From average parameters to statistical resolved resonances

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JEFF Meeting, NEA Paris, April 2012
Motivation

- Improve the global calculations in the resonance range for short-lived nuclides with the TALYS system
- Use CALENDF-2010 to *statistically* reconstruct the URR
- Apply the methodology to TENDL-2012 and proposed isotopes for JEFF-3.2
- Use AVEFIT if possible
Examples of different approaches for $^{90}$Sr ($h_{1/2} = 28$ sec) in the low energy region.

Left: basic optical model calculation for ENDF/B-VII.1 and Single Resonance Approximation (SRA) for EAF-2010. Right: multi-SRA for TENDL-2011 and the present methodology for TENDL-2012.
Schematic approach to use in combination TALYS and CALENDF-2010

- Statistical parameters (Optical model from TALYS)
- Resolved resonances (CALENDF)
- Pointwise cross sections (TALYS)

Cross section (barns) vs. Neutron Energy (eV)

At low energy (below $10^4$ eV) the statistical parameters from the optical model are used.
Necessary parameters

As a starting point energy-dependent statistical parameters as well as specific cross sections are needed in the whole energy range. These parameters are for each orbital angular momentum $l$ and spin of the resonance state $j$:

- the scattering radius $r$,
- the average level spacing $D_0$,
- the average reduced neutron width $\Gamma_n$,
- the average radiation width $\Gamma_\gamma$,
- and if relevant the average fission width $\Gamma_f$.

![Graphs showing thermal cross section $\sigma_{(n,\gamma)}$ and scattering radius $R$ vs. isotopic mass](image)
Necessary parameters

Experiments

Systematics

Isotopic mass

\[ \Gamma_0 \, (eV) \]

\[ 10^4 \times S_0 \]

\[ 10^7 \]

\[ 10^5 \]

\[ 10^3 \]

\[ 10^1 \]

\[ 10^{-1} \]

\[ 10^{-3} \]

50 100 150 200 250

Isotopic mass

Experiments

Systematics

Isotopic mass

Experiments

Systematics

\[ 10^2 \]

\[ 10^1 \]

\[ 10^0 \]

\[ 10^{-1} \]

\[ 10^{-2} \]

50 100 150 200 250

Isotopic mass

Experiments

Systematics

Isotopic mass

Experiments

Systematics

\[ 10^2 \]

\[ 10^1 \]

\[ 10^0 \]

\[ 10^{-1} \]

\[ 10^{-2} \]

50 100 150 200 250

Isotopic mass

Experiments

Systematics

Isotopic mass

Experiments

Systematics

S-wave level spacing \( D_0 \) (eV)

\[ S_0, 1 \]

\[ 10^2 \]

\[ 10^1 \]

\[ 10^0 \]

\[ 10^{-1} \]

\[ 10^{-2} \]

50 100 150 200 250

Isotopic mass

Experiments

Systematics

Isotopic mass

Experiments

Systematics

\[ 10^2 \]

\[ 10^1 \]

\[ 10^0 \]

\[ 10^{-1} \]

\[ 10^{-2} \]

50 100 150 200 250

Isotopic mass

Experiments

Systematics

Isotopic mass

Experiments

Systematics

P-wave
3 groups of isotopes ($t_{1/2} > 1$ sec.)

1. isotopes without any experimental reaction information (about 1600 isotopes). In this case, as no specific information can be used to adjust calculations, we fully rely on systematics, as defined in TALYS.

2. isotopes with scarce experimental data, such as thermal cross sections, resonance integrals, average cross sections at high energy (about 400 isotopes). Such isotopes are for instance $^{40}$K, $^{54}$Mn, $^{60}$Co, $^{90}$Sr, $^{105}$Rh, $^{106}$Ru, $^{109}$Cd, $^{111}$Ag, $^{138,143}$Ce or $^{204}$Hg.

3. isotopes with measured pointwise cross sections, resonances, integral measurements, and resolved resonance parameters (about 400 isotopes).
Converting average parameters to statistical resonances

The idea is to generate random ladders of resonances using the statistical properties (as in the unresolved resonance range):

1. one ladder can be generated for an energy $E$ by randomly selecting a starting resonance energy for one $(l, j)$ sequence, and also randomly selecting a set of widths for that resonance using the appropriate average widths and $\chi^2$ distribution functions.

