Uncertainties in the evaluation of fission observables

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Observables

- Lifetimes ($t_{sf}$)
- Fragments
  - Mass distribution
  - Kinetic energy
  - Excitation energy
- Fission isomer properties
- Barriers (?) Model dependent (?)

both for spontaneous and induced fission
\[ \mathcal{P}_{i \rightarrow f} = \left| \langle \Psi_f | \hat{U}(\infty, -\infty) | \Psi_i \rangle \right|^2 \]

\[ |\Psi_i\rangle \text{ Nuclear ground state, Excited state, Nuclear state and an incident neutron, etc} \]

\[ |\Psi_f\rangle \text{ the final state can be any of the exit channels} \]

\[ |f_1(\alpha_1)\rangle |f_2(\alpha_2)\rangle \]

All the wave functions are the \textbf{exact} ones
but we do not know how to determine the exact wave functions and the evolution operator ....
we end up with a variety of different **mean field based** models used to compute the **observables**

we are interested in **lifetimes**: WKB model

\[
  t_{\text{sf}} = t_0 \exp\left(\frac{2}{\hbar} \int_{a}^{b} ds \sqrt{2B(s)(V(s) - E_0)}\right)
\]

\[
  B(s) = \sum_{ij} B_{ij} \frac{dq_i}{ds} \frac{dq_j}{ds} \quad \text{zero point energy}
\]

\[
  V(s) = \langle \phi(s) | H | \phi(s) \rangle - \epsilon_0(s)
\]

\[|\phi(s)\rangle\] is a constrained HFB mean field wave function
Uncertainties

Effective interaction

- **ph channel (Skyrme, Gogny, relativistic)**
  Influence PES. Under control if the interaction is properly adjusted (D1S, UNDEF1, ...)

- **pp channel (Global or locally adjusted)**
  Influence B(q). Worth to explore

  - Pairing strength gets multiplied by a factor eta

- **“Exotic” terms (Coulomb exchange+antipairing)**
  Relevant at extreme elongations (3rd minimum)
  Antipairing
Gogny
Finite range, density dependent interaction

- **D1S**
  - Fit includes a few selected finite nuclei
  - Fission information in the fit.
  - Poor descriptions of masses
  - Good in describing collective phenomena

- **D1M**
  - Global mass fit
  - No fission information in the fit
  - Very good description of masses (rms 0.7 MeV)
  - Not as thoroughly tested as D1S

BCPM
Density functional inspired in microscopic EoS

- Global (even-even) mass fit
- No fission information in the fit
- Not bad at masses (rms 1.6 MeV, even-even nuclei)
Big differences due to pairing properties
Pairing strength is multiplied by a factor $\eta = 1.05$ (5%) or 1.10 (10%)

Huge impact on lifetimes

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$t_{sf}$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>2.3 E+38</td>
</tr>
<tr>
<td>1.05</td>
<td>8.0E+27</td>
</tr>
<tr>
<td>1.10</td>
<td>6.7E+21</td>
</tr>
</tbody>
</table>

consequence of the reduction of the collective mass

Little impact on binding energies and other properties like deformation
Coulomb repulsion is a fundamental concept in fission that should be treated exactly: Exact Coulomb exchange and Coulomb antipairing

- Exact Coulomb exchange is important for elongated configurations
- Coulomb pairing also important (enhances barriers, even the third one)
- Coulomb antipairing increases collective inertia
- Coulomb antipairing produces bumps in the inertia the favor the localization of wave function in the third minimum

\[ \tau_f \text{ with } ATDHFB \text{ inertias} \]

\[
\begin{align*}
\text{D1S} & : 7.5 \, \text{E}+42 \\
\text{D1S(CE)} & : 3.9 \, \text{E}+43 \quad \text{!!!} \\
\text{D1S(CE+CP)} & : 2.9 \, \text{E}+51 \\
\text{D1M} & : 3.6 \, \text{E}+54 \\
\text{D1M(CE)} & : 4.8 \, \text{E}+56 \quad \text{!!!} \\
\text{D1M(CE+CP)} & : 5.1 \, \text{E}+69
\end{align*}
\]
Inertias

\[ t_{sf} = t_0 \exp\left(\frac{2}{\hbar} \int_a^b ds \sqrt{2B(s)(V(s) - E_0)}\right) \]

Two types of inertias

- ATDHFB: Contains time odd components
- GCM: No time odd components

Both are traditionally computed using the “cranking approximation”

**ATDHFB**

\[ B(Q_{20}) = \frac{1}{2} \frac{M_{-3}}{(M_{-1})^2} \]

**GCM**

\[ B(Q_{20}) = \frac{1}{2} \frac{M_{-2}^2}{(M_{-1})^3} \]

\[ M_{(-n)} = \sum_{\alpha > \beta} \langle 0 | Q_{20} | \alpha \beta \rangle \frac{1}{(E_\alpha + E_\beta)^n} \langle \alpha \beta | Q_{20} | 0 \rangle \]

Both can be computed exactly but the numerical cost involved is rather high (prohibitive up to now).

