Higher-Order Contributions to Capture Processes

Goran Arbanas (ORNL)
Ian Thompson (LLNL)
Jutta Escher LLNL

in collaborations with:
Brett Manning (Rutgers)
Ray Kozub (TTU/ORNL)
Michael Smith (ORNL)
Shisheng Zhang (Beihang Univ./ORNL)

TORUS Collaboration Meeting
Michigan State University, East Lansing, MI
June 9, 2014
Overview

- Computation of capture via collective rotational states (2+, 4+)
  - Higher-order than direct capture
  - Fe-56 (n,g); relevant to CIELO collaboration

- Study of Nickel MACS (Rituparna Kanungo/TRIUMF)
  - Direct capture & compound resonance (s- & p-wave) capture important

- Study of $^{130}\text{Sn}(n,\gamma)^{131}\text{Sn}$ from ($\gamma,n$)
  - B. Manning computed (n,g) G.S. from Adrich’s ($\gamma,n$) data; detailed balance
  - Compute total (n,\gamma) from ($\gamma,n$) $\gamma$-strength function using TALYS

- Quantifying the improvement to MACS that could be hoped for from an improved theory (relative to Hauser-Feshbach) of (n,\gamma):

- Gamow-Shell Model computation of (n,g) near 132-Sn
  - Need effective interaction for tin isotopes (late 2014, or 2015)
Direct \((n, \gamma) +\) coupling to \(2+, 4+\)

- Used FRESCO to consistently couple to 2+ and 4+ states
  - In the incoming and the outgoing states
  - Prior to this work only incoming or outgoing but not both
  - Initiated a study of Ca-\{40,42,44,46,48\} isotopes
  - Computed Fe-56 because relevant to CIELO int.’l collab. nuclear data
    - 0+ (G.S.), 2+, 4+ rotational band states (but not clear for 6+, 8+…)
    - Real vs. Complex Koning-Delarche Opt. Pot. (cf. floor of capture data)
$^{62}\text{Ni}(n,\gamma)^{63}\text{Ni}$: Direct vs. Resonant capture

- **Direct Capture (DC) issues:**
  - $3s1/2$ zero-energy "resonance" of real (e.g. Woods-Saxon) pot. for $A \approx 55-60$
  - May yield unrealistic (too large) DC cross section

- **Resonant capture (RC) issues:**
  - $\gamma$-ray width of the 4.6 keV resonance underestimated:
    - $(0.76 \text{ vs. } 2.895) \text{ eV}$ (plotted below) $\rightarrow$ 30 keV MACS: $(5.2 \text{ vs. } 14.2) \text{ mb}$; 9 mb too small!
    - $p$-wave resonances were omitted from MACS: another 10 mb missing!

![Graphs showing cross-section versus incident energy](image.png)

$\Gamma_\gamma = 0.76 \text{ eV}$

pink: ENDF File 2: s-wave res. only

green: ENDF evaluated data

$\Gamma_\gamma = 2.895 \text{ eV}$

narrow $p$-wave resonances visible in the ENDF data (green);
**$^{62}\text{Ni}(n,\gamma)^{63}\text{Ni}: \text{Direct vs. Resonant capture}**

<table>
<thead>
<tr>
<th>\ MACS 30 keV</th>
<th>Rauscher [mb]</th>
<th>This work</th>
<th>Measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resonant (RC)</td>
<td>$5.2 \pm (5%)$</td>
<td>$24.2 \pm (5%)$</td>
<td>n/a</td>
</tr>
<tr>
<td>Direct (DC)</td>
<td>$5.5 \pm 0.8$</td>
<td>$0.4 \pm (20%)$</td>
<td>n/a</td>
</tr>
<tr>
<td>Total</td>
<td>$10.5 \pm 0.8$</td>
<td>$24.8\pm (&gt;5%)$</td>
<td>$25.8\pm1.8(\text{stat})\pm1.9(\text{sys})$</td>
</tr>
</tbody>
</table>

- **DC in this work computed by CUPIDO (Dietrich, LLNL):**
  - for the real part of the Koning-Delaroche optical potential
    - Its s-wave “resonance” occurs near $A\sim55$, so possibly safer than Rauscher’s potential
  - Analogous computation of MACS on 58,60Ni supported by high-res. data
    - A decreasing trend of DC for $\{58,60,62\}$Ni $\{1.36, 0.54 0.4\}$ mb observed:
      - Expected from a general formula for E1 s-wave neutron capture:
        - $\text{SF}^*(\text{BE}+\text{E}_n)^3 \leftarrow$ both SF and BE slowly decreasing as neutron number increases
      - The above may boost confidence into our DC computations.