2. We can then select the next higher resonance energy by sampling from the Wigner distribution for resonance spacings, and a new set of widths for that resonance can be chosen.

3. The process is continued until a long ladder of resonances for that $(l, j)$ is obtained.

4. The process for the other $(l, j)$ sequences is then repeated, each such sequence being uncorrelated in positions from the others.

5. for each $(l, j)$ couples, a GOE random matrix (Gaussian Orthogonal Ensemble) is used to generate resonance energies (allowing to follow the Wigner law and to include correlations between two successive resonances).
Example 1: short lived isotopes

\[ ^{139}\text{Cs}(n,\gamma) \]
\[ ^{127}\text{Cs}(n,\gamma) \]

Incident neutron energy (eV)

Cross section (b)

\[ ^{10}\text{Mo}(n,\gamma) \]
\[ ^{89}\text{Mo}(n,\gamma) \]

Incident neutron energy (eV)

Cross section (b)

\[ ^{84}\text{Zr}(n,\gamma) \]
\[ ^{100}\text{Zr}(n,\gamma) \]

Incident neutron energy (eV)

Cross section (b)

\[ ^{49}\text{Cr}(n,\gamma) \]
\[ ^{57}\text{Cr}(n,\gamma) \]

Incident neutron energy (eV)

Cross section (b)
Example 2: isotopes with known thermal cross sections

\[ ^{40}\text{K}(n,\gamma) \]

Cross section (b) vs. Incident neutron energy (eV)

\[ ^{111}\text{Ag}(n,\gamma) \]

Cross section (b) vs. Incident neutron energy (eV)

\[ ^{106}\text{Ru}(n,\gamma) \]

Cross section (b) vs. Incident neutron energy (eV)

\[ ^{143}\text{Ce}(n,\gamma) \]

Cross section (b) vs. Incident neutron energy (eV)
Example 3: isotopes with known resonances

\[ ^{132}\text{Xe}(n,\gamma) \]

\[ ^{153}\text{Eu}(n,\gamma) \]

\[ ^{192}\text{Os}(n,\gamma) \]

\[ ^{229}\text{Th}(n,f) \]
Example 4: Thermal cross sections and resonance integrals

Table 1: Comparison of $C/E$ for the thermal capture cross section $\sigma_{\text{th}}(n,\gamma)$ and for the capture integral $I_\gamma$ for a selection of isotopes.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$C/E \sigma_{\text{th}}(n,\gamma)$</th>
<th>$C/E I_\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TENDL-2012</td>
<td>JEFF-3.1.2</td>
</tr>
<tr>
<td>$^{40}$K</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{54}$Mn</td>
<td>1.00</td>
<td>1.02</td>
</tr>
<tr>
<td>$^{60}$Co</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{105}$Rh</td>
<td>0.99</td>
<td>0.76</td>
</tr>
<tr>
<td>$^{106}$Ru</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{109}$Cd</td>
<td>0.99</td>
<td>1.05</td>
</tr>
<tr>
<td>$^{111}$Ag</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{138}$Ce</td>
<td>1.00</td>
<td>0.86</td>
</tr>
<tr>
<td>$^{143}$Ce</td>
<td>1.00</td>
<td>1.33</td>
</tr>
<tr>
<td>$^{192}$Os</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^{204}$Hg</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Extension at high energy with AVEFIT

AVEFIT from M. Moxon works in a similar way compared to CALENDF-2010.

- calculates the capture, fission and inelastic cross-sections from a randomly generated set of resonance parameters,
- single level approximation and the full R-Matrix formalism,
- similar subroutine to that used in the resonance fitting program REFIT,
- cross-section for up to five fission channels per spin and up to 60 inelastic levels,

![Graphs showing cross-sections for different neutron energies](image)
Conclusion

- Combination of TALYS + CALENDF-2010 (+ AVEFIT):
  consistent parameters from 0 to 20(0) MeV,

- Applied to 2400 isotopes for TENDL-2012,

- Sensible improvements compared to JEFF-3.1.2 for short-lived and low abundance isotopes,

- JEFF-3.2 (∼ 400 isotopes) could benefit from this approach.