* of transition state)

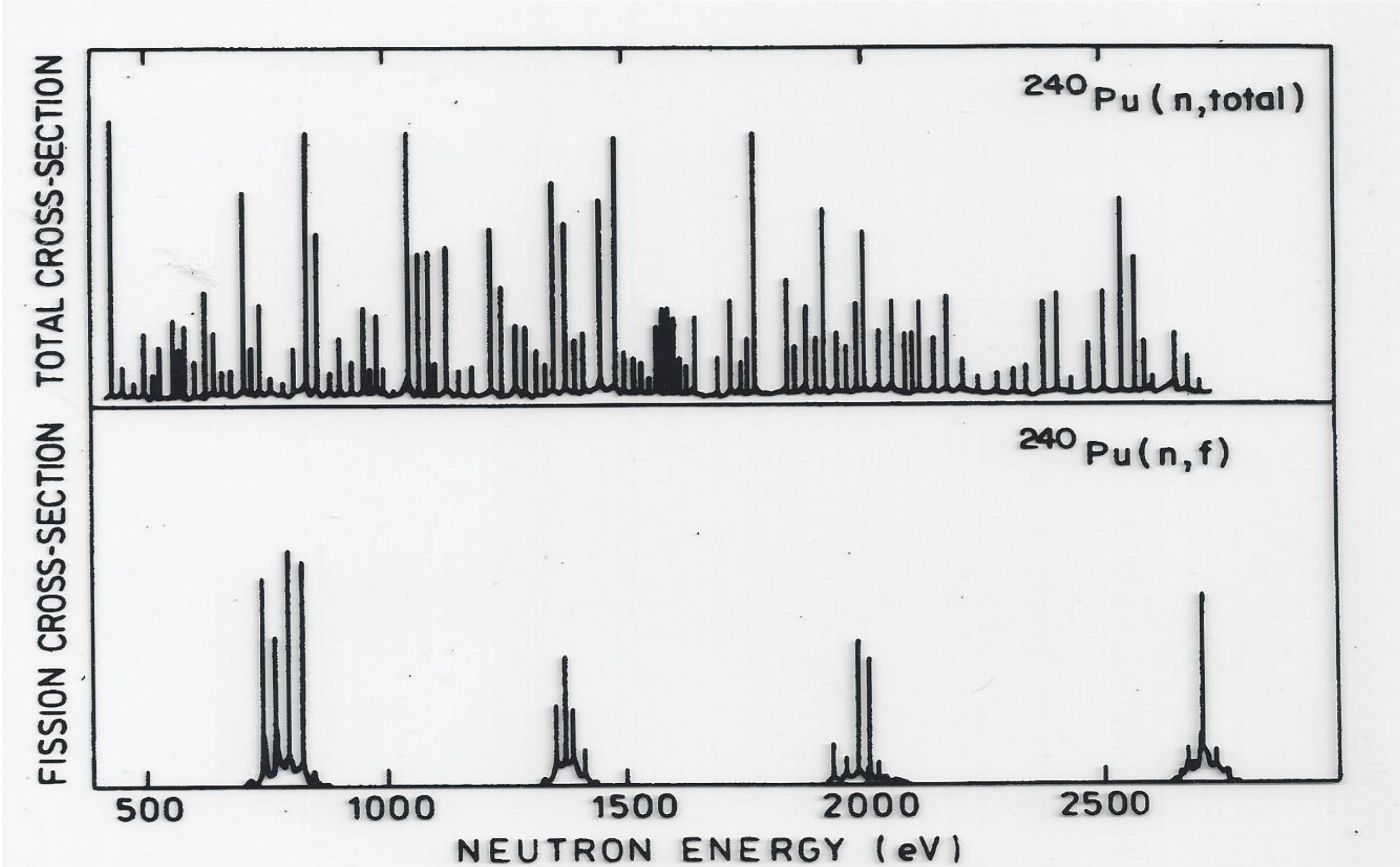
- Hence, concept of 'saddle-point channels'
- Distribution of fission widths

Internal region and channels in nuclear configuration space

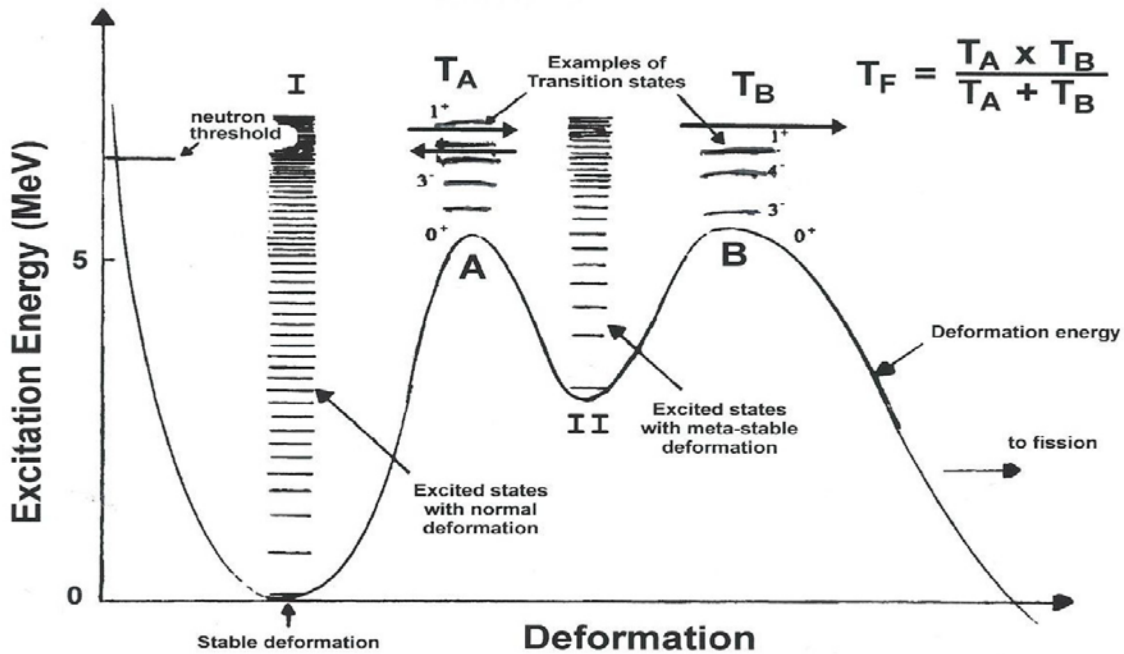


Narrow Intermediate Structure in Fission cross-sections

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



Effect on Fission transmission coefficient

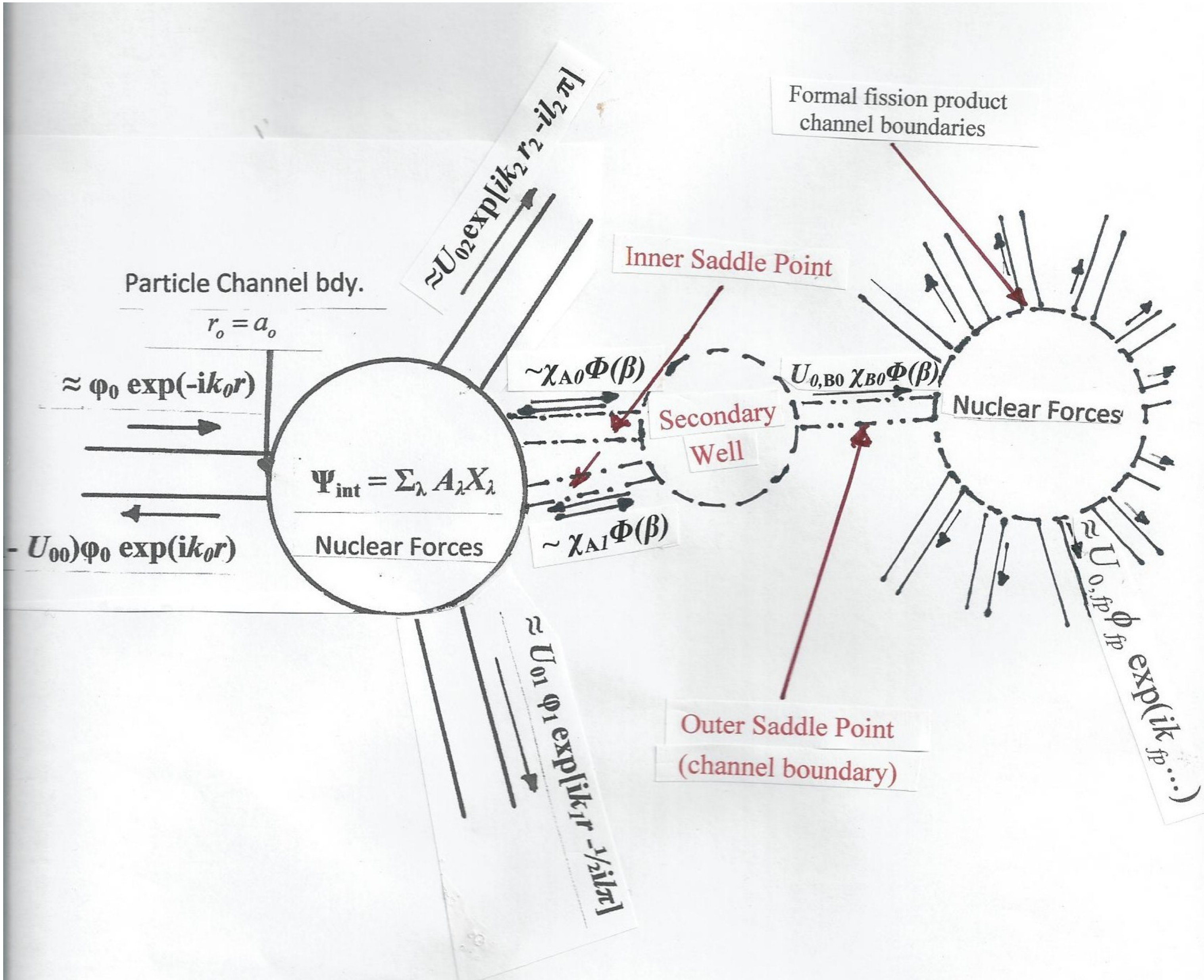


T_A , T_B are transmission coefficients of inner and outer barriers separately

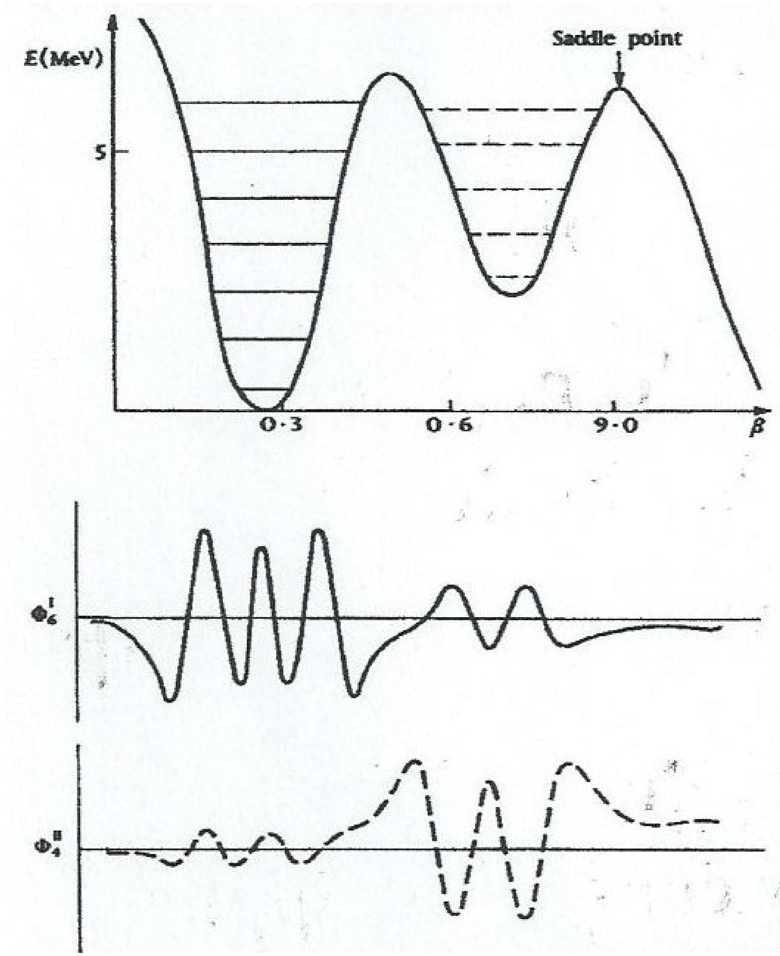
- This is the fission transmission coefficient of the Statistical Model:

