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

15th International Conference on Nuclear Reaction Mechanisms

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11 June 2018

Contents I

Background

- 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 $\langle \text{TKE} \rangle$ 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 δ_i combinations (Usang et al., 2018)
  - natural transition from Fm256 and Fm258 in terms of TKE and fission yield

Anomalous twin transitions from ^{256}Fm to ^{258}Fm

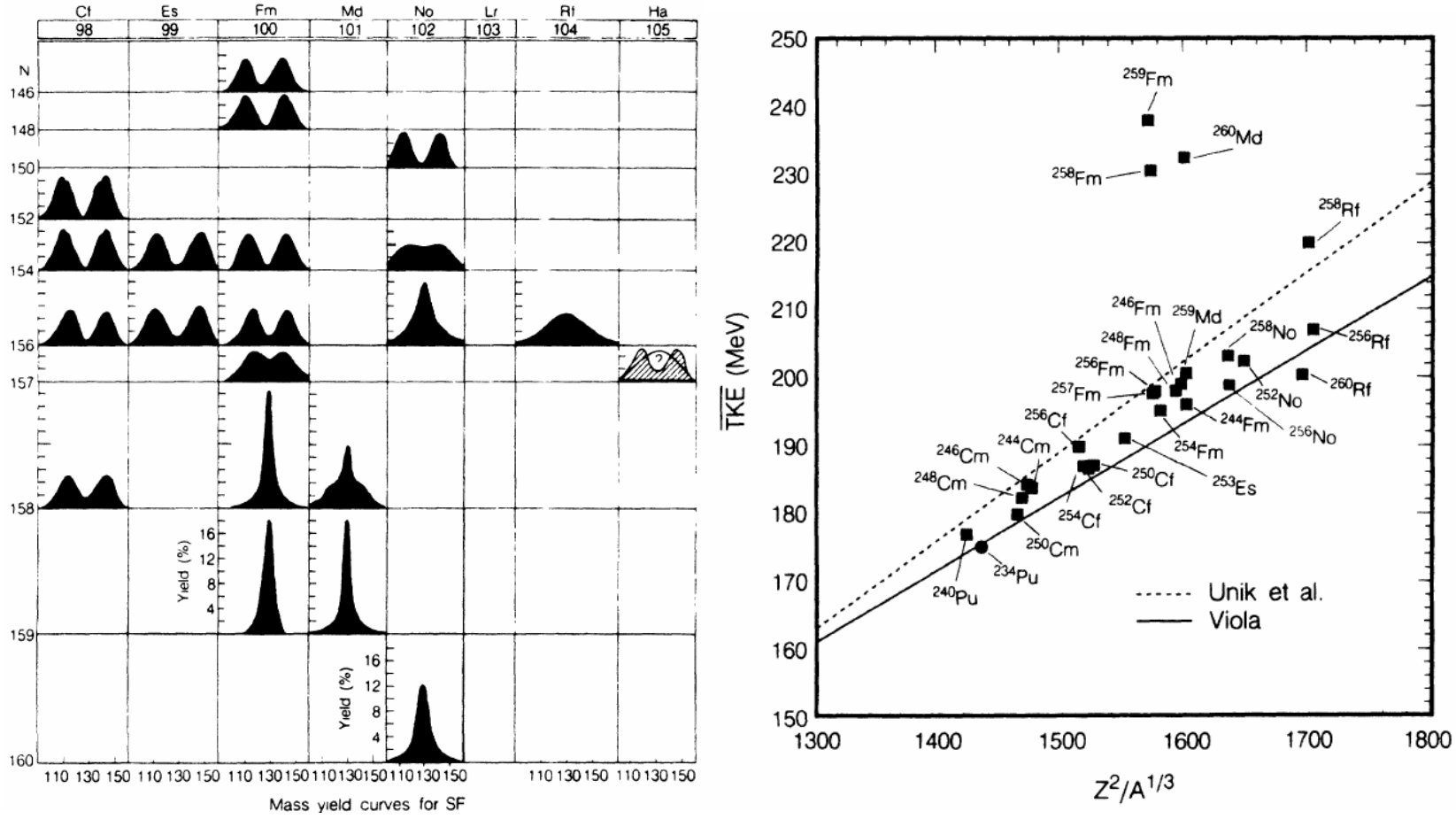


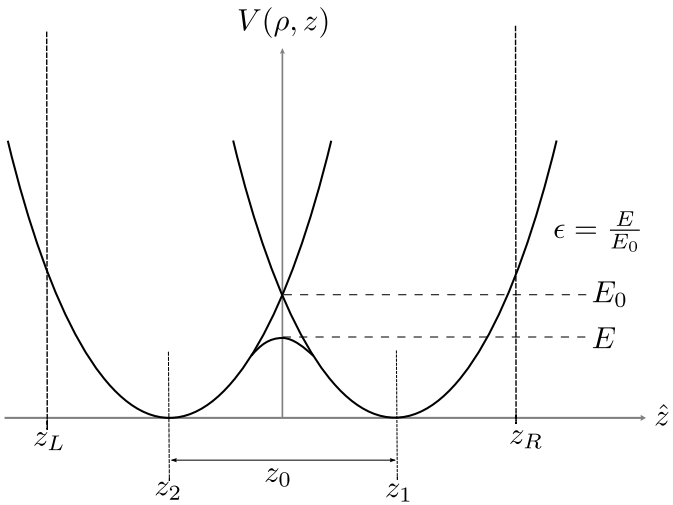
Figure: Hoffman et al. (1990) *Phys. Rev. C*, **41**(2), 631–639

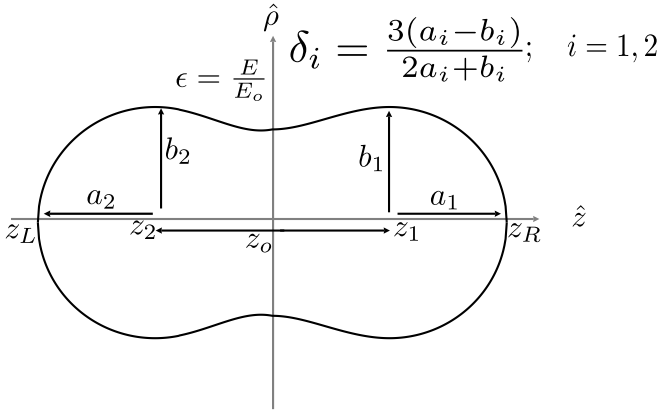
Shape parameterizations

- 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_μ

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

$$zz_0 = \frac{z_0}{R_0}$$
$$\delta_i = \frac{3\,(a_i - b_i)}{2a_i + b_i}$$
$$\alpha = \frac{A_1 - A_2}{A_1 + A_2}$$



