Description and usage of experimental data for evaluation in the resolved resonance region

SG - 36
Objective

Produce **accurate cross section data together with reliable covariance information in the resonance region**

⇒ **Reduce bias effects**

⇒ **Produce reliable and realistic covariance data**
SG36-contributions 2011-2012

- Problems with PPP
- Uncertainty components of experimental data
  - Transmission
  - Capture

- Evaluation models

- Case studies

- Reporting data
  - Reporting experimental data
  - Reporting response functions of TOF-spectrometers
  - *Reporting of RP in a new “AGS-type” format*
\[ \chi^2(\theta) = (T_{\text{exp}} - F_m(x, \theta))^T V^{-1}_{Z,\text{exp}} (T_{\text{exp}} - F_m(x, \theta)) \]

\[
\frac{\delta N}{N} = 10\% \\
\frac{\delta B}{B} = 10\% \\
B = \frac{1}{2} \\
A = 85.0 \\
x_0 = 5 \\
\sigma^2 = 0.0018
\]

**Solution:** include \( N \) in adjustment procedure

Zhao & Perey ORNL/TM-12106

D'Agostini, NIM A346 (1994) 306

Fröhner, NSE 126 (1997) 1 - 18
Uncertainty components of experimental observables

Transmission

\[ T_m \propto e^{-n \times \sigma_{\text{tot}}} \]

\[ T_{\text{exp}} = N \frac{C_{\text{in}} - B_{\text{in}}'}{C_{\text{out}}' - B_{\text{out}}} \]

\[
\frac{\delta N}{N} \approx 0.5\% \quad \frac{\delta B_{\text{out}}}{B_{\text{out}}} \approx 5\% \quad \frac{\delta B_{\text{in}}}{B_{\text{in}}} \approx 5 - 10\% \]

Reaction cross section

\[ Y_m \propto \frac{\sigma_r}{\sigma_{\text{tot}}} (1 - e^{-n \times \sigma_{\text{tot}}}) + \ldots \]

\[ C = \varepsilon_r \Omega_r F_r Y_r A_r \varphi \]

\[ Y_{\text{exp}} = N \frac{\sigma_{\varphi} C_r' - B_r'}{\varepsilon_r C_{\varphi}' - B_{\varphi}'} \]

\[
\frac{\delta N}{N} \approx 2\% \quad \frac{\delta B_{\varphi}}{B_{\varphi}} \approx 5\% \quad \frac{\delta B_r}{B_r} \approx 5 - 10\% \]

Ideal conditions + experimental verification of uncertainties (IRMM, INFN)

Capture: Borella et al., NIMA 577 (2007) 626
Massimi et al., in preparation
Borella et al., NIMA 577 (2007) 626

- Total energy principle: $C_6D_6$ with weighting functions
- Weighting functions which account for the threshold
- Verify experimentally the effect of WF and threshold
- Correction for $\gamma$-ray attenuation in the sample
- Use fixed background filters
- Perform background measurements with additional filters
- Perform additional background measurements with Pb
- Determine neutron flux with a double ionization chamber 2 thin layers of $^{10}$B
- Normalization at a saturated resonance (account for gamma-ray attenuation)
Evaluation methods

LSQ adjustment or Maximum Likelihood (Max. Entropy)

\[ \chi^2(\tilde{\theta}) = (\tilde{Z}_{\text{exp}} - \tilde{Z}_m(\tilde{\theta}))^T V_{\tilde{Z}_{\text{exp}}}^{-1} (\tilde{Z}_{\text{exp}} - \tilde{Z}_m(\tilde{\theta})) \]

\[ \tilde{Z}_m = f(\tilde{\theta}) \]

\[ \tilde{\theta} = (\tilde{\eta}, \tilde{\kappa}) \]