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

Configuration Space: choice of channel boundary



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



Formal exposition of Intermediate Structure

-
- **Hamiltonian**

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

- 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 in basis states of *H(int) +H(def)*:

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

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:

-

$E(\lambda I)$	0	0	……	$\langle \lambda I \| Hc \| \lambda II \rangle$	$\langle \lambda I \| Hc \| \lambda' II \rangle$	……….
0	$E(\lambda' I)$	0	…….	$\langle \lambda' I \| Hc \| \lambda II \rangle$	$\langle \lambda' I \| Hc \| \lambda' II \rangle$	....
0	0	$E(\lambda'' I)$	. ..	$\langle \lambda'' I \| Hc \| \lambda II \rangle$	$\langle \lambda'' I \| Hc \| \lambda' II \rangle$	……..
0	0	0	……			
:						
0	0	0		$\langle \lambda'''' I \| Hc \| \lambda II \rangle$ …….		
$\langle \lambda I \| Hc \| \lambda II \rangle$	$\langle \lambda' I \| Hc \| \lambda II \rangle$	$\langle \lambda'' I \| Hc \| \lambda II \rangle$	..	$E(\lambda II)$	0	0
$\langle \lambda I \| Hc \| \lambda' II \rangle$	$\langle \lambda' I \| Hc \| \lambda' II \rangle$	$\langle \lambda'' I \| Hc \| \lambda'' II \rangle$		0	$E(\lambda' II)$	0
. ……………………………………………				0	0	$E(\lambda'' II)$
:	:	:				

Matrix element core $\langle \nu I | Hc | \nu II \rangle$ is very small

Moderately weak coupling:

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

$$2\pi\gamma^2_{\lambda,F} / D_I = \frac{\Gamma_{\lambda(II),\,C}\ \ \gamma^2_{\lambda(II),\,F}}{(E_{\lambda(II)} - E_\lambda)^2 + (½\Gamma_{\lambda(II),\,C})^2}$$

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 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

$$\Gamma_{\lambda_{II}F} \;\square\; \Gamma_{\lambda_{II}C}$$

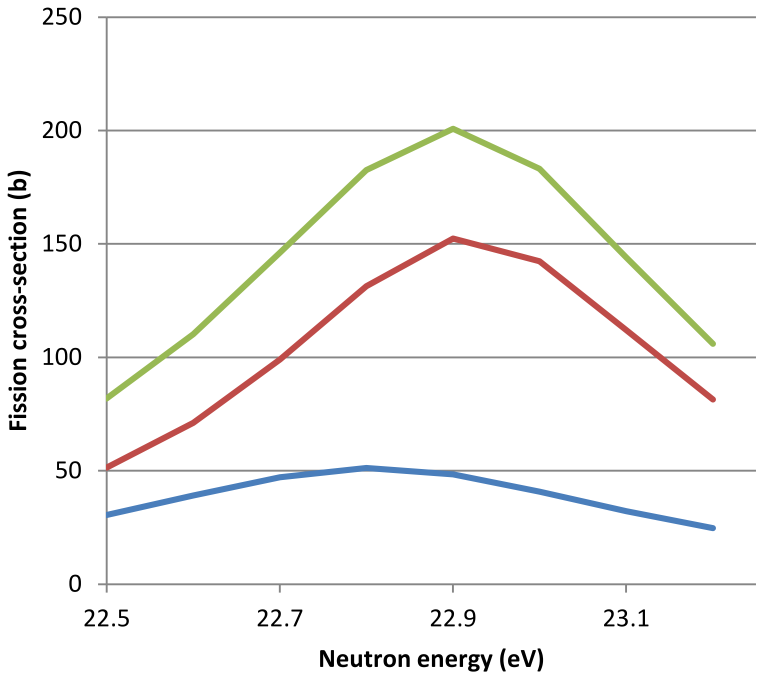
R-matrix fission width profile approximates to intermediate resonance profile.

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

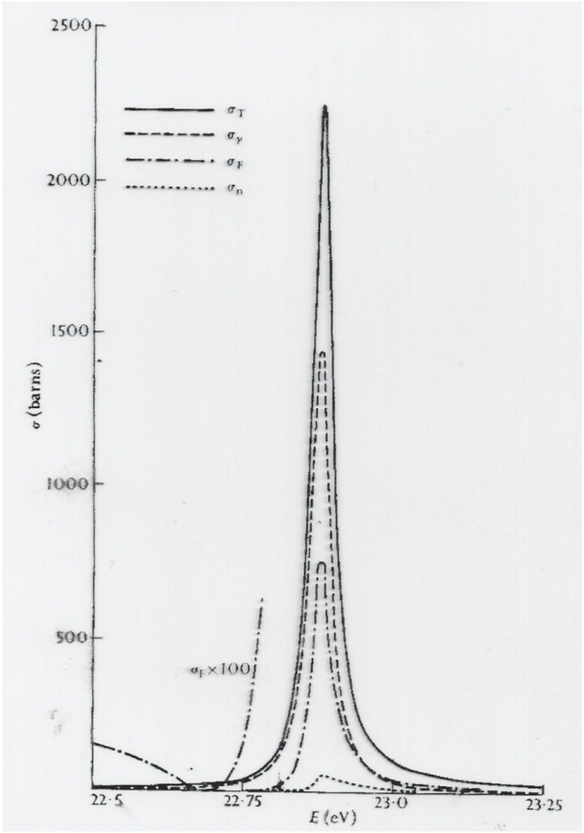
Example:

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

Humblet and Rosenfeld, Nucl. Phys.26**,529 (1961)**

- 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. Note: they are complex.
- $\mathcal{E}$ 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 and penetration factors.

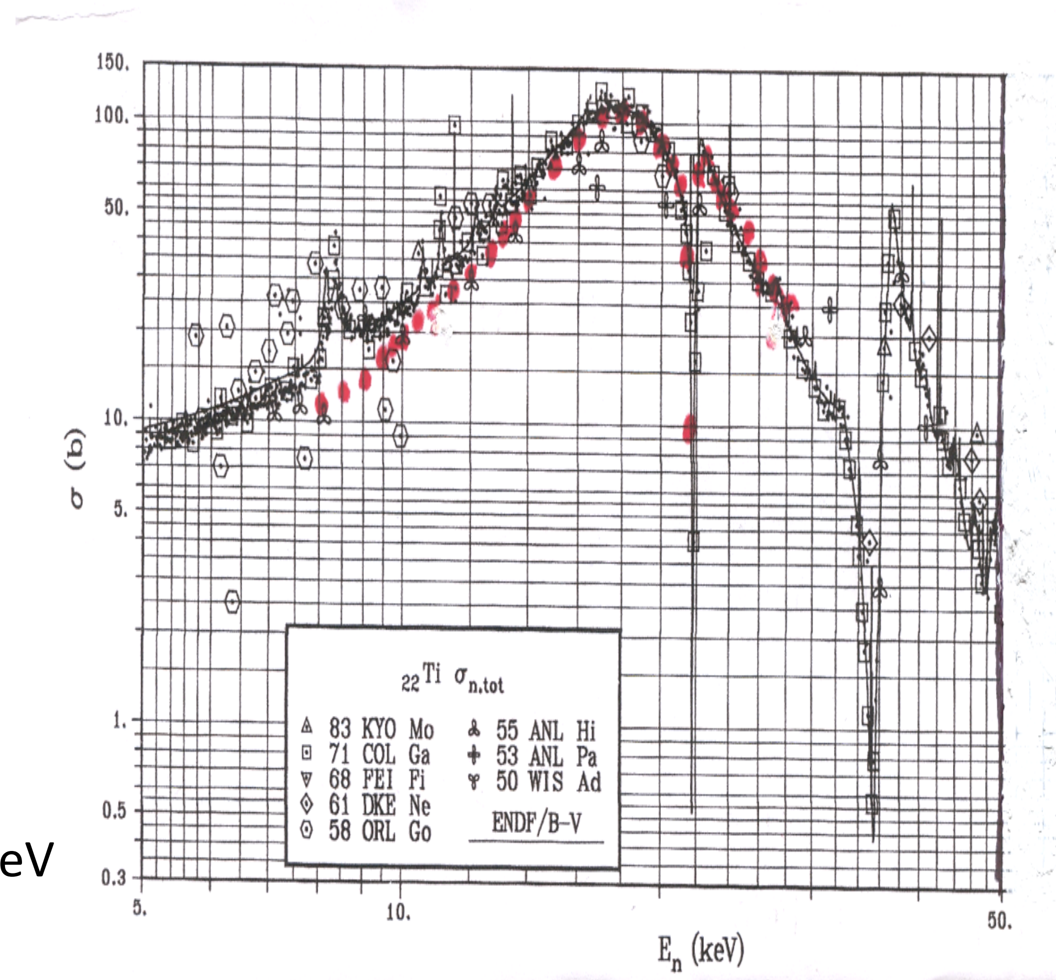
Ti-48 + n

R-matrix parameters

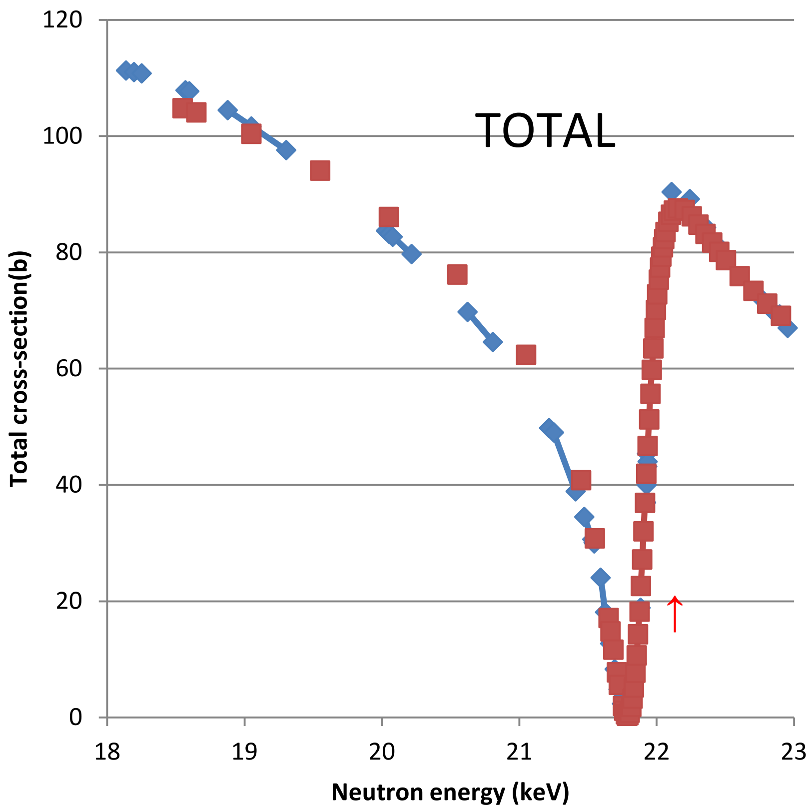
E_λ (keV)	$\Gamma_{\lambda n}$ (keV)
17.8089	8.5714
22.0862	0.792
36.945	1.734