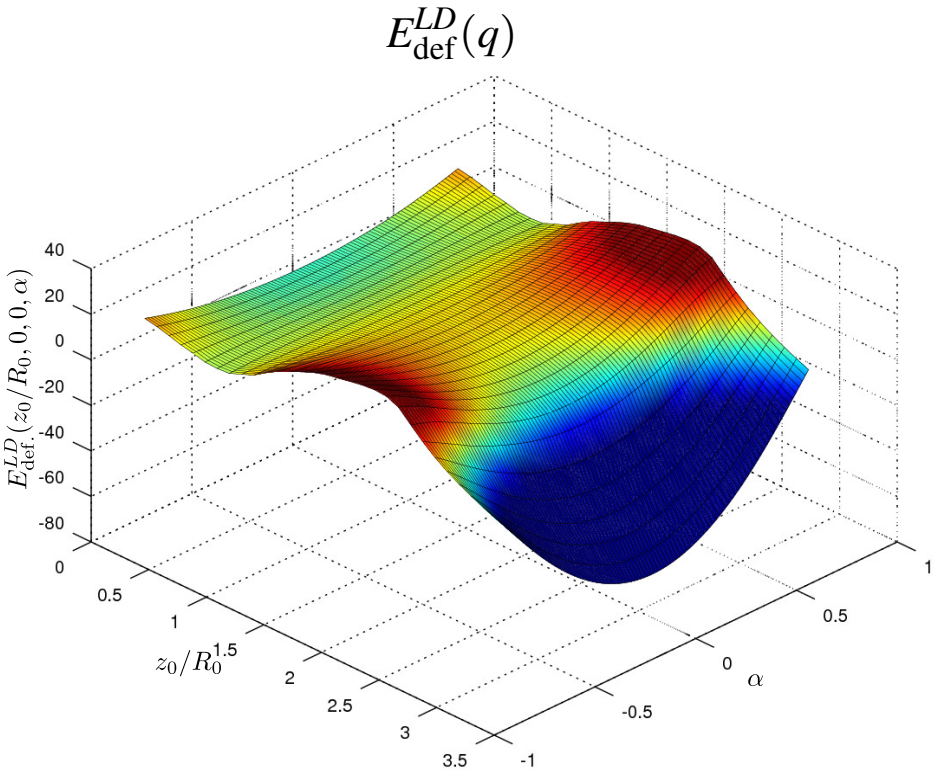


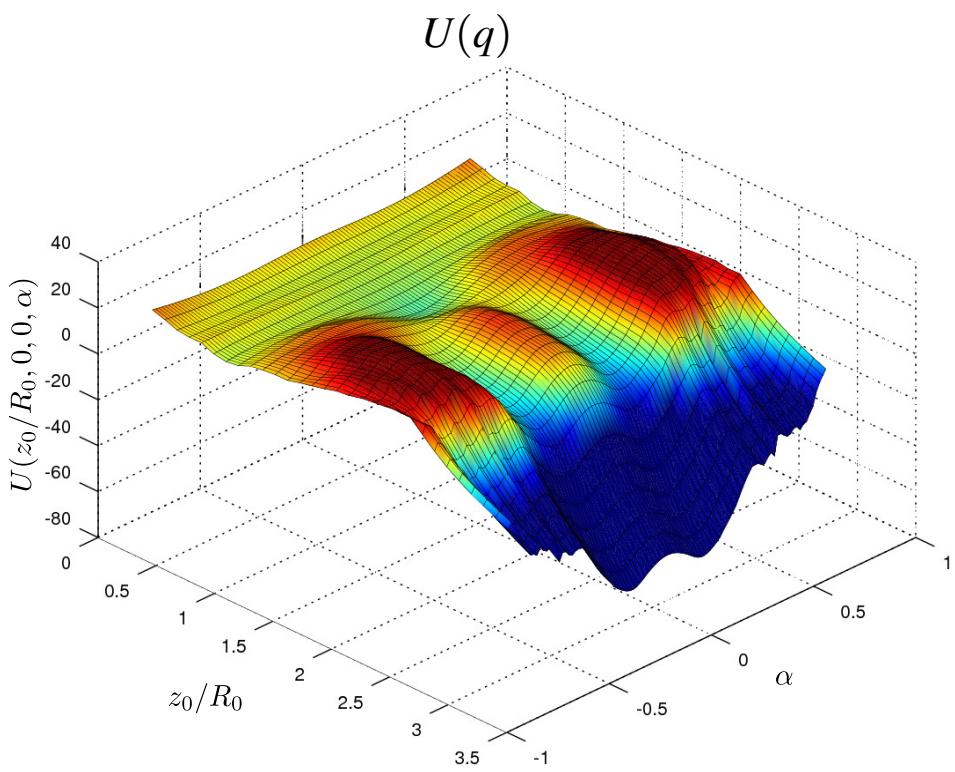
- Two Center Shell Model of Maruhn & Greiner (1972) with the restriction that the neck parameter, $\epsilon = 0.35$

Potential Energy Surface

- 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_μ are evolved from the compound nucleus formation until the radius of the neck connecting the two fragments becomes zero.
- q_μ and its conjugate momentum p_μ are evolved via the Langevin equation,

$$\boxed{\begin{aligned} \frac{dq_\mu}{dt} &= \left(m^{-1}\right)_{\mu\nu} p_\nu \\ \frac{dp_\mu}{dt} &= -\frac{\partial U(q)}{\partial q_\mu} - \frac{1}{2}\frac{\partial}{\partial q_\mu}\left(m^{-1}\right)_{\nu\sigma} p_\nu p_\sigma - \gamma_{\mu\nu}\left(m^{-1}\right)_{\nu\sigma} p_\sigma + g_{\mu\nu} R_\nu(t) \end{aligned}}$$

- 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_ν is the white noise variable. The strength of the random force are calculated via the modified Einstein relation

$$D = T^* \gamma_{\mu\nu} = g_{\mu\sigma} g_{\nu\sigma} \tag{1}$$

- The effective temperature are related to the nuclear temperature by the relationship it has with zero-point energy ($\hbar\varpi$),

$$T^* = (\hbar\varpi/2)\coth[(\hbar\varpi)/(2T)] \tag{2}$$

- We obtain the nuclear temperature T through the Fermi gas relation $E_{\text{int}} = aT^2$ with level density given by Tōke and Światecki (1981).
- E_{int} are calculated at each time step from energy conservation

