Pairing correlations in fissionning nuclei around scission

Krzysztof Pomorski



NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

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Results presented here* are obtained in collaboration with:

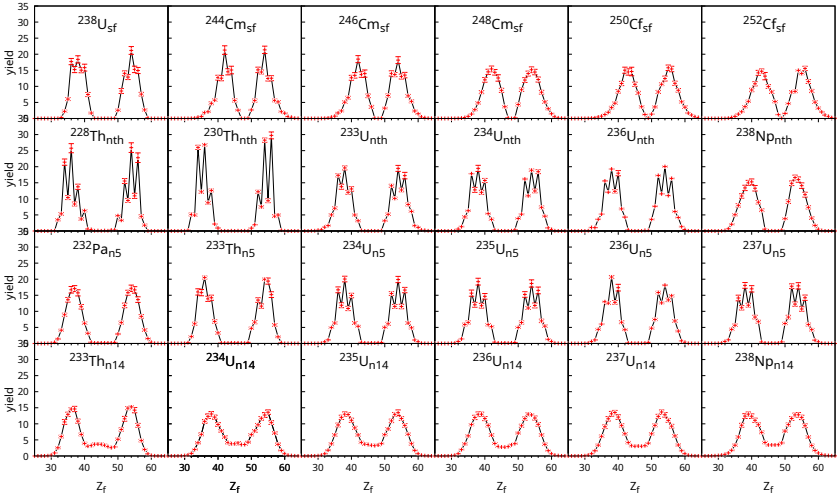
- NCNR - Warsaw:
  A. Augustyn, T. Cap, M. Kowal
- MCSU - Lublin:
  B. Nerlo-Pomorska, M. Warda
- TU - Beijing:
  Z.G. Xiao
- CIAE NDC - Beijing:
  Y.J. Chen, L.L. Liu

Contents:

- Experimental evidence of the odd-even effects around scission[a].
- Simple theoretical explanation origin of this effects[b]
- Potential energy surface (PES) of fissioning nuclei obtained using the Fourier-over-Spheroid (FoS) shape parametrization[c] the macro-micro model based on the Yukawa-folded s.p. potential[d], the Lublin-Strasbourg Drop[e] (LSD) or the ISOscalar Liquid Drop Approximation[f] (ISOLDA).
- Temperature dependence of the microscopic energy correction on the fission fragment mass and charge yields.
- Universal scaling laws for the temperature dependence of the pairing and shell energy corrections[g].
- Does the pairing force strength depend on the nucleus' elongation?
- Summary and conclusions

a) ENDF Database: nfy-version.VIII.1; D. Ramos et al. PRC 99, 024615 (2019).
b) K. Pomorski, B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Phys. Rev. C **107**, 054616 (2023).
c) K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt, Phys. Rev. C **107**, 054616 (2023).
d) A. Dobrowolski, K. Pomorski, J. Bartel, Comp. Phys. Comm. **199**, 118 (2016).
e) K. Pomorski, J.Dudek, Phys. Rev. C **67**, 044316 (2003).
f) K. Pomorski, Z.G. Xiao, Chin. Phys. C 49, 064109 (2025).
g) K. Pomorski, A. Augustyn, T. Cap, Y.J. Chen, M. Kowal, M. Warda, Z.G. Xiao, Phys. Rev. C **114**, 024336 (2026).

Experimental fission-product charge-yields for spontaneous, n_{th}, n(5 MeV), and n(14 MeV) induced fission



s.f.

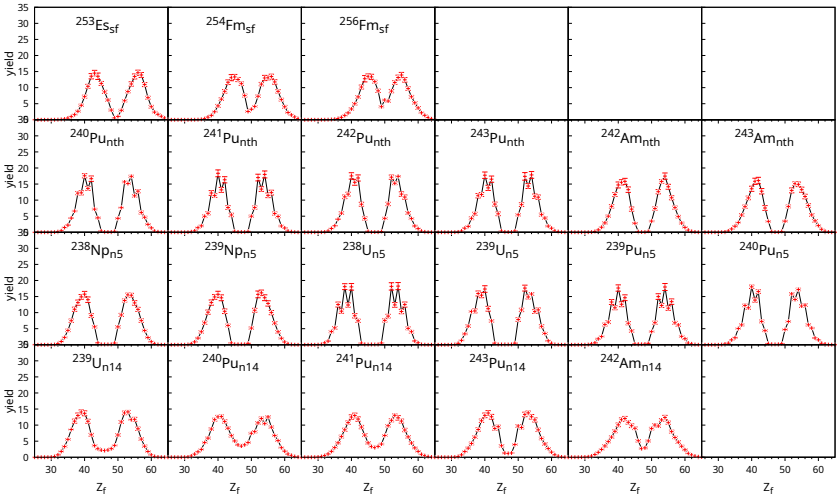
n_{th}

n(5MeV)

n(14MeV)

