Beyond Hauser-Feshbach: the Mazama code

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Outline of talk

1. Original motivation
2. Reminder of Hauser-Feshbach and Bohr-Wheeler.
3. A discrete-basis Hamiltonian model: Mazama
4. Application to cross section fluctuations in $^{235}$U(n,f)
5. Number of fission channels in $^{235}$U(n,f)
My original motivation: are there fission-channel resonances above the barriers?

Some provocative data:

235U(n,f)

Perez, et al. (1971)

Bowman, et al. (1971)

Moore, et al. (1971)
Reminder of Hauser-Feshbach

\[ \sigma_b(E, J, \pi) = \sigma_a(E, J, \pi) \frac{\Gamma_b(E, J, \pi)}{\sum_c \Gamma_c(E, J, \pi)} \]

Base-line formula

Some corrections

\[ \sigma_{ab}^{CN} \equiv < \sigma_{ab}^{fl} > = V_a V_b \left( \sum_c V_c \right)^{-1} [1 + \delta_{ab} (W_a - 1)] . \]

Nuclear Data Sheets 108 2655 (2007)

\[ V_a = T_a \left[ 1 + \frac{V_a}{(\sum_c V_c)} (W_a - 1) \right]^{-1} . \]

\[ W_a = 1 + 2 \left[ 1 + T_a^F \right]^{-1} + 87 \left( \frac{T_a - T_{ave}}{\sum_c T_c} \right)^2 \left( \frac{T_a}{\sum_c T_c} \right) \]

Width fluctuation
It gets even more complicated in fission theory

\[
\langle T_f(\mu) \rangle = \frac{v_A T_{B\text{cst}}}{4} \left( \frac{v_A T_{B\text{cst}}}{2T_A} \right)^{\frac{v_A}{2}} \prod_{\mu'} \left( \frac{T_{B\text{cst}}}{2T_B(\mu')} \right)^{\frac{1}{2}} \int_0^\infty dt \\
\times \left\{ e^{-t} \left[ t + \frac{v_A T_{B\text{cst}}}{2T_A} \right]^{-\frac{(v_A^2+1)}{2}} \left[ t + \frac{T_{B\text{cst}}}{2T_B(\mu)} \right]^{-1} \right. \\
\times \left. \prod_{\mu'} \left[ t + \frac{T_{B\text{cst}}}{2T_B(\mu')} \right]^{-\frac{1}{2}} \right\},
\]

(21)


And remember the Bohr-Wheeler limit

\[
T = 2\pi \frac{\bar{\Gamma}}{D} \quad 0 \leq T \leq 1
\]
A new approach based on a Hamiltonian representation

--The physical input parameters will be Hamiltonian matrix elements.
--The wave function will be represented in a discrete basis, so ordinary linear algebra can be applied to solve the equations.
--The format of the Hamiltonian matrix will be flexible enough to include intermediate structure and explicit exit channels.

The Mazama code: a 250-line Python script

Available to download from Phys. Rev. C Supplementary Material

Fluctuations in the $^{235}\text{U}(n, f)$ cross section

G. F. Bertsch, David Brown, and E. D. Davis
Phys. Rev. C 98, 014611 – Published 18 July 2018

Neutron width statistics in a realistic resonance-reaction model

P. Fanto, G. F. Bertsch, and Y. Alhassid
Phys. Rev. C 98, 014604 – Published 5 July 2018

Thanks to Paul Fanto for help.
Construction of the Mazama code

The Hamiltonian is set up in stages, each one connects only with its neighbors.
- Entrance channel
- Internal stage 1
- Internal stage 2
  -...
The entrance channel is the neutron in a Woods-Saxon potential.

\[ H_n \phi_n = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + V_{WS}(r) \phi_n = E \phi_n \]

Represent it on a discrete mesh: \( r_i = i \Delta r \)

\[ H_n \big|_{i,j} = -\frac{\hbar^2}{2m \Delta r^2} (\delta_{i,j+1} + \delta_{i,j-1} - 2 \delta_{i,j}) + V_{WS}(r_i) \delta_{i,j} \]

Solve it this way

\[ \phi_n(r_i) = \frac{\hbar^2}{2m \Delta r^2} \left( H_n - E \right)^{-1} \phi_n(r_{N+1}) \]

\[ \phi_n(r_N), \phi_n(r_{N+1}) \rightarrow \sin(k_n r + \delta) \]

\[
\begin{array}{c}
V_n \text{ (MeV)} \\
\hline
0 & 10 \\
-10 & -20 \\
-30 & -40 \\
\end{array}
\]

\[
\begin{array}{c}
r \text{ (fm)} \\
0 & 2 & 4 & 6 & 8 & 10 & 12 \\
\end{array}
\]

HmE = la.inv(HmE)
Now include internal states into the matrix Hamiltonian

\[ H = \begin{bmatrix} H_n & \nu \\ \nu^T & H_c \end{bmatrix} \]