$$E_{\text{int}} = E_x - (1/2)[m^{-1}(q)]_{\mu\nu} p_\mu p_\nu - U(q) \tag{3}$$

Brosa Fission Modes

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

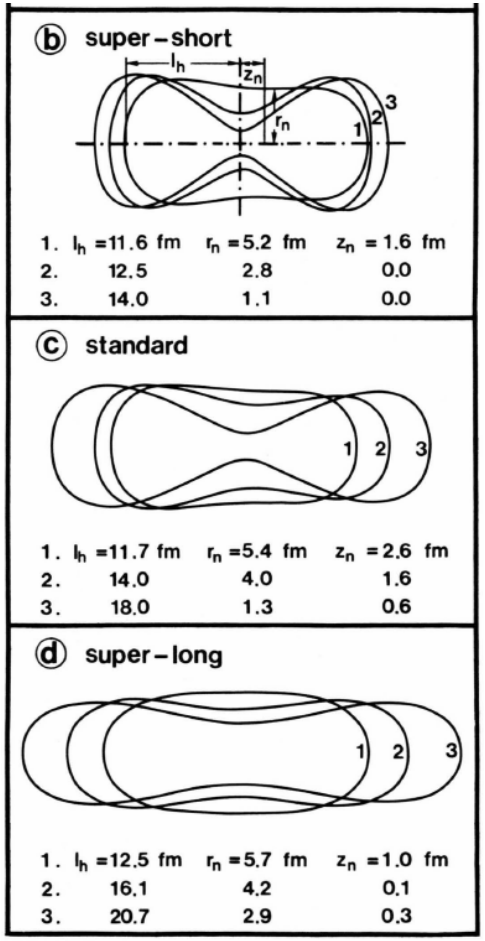
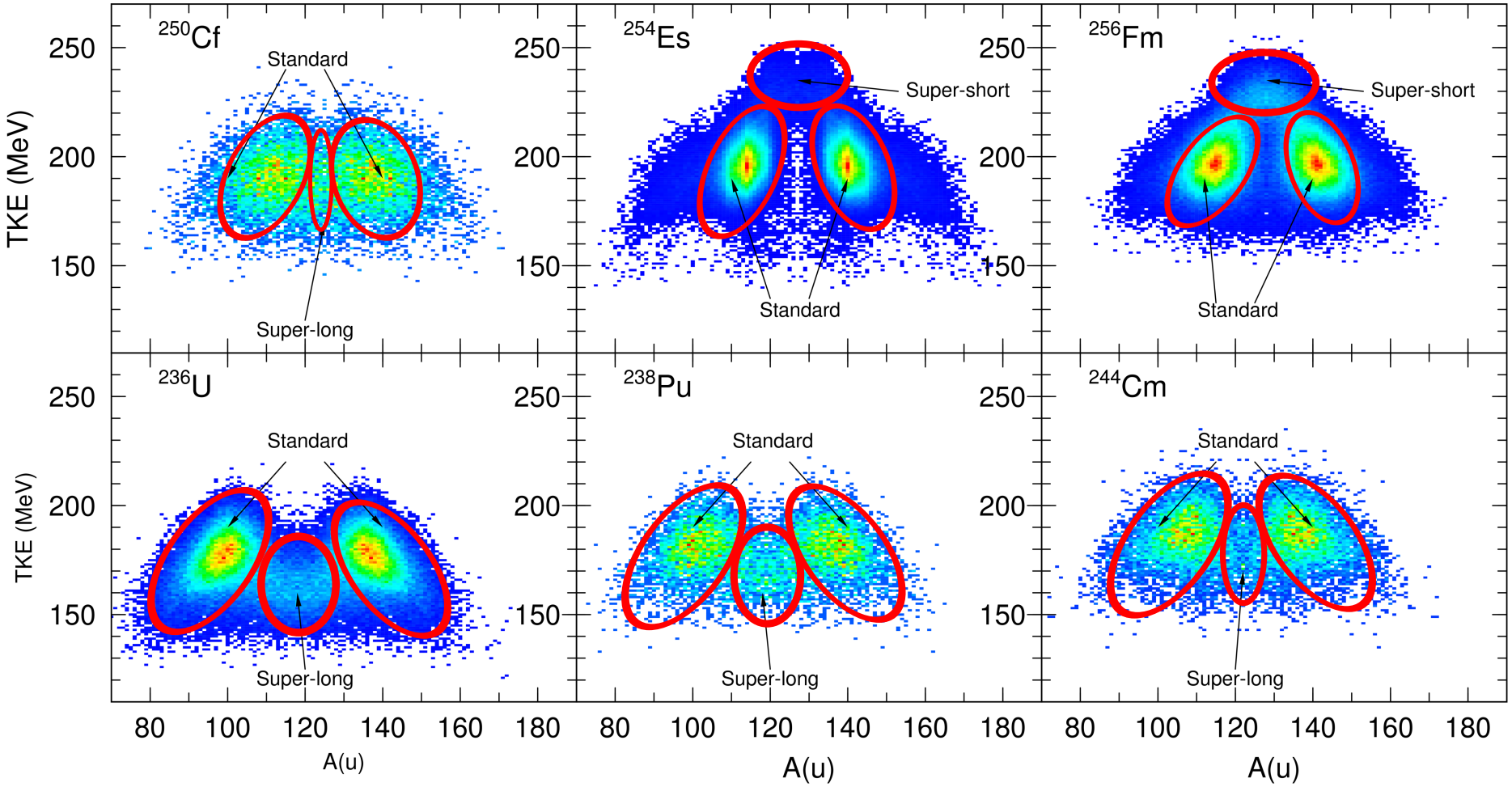