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Experimental fission-product charge-yields



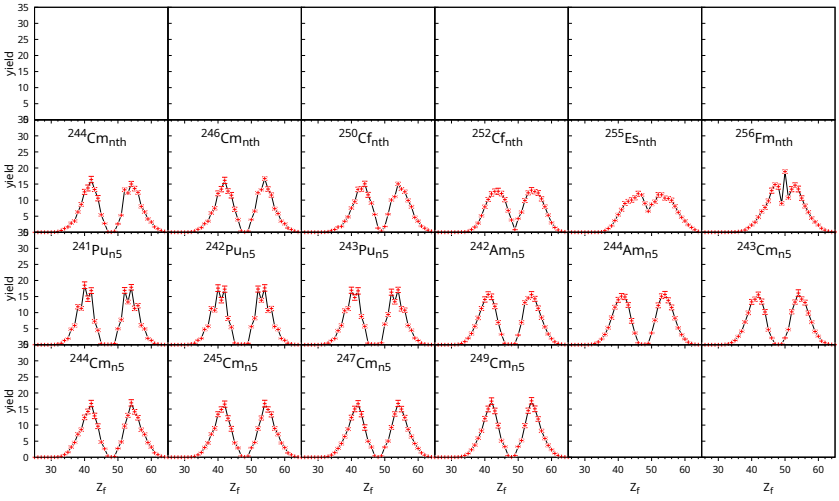
s.f.

n_{th}

n(5MeV)

n(14MeV)

Experimental fission-product charge-yields



sf

n_{th}

n(5MeV)

n(14MeV)

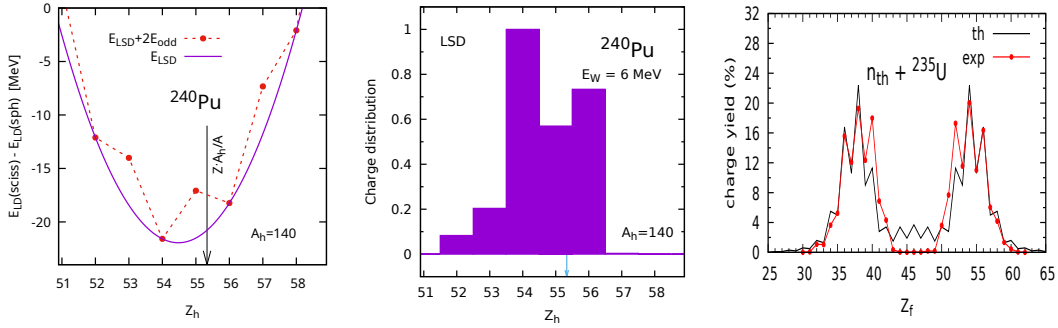
Odd-even effect in FPChY (*) and its correlation with LD scission energies

Z	A	LSD	n_{14}	n_5	n_{th}	sf	ISOLDA	Z	A	LSD	n_{14}	n_5	n_{th}	sf	ISOLDA
		MeV					MeV			MeV					MeV
Th	228	8.5			*		12.6	Pu	243	16.6	*	*	*		21.2
Th	230	8.0			*		12.3	Am	242	19.8	*	*	*		23.9
Th	233	7.4	*	*			12.0	Am	243	19.5			*		23.8
Pa	232	10.4		*			14.6	Am	244	19.3		*			23.7
U	233	13.1			*		17.1	Cm	243	22.6		*			26.6
U	234	12.8	*	*	*		17.0	Cm	244	22.3		*	*	*	26.4
U	235	12.6	*	*			16.8	Cm	245	22.1		*			26.3
U	236	12.3	*	*	*		16.7	Cm	246	21.8			*	*	26.2
U	237	12.1	*	*			16.6	Cm	247	21.6		*			26.0
U	238	11.9		*		*	16.5	Cm	248	21.4				*	25.9
U	239	11.7	*	*			16.5	Cm	249	21.2		*			25.8
Np	238	14.8	*	*	*		19.1	Cf	250	27.0			*	*	31.2
Np	239	14.6		*			19.0	Cf	252	26.5			*	*	30.9
Pu	239	17.5		*			21.6	Es	253	29.4				*	33.6
Pu	240	17.3	*	*	*		21.5	Es	255	28.9			*		33.4
Pu	241	17.0	*	*	*		21.4	Fm	254	32.3				*	36.3
Pu	242	16.8		*	*		21.3	Fm	256	31.8			*	*	36.1

Here: $\Delta E_{\rm LD} = {\rm M(asym.scis)} - {\rm M(sphere)}$ evaluated using the LSD or ISOLDA formula. Odd-even effect survives when $E^{\rm tot}_{\rm scis} = \Delta E_{\rm LD} + B_{\rm n} + e_{\rm n}$ is not larger than 24 MeV (LSD) or 27 MeV (ISOLDA).