\( \nu \) is coupling to entrance channel

\( H_c \) is the Hamiltonian of internal states

Decay widths to other channels are introduced by adding imaginary self-energies

\[ H_c|_{j,j} = \varepsilon_j - i\Gamma_j/2 \]

Solve for \( \phi \) as before

\[ (\phi_n, \phi_c) = \frac{\hbar^2}{2m\Delta r^2} (H - E)^{-1}_{:,N} \phi_n(r_{N+1}) \]

Partial reaction cross section:

\[ \sigma(n, \gamma) = \frac{\pi}{k_n^2} \sum_c \frac{\Gamma_{c,\gamma} |\phi(c)|^2}{\text{Incoming flux}} \]
Each stage is composed of a spectrum of levels following the Gaussian Orthogonal Ensemble. Interactions between levels in neighboring stages are taken from a Porter-Thomas distribution (i.e. a Gaussian distribution).

Examples of models that can be analyzed with Mazama:
Application to cross section fluctuations in $^{235}$U(n,f)


Are there fluctuations beyond those of the compound-nucleus resonances?

ENDF - VII & VIII

Typical Mazama run

Analyze with autocorrelation function

$$R(\varepsilon) = \left\langle \frac{(\sigma(E_+ - \bar{\sigma}(E_+))(\sigma(E_-) - \bar{\sigma}(E_-))}{\bar{\sigma}(E_+)(E_-)} \right\rangle$$

$$E_\pm = E \pm \varepsilon/2$$
The derived autocorrelation function

U-235(n,f) ENDF-VIII  10-30 eV

U-235(n,f) Mazama E = 10-30 eV

Peak height: \( R(0) \approx 4 \)

Peak width at half maximum: \( \Gamma_{HM} = \varepsilon \) at \( R(\varepsilon) = R(0)/2 \)
Results up to 90 eV

<table>
<thead>
<tr>
<th>Energy range</th>
<th>ENDF</th>
<th>Mazama</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\sigma_0(b)$</td>
<td>$\Gamma_{HM}(eV)$</td>
</tr>
<tr>
<td>10 - 30 eV</td>
<td>45.2</td>
<td>4.23</td>
</tr>
<tr>
<td>30 - 50</td>
<td>44.7</td>
<td>2.58</td>
</tr>
<tr>
<td>50 - 70</td>
<td>37.</td>
<td>2.40</td>
</tr>
<tr>
<td>70 - 90</td>
<td>29.9</td>
<td>1.42</td>
</tr>
</tbody>
</table>

Note large fluctuations of derived parameters, except for correlation widths. Experimental energy resolution is probably somewhat degraded in the high range data.

Physics we learned from the multi-keV data:
1) The compound-nucleus fluctuations are visible up to tens of keV, even though individual resonances cannot be resolved.
2) There is no systematic evidence for fluctuations on the one-keV energy scale in the 10-90 keV data.
Application 2:
How many fission channels are needed to describe $^{235}\text{U(n,f)}$ in the resolved resonance region? Bertsch and Kawano, Phys. Rev. Lett. 119 222504 (2017)

$$K = \pi \gamma T \frac{1}{E - H} \gamma,$$

$$S = \frac{1 - iK}{1 + iK},$$

the nonelastic cross sections [10]

$$\sigma_{nf} = \frac{\pi}{k_n^2} \sum_{c \in f} |S_{nc}|^2.$$  

(1)

(2)

(3)

FIG. 1. Cross section ratio $\alpha^{-1} = \langle \sigma_F \rangle / \langle \sigma_{cap} \rangle$ as a function of average fission width $\Gamma_F^K$ assuming a single fission channel. Solid line: Eqs. (1)–(3). Dotted line: Hauser-Feshbach approximation, i.e., $\alpha^{-1} = \Gamma_F^K / \Gamma_{cap}^K$. Dashed line: Hauser-Feshbach including the WFC correction, Eq. (8). Blue band: experimental range, taking uncertainty from Table I. Widths are the statistical errors associated with the 1-keV cross section averaging interval.

Conclusion: Full reaction calculation needed when only few channels present.
$^{{235}}\text{U}(n,\gamma)$ in the resolved resonance region.

Assume fission goes through a single transition state.

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- 7 physical input parameters (3 Woods-Saxon, 4 couplings, 1 compound nucleus.
- 2 numerical input parameters (Delta r, N_goe)

$$\langle \frac{\Gamma_n}{D} \rangle = 10^{-4} \left( \frac{E_n}{1\text{eV}} \right)^{1/2}$$

$\Gamma_{\gamma} \approx 35\text{ meV}$

$\Gamma_F \approx 100\text{ meV}$

$\alpha^{-1} \approx 2.8$

Output: $\alpha_{sts}^{-1} \approx 0.9$ 😞
Autocorrelation function up to 100 keV


$R_{\Delta E} \approx R(0) \frac{\pi \Gamma}{\Delta E}$
The effect of compound-nucleus fluctuations are clearly visible at tens of keV, but there is no structure beyond that in 6 out of 7 energy intervals.