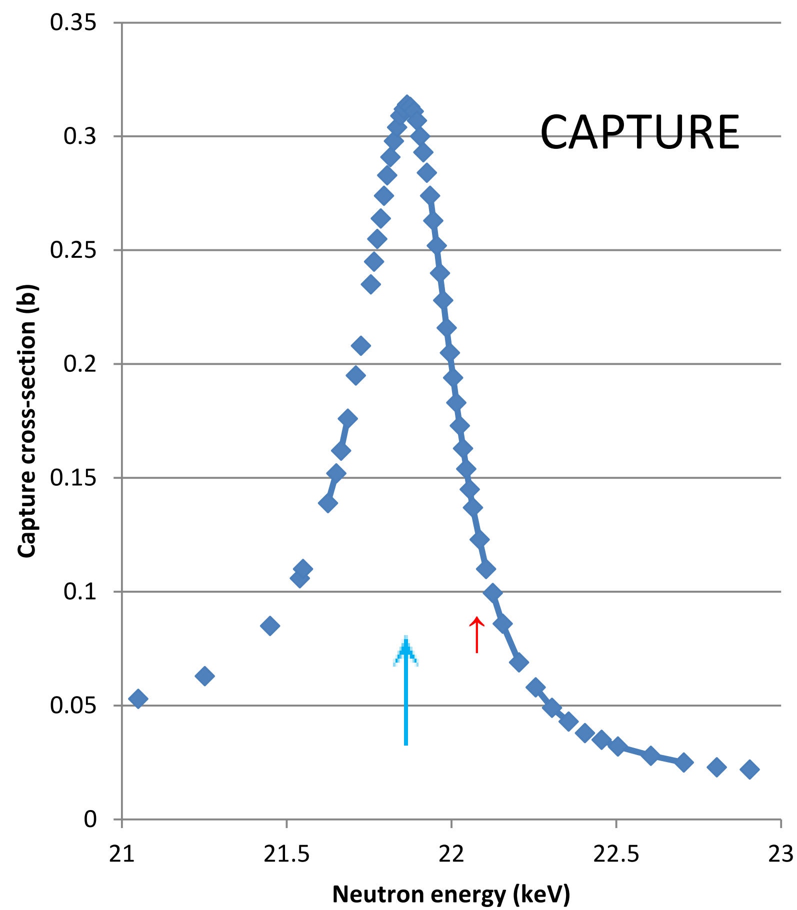
- **S-matrix parameters**
- E_1 = 18.142 - i 4.544 keV,
- G_{11} =√[9.697exp(i1.41π)] keV

- E_2 = 21.8818 - i 0.1749 keV,
- G_{21} =√[0.3626exp(i0.823π)] keV



Calculated cross-sections of Ti-48

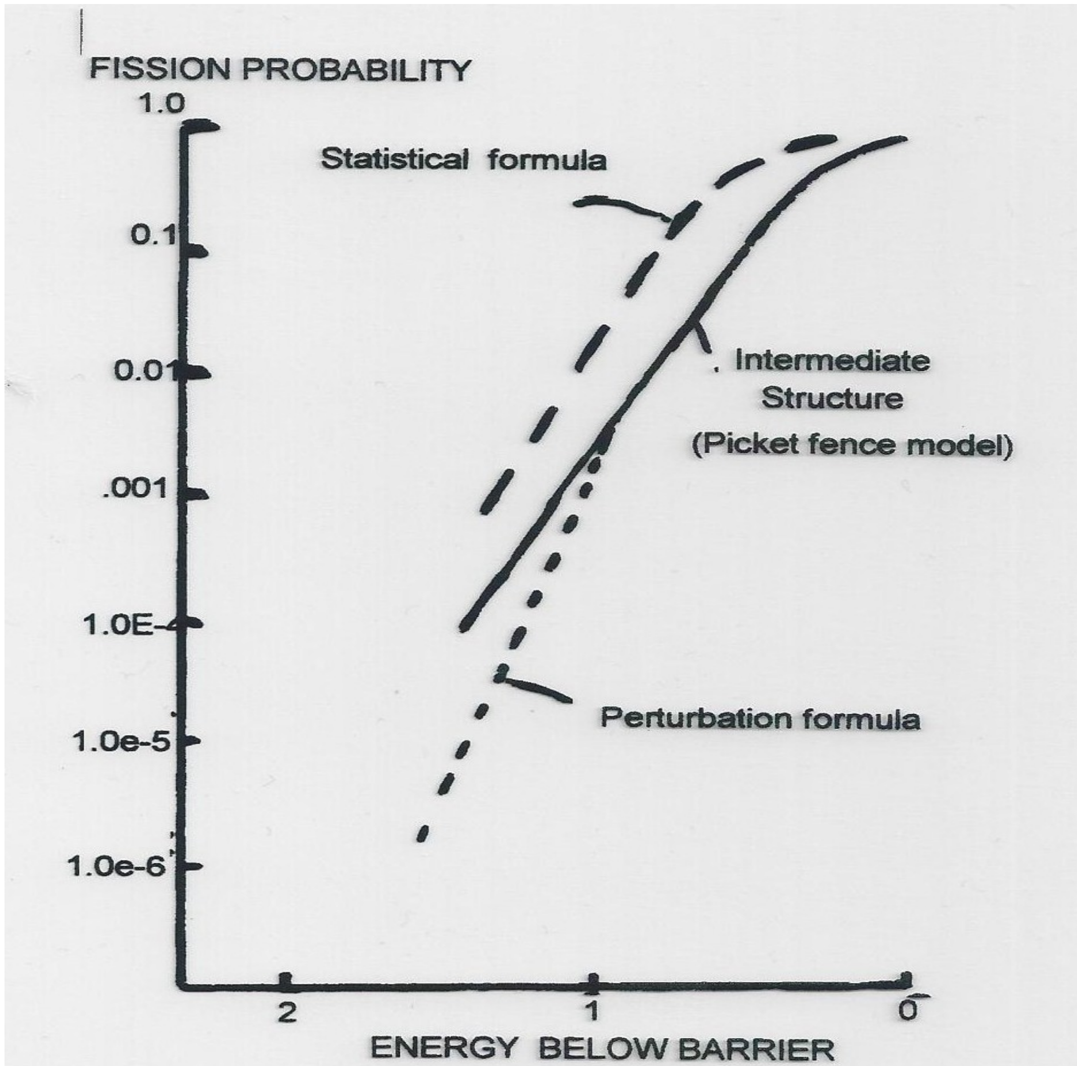




Averaging for different intermediate structure models

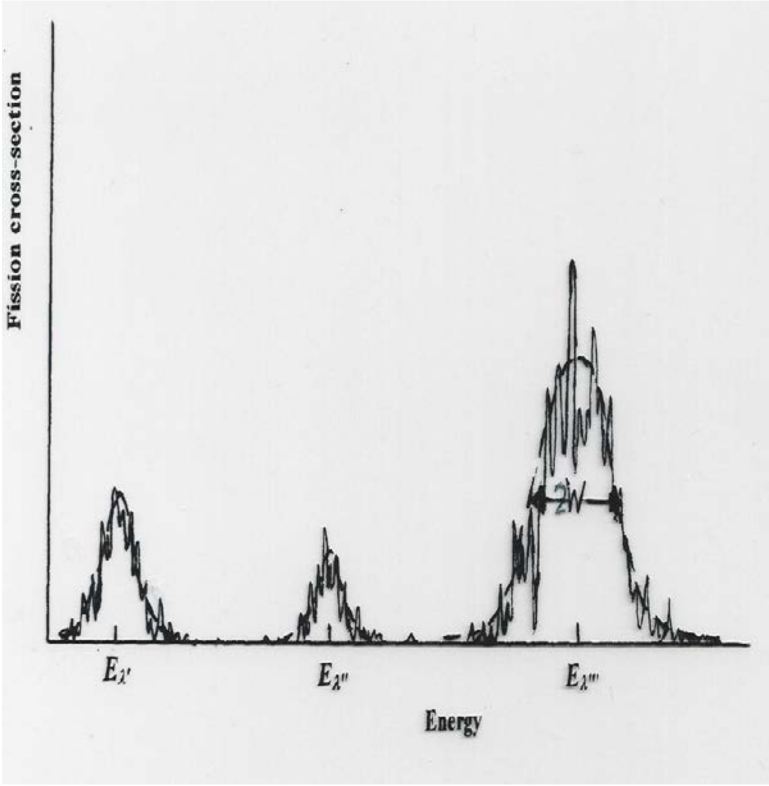
- Fission probability in different models. (σ_{CN} is compound nucleus formation cross-section).

