Analysis of the Neutron-Induced Fission Reaction in the plutonium isotopes

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Present purpose and challenge

From classic $R$-matrix to deformation channels

Procedure followed and present results with our AVXSF-LNG code
(Average CROSS SECTION Fission – Lynn & Next Generation)

Fission cross section prediction capability of short-lived plutonium isotopes?

But now you have to tackle the actual part of the iceberg ....
Our purpose is an accurate modeling of the fission cross section up to the second-chance fission threshold of the nuclides for which measurements are either available or very poor.

- The inclusion of the best knowledge we have of the physics of fission,
- Reconcile evaluation techniques and microscopic physics (i.e.; less adjusted parameters, phenomenology and, dependency on experimental fits).

Framework: on-going CEA-LANL collaboration involving modern writing (Fortran 95) of a code based on Eric Lynn’s theory of the $R$-matrix extended into deformation channels.
Classic R-matrix theory in Resonance analyses

- Involve

- an exterior region (nuclear interactions neglected, Schrödinger eq.)

- an internal spherical region ($\varphi_\lambda$, $E_\lambda$ unknown),

\[ R_{cc'} = \sum_{\lambda} \frac{\gamma_\lambda c \gamma_\lambda c'}{E_\lambda - E}, \]

- boundary conditions on reaction channels insure the connection.

\( c = [\alpha, l, s, J] \)
RM implicit fission hypothesis

Relies on the experimental evidence of a few number of degrees of freedom in fission and so implicitly on A. Bohr’s concept (1955) of ‘cold’ deforming nucleus

Analyses of fission cross section measurements in classic R-matrix codes

\[ \Gamma_{f_c} = 2P_{f_c} \gamma_{f_c}^2 \approx 2\gamma_{f_c}^2 \]

“Apparent” fission widths

\[ E_\lambda, g_J \Gamma_{\lambda_n}, \Gamma_{\gamma_{tot}}, \Gamma_{\lambda_f1}, \Gamma_{\lambda_f2} \]
Unresolved range and continuum

Standard Hauser-Feshbach theory:

\[
\bar{\sigma}_{c,c'}(E) = \sigma_{c,CN}(E) \sum_{s'} |i' - i'| \sum_{l'} |J - s'| \frac{T_{c'}^{J}(l's') (E)}{\sum_{c''} T_{c''}^{J}(l''s'') (E)} W_{nc'}
\]

With

\[
\sigma_{n, CN}(E) = \pi \chi^2 \sum_{J} \sum_{s=|I - \frac{1}{2}|} |J + s| g_{J,I} T_{n}^{J}(1s) (E)
\]

and

\[
T_{c}^{J}(1s) = 2\pi \frac{\bar{\Gamma}(c)}{D_{J}}, \quad \left\langle \frac{\Gamma_{n}^{J}(1s) \Gamma_{c'}^{J}(l's')}{\sum_{c''} \Gamma_{c''}^{J}(l''s'')} \right\rangle = \frac{\Gamma_{n}^{J}(1s)}{\sum_{c''} \Gamma_{c''}^{J}(l''s'')} \times W_{nc'}
\]
Shape classification of vibrational states

Exp. Proof of intermediate states has required the explicit inclusion of deformation modes in the Schrödinger eq. of the system:

\[
H = H_\eta + H_{int}(\zeta, \eta_0) + H_c(\eta, \zeta; \eta_0) \quad \Rightarrow \quad H X_\lambda = E_\lambda X_\lambda
\]

\[
\Phi_\nu(\eta), \epsilon_\nu \quad \chi_\mu(\eta), \epsilon_\mu(\eta)
\]

\[
X_\lambda = \sum_{\nu\mu} C_{\lambda(\nu\mu)} \Phi_\nu^{(\mu)} \chi_\mu
\]

\[
(\epsilon_\nu + \epsilon_\mu - E_\lambda) C_{\lambda(\nu\mu)} + \sum_{\nu'\mu'} C_{\lambda(\nu'\mu')} < \Phi_\nu^{(\mu)} \chi_\mu | H_c | \Phi_\nu^{(\mu')} \chi_{\mu'} >= 0
\]
Eventually, if the eigenvalues $\epsilon_\nu$ lower than the intermediate barrier, they fall into class-I and class-II categories.