- **RC in this work: corrected $\Gamma_\gamma$ of 4.6 keV res. + p-wave resonances**


Estimating errors of Hauser-Feshbach (HF)

- HF uses optical potential transmission coefficients
  - Yields energy-averaged cross-sections (*gross* structure)
    - Energy-averaging interval is on the order of 1 MeV

- What if we had an *intermediate* structure theory?
  - s.t. yields energy-averaged cross sections averaged over ~0.1 MeV
    - Corresponding to the width of nominal doorway states; e.g. 2p-1h states

- Performed a numerical estimate by energy-averaging $^{62}$Ni(n,$\gamma$) data
  - Followed by Maxwellian averaging for KT= 30 keV; cf. TALYS HF MACS

<table>
<thead>
<tr>
<th>E-avg. interval [MeV]</th>
<th>MACS [mb] kT=30 keV</th>
<th>TALYS $\Gamma_\gamma$-strength</th>
<th>renormalized</th>
<th>unrenor.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>24.2</td>
<td>Kopecky-Uhl Lorentz.</td>
<td>31</td>
<td>8</td>
</tr>
<tr>
<td>0.1</td>
<td>24.7</td>
<td>Brink-Axel Lorentzian</td>
<td>29</td>
<td>35</td>
</tr>
<tr>
<td>0.2</td>
<td>20.3</td>
<td>Hartree-Fock BCS</td>
<td>n/a</td>
<td>13</td>
</tr>
<tr>
<td>0.5</td>
<td>8.8</td>
<td>Hartree-Fock-Bogol.</td>
<td>n/a</td>
<td>13</td>
</tr>
<tr>
<td>1.0</td>
<td>7.0</td>
<td>Goriely’s hybrid model</td>
<td>30</td>
<td>12</td>
</tr>
</tbody>
</table>

- The improvement in accuracy may be appreciable in this case.
Intermediate Struct. Theory of Reactions

- How would an ideal Intermediate Structure Theory improve MACS
  1. Compute MACS of the Hauser-Feshbach (OMP) vs. MACS of the data
  2. Compute MACS of the averaged data 100 keV vs MACS of

- KKM formally extended to intermediate structure (UNEDF)
  - Via doorway projection operators

Atomic Data and Nuclear Data Tables 76, 70–154 (2000)

**FIG. 3.** Comparison of Maxwellian-averaged \((n, \gamma)\) cross sections for 30 keV thermal energy calculated with the statistical model code NON-SMOKER [3] with experimental data. The dashed lines are drawn to illustrate that the calculations tend to overestimate the cross sections near magic neutron numbers by up to a factor two, but are much more reliable elsewhere.
DC vs RC near closed shell nuclei

• Motivated by our computation of $^{130,132}\text{Sn}(n,\gamma)$ Direct Capture (DC)
  – $^{132}\text{Sn}(n,\gamma)$: DC $\gg$ RC is generally accepted
  – $^{130}\text{Sn}(n,\gamma)$: DC $\ll$ RC is estimated by Hauser-Feshbach models
    • But not confirmed experimentally
    • For $^{48}\text{Ca}$ and $^{208}\text{Pb}$ data suggest DC $\gg$ RC (in support of 132Sn DC $\gg$ RC above)
    • For $^{46}\text{Ca}$ and $^{206}\text{Pb}$ data suggest DC $\ll$ RC; does this imply $^{130}\text{Sn}(n,\gamma)$ DC $\ll$ RC too?
    • $^{124}\text{Sn}(n,\gamma)$ (the heaviest stable tin) plotted; shows many compound resonances
      – Its $kT=30\text{keV}$ MACS is $\sim10$ mb
      – consistent with some HF models
      – but still inconclusive Re: $^{130}\text{Sn}(n,\gamma)$
    – Could an intermediate structure model give answer?