Figure: Brosa et al. (1986) *Z. Naturforsch* **41**(a), 1341–1346

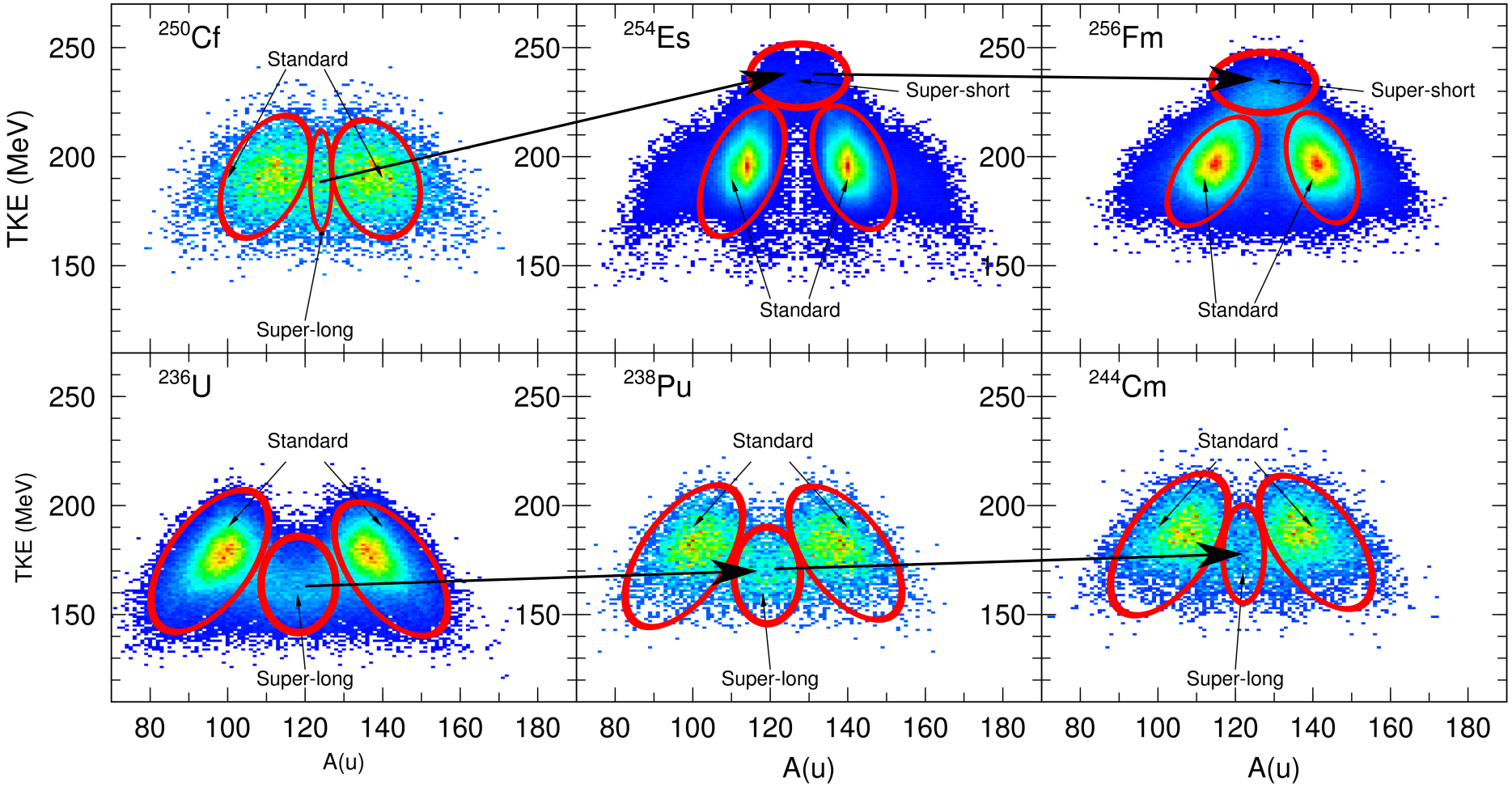
U236 to Fm256

Neck parameter, $\epsilon = 0.35$



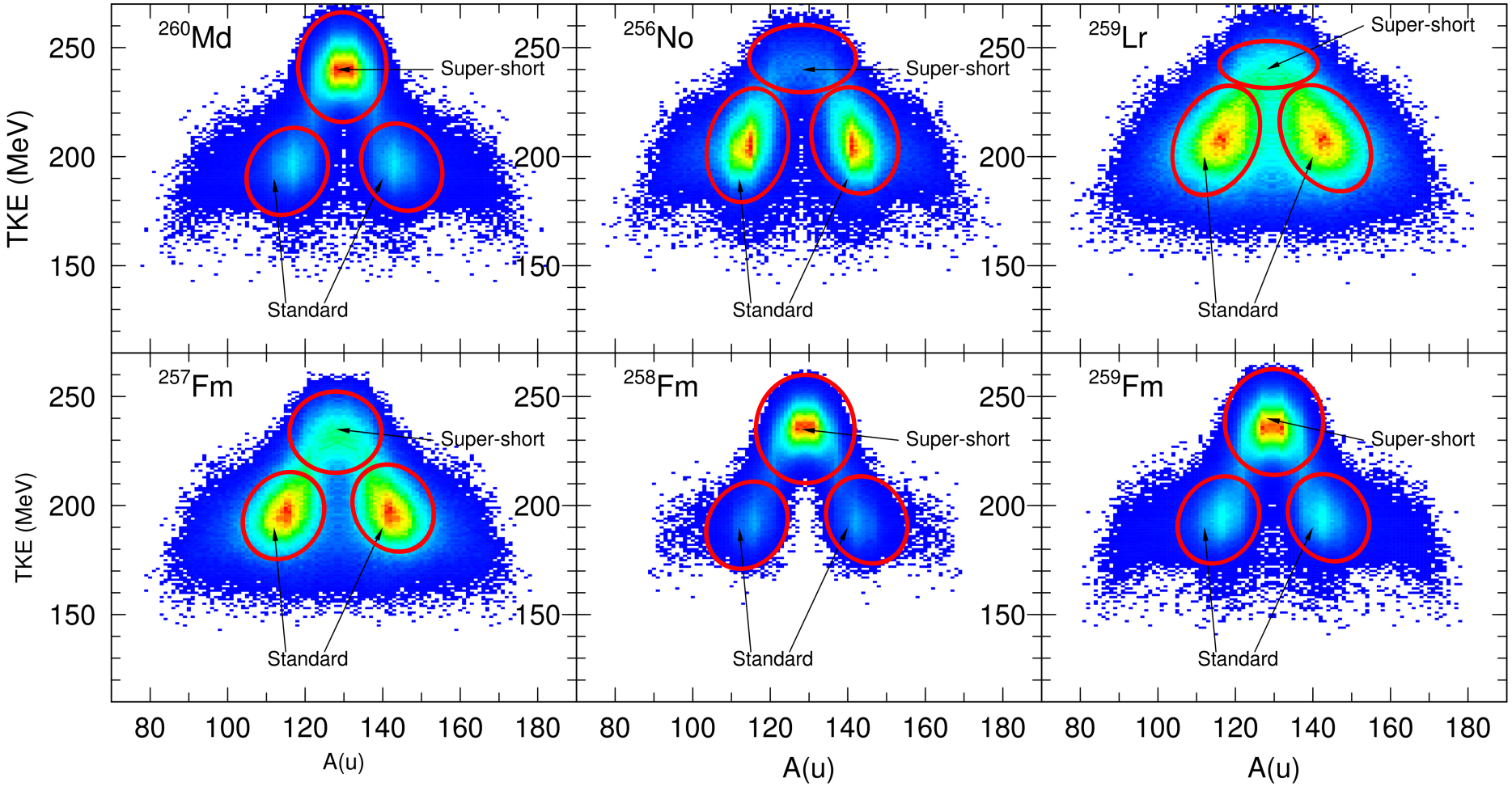
