Density functional theory of spontaneous fission life-times

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Fission

**Experimental results**

- 239Pu thermal
- Fission
- Microscopic understanding

**Equations**

\[ N = N_1 + N_2 \]
\[ Z = Z_1 + Z_2 \]

**Diagram Elements**

- Elongation
- Necking
- Split
- \( N_1, Z_1 \)
- \( N_2, Z_2 \)
Fission: our strategy

Stability of the heaviest nuclei, r-process, advanced fuel cycle

Quality Input

Large-scale Simulations on Leadership-class Computers

Dynamics

Collective potential and inertia in 2D \((Q_{20}, Q_{22})\) for \(^{264}\text{Fm}\)

\((^{264}\text{Fm} \text{ undergoes symmetric fission})\)

ph channel:
Skyrme functionals
SkM* parametrization

pp channel:
mixed pairing interaction

Numerical

Symmetry unrestricted DFT solver: HFODD (v2.49t)

HFB for potential
ATDHFB for cranking inertia

Action minimization technique

Spontaneous fission pathways & \(T_{1/2}\)

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Plan

- Hetree-Fock-Bogoliubov (HFB) method → Potential Energy Surface (PES)
- A diabatic Time Dependent HFB formalism → Collective Inertia (M)
- Action minimization techniques

Dynamic Programming Method (DPM)
Ritz Method (RM)

Results: Spontaneous Fission (SF) paths and Half-lives (T_{1/2})
**HFB formalism**


- **HFB equation**
  \[ [\mathcal{W}, \mathcal{R}] = 0 \]

- **Generalized density**
  \[ \mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} \]

- **Single particle Routhian**
  \[ \mathcal{W} = \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \]

- **Non-linear eigenvalue equation**
  \[ \mathcal{W} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} E \]

  - *E* → Diagonal matrix of quasiparticle energies
  - *A*, *B* are quasiparticle wavefunctions

- **Particle density**
  \[ \rho = B^* B^T \]

- **Pairing density**
  \[ \kappa = B^* A^T \]

- **Chemical potential**
  \[ \Delta = \Gamma_{pp}[\kappa] = f_{\kappa} \]

- **Paring form factor**
  \[ \Gamma_{ph}[\rho] + \text{constraint}(<Q>) \]

- **Calculation can be constraint at a particular value of quadrupole moment* \(<Q>\)**

- **Converged solutions** \(\rho_0\) & \(\kappa_0\) are achieved after solving HFB equation iteratively

- **Total energy**
  \[ E_{tot}(Q) = Tr(T\rho_0) + Tr(\Gamma_{ph}[\rho_0]\rho_0) + Tr(\Gamma_{pp}[\kappa_0]\kappa_0) + \text{Coulomb} \]
Calculated potential energy

\[ \Gamma[\rho] \rightarrow \text{Skyrme functional with SkM* parametrization} \]


\[ f(r) = V_{0}^{(n,p)} \left[ 1 - \frac{1}{2} \rho(r) \rho_{c} \right] \]


\[ \rho_{c} = 0.16 \text{fm}^{-1} \quad V_{0}^{n} = -268.9 \text{MeV fm}^{3} \]
\[ V_{0}^{p} = -332.5 \text{MeV fm}^{3} \]

Adjusted to reproduce the ‘n’ & ‘p’ pairing gaps of \(^{252}\text{Fm}\)


\[ V = E_{\text{tot}} - E_{\text{ZPE}} \]

Vibrational Zero Point Energy (GOA)


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ATDHFB formalism

Introducing dynamics:

\[ i\dot{\mathcal{R}}(t) = [\mathcal{W}, \mathcal{R}(t)] \]

Adiabatic approximation:

\[ \mathcal{R}(t) = e^{(i/\hbar)\chi(t)}\mathcal{R}_0(t)e^{(1978/\hbar)\chi(t)} \]

(dynamics is quasi-stationary)

Expansion in powers of collective momentum $\chi$

Comparing with the classical expression of KE

Collective Inertia:

\[ \mathcal{M}_{ij} = \frac{i}{2\dot{q}_j} Tr \left( \frac{\partial \mathcal{R}_0}{\partial q_i} [\mathcal{R}_0, \mathcal{R}_1] \right) \]


$q_i$s are collective coordinates, quadrupole moment $Q$ for the present purpose

M. Baranger M. Veneroni, Ann. Phys. 114, 123

…… talk by J. Dobaczewski
Calculated Inertia

After a few steps:-

\[ -\mathbf{F}^{\dagger} = \left( B^T \frac{\partial \rho_0}{\partial q_i} A + B^T \frac{\partial \rho_0}{\partial q_i} A + B^T \frac{\partial \rho_0}{\partial q_i} A \right) \]

\( A, B \) are quasiparticle energies

Derivatives of densities can be calculated using Lagrange three-point formula

Derivatives calculated approximately in terms of collective variables

Cranking Approximation

more simplified way (perturbative approximation)

\[ \hat{M}^{\dagger} = \hat{M}^{(1)} - \hat{M}^{(2)} \]

\[ \hat{M}^{(2)} \]

Unit = \( 10^{-3} \hbar^2/M \text{eV b}^2 \)

\[ E_1 \]

\[ E_1 \]

\[ \mathbf{W}_1 \]

\[ \mathbf{W}_1 \]

\[ \mathbf{W}_1 \]

\[ \mathbf{W}_1 \]

\[ \mathbf{W}_1 \]

\[ \mathbf{W}_1 \]
Understanding calculated Inertia

$$|\mathcal{M}|^{1/2} = (\mathcal{M}_{11}\mathcal{M}_{22} - \mathcal{M}_{12}^2)^{1/2}$$