$^{124}\text{Sn}(n,\gamma)$ ENDF evaluated data
\textbf{\(^{130}\text{Sn}(n,\gamma)^{131}\text{Sn}_{\text{g.s.}}\) from \(^{131}\text{Sn}_{\text{g.s.}}(\gamma,n)^{130}\text{Sn}\)}

- Using principle of detailed balance (g.s. only)
  - \((\gamma, n)\) a surrogate reaction for \((n, \gamma)\); usually applied to lighter nuclei
  - Adrich (2005) \(^{131}\text{Sn}_{\text{gs}}(\gamma, n)\) data yields \(^{130}\text{Sn}_{\text{gs}}(n, \gamma)\) \(E_n < 1.2\) MeV, ~ 10 x DC
  - even with large uncertainties; and without pygmy dipole resonance
  - A. Tonchev (TUNL) monochromatic laser (1-3)% energy variance
    - Stable nuclei.

\[\text{Diagram}\]
\( (n,\gamma) \) from \((\gamma,n)\) \(\gamma\)-strength function method

- Goriely, Hillaire, Koning (TALYS)
  - \(\gamma\)-strength function method to compute \((n,\gamma)\) from \((\gamma,n)\) & \((\gamma,\gamma')\) data
  - Total capture cross section (not just capture c.s. to g.s.)
  - Correspondence in progress. References
Proposal for \( (n, \gamma) \) in Gamow Shell Model

- Higher order (2p1h, 3p2h, ...) components in bound/resonant states
  - More complex than direct capture toward compound resonant capture
  - Comparison with Hauser-Feshbach

\[
\frac{d\sigma_{fc}}{dE_\gamma d\Omega_\gamma} = \frac{1}{\phi_{inc}} \frac{2\pi}{\hbar} \frac{E_\gamma^2}{(hc)^3} |T_{fc}|^2 \delta(E - E_f).
\]

- Coupled channels

- Proposal is nearly finalized
  - Pending effective interaction

\[
T_{fc} = \langle \Psi_f^{(A)} | H_\gamma | \Phi_c \rangle
\]

Table 1. Computational requirements of GSM on truncated space of tin isotopes near \(^{132}\)Sn needed for neutron capture computations. The columns display the mass number \( A \), dimension of the GSM truncated space, the memory requirements of the Slater determinants (SD) in kilobytes, the memory requirement of number-density matrices (SD|\( a^\dagger a \rangle SD \rangle \) in kilobytes, the number of Hamiltonian’s \( N \)-body matrix elements (NBME), and the percentage of these NBMEs that are not zero.

| \( A \) | Dimension | SD [kB] | \( \langle SD|a^\dagger a|SD \rangle \) [kB] | NBME’s\( \neq 0 \) \( \times 10^3 \) | \text{fraction NBME’s\( \neq 0 \) \%} |
|---|---|---|---|---|---|
| 129 | 379,430 | 563,421 | 467,232 | 651,549 | 0.5 |
| 130 | 59,886 | 80,382 | 58,667 | 41,271 | 1.2 |
| 131 | 7,294 | 8,305 | 5,629 | 7,532 | 14.2 |
| 132 | 691 | 553 | 395 | 239 | 50.1 |
| 133 | 46 | 1 | 15 | 2 | 100.0 |
| 134 | 662 | 51 | 676 | 226 | 51.7 |
| 135 | 13,078 | 1,612 | 16,076 | 18,409 | 10.8 |
| 136 | 136,805 | 29,693 | 219,202 | 122,790 | 0.7 |
| 137 | 1,289,881 | 377,388 | 2,512,421 | 3,147,875 | 0.2 |
Review and Outlook

• Direct neutron capture on non-spherical nuclei was modeled by rotational band states 2+, 4+ in incoming and outgoing partitions, and their effect, computed by Fresco, was significant for $^{56}$Fe.

• The improvement to stellar MACS that could be achieved by an ideal intermediate structure reaction theory over Hauser-Feshbach
  – The upper-limit promising, but a realistic theory would not do quite as well

• Used detailed balance and Adrich’s $^{131}$Sn($\gamma$,n) to estimate the lower limit of compound resonant capture on $^{130}$Sn(n,$\gamma$)$^{131}$Sn_{g.s.}
  – It appears to be greater than the Direct Capture component
  – Exploring the prospect of using g-strength function to compute total compound resonant capture, to all states (not just the g.s.)

• Gamow Shell Model; an intermediate structure theory of reactions?
  – An attempt to apply it to $^{132}$Sn(n,$\gamma$) is planned for 2015