U236 to Fm256

Neck parameter, $\epsilon = 0.35$



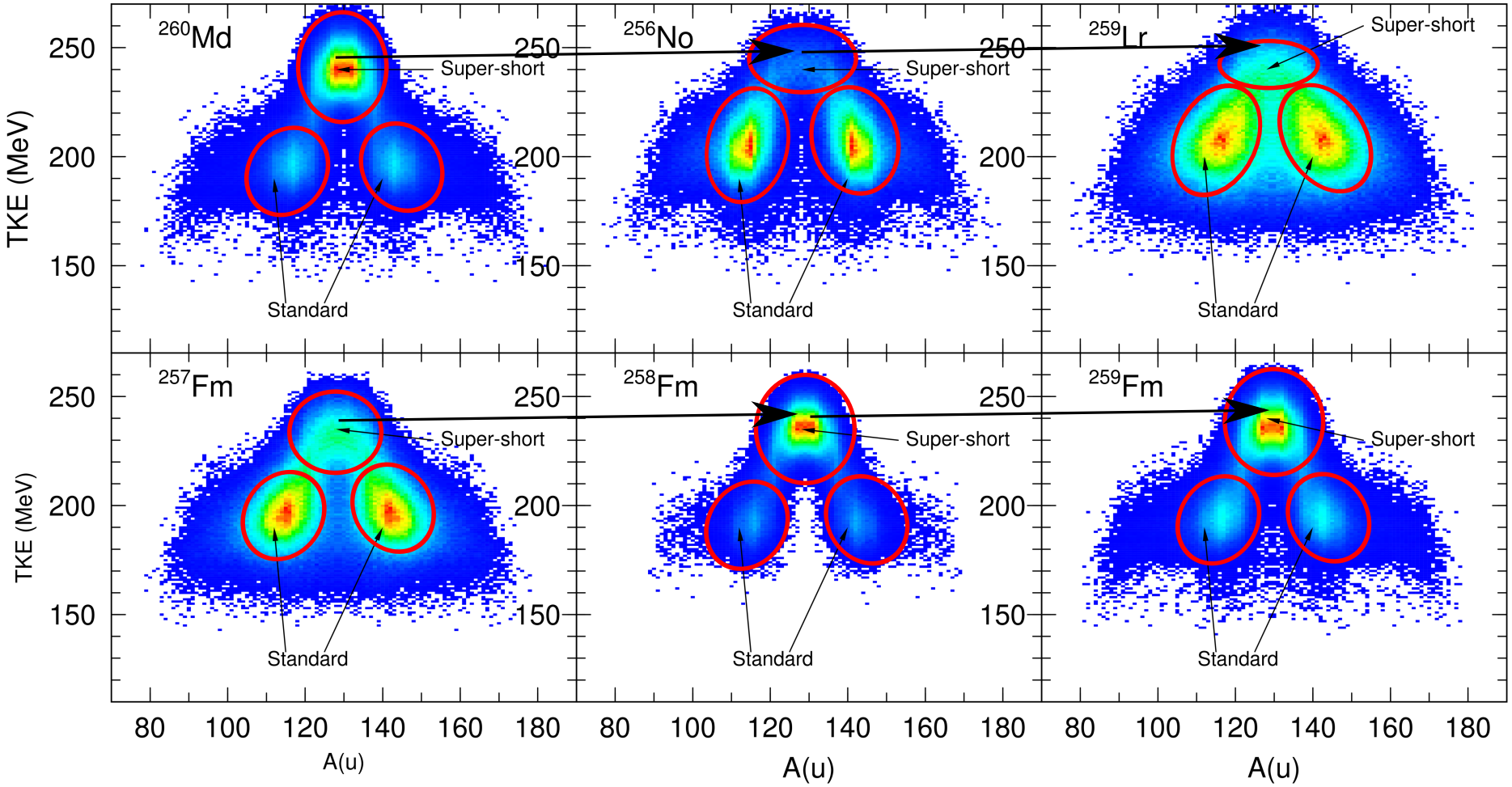
From Fm257 to Lr259

Neck parameter, $\epsilon = 0.35$

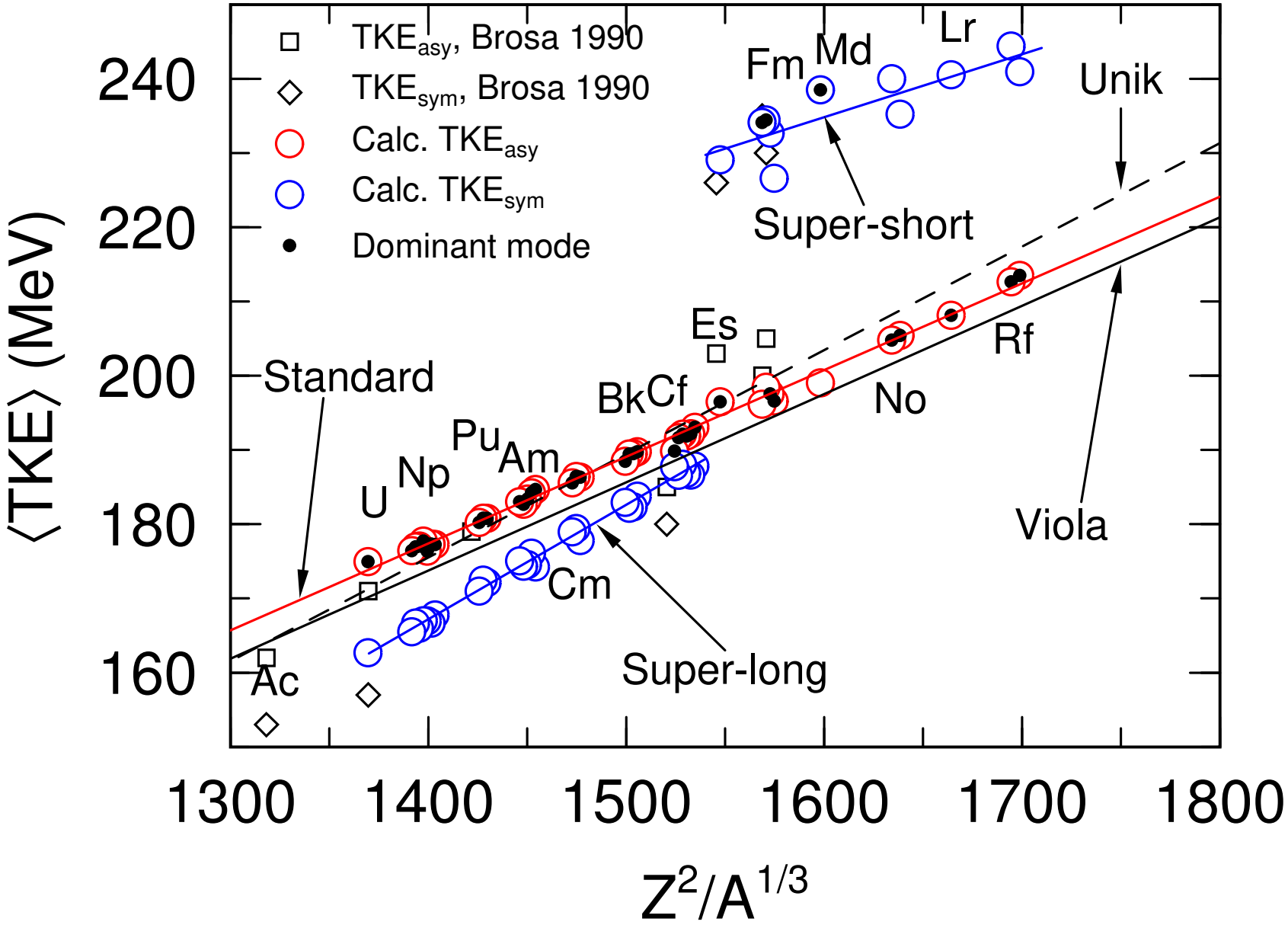