\( \eta \): theoretical model parameters

\( \kappa \): experimental parameters

\[ \tilde{\theta} = \left( G^T_{\tilde{\theta}} V^{-1}_{\tilde{Z}_{\text{exp}}} G_{\tilde{\theta}} \right)^{-1} \left( G^T_{\tilde{\theta}} V^{-1}_{\tilde{Z}_{\text{exp}}} \tilde{Z}_{\text{exp}} \right) \]

\[ V_{\tilde{\theta}} = \left( G^T_{\tilde{\theta}} V^{-1}_{\tilde{Z}_{\text{exp}}} G_{\tilde{\theta}} \right)^{-1} \]

(linear model)

Methods to account for all uncertainty components and avoid PPP

- Include all model parameters in adjustment procedure Fröhner, NSE 126 (1997) 1 – 18
- Monte Carlo De Saint Jean et al., NSE 161 (2009) 363 - 370
- Marginalization Habert et al., NSE 166 (2010) 276 - 287

Differ in the way the uncertainty of experimental parameters are taken into account

⇒ At IRMM all tools available
$E = 4.9 \text{ eV}$

$\Gamma_\gamma = 122 \text{ meV}$

$\Gamma_n = 15 \text{ meV}$

Problem related to LSQ + GLUP
Comparison 3 methods : 4.9 eV $^{197}$Au(n,γ)

$E = 4.9$ eV
$\Gamma_\gamma = 122$ meV
$\Gamma_n = 15$ meV

<table>
<thead>
<tr>
<th>Sample thickness</th>
<th>0.001 mm</th>
<th>0.01 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fit -all</td>
<td>MC</td>
</tr>
<tr>
<td>$E$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$\Gamma_\gamma$</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>$\Gamma_n$</td>
<td>2.3</td>
<td>2.3</td>
</tr>
<tr>
<td>N (2%)</td>
<td>2.0</td>
<td></td>
</tr>
</tbody>
</table>

Peak uncertainty (counting statistics) : 1%

Relative uncertainty in %
Transmission, PbI\textsubscript{2} sample: Least-squares fit of R’ with SAMMY and CONRAD.

$N_T = 1.163 \pm 0.006 \text{ (0.5\%)}$

<table>
<thead>
<tr>
<th>Method</th>
<th>$R'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SAMMY+GLUP</td>
<td>6.690±0.001 fm</td>
</tr>
<tr>
<td>CONRAC+GLUP</td>
<td>6.697±0.001 fm</td>
</tr>
<tr>
<td>CONRAD+Marginalization</td>
<td>6.68 ± 0.16 fm</td>
</tr>
<tr>
<td>Direct perturbation</td>
<td>$\Delta R' \approx 0.14$ fm</td>
</tr>
</tbody>
</table>
Case studies: experimental data base created

- Resonance parameters
  - $T_{exp} = 0.1, 0.5 \text{ and } 0.9$
  - $Y_{exp} = 10^{-4}, 0.3 \text{ and } 0.9$

- Counting statistics uncertainty
  - 0.1, 1.0, 10% in peak (or baseline)

- Experimental parameters
  - Data reduction (GELINA)
    - Dead time
    - Background
  - Data analysis
    - Normalization
    - $\Delta n/n = 0.2\%$
    - $\Delta T_{\text{eff}} = 5 \text{ K}$
    - Response function

- Recommendation: repeat study and verify the effect of self-shielding

<table>
<thead>
<tr>
<th>E / eV</th>
<th>$\Gamma_\gamma$ / meV</th>
<th>$\Gamma_n$ / meV</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>100</td>
<td>1</td>
<td>100</td>
</tr>
</tbody>
</table>

With:

$(\Delta_D + \Delta_R) < \Gamma$

$(\Delta_D + \Delta_R) > \Gamma$
Reporting of results + experimental conditions

- **Facility/Neutron production (response function)**
  - Discuss with N. Otsuka
  - Input from nTOF, RPI, ORELA and IRMM,
  - Contact POHANG, LANL