Invariant under rotation in 2D

Sharp variations

variations similar to $|\mathcal{M}^c|$ 

Large fluctuations of mass parameters are manifestations of crossings of single-particle levels near the Fermi energy

Unit = $10^{-3} \ h^2/\text{MeV b}^2$
Numerical test

\[ M_{\text{eff}}(s) = \sum_{i,j} M_{i,j} \frac{dq_i}{ds} \frac{dq_j}{ds} \]

‘s’ describes the path on 2D surface

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Step 1: 
\( M_{\text{eff}} \) is calculated along \( \gamma = 180^0 \)

Step 2: 
Densities are rotated by Proper Eulerian angles

Step 3: 
\( M_{\text{eff}} \) is calculated along \( \gamma = 60^0 \)
Spontaneous fission half-life

\[ T_{1/2} = \frac{\ln 2}{nP} \]

\( n \) is the number of assaults on the fission barrier per unit time \( \approx 10^{20.38} \text{ s}^{-1} \)

Penetration probability \( \rightarrow P = (1 + \exp 2S(L))^{-1} \) \( \text{(WKB)} \)

Action integral along the fission path \( L(s) \)
\[ S(L) = \int_{s_1}^{s_2} \frac{1}{\hbar} [2\mathcal{M}_{\text{eff}}(s) (V_{\text{eff}}(s) - E_0)]^{1/2} ds \]

Most probable fission path = Minimum action path
Action minimization techniques

Two numerical methods

Ritz method (RM):

\[ y(L) = \sum_{k} a_k \sin \left( \pi k \frac{x - x_1}{x_2 - x_1} \right) + \text{b.c.} \]

b.c. decided by \( s_1(x_1, y_1) \) and \( s_2(x_2, y_2) \)

\[ S(L) = \int_{s_1}^{s_2} \frac{1}{\hbar} [2\mathcal{M}_{\text{eff}}(s)(V_{\text{eff}}(s) - E_0)]^{1/2} \, ds \]

\[ S(L) \rightarrow S(a_1, a_2, \ldots a_n) \]

path is decided by varying \( a_i \)s

For the present calculation \( a_1, a_2 \) and \( a_3 \) are sufficient
Action minimization techniques

Dynamic programing method (DPM) :-

Select $s_1$ & $s_2$

Surface between $s_1$ & $s_2$ is divided into 2D mesh

$S$ is calculated between $s_1$ & each point in 1$^{st}$ column

$S$ is calculated for each point in 2$^{nd}$ column with all points in 1$^{st}$ column &

Minimum action path is retained

Repeated for all points in column 2: - minimum action paths up to column 2

Repeated for all columns

Finally we get the minimum action path between $s_1$ & $s_2$
5. Conclusions

Non-axial quadrupole shapes seem to play a minor role in the spontaneous fission of the SHE nuclei around $^{298}$114, in spite of the fact that they can considerably lower the static fission barriers. Fission paths which exploit a non-axial saddle are rather long. The probability of the occurrence of triaxial fission trajectories is reduced by the tendency towards the minimal length of the fission path, following from the principle of the least action.

Fig. 1. The energy contour maps with drawn static (dashed) and dynamic (solid) fission trajectories for selected systems. The minimization over $\beta_4$ was performed at each $(\beta, \gamma)$. Contour lines are 1 MeV apart. Provided contour labels help to reveal topography.
Results (existing)

J.-P. Delaroche, M. Girod, H. Goutte, J. Libert
Nuclear Physics A 771 (2006) 103–168

Microscopic HFB calculation
With Perturbative-cranking inertia $M^{CP}$
Results (present calculation)

$E_0 = 1.0 \text{ MeV}$

Static path
(minimum potential path)

Dynamic path with cont. $M$
$M = M_{2020}^{C_p}$ at ground state
(DPM)

Dynamic path with $M^C$
(DPM & RM)

Dynamic path with $M^{C_p}$
(DPM & RM)

Dynamical effects due to action minimization is not very prominent

With $M^C$: dynamics is favoring triaxial saddle, similar to static path

With $M^{C_p}$: Strong dynamical effects, triaxiality becomes unimportant

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Results (present calculation)

Orders of magnitude difference in $T_{1/2}$ calculated with $M^C$ and $M^{Cp}$

<table>
<thead>
<tr>
<th>path</th>
<th>$S(L)$</th>
<th>log($T_{1/2}$/yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Static+$M^C$</td>
<td>23.4</td>
<td>-7.7</td>
</tr>
<tr>
<td>Static+$M^{Cp}$</td>
<td>20.8</td>
<td>-10.0</td>
</tr>
<tr>
<td>DPM+$M^C$</td>
<td>19.1</td>
<td>-11.4</td>
</tr>
<tr>
<td>DPM+$M^{Cp}$</td>
<td>16.8</td>
<td>-13.4</td>
</tr>
<tr>
<td>RM+$M^C$</td>
<td>18.9</td>
<td>-11.6</td>
</tr>
<tr>
<td>RM+$M^{Cp}$</td>
<td>16.8</td>
<td>-13.4</td>
</tr>
</tbody>
</table>
Summary & conclusion

Spontaneous fission lifetimes have been studied within a dynamic approach based on the minimization of the collective action in a two-dimensional collective space of elongation and triaxiality.

A strong dynamical effect has been predicted. Although it offsets the static reduction of the inner barrier by triaxiality when the approximate perturbative cranking inertia is used, the strong effect of triaxiality is observed with the more appropriate non-perturbative cranking inertia.

A more detailed study of dynamical effects due to triaxial and reflection asymmetric degrees of freedom is in progress.
Collaborators:
W. Nazarewicz
J. Dobaczewski
A. Baran
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J. A. Sheikh

Thank you...