From Fm257 to Lr259

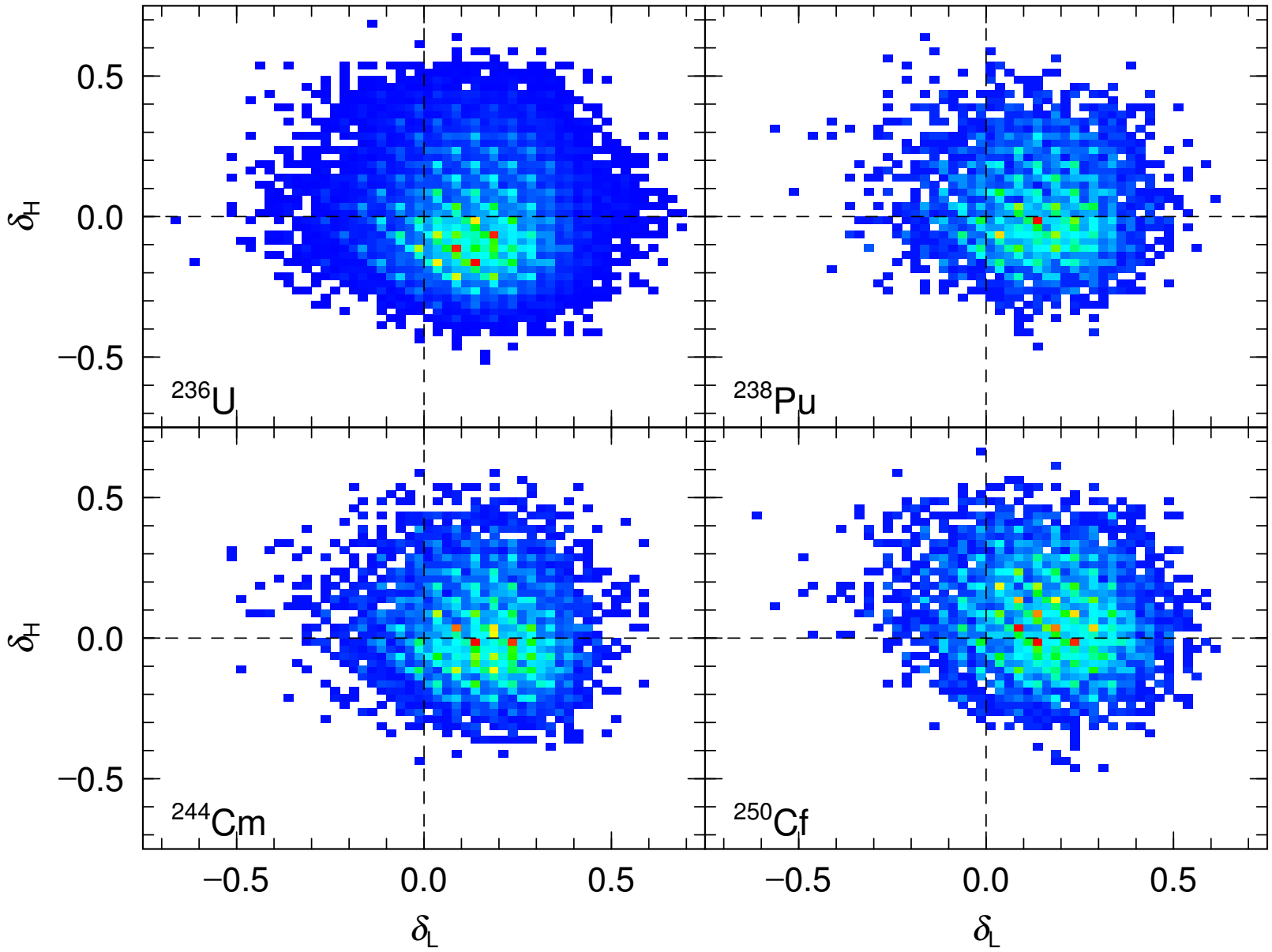
Neck parameter, $\epsilon = 0.35$



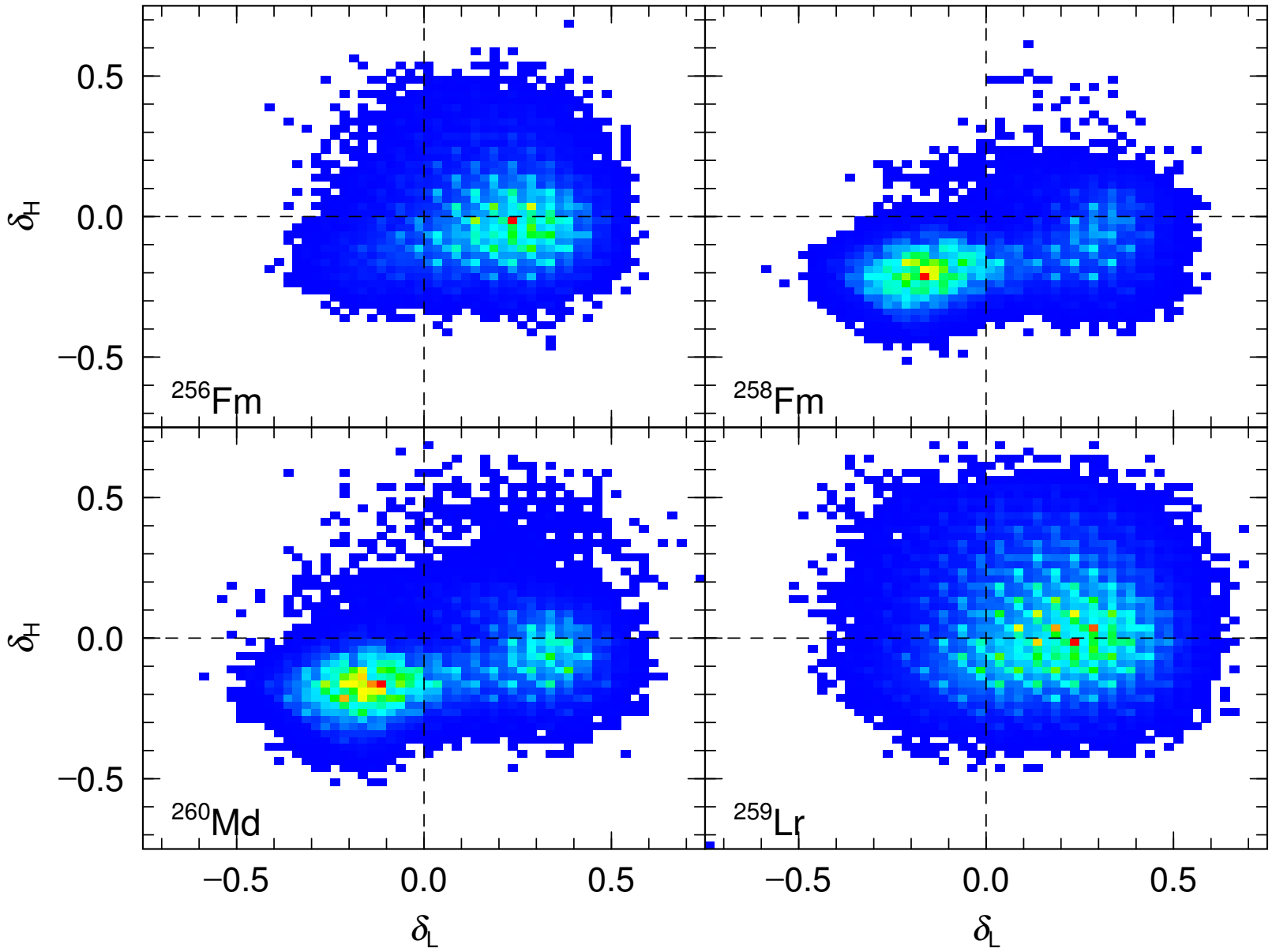
TKE Systematics: fission mode components