- **Target characteristics**
  - Areal density distribution, contact N. Otsuka

- **Flux** *(recommend to provide the flux used for reaction data)*

- **Data Uncertainties**
  - Recommendation on dead time correction (< 1.2)
  - Report TOF
  - Report E + how it was deduced
  - Ideally: AGS-concept
  - In any case report separately
    - Uncorrelated component (due to counting statistics)
    - Normalization uncertainty
Response function $R'(L,E_n)$

- $1 - 5$ eV
- $100 - 500$ eV
- $1000 - 2000$ eV
- $6000 - 8000$ eV
- $10000 - 20000$ eV
- $60000 - 80000$ eV

Distance / cm

Probability density

$10^0$
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$

Distance / cm

Probability density

$10^0$
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$

2 cm
Analytical description of response

Order of magnitude of the parameters:

\[ \lambda_0 = 7 \pm 2 \text{ mm} \]
\[ \lambda_T = 24 \pm 5 \text{ mm} \]
\[ D_c = 10 \pm 2 \text{ cm} \]
Reporting of results + experimental conditions

- **Facility/Neutron production (response function)**
  - Discuss with N. Otsuka
  - Input from nTOF, RPI and IRMM

- **Target characteristics**
  - areal density distribution, contact N. Otsuka

- **Flux** *(recommend to provide the flux used for reaction data)*

- **Data Uncertainties**
  - Recommendation on dead time correction (< 1.2)
  - Ideally : AGS-concept
  - In any case report separately
    - Uncorrelated component (due to counting statistics)
    - Normalization uncertainty
Data reduction process

**Reaction yield + Self-indication**

\[ Y_{\text{exp}} = N \frac{Y_{\varphi} C' - B'_{w}}{\varepsilon_r C' - B'_{\varphi}} \]

- **C'** dead time corrected counts
- **B'** background contribution
- **N** normalization factor

**Transmission**

\[ T_{\text{exp}} = N \frac{C'_{\text{in}} - B'_{\text{in}}}{C'_{\text{out}} - B'_{\text{out}}} \]

**Histogram operations + Covariance information**

- **\( Y_{\text{exp}} \)** + covariance
- **\( Y_{\text{SI,exp}} \)** + covariance
- **\( T_{\text{exp}} \)** + covariance

**Models**
Observable $Z$ (dimension $n$) with $k$ sources of correlated uncertainties

$$V_Z = D_Z + S_Z S_Z^T$$

$D_Z$: uncorrelated part
$n$ values

$S_Z$: correlated part
dim. $(n \times k)$
Data reduction by AGS

\(^{235}\text{U}(n,f)\) measured at the GELINA facility\(^*\), \(L=10\) m, 100Hz, 800Hz

\[\text{Energy (eV)}\]

\[\text{Fission cross section (barns)}\]

\(100\) Hz  
\(800\) Hz

JEFF–3.1.1

\(*\)Olivier Serot, Cyrille Wagemans
Implicit Data Covariance Matrix with AGS methodology
## Link with AGS formalism

\[
\Sigma = \begin{pmatrix}
\Sigma_{11} & \Sigma_{12} \\
\Sigma_{21} & \Sigma_{22}
\end{pmatrix}
\]

\[
\begin{aligned}
\Sigma_{11} &= M_x + \left(\left(G_x^T G_x\right)^{-1} G_x^T G_\theta M_\theta G_\theta^T G_x \left(G_x^T G_x\right)^{-1}\right) \\
\Sigma_{12} &= -(G_x^T G_x)^{-1} G_x^T G_\theta M_\theta \\
\Sigma_{22} &= M_\theta
\end{aligned}
\]

Cholesky decomposition of the positive-definite matrix \( M_x \) into the product of a lower triangular matrix and its conjugate transpose lead to:

\[
\Sigma_{11} = M_x + S S^T
\]

If the contribution of the « statistical » uncertainties (from the fit) are negligible compared to the « systematic » uncertainties

\[
M_x \approx \text{diag(var}(x_1) \ldots \text{var}(x_n))
\]

Has to be verified: mathematics and also the impact of neglecting correlated terms in \( M_x \)