\[
X^{(I)}_{\lambda_I} = \sum_{\nu\mu} C_{\lambda_I(\nu\mu)} \Phi^{(\mu)}_{\nu_I} \chi_{\mu}
\]

\[
X^{(II)}_{\lambda_{II}} = \sum_{\nu\mu} C_{\lambda_{II}(\nu\mu)} \Phi^{(\mu)}_{\nu_{II}} \chi_{\mu}
\]

\[
\Gamma_{\lambda_{I},tot} = \Gamma_{II,f} + \Gamma_{II,c}
\]
$^{241}$Pu: best known class-II parameters

- Analyzed class-II clusters by Auchampaugh et al. (PRC12 (1975))

<table>
<thead>
<tr>
<th>Target nucleus</th>
<th>$D_{II}$ [eV]</th>
<th>$E_{II}$ [eV]</th>
<th>$\Gamma_{II}(f)$ [eV]</th>
<th>$\Gamma_{II}(c)$ [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{240}$Pu</td>
<td>450 ± 50</td>
<td>782</td>
<td>1.92 ± 0.04</td>
<td>0.86 ± 0.17</td>
</tr>
<tr>
<td></td>
<td>1405</td>
<td>3.5 ± 0.4</td>
<td></td>
<td>0.15 ± 0.13</td>
</tr>
<tr>
<td></td>
<td>1937</td>
<td>1.9 ± 0.2</td>
<td></td>
<td>1.37 ± 0.26</td>
</tr>
<tr>
<td>average</td>
<td>2.5 ± 1.008 ± 0.6</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Note: resonances outside clusters $\Gamma_{f1}[eV] \approx \text{meV}$
Statistical regime Vs sub-barrier moderately weak coupling

\[
\sigma_{c,c'}(E) = \sigma_{c,CN}(E) \sum_{s'=|I'-i'|} \sum_{l'=|J-s'|} \frac{T_{c'}^{J_{\pi}(l's')}(E)}{\sum_{c''} T_{c''}^{J_{\pi}(l''s'')(E)}} \times W_{c,c'} \times W_{II}
\]

- **Complete mixing** \( (T_A + T_B) \gg 1 \)

\[
T_f(\beta) = \frac{T_A T_B(\beta)}{T_A + T_B + T_{II,\gamma} + T_{II,x}}
\]

- **Sub-barrier energies**

\[
\bar{P}_F = \left[ 1 + \left( \frac{T_I}{T_F} \right)^2 + \left( \frac{2T_I}{T_F} \right) \coth \left( \frac{T_A + T_B}{2} \right) \right]^{-1/2}
\]

I.S lower the average cross section,
IS effect might be \( \geq \) fluctuations effect

**Alternative to analytic formulae ARE Monte Carlo calculations**
Individual treatment of class-I and –II coupling

- Sub-barrier energies case: narrow central class-II state

\[
\begin{align*}
\varepsilon^{II} & \quad < \lambda_{II} | H_c^2 | \lambda_{I_1} > \quad \cdots \quad < \lambda_{II} | H_c^2 | \lambda_{I_N} > \\
< \lambda_{I_1} | H_c^2 | \lambda_{II} > & \quad \varepsilon_I^{I_1} \quad \cdots \quad 0 \\
. & \quad 0 \quad \cdots \quad . \\
. & \quad 0 \quad \cdots \quad . \\
< \lambda_{I_N} | H_c^2 | \lambda_{II} > & \quad 0 \quad \cdots \quad \varepsilon_I^{I_N}
\end{align*}
\]

Exact diagonalization of the Hamiltonian matrix to get \( E_\lambda \)
Discrete and continuum sequences: vibrational and intrinsic states

- 2 types of states might be present at the same excitation energy $E_{\text{exc}}$
  - The vibrational states of collective nature \( (500 \text{ keV} \leq D_{\phi}^{(\nu,\mu)} \approx \hbar \omega \leq 1200 \text{ keV} ) \)
  - The intrinsic states from combinations of single particle or hole states (D~100keV)

- Combined together to form band heads for rotational levels. It results in:
  - the “Compound Nucleus” state sequences in the wells,
  - transition state sequences on top of the barriers.

\[
E_N = (E_\nu + E_{\nu'} + \ldots + E_{\nu^*}) + (E_{Vib} + E_{Vib'} + \ldots + E_{Vib^*})
\]
\[
K_N = (\Omega_\nu \pm \Omega_{\nu'} \pm \ldots \pm \Omega_{\nu^*}) \pm (K_{Vib} \pm K_{Vib'} \pm \ldots \pm K_{Vib^*})
\]
\[
\pi_N = \pi_\nu \times \pi_{\nu'} \times \ldots \times \pi_{\nu^*} \times \pi_{Vib} \times \pi_{Vib'} \times \ldots \times \pi_{Vib^*}
\]
Even-even CN vs. e-odd, odd-e and o-o