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



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:

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

General formula for fission widths of resonances

- Fine structure fission widths

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

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 $\mu'\nu_{II}$)

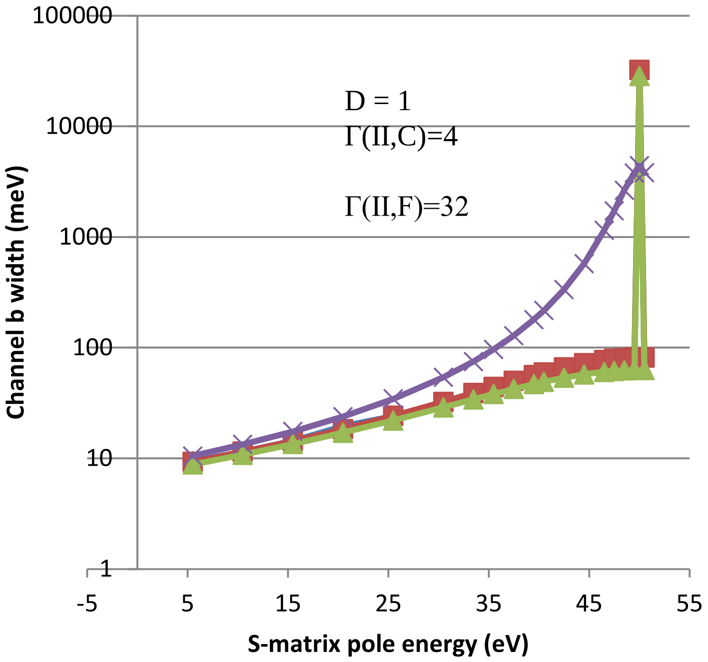
- This formula is approximate.
- General prescription:

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

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

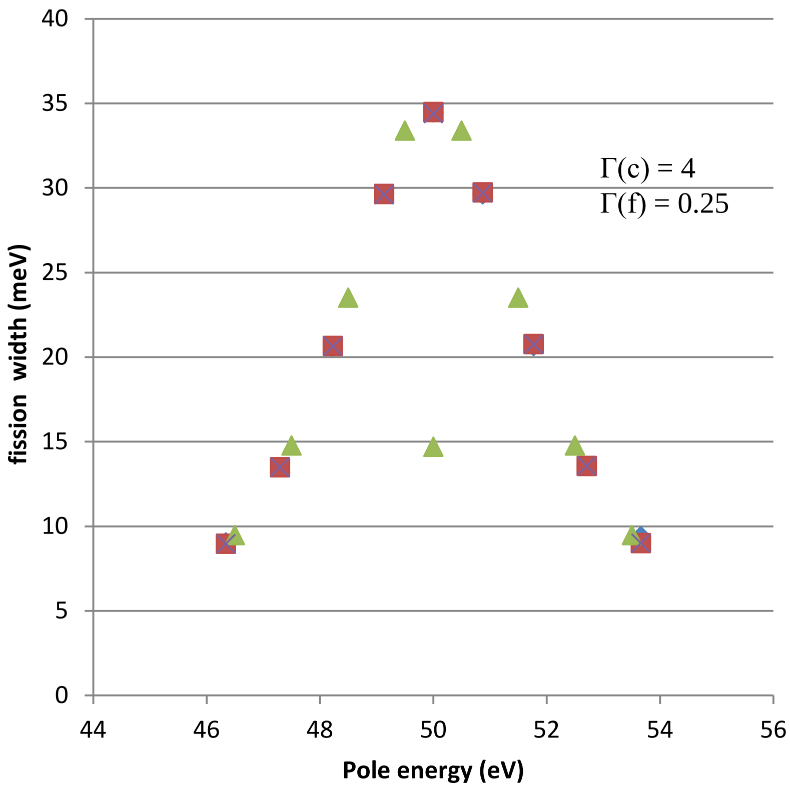
- Red : S-matrix pole fission widths Green: from hypothesis formula;

Purple : R-matrix fission widths.

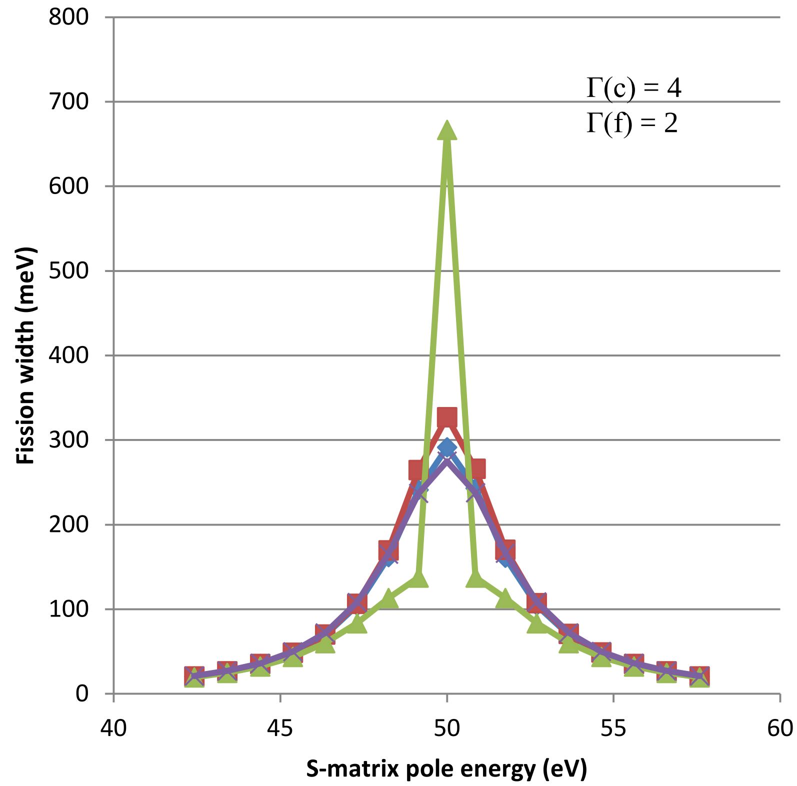


Class-II fission width < coupling width

Red – S-matrix pole width (from residues)
Green – Lorentzian model

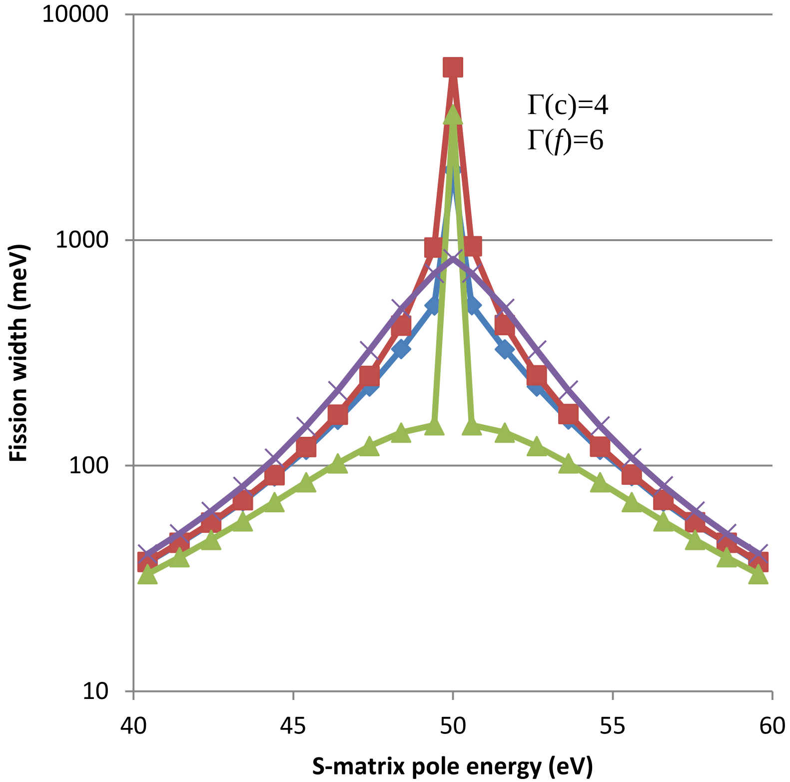


Blue – S-matrix pole width
Purple – R-matrix fission widths

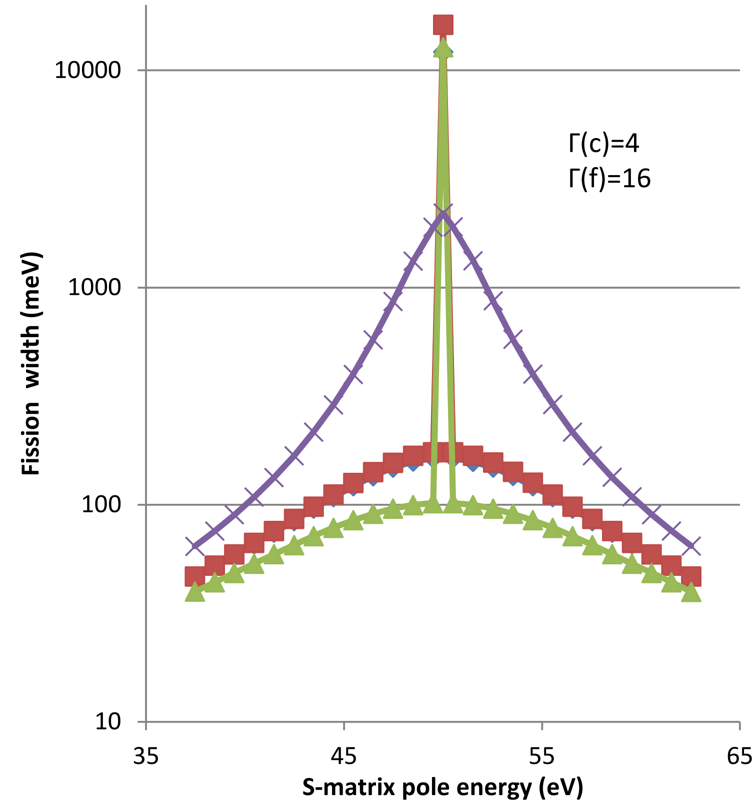


Class-II fission width > coupling width

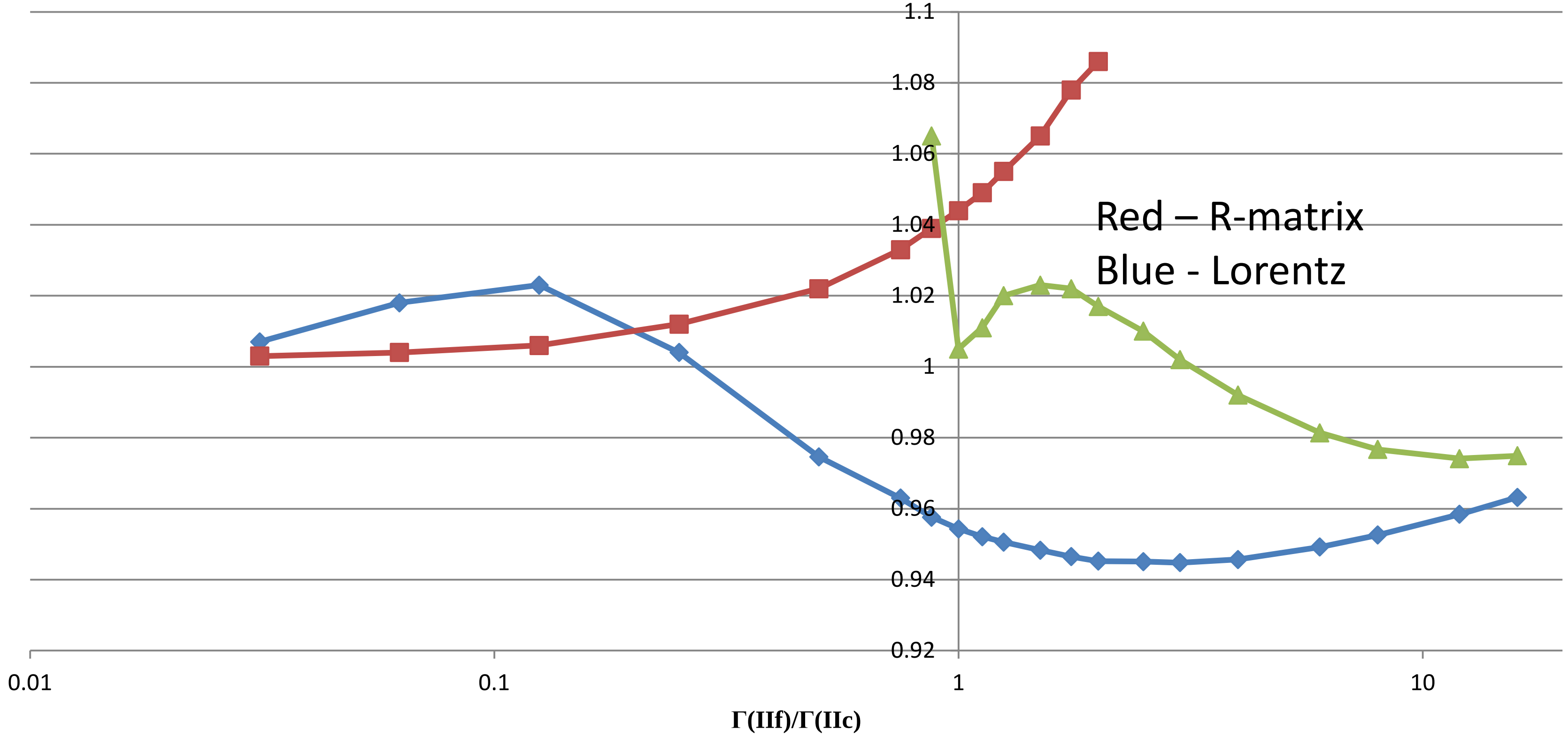
Blue – S-matrix pole width
Purple – R-matrix fission widths



