Toward a microscopic calculation of induced fission cross sections

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Introduction

- Surrogate technique for (n,f) reactions that can't be measured
  - use surrogate reactions, e.g., (t,p), to populate same compound nucleus
  - Use model to compensate between (t,p) and (n) reactions

- Younes et al., 67 024610 (2003), ...
- Phenomenological treatment of fission
- Extend to $E_n = 20$ MeV

- Microscopic treatment of fission
  - Self-consistent barrier properties
    e.g., Bonneau et al., EPJA 21, 391 (2004)
Surrogate-reaction technique: formalism I

**Basic technique:**

<table>
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<tr>
<th>Measure</th>
<th>Calculate</th>
<th>Fit model</th>
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<td>$P_{(t,p)}(E_x) = \sum_{J^\pi} P_{(t,p)}(J^\pi) \times P_f(E_x, J^\pi)$</td>
<td>$\sigma_{(n,f)}(E_n) = \sum_{J^\pi} \sigma_{CN}(E_n, J^\pi) \times P_f(E_x, J^\pi)$</td>
<td>$\rightarrow P_f(E_x, J^\pi)$</td>
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**Basic ingredients:**

- $(t,p)$ reaction population
- $(n)$ reaction cross section
- **Fission model**
  - $P_f(E_x, J^\pi)$

Deduce, Calculate, Reuse
Double-humped fission model

Procedure:
- adjust barrier A & B heights to fit measured $P_{(t, pf)}$

Discrete levels:
- based on experiment

Continuous level density:
- micro/macro model
  + grand-partition func

Width fluctuations
Non-resonant barrier coupling
No class-II states
Surrogate-reaction technique: formalism II

### Basic technique:

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<td>$E_x$ (MeV)</td>
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<tr>
<td>Reuse</td>
<td>Deduce</td>
<td>Calculate</td>
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- Fit is not perfect
  - Model is over-constrained
  - Relative $P_f(E_x, J^\pi)$ are robust
- Renormalize to $P_{(t,\text{pf})}$ data

![Graph showing best fit to fission probabilities for $^{234}\text{U}(t,\text{pf})$.](image)

- Britt et al.
- This work
Surrogate reaction technique: proof-of-principle

Fission Probability

\[
\sigma_{n,t}(E_n) \times \frac{P_{t,p}^{(expt)}(E_x)}{P_{t,p}^{(calc)}(E_x)}
\]

Very good agreement, but limited to range of surrogate data

\[
235U(n,f) \text{ cross section}
\]
Surrogate technique: extension to $E_n = 20$ MeV

- **1\textsuperscript{st}-chance fission**: $^{235}\text{U}(n,0nf)$
  - $E_n \sim \text{few MeV} \rightarrow \text{use surrogate result}$
  - Higher $E_n \rightarrow \text{smooth (linear) extrapolation}$

- **2\textsuperscript{nd}+higher-chance fission**: $^{235}\text{U}(n,xnf) \times \geq 1$
  - Assume for 2\textsuperscript{nd} chance:
    $P[\text{fission, given } ^{235}\text{U}^* = ^{235}\text{U}(n,n')] = P[\text{fission, given } ^{235}\text{U}^* = n+^{234}\text{U}]$
  - Then:
    Calculated $\sigma_{(n,n')}(^{235}\text{U},E_n)$ is sum of two contributions
      - $\sigma_{(n,n')}(^{235}\text{U},E_n)$ folded with EQ neutron distribution (Maxwell)
      - $\sigma_{(n,n')}(^{235}\text{U},E_n)$ folded with PEQ neutron distribution (HMS calculation)

**Only one free parameter for 2\textsuperscript{nd}-chance fission:**
$\rightarrow \text{Maxwell-distribution temperature}$
Extended surrogate technique: proof-of-principle

\[ ^{235}\text{U} (n,f) \text{ cross section} \]

