Effects of temperature on nuclear deformation energy and the predictions of fission observables with calculation using Langevin equation

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Contents I

1 Background
2 Shape parameterizations
3 Potential Energy Surface
4 Fission Dynamics
5 Brosa Fission Modes
6 Results
   • From U236 to Fm256
   • From Fm257 to Lr259
   • TKE Systematics
   • Effects of Temperature on Potential Energy Surface
7 Conclusion
8 References
9 Appendix
There has been considerable success in the calculation with 3-D Langevin equation especially in the calculation of low energy fission to obtain observables such as:

- fission fragment yield \(Y(A)\)
- total kinetic energy (TKE).

We have been able to extend 3-D Langevin equation that traditionally use macroscopic transport coefficients (Aritomo and Chiba, 2013; Aritomo et al., 2014) into microscopic transport coefficients (Usang et al., 2016).

This has allowed us to observe:

- the dependence of the fission fragment \(\langle TKE \rangle\) on \(E_x\) (Usang et al., 2017).
- the effects of pairing on fission observables,
- to see the emergence of standard, super-long and super-short fission modes,
- that 3-D Langevin will never produce the twin-transition seen in Fm256 to Fm258.

After Ishizuka et al. (2017) [Phys. Rev. C 96, 064616] has introduced 4-D Langevin equation

- improved TKE(A)
- relationship of TKE with \(\delta_i\) combinations (Usang et al., 2018)
- natural transition from Fm256 and Fm258 in terms of TKE and fission yield.
Anomalous twin transitions from $^{256}\text{Fm}$ to $^{258}\text{Fm}$

**Figure:** Hoffman et al. (1990) *Phys. Rev. C*, 41(2), 631–639
Shape parameterizations

- The shape of the nucleus are defined by the collective variable $q_\mu = \{z_0/R_0, \delta_1, \delta_2, \alpha\}$, and each collective variable has the momentum conjugate $p_\mu$.

- We define the following collective coordinates (with $R_0 = 1.2 \sqrt[3]{A}$ and $A = A_1 + A_2$),

  - $z_0 = \frac{z_0}{R_0}$
  - $\delta_i = \frac{3(a_i - b_i)}{2a_i + b_i}$
  - $\alpha = \frac{A_1 - A_2}{A_1 + A_2}$

- Two Center Shell Model of Maruhn & Greiner (1972) with the restriction that the neck parameter, $\epsilon = 0.35$.
The Potential energy surface $U(q)$ are usually defined as,

$$U(q) = E_{\text{def}}^{LD}(q) + \sum_{n,p} \left[ \Phi_{\text{shell}} \delta E_{\text{shell}}(q, T = 0) + \Phi_{\text{pair}} \delta E_{\text{pair}}(q, T = 0) \right]$$
Fission Dynamics

- The collective variables $q_\mu$ are evolved from the compound nucleus formation until the radius of the neck connecting the two fragments becomes zero.
- $q_\mu$ and its conjugate momentum $p_\mu$ are evolved via the Langevin equation,
  \[
  \frac{dq_\mu}{dt} = \left(m^{-1}\right)_{\mu\nu} p_\nu \\
  \frac{dp_\mu}{dt} = -\frac{\partial U(q)}{\partial q_\mu} - \frac{1}{2} \frac{\partial}{\partial q_\mu} \left(m^{-1}\right)_{\nu\sigma} p_\nu p_\sigma - \gamma_{\mu\nu} \left(m^{-1}\right)_{\nu\sigma} p_\sigma + g_{\mu\nu} R_\nu(t)
  \]
- The collective inertia $(m^{-1})_{\mu\nu}$ are calculated using Werner-Wheeler approximation to the mass tensor and the friction $\gamma_{\mu\nu}$ from the wall-window approximation.
- $R_\nu$ is the white noise variable. The strength of the random force are calculated via the modified Einstein relation
  \[
  D = T^* \gamma_{\mu\nu} = g_{\mu\sigma} g_{\nu\sigma}
  \]
- The effective temperature are related to the nuclear temperature by the relationship it has with zero-point energy ($\hbar \bar{\omega}$),
  \[
  T^* = (\hbar \bar{\omega}/2) \coth[(\hbar \bar{\omega})/(2T)]
  \]
- We obtain the nuclear temperature $T$ through the Fermi gas relation $E_{\text{int}} = aT^2$ with level density given by Tőke and Światecki (1981).
- $E_{\text{int}}$ are calculated at each time step from energy conservation
  \[
  E_{\text{int}} = E_x - (1/2)[m^{-1}(q)]_{\mu\nu} p_\mu p_\nu - U(q)
  \]
Brosa calculated the average TKE of the fission mode for given possible shapes of the nuclei. The following are a summary of basic Brosa fission modes:

