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Colloque GANIL

How the octupole structure determines the fission asymmetry

Guillaume SCAMPS

Collaboration : C. Simenel
Motivation: to understand the shell effects on fission

Empirical behaviour of actinide nuclei


Data from D. A. Brown et al., Endf/b-viii.0, Nucl. Data Sheets 148, 1 (2018), (spontaneous and thermal neutron-capture).
Systematic comparison for actinide
Empirical behavior of actinide nuclei


C. Bückstiegel et al. / Nuclear Physics A 802 (2008) 12–25

Motivation
How can we understand this behaviour? Interplay between structure and reactions?
Mean-field dynamics with pairing

**TDHF+BCS**
- Based on TDHFB with the approximation: $\Delta_{ij} = \delta_{ij}\Delta_i$
- Initialisation from ev8 (HF+BCS)
- Evolution:
  
  \[ i\hbar \frac{d\varphi_i}{dt} = (\hat{\mathcal{H}}_{MF} - \epsilon_i)\varphi_i \]
  \[ i\hbar \frac{dn_i}{dt} = \Delta^*_i \kappa_i - \Delta_i \kappa^*_i \]
  \[ i\hbar \frac{d\kappa_i}{dt} = \kappa_i(\epsilon_i - \epsilon_{\bar{i}}) + \Delta_i(2n_i - 1) \]

**Details of the calculation**
- Skyrme functionnal Sly4d
- Surface pairing interaction
- $\Delta x = 0.8$ fm; $\Delta t = 1.5 \times 10^{-24}$ s
- Lattice: $L_x \times L_y \times 2L_z = 40 \times 19.2 \times 19.2$ fm$^3$
Why does we need pairing?

Fission barrier: $^{258}\text{Fm}$

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Fission barrier: $^{258}_{\text{Fm}}$

$E [\text{MeV}]$

$R [\text{fm}]$

TDHF

TDHF + BCS

Why does we need pairing?

Fission barrier: $^{258}\text{Fm}$

Influence of pairing on fission process
Influence of pairing on fission process
New systematic study

First: CHF+BCS

Example: $^{240}$Pu

Second: TDHF+BCS
New systematic study

First: CHF+BCS

Example: $^{240}\text{Pu}$

Second: TDHF+BCS
New systematic study

First: CHF+BCS

Example: $^{240}\text{Pu}$

Second: TDHF+BCS
TDHF+BCS systematics results

TDHF+BCS

Comparison with experimental data
The TDHF+BCS calculation reproduces well the \( Z = 54 \) behavior. But why?
Nucleon localization function

Fermion localization function

\[ C_{q\sigma}(\mathbf{r}) = \left[ 1 + \left( \frac{\tau_{q\sigma} \rho_{q\sigma} - \frac{1}{4} |\nabla \rho_{q\sigma}|^2 - j_{q\sigma}^2}{\rho_{q\sigma} \tau_{q\sigma}^{TF}} \right)^2 \right]^{-1} \]


Physical meaning :
\[ C \in [0 : 1] \]
\[ C_{q\sigma}(\mathbf{r}) = 1 \] Probability to find another particle with the same \( q \) and \( \sigma \) very low.
\[ C_{q\sigma}(\mathbf{r}) = 0.5 \] Limit of uniform-density Fermi gas.

Mask function :
\[ \rightarrow \frac{C_{q\sigma}(\mathbf{r}) \rho_{q\sigma}}{\rho_{q\sigma}^{\text{max}}} \]
Nucleon localization function

Fermion localization function

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Physical meaning:
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Example of $^{240}\text{Pu}$
Example of $^{240}\text{Pu}$
Example of $^{240}\text{Pu}$
Example of $^{240}\text{Pu}$
Hypothesis

The octupole shell effects are important in the fission fragment
Other systems
Other systems
Why the fragments have octupole deformation?