Red – S-matrix pole width (from residues)
Green – Lorentzian model



Ratio of model average to true (numerical) average



Conclusions

- R-matrix theory is general and flexible enough that, with suitable insight and statistical methods, it can be used for highly complex phenomena such as fission.
- With R-matrix theory, fine structure, intermediate and vibrational resonances can all be treated. R-matrix theory is at the basis of the AVXSF code
- Conversion to S-matrix parameters reveals new phenomena and can facilitate averaging processes. More work is required to understand systematics of S-matrix parameters

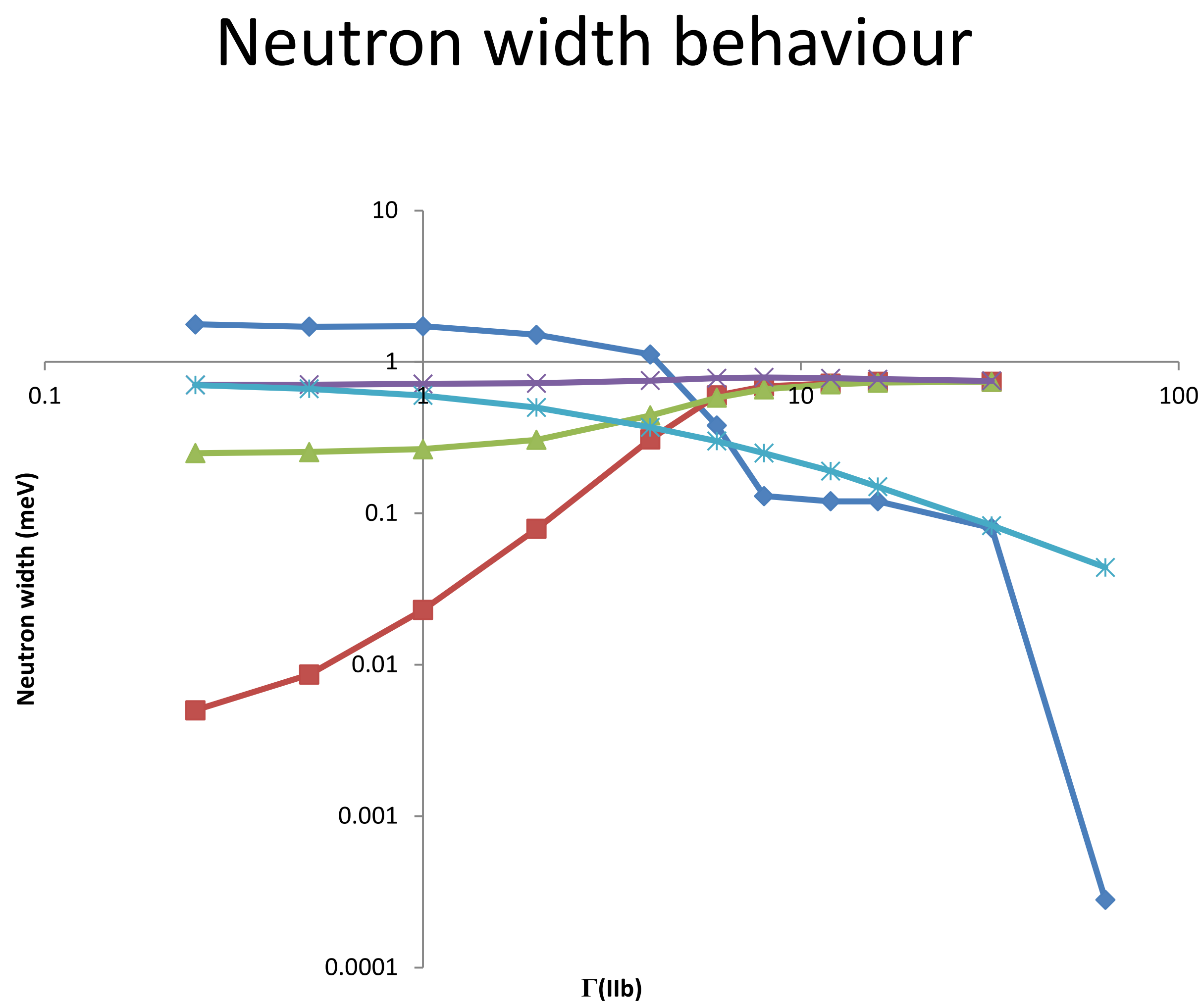
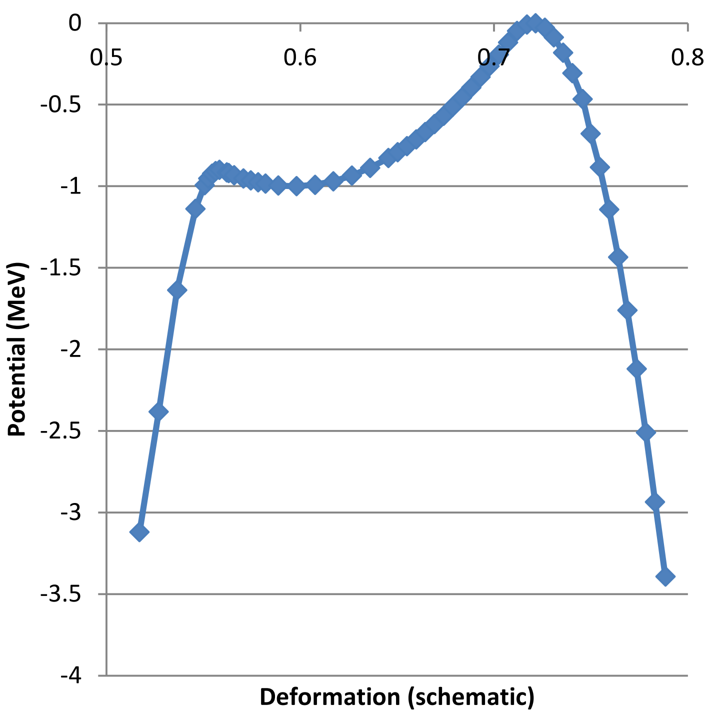


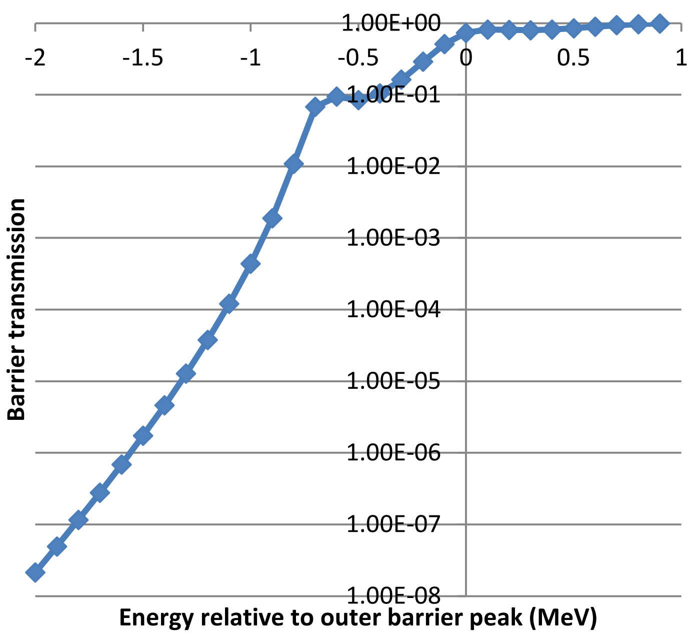
Figure 17. Example of entrance channel width behaviour for $\Gamma_{IIC} = 4$. Rhomboids (blue) represent the central pole, squares (red) the next neighbour, triangles (green) the second neighbour, crosses (purple) third neighbour, crosses (pale blue) the Lorentzian model for the central pole.