- **Even-Even** ($^{240*}$Pu): band heads (mainly vibrations $\beta$, bending, mass ass. and combinations of them) with rotational band build-up.

  \[
  E_{\text{rot}}(J^\pi) = \frac{\hbar^2}{2\Sigma} \left[ J(J + 1) - K(K + 1) \right]
  \]

  with $J^\pi = \begin{cases} \frac{K^\pi, (K + 1)^\pi, (K + 2)^\pi, \text{etc.} \text{ if } K \neq 0}{0^+, 2^+, 4^+, \text{etc.} \text{ if } K = 0^+} \\ \frac{1^-, 3^-, 5^-, \text{etc.} \text{ if } K = 0^-} \end{cases}$

- **Odd (N)–Even (P)** ($^{241*}$Pu): vibrations + independent particles (Nilsson orbitals) spectrum neutron quasi-particle and vibration spectra combination; then rotational build up.

  \[
  E_{\nu}^{\text{qp}}(\eta) = \sqrt{\left( e_{\nu}^{p(n)}(\eta) - \lambda_{p(n)}(\eta) \right)^2 + \Delta_{p(n)}^2(\eta)}
  \]

  with \( \lambda_{p(n)} = \) Fermi energy \( \Delta_{p(n)} = \) pairing energy \( e_{\nu}^{p(n)} = \) single particle energy (\( \hbar \omega_0 \) unit)
Combination of multi-quasi-particle states combinatorial + multi-vibrations and rotational band build-up,

\[ U_N = E_N - \frac{1}{4} \sum_{i=n,p} \rho_i \Delta_i^2(\eta) \]

'Tracking' : \( \Delta'_{p(n)}(\eta) = \Delta_{p(n)} \exp \left[ -\frac{q_{p(n),\text{eff}}^2}{b_{p(n)}} \right] \)

\[ \begin{align*}
    &\text{\textbf{239Pu target}} \\
    &\text{\textbf{240Pu compound}} \\
    \end{align*} \]
Demarche adopted for this series of plutonium

- Model a ‘complete’ series of isotopes of a same element (plutonium) to supply ‘comprehensive’ information for each compound nucleus studied.
  - Consistent cross section calculations,
  - Possible reliable prediction of fission cross sections of the short-lived isotopes of the series.

- Work hypotheses
  - Outer barrier somewhat lower than the inner barrier,
  - Fission xs at lower energy dominated by specific barrier level schemes,
  - Normal deformation: specific scheme and combinatorial level density,
  - Inner barrier: specific scheme and combinatorial level density,
  - Outer barrier: empirical phase level density fitted on data.
Even-even excited nuclide ($^{240}\text{Pu}^*$) Example of individual states input

$$E_A = 5.80 \text{ MeV} \quad E_B = 5.00 \text{ MeV}$$

Pu-240 $^*$

$S_n$

Energy (MeV)

Fission Barrier 1 \hspace{2cm} Fission Barrier 2
Calculated average neutron-induced fission cross sections

- Level densities and barrier heights play an anti-correlated key role,
- Level density information extracted from the evaluation of the fission cross section of syst. (A+1) is used as input for the inelastic level density of target A.
Calculated average fission cross sections

Independent estimate of barrier heights for target nuclides which barrier(s) lie(s) below Sn was sought in this work.
Systematic trends extracted from this study (1)

Fundamental barrier heights vs. mass number

Inner

Outer
Systematic trends extracted from this study (2)

Proton and neutron pairing vs. mass number

Outer barrier combinatorial level density extraction from fitted empirical level barrier.
Capability of fission cross section prediction of short-lived nuclides
Conclusion

- We are now able to make more accurate fission average $\times s$ calculation starting from a microscopic basement in the energy range where the extended R-matrix is relevant,

- This consistent study of a series of isotopes involving a significant data base, including measurements data of same compound nuclei, is promising,

- Although we know that the results are likely, for now, not competitive with the evaluated data of ‘reference’.

And after ....
… we have to tackle the actual part of the iceberg

Update our Nilsson-type spectrum (and inertia momentum values),

Move from parabolic barrier shapes to actual ones,

Test our ‘transfer’ reaction and explicit class-II states models subsequently,

Explore parity dependence of level densities, etc.
Thank you for your kind attention