- Excellent agreement with measured \( \sigma_{(n,f)} \)
- Slope of 1st-chance fission depends on
  - Fission barriers
  - Level densities

\[
\frac{\Gamma_n}{\Gamma_f} \propto \frac{\exp \left( 2\sqrt{a_n (E - B_n)} \right)}{\exp \left( 2\sqrt{a_f (E - B_f)} \right)}
\]

(very roughly)

Need consistent calculations of barriers, level densities
Details of the HF+BCS calculations

• Code:
  ➔ HFODD v2.09i (Dobaczewski et al., CPC 1997-2005)
  ➔ Modified to print out single-particle wave functions in cylindrical basis

• Force:
  ➔ SKM* (standard)
  ➔ Pure pairing BCS, $G_p$ and $G_n$ adjusted to match experimental gaps

• Basis:
  ➔ Up to 31 oscillator quanta in cartesian directions
  ➔ Up to 1140 basis states
Check of the single-particle wave functions

- Calculated ground-state $<Q_{20}>$:

\[
\langle \text{G.S.} \mid \hat{Q}_{20} \mid \text{G.S.} \rangle = 2 \sum_{i>0} \langle i \mid \hat{Q}_{20} \mid i \rangle v_i^2
\]

\[
\left| i \right\rangle = \sum_{j>0} C_{j,i} \left| N^j, n_z^j, \Lambda^j, \Sigma^j \right\rangle
\]

- Within HFODD (internal)
- From s.p. Wave functions (external)

Very good agreement
\( ^{236}U \) potential surface along the symmetric path

- Barriers along symmetric path
  - \( E_A \approx 7.8 \text{ MeV} \)
    (accepted \( \approx 5.75 \text{ MeV} \))
  - \( E_B \approx 11.8 \text{ MeV} \)
    (accepted \( \approx 5.75 \text{ MeV} \))

Next: Explore \( Q_{22} \), \( Q_{30} \)
Barriers with $Q_{22}, Q_{30}$ degrees of freedom

- Barriers
  - $E_A \approx 6.92 \text{ MeV}$
    (accepted $\approx 5.75 \text{ MeV}$)
  - $E_B \approx 6.37 \text{ MeV}$
    (accepted $\approx 5.75 \text{ MeV}$)

Next: zero-point corrections
ATDHF + Belyaev cranking

• Libert *et al.*, PRC 60, 054301 (1999)

• Parameterize
  • Nuclear shape
    \[ q_0 \equiv \langle 2z^2 - x^2 - y^2 \rangle \]
    \[ q_2 \equiv \langle x^2 - y^2 \rangle \]
    Not used presently

• Nuclear orientation
  \[ q_1 \equiv \langle -2 iyz \rangle \]
  \[ q_{-1} \equiv \langle -2 xz \rangle \]
  \[ q_{-2} \equiv \langle 2 ixy \rangle \]

• Study response to slowly-varying field
Zero-Point-Energies from ATDHF + cranking

- Define:

\[ \Delta V_{ij} \equiv \frac{M_{ij}^{(-2)}}{M_{ij}^{(-3)}} \]

\[ M_{ij}^{(-k)} \equiv \sum_{\mu\nu} \frac{\langle \phi | \tilde{Q}_i | \mu\nu \rangle \langle \mu\nu | \tilde{Q}_j | \phi \rangle}{(E_\mu + E_\nu)^k} \]

- Zero-point vibrational energy:

\[ \Delta V_{vib} = \Delta V_{0,0}, \quad \tilde{Q}_0 \equiv \tilde{Q}_{20} \]

- Zero-point rotational energy:

\[ \Delta V_{rot} = \Delta V_{-2,-2} + \Delta V_{-1,-1} + \Delta V_{1,1} \]

\[ \tilde{Q}_{-2} \equiv 2i x y, \quad \tilde{Q}_{-1} \equiv -2x z, \quad \tilde{Q}_1 \equiv -2i y z \]
Zero-Point-Energies from ATDHF + cranking

• Define:

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• Zero-point rotational energy:

\[
\Delta V_{rot} = \Delta V_{-2,-2} + \Delta V_{-1,-1} + \Delta V_{1,1}
\]

\[
\bar{Q}_{-2} \equiv 2ixy, \quad \bar{Q}_{-1} \equiv -2xz, \quad \bar{Q}_1 \equiv -2iyz
\]

Calculated ZPEs are too large!
Zero-point energies at the barriers

- Assume 1D motion in $Q_{20}$ only at
  - 1st barrier ($\langle Q_{22} \rangle \neq 0$)
  - 2nd barrier ($\langle Q_{30} \rangle \neq 0$)

<table>
<thead>
<tr>
<th></th>
<th>1st min</th>
<th>1st barrier</th>
<th>2nd barrier</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta V_{\text{vib}}$ (MeV)</td>
<td>9.75</td>
<td>10.32</td>
<td>8.78</td>
</tr>
<tr>
<td>$\Delta V_{\text{rot}}$ (MeV)</td>
<td>11.85</td>
<td>15.88</td>
<td>17.84</td>
</tr>
<tr>
<td>$\Delta V_{\text{tot}}$ (MeV)</td>
<td>21.60</td>
<td>26.20</td>
<td>26.62</td>
</tr>
</tbody>
</table>

- Yields ZPE corrections
  - At 1st barrier: 4.60 MeV
  - At 2nd barrier: 5.02 MeV

Barriers are lowered too much!
Collective mass from ATDHF + cranking

- For $Q_{20}$ only:

$$M_{22} \equiv \frac{M(-3)}{[M(-1)]^2}$$

$$M(-k) \equiv \sum_{\mu\nu} \left| \left\langle \mu\nu \left| \hat{Q}_{20} \right| \phi (q_{20}) \right\rangle \right|^2 \left( E_\mu + E_\nu \right)^k$$

$$B_{22} = \frac{1}{M_{22}}$$

- At 1st barrier ($<Q_{22}> \neq 0$):
  - $B_{22} = 280.24$ MeV b²

- At 2nd barrier ($<Q_{30}> \neq 0$):
  - $B_{22} = 408.95$ MeV b²

\[ ^{236}\text{U, along symmetric path} \]
Collective mass and pairing gaps

$^{236}$U, along symmetric path

$^{236}$U, along symmetric path
Calculated barrier properties for $^{236}$U

• Barrier heights:
  → $E_A \approx 6.92 - 4.60 = 2.32$ MeV (compared to 5.75 MeV)
  → $E_B \approx 6.37 - 5.02 = 1.35$ MeV (compared to 5.75 MeV)

  
  
  Too low!

• Barrier curvatures:
  
  $$V(q) = E_i - \frac{1}{2} \mu(q)(\hbar \omega_i)^2 (q - q_i)^2$$

  → $\hbar \omega_A \approx 2.89$ MeV (compared to 0.90 MeV)
  → $\hbar \omega_B \approx 1.22$ MeV (compared to 0.50 MeV)

  
  
  Too large!
What's wrong?

- Mistake (phases?)
- Wrong prescription for pairing interaction
  - Test: vary energy cutoff ($\Delta E$) in calculation of moments

\[ \Delta V_{\text{rot}} \]
\[ \Delta V_{\text{vib}} \]

\[ \Delta V_{\text{rot}} \]
\[ \Delta V_{\text{vib}} \]

\[ \Delta V_{\text{rot}} \]
\[ \Delta V_{\text{vib}} \]

- Note slow convergence
- $G_n$, $G_p$, not constant with deformation
Conclusion

- Calculated
  - Microscopic energy surface

- Need to fix
  - Zero-point corrections
  - Collective mass

- Next:
  - Level densities
  - Fission probabilities \(\Rightarrow\) (n,f) cross sections

Thanks to A. Staszczak, H. Goutte, D. Gogny, J. Dobaczewski
Evolution of $\langle Q_{22} \rangle$ and $\langle Q_{30} \rangle$