Fission path



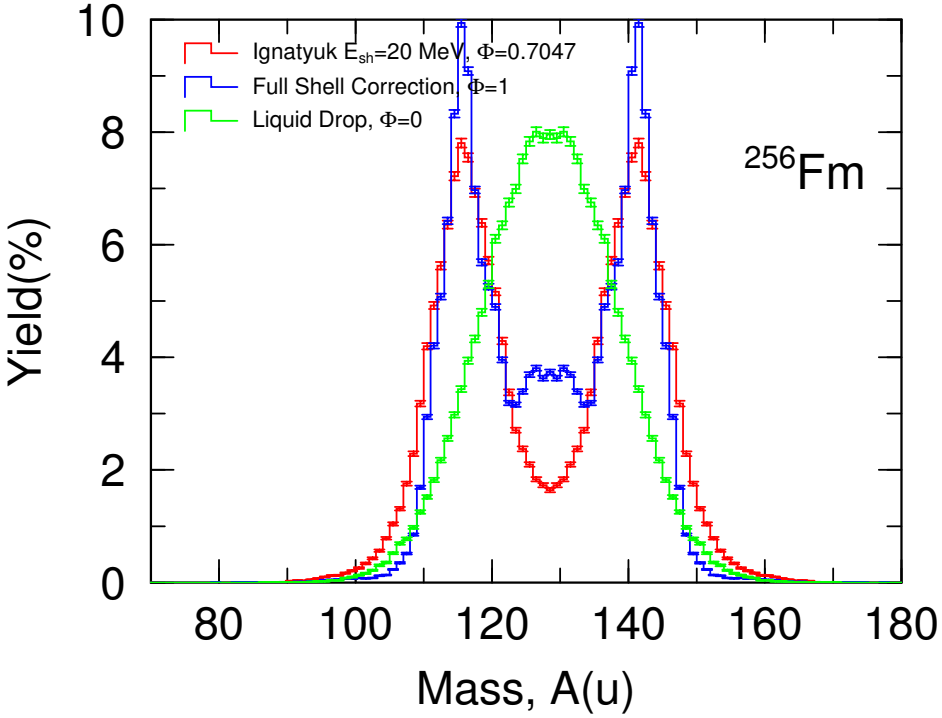
Fission path

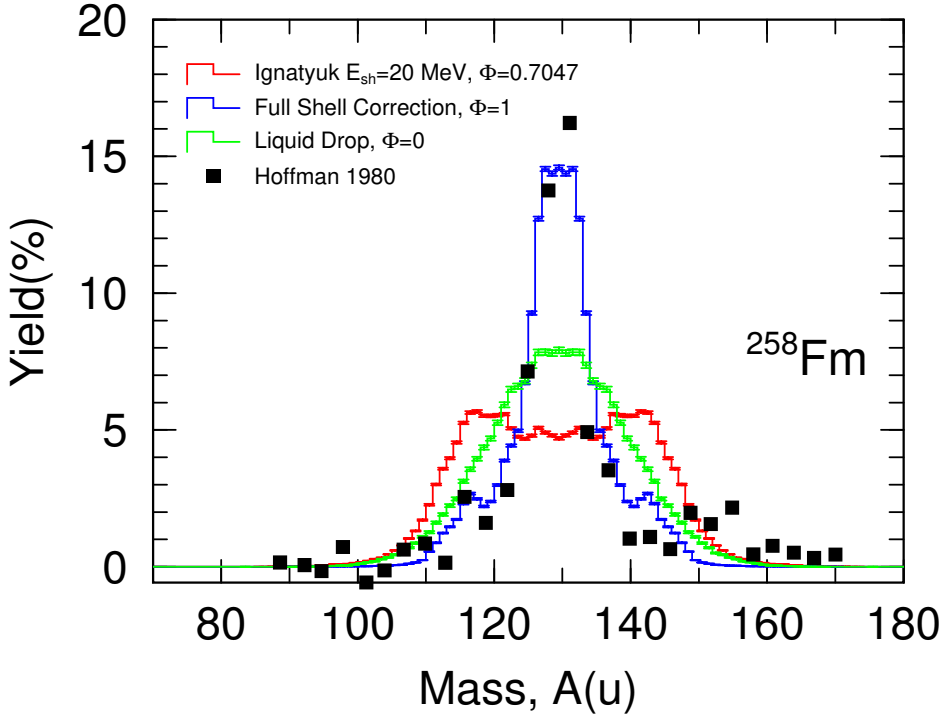


Shell correction factor

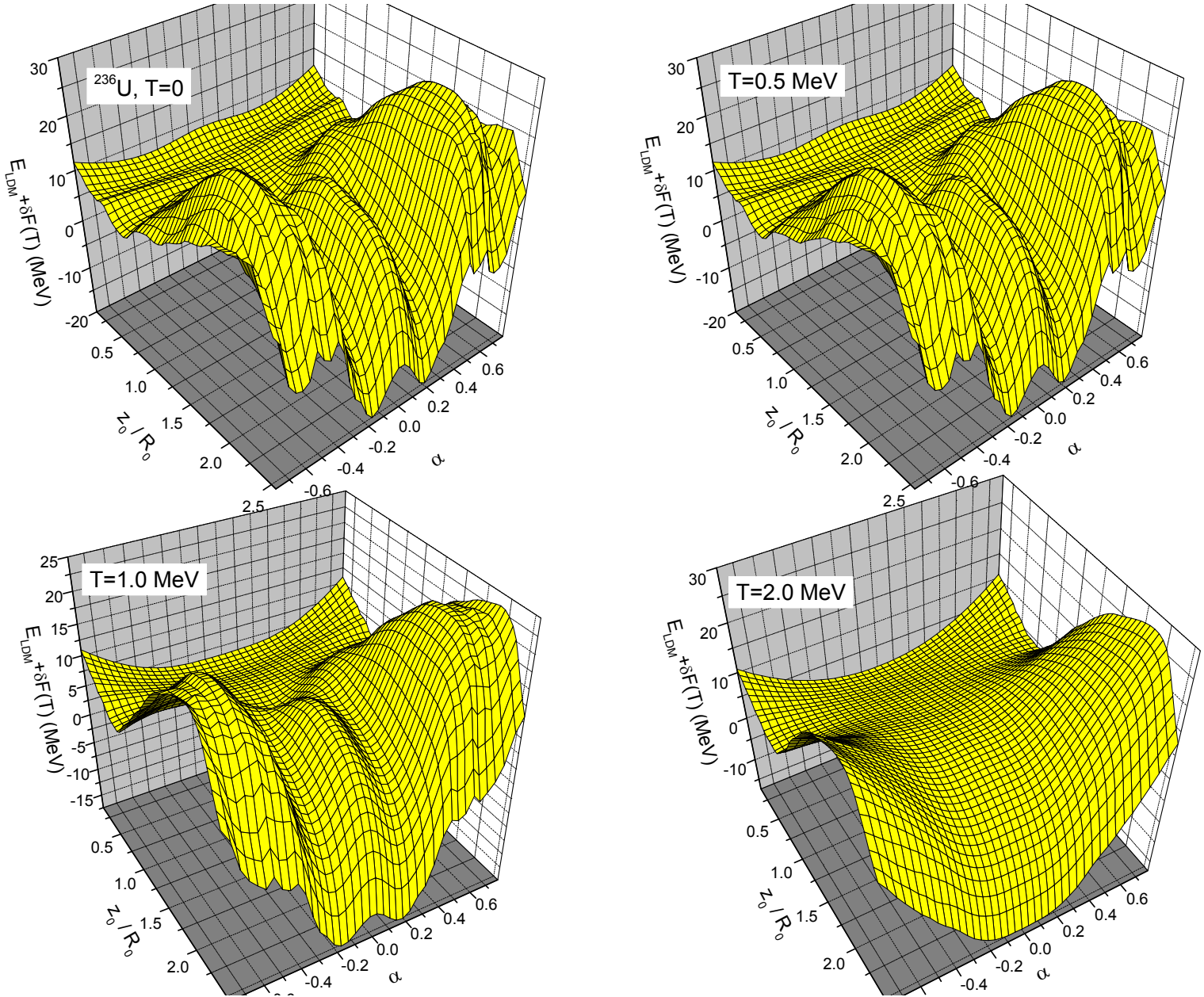
- Most approximation of higher temperature is by shell correction factor
- However careless application of shell correction factor, Φ in calculations will sometime suppress important fission modes.

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





Effects of Temperature on Potential Energy Surface



Conclusion and way forward

- Our 4-D Langevin calculations reveals that:
  - the standard fission modes are dominant except ^{258}Fm, ^{259}Fm and ^{260}Md
  - the symmetric component switches from super-long to super-short fission mode from Es to larger fissioning system.
  - when the fragments of ^{258}Fm, ^{259}Fm and ^{260}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}Fm to ^{258}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
  - Ivanyuk et al. (2018) [*Phys. Rev. C* **97**, 054331] shell correction factors for various fissioning systems
  - calculate shell corrections for a given temperature.

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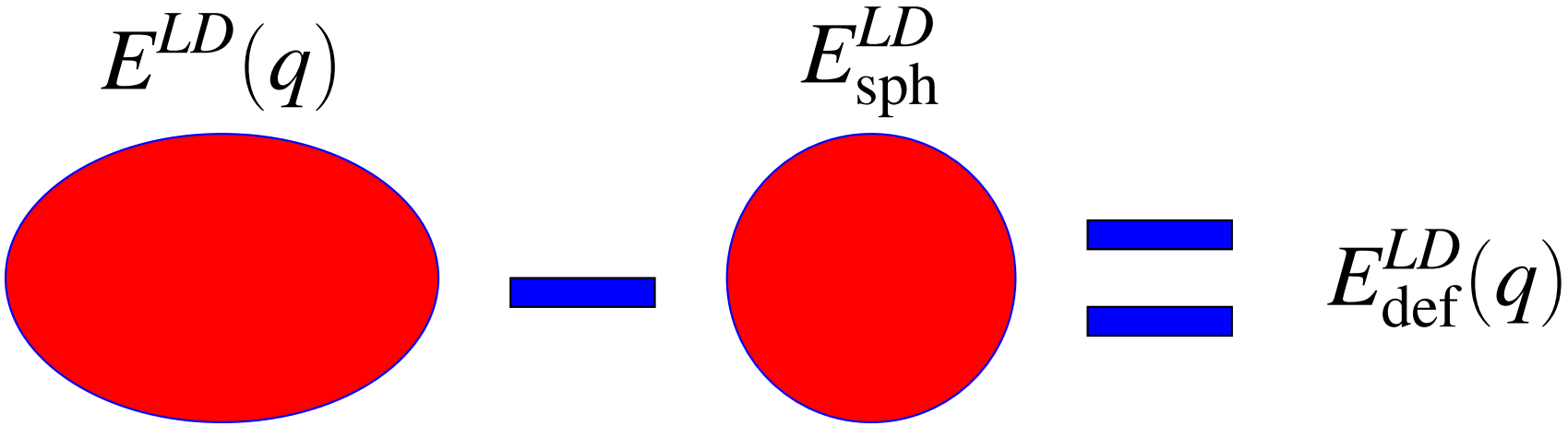
Deformation Energy



- The liquid drop energy are calculated using finite-range liquid drop model (Krappe et al., 1979)
- δE_{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

$$\delta E_{\text{shell}} = \sum_i 2E_i - 2\int_{-\infty}^{E_F} E\tilde{g}(E,q)dE \tag{4}$$

- $\tilde{g}$ is the occupation number for uniform energy levels.
- Contribution of δE_{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,