Similar effect on fusion reaction

$^{40}\text{Ca} + ^{40}\text{Ca}, \ E3^- = 3.7 \text{ MeV}$

\[
\begin{align*}
t &= 2.25 \text{ zs} \\
D &= 11.08 \text{ fm}
\end{align*}
\]

\[
\begin{align*}
t &= 2.5 \text{ zs} \\
D &= 10.56 \text{ fm}
\end{align*}
\]

\[
\begin{align*}
t &= 2.75 \text{ zs} \\
D &= 10.54 \text{ fm}
\end{align*}
\]

\[
\begin{align*}
t &= 3 \text{ zs} \\
D &= 10.18 \text{ fm}
\end{align*}
\]

$^{56}\text{Ni} + ^{56}\text{Ni}, \ E3^- = 7.5 \text{ MeV}$

\[
\begin{align*}
t &= 2 \text{ zs} \\
D &= 11.26 \text{ fm}
\end{align*}
\]

\[
\begin{align*}
t &= 2.3 \text{ zs} \\
D &= 10.98 \text{ fm}
\end{align*}
\]

\[
\begin{align*}
t &= 2.6 \text{ zs} \\
D &= 11.10 \text{ fm}
\end{align*}
\]

\[
\begin{align*}
t &= 2.9 \text{ zs} \\
D &= 10.72 \text{ fm}
\end{align*}
\]

Why the fragments have octupole deformation?

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$t=2.9 \text{ zs} \\
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Octupole deformation systematics

**Skyrme Skm*.**


**Gogny D1S**


Results from systematic calculation

In both calculations, the region $Z \approx 56$, $N \approx 88$ is favorable for octupole deformation.

Experimental results

$^{144}$Ba is found to be octupole in its groud state. Burcher et al. PRL 116 (2016).
Octupole deformation systematics


Results from systematic calculation
In both calculations, the region $Z \simeq 56$, $N \simeq 88$ is favorable for octupole deformation.

Experimental results
$^{144}$Ba is found to be octupole in its ground state. Burcher et al. PRL 116 (2016).
Constraint HF+BCS octupole deformation with Sly4d

Result from constraint calculation of the heavy fragment

The gain in energy due to the octupole softness drives the fission to the $Z \approx 54$
Structure, $^{144}\text{Ba}$, $Z=56$, $N=88$

$Q_2 - Q_3$ potential energy surface

Single particle energy

![Graph showing the potential energy surface and single particle energy levels for $^{144}\text{Ba}$](image-url)
Structure

Single particle energies

Experimental results

C. Böckstiegel et al./Nuclear Physics A 802 (2008) 12–25

Position in Z

Position in N

Mass number
We need Z and N identification pre-evaporation → VAMOS at GANIL (see next talk by Diego Ramos).
Deformation energy at the scission. Simple scission point model

\[ E(N, Z) = E_{\beta^3=0.35}(N, Z) + E_{\beta^2=0.8}(N_{\text{tot}} - N, Z_{\text{tot}} - Z) + \epsilon^2 \frac{Z(Z_{\text{tot}} - Z)}{D_{\text{sc}}} \]

With \( D_{\text{sc}} = 17 \text{ fm} \). On the map, \( E(N, Z) - E_{\text{min}} \) is shown. For \(^{240}\text{Pu}\), \( N_{\text{tot}} = 146 \) and \( Z_{\text{tot}} = 94 \)

The energies have been calculated with the CHF+BCS theory Sly4d
Identification method with the nucleon localisation function

This method assumes that the pre-fragments have reflexion symmetry.
Identification with density


Green contour line: density of a $^{144}$Ba with a constraint $\beta_3=0.42$
Red contour line: density of a fissioning $^{258}$Fm (asymmetric mode)
Identification with nucleon localisation function

Top: NLF of a $^{144}$Ba with a constraint $\beta_3 = 0.42$
Bottom: NLF of a fissioning $^{258}$Fm (asymmetric mode)
Identification with nucleon localisation function
Identification method with octupole degree of freedom

Identification of the fragments as a function of time for the fission of $^{258}\text{Fm}$

All of the systems are identified as $^{144}\text{Ba}$ with different $\beta_3$ values (resp. 0.14, 0.39, 0.39 and 0.42)
Identification method with octupole degree of freedom

Identification of the fragments at the scission for the different elements.