Other topics (1): Vibrational resonances

- Quasi-tertiary well effects in outer barrier

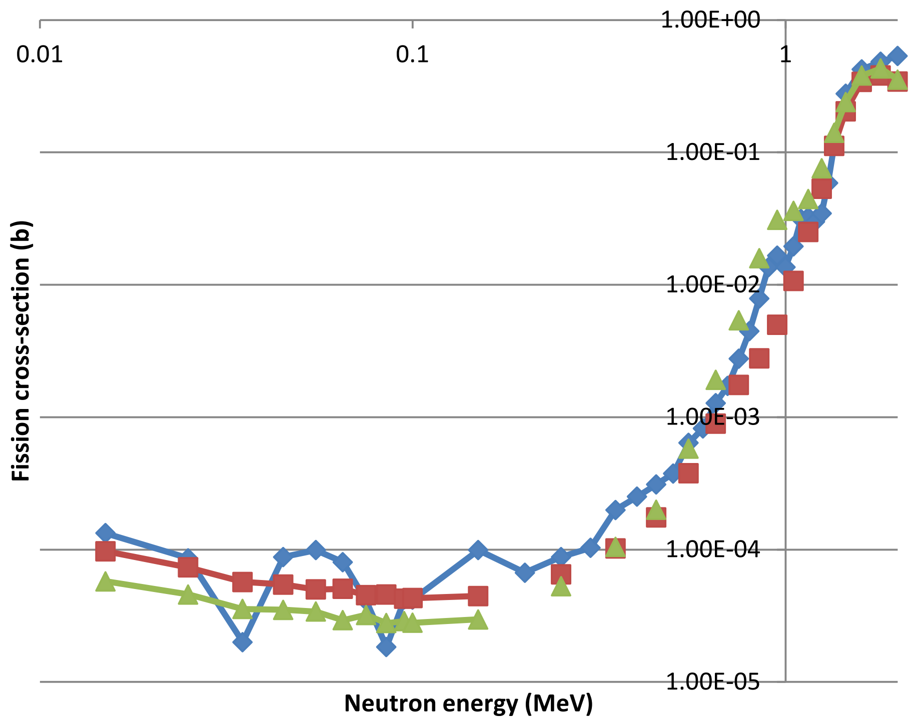


- Penetration function



Vibrational resonance in cross-section of U-238 + n

- Blue – exptl. data; Red – inverse harmonic barrier; Green – barrier with quasi-well



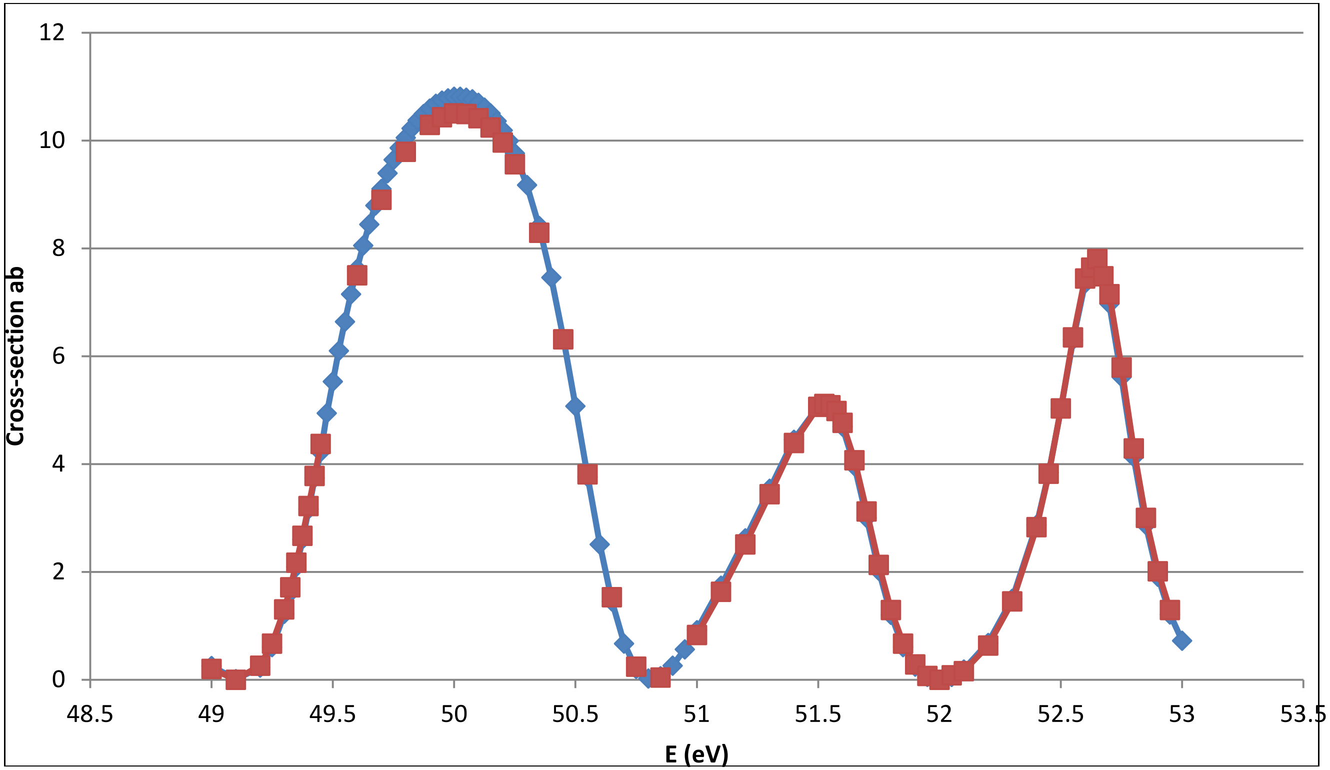
Other topic (2) Example of R- to S-matrix conversion

- Table of R-matrix and corresponding S-matrix parameters

E_λ (eV)	$\Gamma_{\lambda a}$ (meV)	$\Gamma_{\lambda b}$ (meV)	E_l - E_λ (meV)	$\Gamma_{l\, b}$ (meV)	$G_{la}\, G_{lbb}$ (eV)	q
44.3017	0.109	263.9	63	194	.00291-i.00353	0.951
45.2729	0.041	329.9	101	238	-.00168+i.00332	1.007
46.2368	0.134	413.4	112	298	.00498- i.00440	1.089
47.1917	0.021	513.2	151	380	.00226- i.00490	1.223
48.1365	0.101	618.4	211	505	-.00751+i.00545	1.503
49.0718	4.10^{-7}	704.1	317	722	-.00150+i.01559	2.438
50.0009	0.207	738.4	10	2038	-.00660 -i.05186	4.454
50.9300	7.10^{-6}	705.8	-322	730	.00026 +i.0185	2.482
51.8650	9.10^{-6}	620.9	-257	509	.00334+i.00767	1.514
52.8096	0.057	516.0	-153	383	.00457+i.00532	1.229
53.7642	0.188	415.9	-113	299	.00615+i.00450	1.091
54.7279	6.10^{-6}	331.8	-84	239	-.00007 -i.00532	1.008
55.6990	0.039	265.4	-64	195	-.00139 -i.00330	0.953
56.6757	0.077	214.2	-49	160	-.00192 -i.00333	0.910

Comparison of calculated cross-sections

- Red – R-matrix; Blue – S-matrix

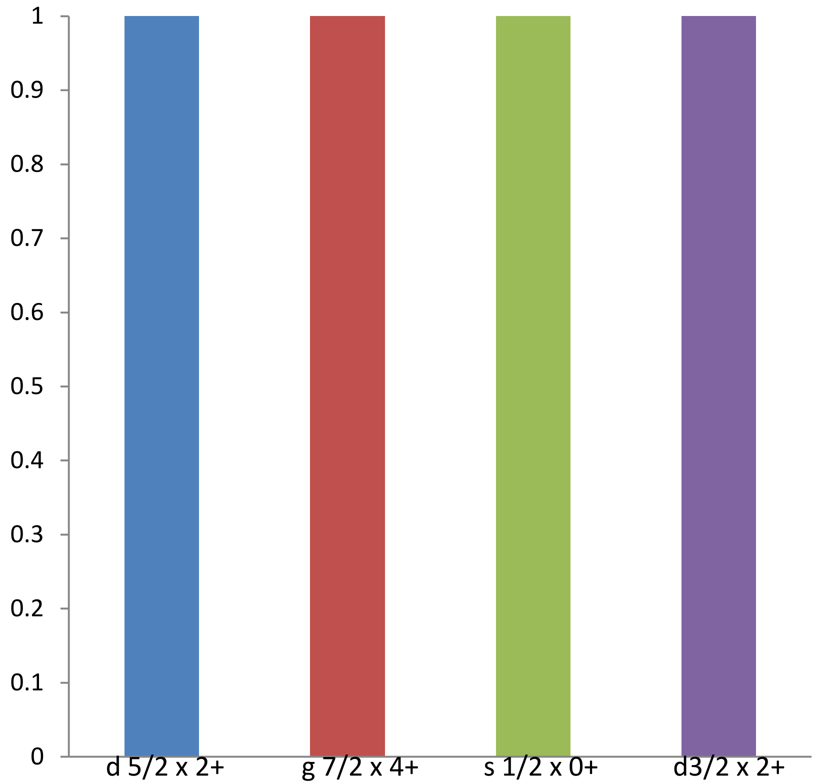


Other Topic (3) Inelastic scattering; R-matrix treatment

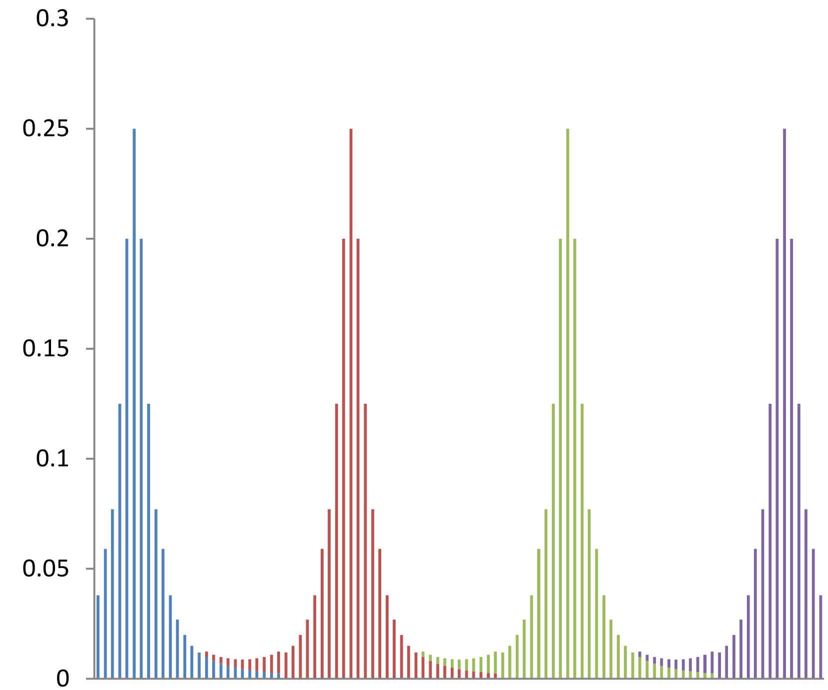
- Other uncertainties in average fission cross-section calculations
- a) Compound nucleus formation cross-section
- b) Strength functions for inelastic scattering
- Estimates for above made from optical model, or, in case of main inelastic terms, from its coupled channel extension.
- The latter produces enhancements which are interpreted as “direct inelastic scattering”
- An R-matrix approach may produce a fresh insight into this