**Exact inertias can be a factor 1.5 larger than the approximate ones.**
Full line: ATDHFB (Cranking) mass
Dashed: GCM (Cranking) mass

ATDHFB is a factor of 1.8 larger than GCM

<table>
<thead>
<tr>
<th>$t_{sf}$</th>
<th>ATDHFB</th>
<th>GCM</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1S</td>
<td>4.3 E+32</td>
<td>5.7 E+23</td>
</tr>
<tr>
<td>D1M</td>
<td>6.0 E+46</td>
<td>6.6 E+34</td>
</tr>
<tr>
<td>BCPM</td>
<td>3.0 E+54</td>
<td>1.6 E+40</td>
</tr>
</tbody>
</table>

Up to 14 orders of magnitude difference
Exact versus approximate GCM masses

- Exact GCM is computed with second derivatives of energy overlap
- Approximate GCM using the “cranking” formulas. Red curve: approximate x 1.6
- ATDHFB computed using “cranking” formulas

Quadrupole inertia

If inertia gets multiplied by a factor f the actions is multiplied by $\sqrt{f}$ as the expected change in the exponent of $t_{sf}$
Zero point energies

- Symmetry restoration
  (Rotational, PNP, parity, Center of mass)
- Fluctuations on quadrupole, octupole, etc

Typically, symmetry restoration energies are considered in the spirit of Projection After Variation

\[
\frac{\langle \Delta \vec{J}^2 \rangle}{2 J Y_{occ}}
\]

Rotational energy correction well approximated by rotational formula if exact Yoccoz is used.

A good approximation to Yoccoz is to use “cranking” formula and multiply by a phenomenological factor

Rotational correction substantially modifies energy landscape (3 - 7 MeV)

Parity projection and PNP-PAV have little impact on energy landscapes

PNP-VAP increases pairing correlations: the inertia decreases!
**PNP-RVAP**: Minimize projected energy on a restricted subspace (fluctuations in proton and neutron number)

Coulomb exchange and antipairing has to be considered to avoid pathologies in the evaluation of overlaps.

PES affected by PNP-RVAP

Collective mass similar to HFB one!

Effect of Coulomb antipairing cancels out.
The $E_0$ parameter

$$t_{\text{Sf}} = t_0 \exp\left(\frac{2}{\hbar} \int_a^b ds \sqrt{2B(s)(V(s) - E_0)}\right)$$

$E_0$ is taken as the HFB ground state energy plus the zero point energy of the quadrupole motion: typically some value in between 0.5 and 1.5 MeV

Increasing $E_0$ makes the integration interval in the action sorter and the action smaller. Reduces lifetimes (up to 5 orders of magnitude)
Some physics with BCPM

Nuclei with known experimental data on $t_{sf}$

GCM inertias

Large variability with eta and $E_0$

Isotopic trend reproduced

Trend with mass number reproduced
Z, N of each fragment

Consider a large Q20 value

Constrain the neck to a small value

Release the constraint to obtain a solution with two fragments

Use that solution to seed a calculation for larger values of Q20 (i.e. increase the separation between fragments)

Continue the calculation until the Z and N values of the fragments do not change significantly as Q20 is increased
Neutron rich uranium (predictions!)

From $^{230}\text{U}$ up to $^{282}\text{U}$

Emergence and evolution of the third minimum

Barriers increase and become wider
alpha decay from Viola’s formula  (BCPM is good with masses)

Peak at $^{276}$ U
Fragments
Gogny D1S, D1M and D1N
Minimizing the action

Long ago (Funny hills paper) the minimization of the action was proposed

\[ t_{sf} = t_0 \exp\left(\frac{2}{\hbar} \int_a^b ds \sqrt{2B(s)(V(s) - E_0)}\right) \]

Later, Moretto proposed a simple model of fission where the pairing gap is a relevant degree of freedom

\[ B \sim \frac{1}{\Delta^2} \quad V(s) = V_0(s) + 2g(\Delta - \Delta_0)^2 \]

Minimization of the action using the pairing gap as degree of freedom decreases \( t_{sf} \) by several orders of magnitude

Pursued by Pomorski and others in the 80’s
We have explored the idea using \( \langle \Delta N^2 \rangle \) instead of the gap to search for a minimum of the action for each quadrupole moment.

Strong quenching of the collective mass at the minimum of S.

Moderate increase of the potential energy (meaning of barrier heights here?).

The action gets reduced by 20 \% - 30 \% implying a similar reduction of the exponent in \( t_{sf} \).
A reduction of many orders of magnitude is observed. The ATDHF and GCM results seem to “converge.”
also

- Numerical convergence with basis size, box size, step size, etc should be assessed

- An easy to implement extrapolation scheme to “infinite” basis will be beneficial

- Numerical accuracy of matrix elements, algorithms, etc should be tested (specially Coulomb)
Conclusions

- For a **qualitative** description of fission the present mean field methods are still valid

- To reach the “**quantitative**” level the dynamical aspects of fission have to be addressed

  - Pairing as a new degree of freedom
  - Least action versus Minimum energy
  - Exact evaluation of inertias
  - Particle number restoration
  - Full treatment of Coulomb
Thanks to ...

Previous studies
Michal Warda, K. Pomorski, S. Pérez, V. Martín and F de la Iglesia

Cluster radioactivity
Michal Warda

Present (in progress) studies
Samuel Giuliani (BCPM) and R.R. Rodriguez-Guzman (Gogny)