All systems are identified as $^{144}$Ba with different $\beta_3$ values (resp. 0.28, 0.28, 0.27 and 0.44)
Conclusion

Mechanism

- The Nucleus-Nucleus interaction at the scission configuration favors the octupole shapes
- Shell structure favors octupole shape in the region $Z \approx 52-56$, $N \approx 84-88$
- Actinide fission fragments are driven in the region $Z \approx 54$, $N \approx 86$

Similar effect for other systems?

P. A. Butler.

Experimental data of $^{180}\text{Hg}$

Experimental data of $^{178}\text{Pt}$


(a) $TKE_{\text{high}}^{\text{mass}}$ vs Counts
(b) $TKE_{\text{mean}}$ vs Mass (amu)
(c) $TKE_{\text{low}}$ vs Mass (amu)

$^{178}\text{Pt}$

$N=56$
$N=50$
$Z=34$
$Z=28$

exp.
sym.
Similar effect of the octupole deformation?
CHF + BCS calculation
Comparison with experimental data


and the fission-fragment mass is shown in Fig. 4. The mass distribution is clearly asymmetric, with the most probable heavy and light masses of $A_H = 100(1)$ and $A_L = 80(1)$, having a width of $\sigma = 4.0(3)$ amu. The most probable $Z$ values of the heavy and light fission fragments are deduced to be $Z_H = 44(2)$ and $Z_L = 36(2)$, respectively, assuming that the $N/Z$ ratio of the parent nucleus $^{180}$Hg is preserved in the fission fragments. Thus, the most abundantly produced fission fragments are $^{100}$Ru and $^{80}$Kr and their neighbors. Although 75% of the fission events are
Single-particle energies in the heavy fragment

Structure of $^{100}\text{Ru}$ ($Z=44$ and $N=56$)

Structure of pre-fragment (Z=34 and N=44)
CHF+BCS calculations : Hg isotopic chain
Conclusion

The fission process magnifies the octupole shell structure
Thank you
## Comparison TDHFB - TDHF+BCS

### TDHFB
- **Quasi-particles**: \(|\omega_\alpha\rangle = (U_\alpha V_\alpha)\)
- **Evolution**: \(i\hbar \frac{d|\omega_\alpha\rangle}{dt} = (\frac{h}{\Delta} \Delta^* - h^* h) |\omega_\alpha\rangle\)

### TDHF+BCS
- Based on TDHFB with the approximation: \(\Delta_{ij} = \delta_{ij} \Delta_i\)
- **Evolution**: \(i\hbar \frac{d\varphi_i}{dt} = (\hat{h}_{MF} - \epsilon_i) \varphi_i\)
  
  \[
  i\hbar \frac{dn_i}{dt} = \Delta_i^* \kappa_i - \Delta_i \kappa_i^* \\
  i\hbar \frac{d\kappa_i}{dt} = \kappa_i (\epsilon_i - \epsilon_i^*) + \Delta_i (2n_i - 1)
  \]

### Theoretical difference
- **Numerical cost**: TDHFB requires 1000 times more numerical resources
- **Treatment of continuum states**: BCS gas problem
- **Continuity equation**
- **Number of pairing degrees of freedom** (HFB \(\Delta(r)\), BCS: \(\Delta_{i\bar{i}}\))
- **Spatial dependence of the pairing correlation**
Comparison for fission of $^{240}\text{Pu}$


<table>
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<tr>
<th>S no.</th>
<th>$\eta$</th>
<th>$E^*$</th>
<th>$E_n$</th>
<th>$q_{zz}$</th>
<th>$q_{zzz}$</th>
<th>$t_{SS}$</th>
<th>TKE_{syst}</th>
<th>TKE</th>
<th>$A_L^{syst}$</th>
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<td>62.6</td>
<td>41.3</td>
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**Table** — TDHF+BCS results for $^{240}\text{Pu}$

<table>
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<tr>
<th>#</th>
<th>$Q_0$ [b]</th>
<th>$E_0^*$ [MeV]</th>
<th>$T_{fis}$ [fm/c]</th>
<th>$Z_L$</th>
<th>$N_L$</th>
<th>TKE [MeV]</th>
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<td>6480</td>
<td>40.21</td>
<td>60.77</td>
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