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

- 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,

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

- 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,

$$\gamma_{\mu\nu}^{w+w} = \gamma_{\mu\nu}^{\text{wall2}} + \gamma_{\mu\nu}^{\text{window}};$$

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

TKE Systematics

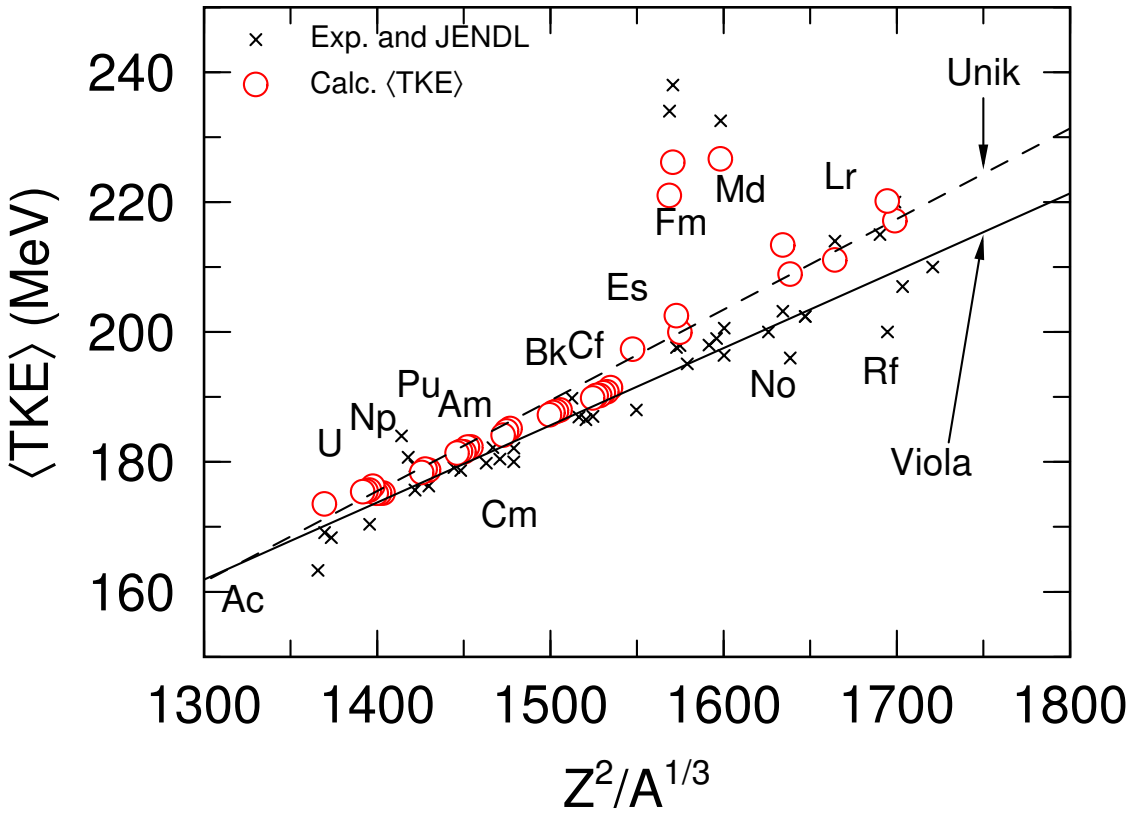


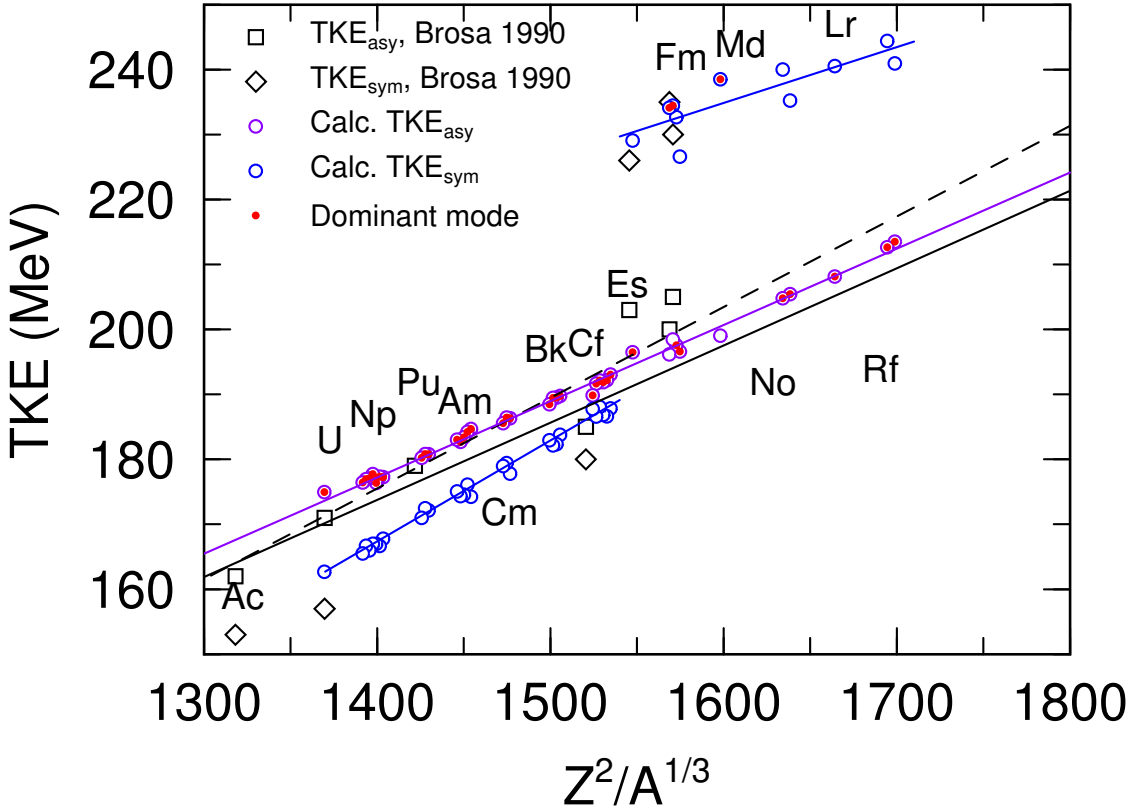
Figure: Calculated ⟨TKE⟩ (○) distribution with respect to Viola (——) systematics ; and Unik (– – –) systematics.

$$\mathrm{TKE_{Viola}} = 0.1189 Z^2 A^{-1/3} + 7.3 \text{ MeV}$$
$$\mathrm{TKE_{Unik}} = 0.1396 Z^2 A^{-1/3} - 19.9 \text{ MeV}$$

Calculated values;

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

TKE Systematics: fission mode components



$$\mathrm{TKE_{Viola}} = 0.1189 Z^2 A^{-1/3} + 7.3\ \mathrm{MeV}$$
$$\mathrm{TKE_{Unik}} = 0.1396 Z^2 A^{-1/3} - 19.9\ \mathrm{MeV}$$

$$\mathrm{TKE_{asy}^{calc.}} = 0.1168 Z^2 A^{-1/3} + 13.9\ \mathrm{MeV}$$

In the range $1300 < Z^2/\sqrt[3]{A} < 1550$,
$$\mathrm{TKE_{SL}^{calc.}} = 0.1542 Z^2 A^{-1/3} - 48.7\ \mathrm{MeV}$$

In the range $Z^2/\sqrt[3]{A} > 1550$,
$$\mathrm{TKE_{SS}^{calc.}} = 0.0849 Z^2 A^{-1/3} + 99.0\ \mathrm{MeV}$$

Figure: Viola (——) and Unik (– – –) systematics are compared with our calculation for TKE$_{asy}$ (——) and TKE$_{sym}$ (——)

Effects of Temperature on Potential Energy Surface