Basis states: single-particle+target rotational state

- No coupling term
- d5/2 x 2+ g7/2x4+ s1/2x0+ d3/2x2+

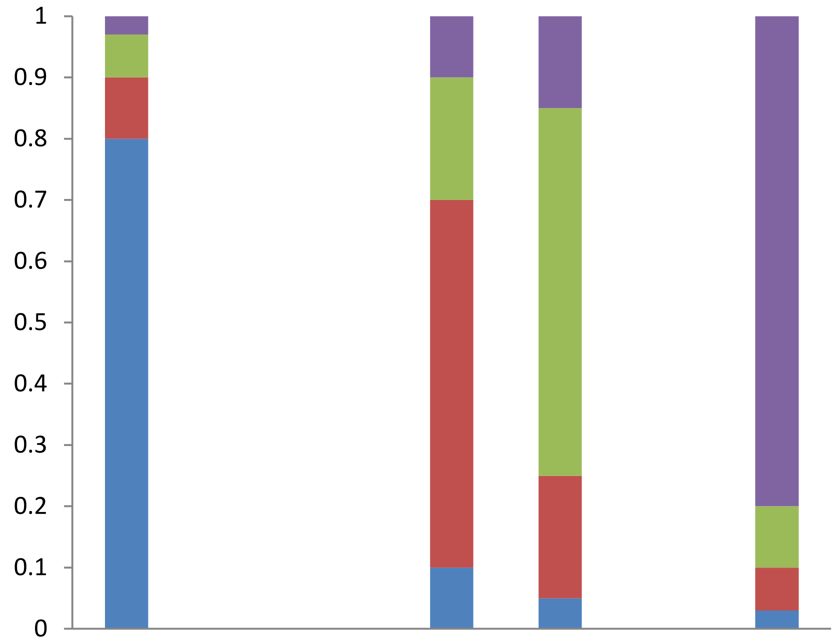


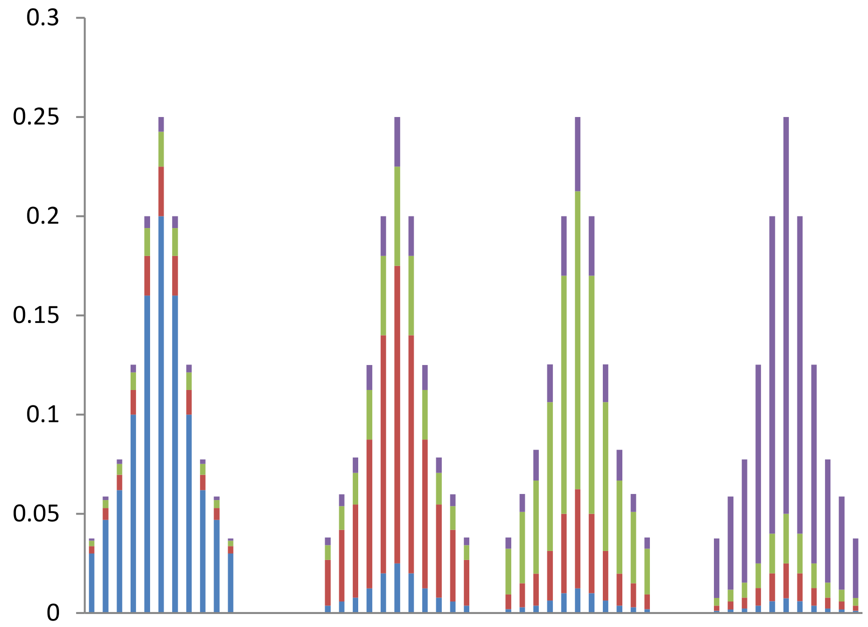
- "Optical model" spreading



Effect of coupling term

- With “optical model” mixing
- Green – el. scattg.; blue & purple –inel. to 2+; red – inel. to 4+





Basics of R-matrix theory

- 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

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

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

Amplitudes of outgoing waves in this system are denoted by <u>collision matrix</u> element

$$U_{cc'}$$

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 :

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

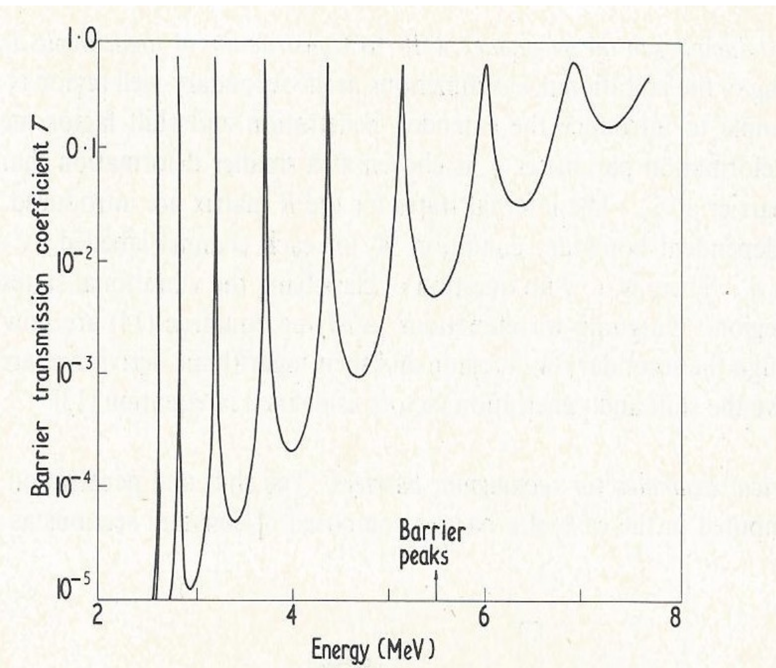
$\mathcal{I}$ and $\mathcal{O}$ are incoming and outgoing wave functions generalized to specific channels by incorporating intrinsic excitation and angular momentum couplings

- The cross-section is

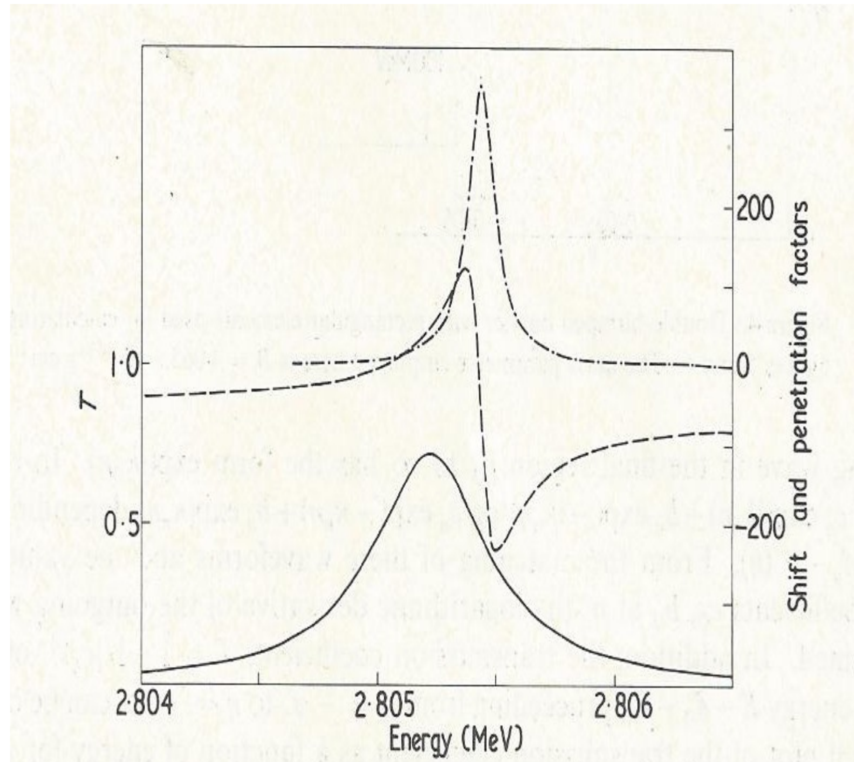
$$\sigma_{cc'} = \left| \left\langle \Psi_{ext} - \Psi_{plane} \mid c' \right\rangle \right|^2$$

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

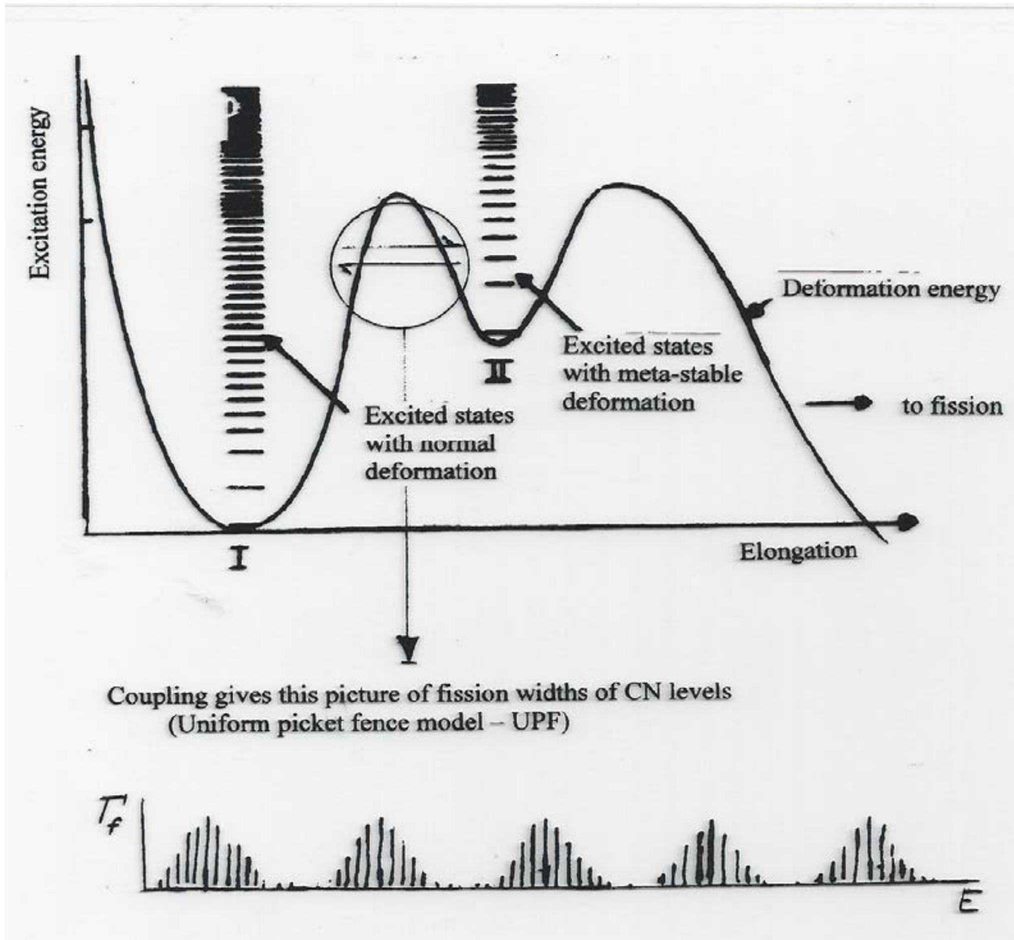
- Transmission coefficient



- Shift and penetration factors



CN states in double well



Transforming R-matrix parameters to S-matrix parameters

- “Broad” class –II R-matrix state:

  $$\Gamma_{\lambda(II)F} \square \; D_I \qquad \text{and} \qquad \Gamma_{\lambda(II)F} \square \; \Gamma_{\lambda(II)C}$$

  Fine structure resonance fission widths

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

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

- Remaining class-II fission strength is

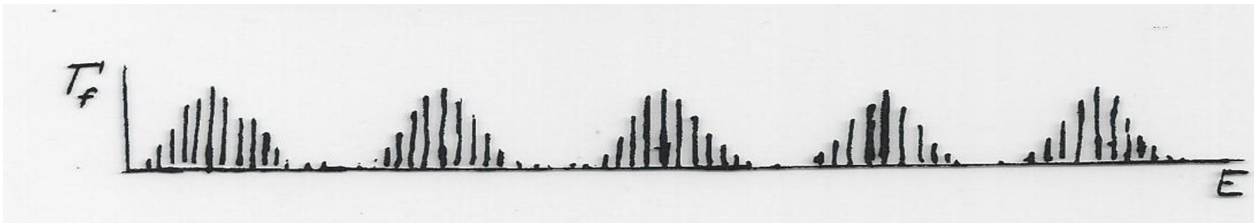
  $$\mathbf{[1 - \Gamma_{\lambda(II),C} / \Gamma_{\lambda(II),F}] \, \Gamma_{\lambda(II),F}}$$

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

Essentially, the relatively strong mixing of class-I and class-II wave functions in the R-matrix states is decoupled by their broad spreading into the fission continuum, and the fission widths of the quasi-class-I resonances are picked up by weak perturbation from the class-II state

Averaging over Intermediate Structure

- Uniform picket fence model.