Super-short Fission Modes
- Average TKE bigger than standard fission modes
- Both fragments are oblate

Standard Fission Modes
- Average TKE that scales with Coulomb repulsion systematics of Viola and Unik.
- One fragment is oblate and the other fragment is prolate.

Super-long Fission Modes
- Average TKE smaller than standard fission modes
- Both fragments are prolate

Figure: Brosa et al. (1986) Z. Naturforsch 41(a), 1341–1346
U236 to Fm256

Neck parameter, $\epsilon = 0.35$
Results

From U236 to Fm256

Neck parameter, $\epsilon = 0.35$
From Fm257 to Lr259

Neck parameter, $\epsilon = 0.35$
Neck parameter, $\epsilon = 0.35$
TKE Systematics: fission mode components

\[ \langle TKE \rangle \text{ (MeV)} \]

- TKE\textsubscript{asy}, Brosa 1990
- TKE\textsubscript{sym}, Brosa 1990
- Calc. TKE\textsubscript{asy}
- Calc. TKE\textsubscript{sym}
- Dominant mode

Figure: Viola ( ) and Unik ( ) systematics are compared with our calculation for TKE\textsubscript{asy} and TKE\textsubscript{sym}.
Fission path

\[
\begin{align*}
\delta_H &\quad 236\text{U} &\quad 238\text{Pu} \\
\delta_L &\quad 244\text{Cm} &\quad 250\text{Cf}
\end{align*}
\]
Fission path
Shell correction factor

- Most approximation of higher temperature is by shell correction factor
- However careless application of shell correction factor, \( \Phi \) in calculations will sometime suppress important fission modes.

\[
U(q) = E_{\text{def}}^{LD}(q) + \sum_{n,p} \left[ \Phi_{\text{shell}} \delta E_{\text{shell}}(q, T = 0) + \Phi_{\text{pair}} \delta E_{\text{pair}}(q, T = 0) \right]
\]
Effects of Temperature on Potential Energy Surface

- $^{236}\text{U, T}=0$
- $T=0.5 \text{ MeV}$
- $T=1.0 \text{ MeV}$
- $T=2.0 \text{ MeV}$
Conclusion and way forward

Our 4-D Langevin calculations reveals that:

- the standard fission modes are dominant except $^{258}\text{Fm}$, $^{259}\text{Fm}$ and $^{260}\text{Md}$
- the symmetric component switches from super-long to super-short fission mode from Es to larger fissioning system.
- when the fragments of $^{258}\text{Fm}$, $^{259}\text{Fm}$ and $^{260}\text{Md}$ prefers double magic configuration, the only channel available in the symmetric component is super-short
- 4-D Langevin equation allow natural transition from $^{256}\text{Fm}$ to $^{258}\text{Fm}$.

Shell correction factor approximates higher temperature potential energy surfaces by moderating the contribution of shell correction.

However, we noticed that careless applications of shell correction may give misleading conclusions. Thus we suggest either

- judicious choice of shell corrections depending on experimental situations
- calculate shell corrections for a given temperature.