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

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

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.

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.
- Too much overlap in cross-sections of fissile nuclei to find good experimental examples. Therefore, we seek examples in multi- keV region of intermediate mass nuclei.

R-matrix Theory in the analysis of fission cross-sections

SLIDE 2

INTRODUCTION.

First, I want to acknowledge my friends and colleagues, Patrick Talou of LANL and Olivier Bouland of Cadarache, my collaborators in the project on which this paper is based.

Our aim was to provide a code, AVXSF, with analytical and predictive capability for calculating average fission cross-sections and was based on the soundest theoretical basis available and as little phenomenology as possible.

For describing the underlying resonances from the properties, such as barrier height and penetrability, of the fissioning compound nucleus we based the code on R-matrix theory. The project resulted in a paper in 2013 on the fission cross-sections of a series of plutonium isotopes, and helped understand barrier height and pairing gap systematics.

In this paper I propose to give an overview, partly historical, on the use of R-matrix theory in fission. R- matrix theory has been an important tool in analysis of fission cross-sections since the early 1950s when measurements of the resonances in the cross-sections of fissile nuclei revealed that they were often very broad and quite asymmetric in shape. A formalism, such as R-matrix, that was much more generalized than simple Breit-Wigner was required.

This slide shows the topics I propose to cover

SLIDE 3

So how do we put fission into R-matrix theory?

This is a schematic diagram of configuration space. Here on the left we have an incoming wave, the incident projectile, with a returning outgoing wave. At the centre is the combined system of projectile and target nucleus with binding energy available as excitation energy, which we

call the internal nuclear region. The nuclear interactions within this modify the returning outgoing wave and create new waves in other channels (to the right) defined by various ejectiles and a residual nucleus in various states of internal excitation and angular momentum .

In this picture the multiple combinations of fission products in different states of excitation and angular momentum and parity beyond the scission point are all defined as channels.

However, this straightforward idea is confounded by observation of the statistical properties of resonances. Neutron widths vary widely from resonance to resonance - the Porter-Thomas distribution. Radiation widths are constant within experimental uncertainty. This can be understood by the total radiation width being composed of a large number of primary transitions, each with an independent P-T distribution; the distribution therefore converges to a narrow Gaussion. The same argument should hold for fission widths.

SLIDE 4

Let us look now to the formal theory. At the top we show the wave-function of the internal region expanded over the basis R-matrix states X_λ defined as the eigenstates of the full Hamiltonian with real, energy independent boundary conditions applied at the channel entrances. Matching at the channel entrances gives the central relation between the collision matrix and the R-matrix states, involving hard-sphere phase shifts, penetration, shift and boundary conditions (all diagonal matrices). The central quantity is the R-matrix, a typical element of which is shown at the bottom, featuring eigenvalue E_λ and reduced width amplitudes $\gamma_{\lambda c}$ (projections of the internal wave-function on the channel wave functions at the channel boundaries).

SLIDE 5

Let us look more closely at the fission process. Here we see the classical fission barrier in the collective variable defining deformation towards fission.

Beyond the saddle point the nucleus becomes internally excited, unlike angular momentum and Coulomb barriers in the particle channels, and this why we have included the barrier and saddle point within the internal region. In their 1939 paper Bohr and Wheeler pointed out that the nucleus can deform over the barrier in one of possibly many states of internal excitation and these all need to be counted in evaluating the transmission coefficient (which can be used in Hauser-Feshbach theory or to give an estimate of the fission width). Aage Bohr later recognized that these "transition states" were not simply a counting device but are widely enough separated to be able to stamp their own properties on the ultimate pattern of fission product division.

SLIDE 6

On the left is a table of possible barrier transition states (largely compiled by Wheeler) for an even nucleus with estimates of their excitation energy and their K, parity and total angular momentum numbers. With these Aage Bohr could explain photofission and neutron-induced fission product angular distributions through the K, J and M quantum numbers.

What we realize from this is that the barrier transition state could be controlling the amplitudes of the fission products at the scission point and they are correlated; if the nucleus is constrained by energy to pass through only one or few transition states then the total fission widths will be governed by the amplitudes of the transition states in the wave function of the resonance state. Hence the wide distribution of fission widths.

SLIDE 7.

So this is the picture we now have of configuration space. The classic internal region is separated by a relatively nuclear interaction-free zone at the saddle point deformation from another interaction region at higher deformation with the fission product channels leading off from the latter. For application of R-matrix theory to fission we now place the

channel entrances at the saddle point deformation, and this works well - the SAMMY code and other codes are based on this device.

SLIDE 8.

In the late 1960s a new chapter opened in the understanding of fission. From the neutron resonance point of view this was the discovery of narrow intermediate structure in fission cross-sections of fissionable actinide nuclides, originally in Pu-240 (Geel) and Np-237 (Saclay).. The Pu-240 total cross-section is shown above with resonances spaced at about 14eV, and the fission cross-section below with narrow clusters at intervals of about 700eV.

This was the clinching proof for Strutinsky's theory that the fission barrier could be split owing to shell effects in deformed nuclei.

SLIDE 9.

The double-humped barrier is shown schematically here. Notice that while we still have a region of strong nuclear interactions beyond the outer saddle that can knock things about a bit about but eventually still spits the system out as fission products, we also have an intermediate region in the secondary well where the available internal excitation energy is sufficient to regurgitate the system back into the primary well. This is the basis of Strutinsky's formula for the fission transmission coefficient for use in Hauser-Feshbach calculations, but is nowhere nearly sufficient to deal with sub-barrier or near-barrier cross-sections.

It is clear that, in general, we must place the fission channel boundaries at the outer barrier.

SLIDE 10.

Our new situation is shown in this version of configuration space, with the secondary well placed in our effective internal region.

SLIDE 11.

To develop this by R-matrix theory, we first consider discrete vibrational states within the double well potential (with suitable boundary conditions applied at the outer barrier deformation).

There are clearly two classes, one class with near-zero amplitude in the secondary well (these include the zero-point state, which is essential to the overall ground state of the compound nucleus), and the other set with major significant amplitude in the secondary well.

From these we can form two classes of R-matrix basis states, which are described in the following slides.

SLIDE 12.

SLIDE 13.

SLIDE 14

SLIDE 15.

SLIDE 16

SLIDE 17.

This shows schematically the form of the matrix that has finally to be diagonalized to obtain the final R-matrix states. The matrix elements in the off-diagonal sub-matrices are small because they involve the overlap of class-I and class-II vibrational states. hence the coupling between class-I and class-II R-matrix states can be achieved by perturbation methods or the mixing of a single class-II state with a neighbouring group of class-I levels.

SLIDE 18.

The Lorentzian form of the fission widths of a group of final R-matrix levels can be demonstrated exactly. Notice that the width of the Lorentzian is the coupling width across the inner barrier, which can be related to the transmission coefficient across that barrier.

SLIDE 19.

We still have to couple to the continuum to obtain the collision matrix which gives, finally, the cross-section. This can alter the profile of resonances dramatically.

SLIDE 20.

Take the case of two overlapping R-matrix states. On the left we see two R-matrix levels with their parameters treated as a couple of Breit-Wigner resonances. On the right is the R-matrix calculation, giving a much narrower peak in the cross-section.

SLIDE 21.

We can understand this by casting the R-matrix parameters into S-matrix theory, shown on this slide. In this theory, developed by Humblet and Rosenfeld in the early 1960s, the S-matrix, which is essentially the collision matrix, is expanded directly in the poles that occur in the complex energy field. Those poles give directly the location (real part) and half-width (imaginary part) of the observed resonances in the cross-section and the residues give their magnitude.

In the case shown in the last slide we find two poles, closer in real energy than the R-matrix states, one with very narrow width and one very broad, comprising in fact most of the summed widths of the two R-matrix states.

SLIDE 20.

Because there are normally two overlapping spin cases in the s-wave cross-sections of the fissile nuclei, it is difficult to find good clear experimental examples of this phenomenon, but they do occur in the keV region of much lighter nuclei.

Here is the total (almost pure elastic) cross-section of titanium, 74% Ti-48. The R-matrix fit has levels at the two main peaks shown with an interference dip between them.

SLIDE 23.

Let us look at the central energy region more closely. The S-matrix energy of the first pole is moved up a little to just above 18 keV, while that of the second has moved down from the red arrow signifying the R-matrix energy to directly under the interference dip. The width of the first pole is greater than the R-matrix width and that of the second is greatly decreased. The S-matrix description is that of a broad resonance embracing both peaks and a negative resonance near the middle of it. This seems unrealistic until you look at the capture cross-section which shows a positive peak virtually coinciding with the "negative" scattering resonance. The negativity is due to the phase difference in the residues of the two poles.

SLIDES 24

To return to our intermediate structure fission problem, already at near-barrier and sub-barrier energies the intermediate structure, even if represented as a uniform picket-fence model, causes large reductions below the Hauser-Feshbach (statistical) model.

SLIDE 25

We can now attempt to construct a formula to obtain easily the resonance parameters; from these we can calculate simply the average cross-sections for the AVXSF code. This is important because of the highly stochastic nature of the resonances, both fine-structure and intermediate. To take this into account we perform Monte Carlo type generation of R-matrix parameters. Numerical point-by-point averaging over the resulting detailed cross-sections would be very time-consuming. We aim to calculate the average cross-section over each resonance simply from its S-matrix parameters.

SLIDE 26.

In the limit of the class-II fission width being much greater than the coupling width, we can find analytically that the profile of S-matrix fission widths is Lorentzian with the width of the class-II fission width and other widths close to the R-matrix values. In addition there is a very broad pole having most of

the class-II fission width and a greatly reduced neutron width (compared with the average class-I value).

SLIDES 27-28

These slides show the S-matrix fission widths generated numerically from R-matrix states for a range of ratios of Class-II fission to coupling widths. We see that in the intermediate cases the S-matrix widths are very different from both their R-matrix fission widths and our simple Lorentzian hypothesis.

SLIDE 29

This shows the ratio of model cross-section to numerical point-by-point averaging. It is clear that use of the R-matrix parameters is reasonably good (and better than the S-matrix representation) for class-II fission width less than the coupling width, but our simple model is better (and good to within about 5%) above that. . The green curve is the result of an empirical construct that describes the condensation of a central group of states toward the final re-emergence of the class-II state as a broad underlying resonance.

SLIDE 30.

Conclusions.

SLIDES 31 etc.

Additional slides that were not shown in the lecture. These may be of some interest to those who wish to follow this subject more closely. (A few were shown in the following discussion session)