Deformation Energy

\[ E^{LD}(q) = E^{LD}_{sph} = E^{LD}_{def}(q) \]

- The liquid drop energy are calculated using finite-range liquid drop model (Krappe et al., 1979)
- \( \delta E_{\text{shell}} \) are calculated according to (Strutinsky, 1967)(Strutinsky, 1968) by calculating the difference between the sum of the single particle energies, \( E_i \) against the average

\[
\delta E_{\text{shell}} = \sum_i 2E_i - 2 \int_{-\infty}^{E_F} E\tilde{g}(E, q)\,dE
\]

- \( \tilde{g} \) is the occupation number for uniform energy levels.
- Contribution of \( \delta E_{\text{pair}} \) are calculated using the procedure by (Brack et al., 1972)
- The shell correction factor are usually
  - \( \Phi = 1 \) for spontaneous fission (Full shell),
  - \( \Phi = \exp(-E_x/E_d) \) with \( E_d \) between 16 MeV to 20 MeV for induced fission (Ignatyuk et al., 1979).
Macroscopic Transport Coefficients

- Werner-Wheeler approximation of macroscopic mass,

\[
m_{\mu\nu} = \pi \rho_0 \int \rho^2 \left[ A_\mu A_\nu + \frac{\rho^2}{8} A'_\mu A'_\nu \right] dz;
\]

\[
A_\mu(z; Q) = \frac{1}{\rho^2(z, Q)} \frac{\partial}{\partial Q_\mu} \int_z^{z_R} \rho^2(z', Q) dz'.
\]

- Wall friction,

\[
\gamma_{\mu\nu}^{\text{wall}} = \pi \rho_0 v_F \int_{z_L}^{z_R} \frac{dz}{\sqrt{4\rho^2 + \left( \frac{\partial \rho^2}{\partial z} \right)^2}}.
\]

- For two separating fragments

\[
\gamma_{\mu\nu}^{\text{wall2}} = \frac{\pi \rho_0 \bar{v}}{2} \left( \int_{z_L}^{0} I_L(z) \, dz + \int_{0}^{z_R} I_R(z) \, dz \right),
\]

with,

\[
I_{L,R}(z) = \prod_{i=\mu,\nu} \left( \frac{\partial \rho^2}{\partial Q_i} + \frac{\partial \rho^2}{\partial z} \frac{\partial \rho_{cm}(L,R)}{\partial Q_i} \right) \frac{1}{\sqrt{4\rho^2 + \left( \frac{\partial \rho^2}{\partial z} \right)^2}}.
\]

- Window term

\[
\gamma_{\mu\nu}^{\text{window}} = \frac{\rho_0 \bar{v}}{2} \left[ \Delta \sigma \frac{\partial R_{12}}{\partial Q_\mu} \frac{\partial R_{12}}{\partial Q_\nu} \ldots + \frac{32}{9\Delta \sigma} \frac{\partial V_L}{\partial Q_\mu} \frac{\partial V_L}{\partial Q_\nu} \right],
\]

- Wall-window friction,

\[
\gamma_{\mu\nu}^{\text{wall+w}} = \gamma_{\mu\nu}^{\text{wall2}} + \gamma_{\mu\nu}^{\text{window}};
\]

\[
\gamma_{\mu\nu}^{\text{total}} = \sin^2 \left( \frac{\pi \alpha}{2} \right) \gamma_{\mu\nu}^{\text{wall}} + \cos^2 \left( \frac{\pi \alpha}{2} \right) \gamma_{\mu\nu}^{\text{wall+w}}.
\]
**TKE Systematics**

![Graph showing TKE distribution with Viola and Unik systematics]

**Figure:** Calculated $\langle TKE \rangle$ (○) distribution with respect to Viola (——) systematics; and Unik (−−−) systematics.

<table>
<thead>
<tr>
<th>Nuclei</th>
<th>$\langle TKE \rangle$</th>
<th>TKE$_{Viola}$</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{236}\text{U}$</td>
<td>173.57</td>
<td>170.15</td>
<td>169.1</td>
</tr>
<tr>
<td>$^{238}\text{Np}$</td>
<td>175.70</td>
<td>173.24</td>
<td>170.4</td>
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<tr>
<td>$^{238}\text{Pu}$</td>
<td>178.41</td>
<td>176.83</td>
<td>177.0</td>
</tr>
<tr>
<td>$^{240}\text{Am}$</td>
<td>182.32</td>
<td>179.97</td>
<td></td>
</tr>
<tr>
<td>$^{244}\text{Cm}$</td>
<td>184.80</td>
<td>182.66</td>
<td>183.7</td>
</tr>
<tr>
<td>$^{246}\text{Bk}$</td>
<td>187.64</td>
<td>185.84</td>
<td></td>
</tr>
<tr>
<td>$^{250}\text{Cf}$</td>
<td>189.88</td>
<td>188.57</td>
<td>187.0</td>
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<tr>
<td>$^{254}\text{Es}$</td>
<td>197.39</td>
<td>191.31</td>
<td></td>
</tr>
<tr>
<td>$^{256}\text{Fm}$</td>
<td>200.01</td>
<td>194.56</td>
<td>197.9</td>
</tr>
<tr>
<td>$^{257}\text{Fm}$</td>
<td>202.55</td>
<td>194.31</td>
<td>197.6</td>
</tr>
<tr>
<td>$^{258}\text{Fm}$</td>
<td>226.17</td>
<td>194.07</td>
<td>238.0</td>
</tr>
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<td>$^{259}\text{Fm}$</td>
<td>221.06</td>
<td>193.83</td>
<td>242.0</td>
</tr>
<tr>
<td>$^{260}\text{Md}$</td>
<td>226.69</td>
<td>197.33</td>
<td>232.5</td>
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<tr>
<td>$^{256}\text{No}$</td>
<td>208.95</td>
<td>202.12</td>
<td>202.4</td>
</tr>
<tr>
<td>$^{259}\text{Lr}$</td>
<td>211.13</td>
<td>205.19</td>
<td>214.0</td>
</tr>
<tr>
<td>$^{258}\text{Rf}$</td>
<td>226.17</td>
<td>209.31</td>
<td>220.0</td>
</tr>
</tbody>
</table>

$\text{TKE}_{Viola} = 0.1189Z^2A^{-1/3} + 7.3 \text{ MeV}$

$\text{TKE}_{Unik} = 0.1396Z^2A^{-1/3} - 19.9 \text{ MeV}$
TKE Systematics: fission mode components

![Graph showing TKE systematics]

TKE\textsubscript{Viola} = 0.1189Z^2A^{-1/3} + 7.3 \text{ MeV}
TKE\textsubscript{Unik} = 0.1396Z^2A^{-1/3} - 19.9 \text{ MeV}
TKE\textsubscript{calc.}\textsubscript{asy} = 0.1168Z^2A^{-1/3} + 13.9 \text{ MeV}

In the range 1300 < Z^2/\sqrt[3]{A} < 1550,
TKE\textsubscript{calc.}\textsubscript{SL} = 0.1542Z^2A^{-1/3} - 48.7 \text{ MeV}
In the range Z^2/\sqrt[3]{A} > 1550,
TKE\textsubscript{calc.}\textsubscript{SS} = 0.0849Z^2A^{-1/3} + 99.0 \text{ MeV}

**Figure:** Viola (——) and Unik (−−−) systematics are compared with our calculation for TKE\textsubscript{asy} (-----) and TKE\textsubscript{sym} (———)
Effects of Temperature on Potential Energy Surface

- $T = 0.0 \text{ MeV}$
- $T = 0.6 \text{ MeV}$
- $T = 1.0 \text{ MeV}$
- $T = 1.5 \text{ MeV}$