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On origin of the odd-even effect in the fission fragment charge yield



The liquid drop energy of nucleus at scission is a function of the heavy fragment charge:

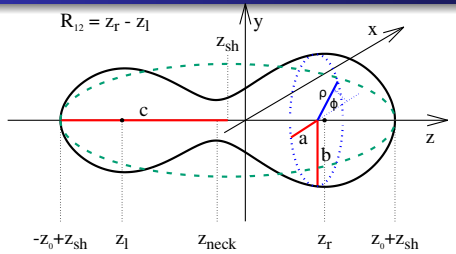
$$V_{\rm sc}(Z_{\rm h}) = E_{\rm LSD}(Z_{\rm h}, A_{\rm h}; \vec{q}_{\rm h}) + E_{\rm LSD}(Z - Z_{\rm h}, A - A_{\rm h}); \vec{q}_{\rm l}) + e^2 Z_{\rm h}(Z - Z_{\rm h})/R_{12} - E_{\rm LSD}(Z, A; 0) \ .$$

The proton odd-even energy is $E_{\rm odd} = 4.8/Z^{1/3}$ MeV in the case of cold nuclei. It gives the odd-Z energy effect of around 1.45 MeV and 1.25 MeV for light and heavy fragments, respectively. Probability distribution is approximated here by a Wigner type function:

$$W(Z_{\rm h}) = \exp\{-[V_{\rm sc}(Z_{\rm h}) - V_{\rm sc}(Z_{\rm min})]^2/E_0^2\} \quad \text{with} \quad E_0 \sim \hbar\omega_z \ .$$

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Fourier over Spheroid shape parametrization*



Non-axial shapes:

$(x, y, x) \quad \rightarrow \quad (\rho, \varphi, z)$

$$\eta = \frac{b-a}{a+b}\ ; \qquad a(z)b(z) = \rho_s^2(z)$$

The parameter η is similar, but more general, than the γ-deformation of Åge Bohr.

The distance from the z-axis to the surface is given by:

$$\rho^2(z,\varphi) = \frac{R_0^2}{c}\, f\left(\frac{z-z_{\rm sh}}{z_0}\right) \frac{1-\eta^2}{1+\eta^2+2\eta\cos(2\varphi)}\ .$$

where

$$f(u) = 1 - u^2 - \sum_{k=1}^{n} \left\{ a_{2k}\cos\left(\tfrac{k-1}{2}\pi u\right) + a_{2k+1}\sin(k\pi u)\right\}\ ,$$

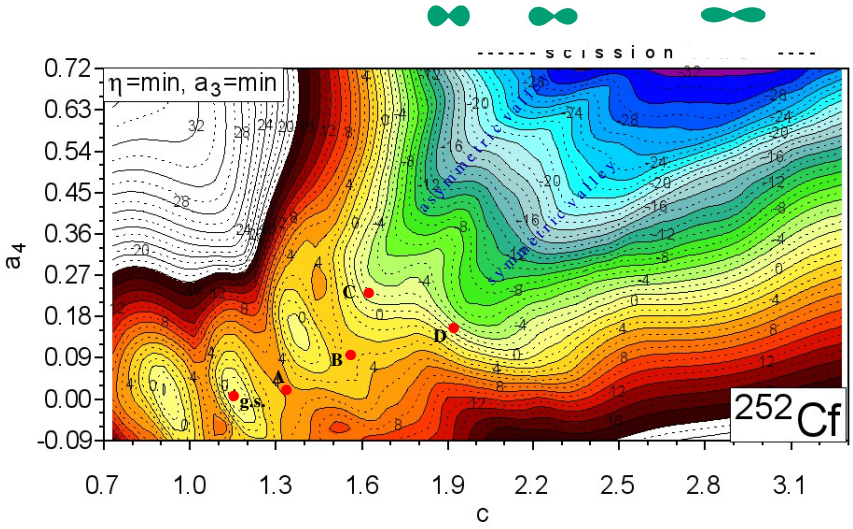
Here $u = (z - z_{\rm sh})/z_0$ and $-1 \le u \le 1$, $z_0 = cR_0$ is the half-length of nucleus, R_0 is the radius of spherical nucleus, $z_{\rm sh} = -3/(4\pi)\, z_0(a_3 - a_5/2 + \dots)$ is the shift to keep the mass-center at the coordinate origin, and a_i play a role of the deformation parameters.

The volume conservation is ensured by assuming $a_2 = a_4/3 - a_6/5 + \dots$.

* K. Pomorski, B. Nerlo-Pomorska, Acta Phys. Pol. B Proc. Suppl. **16**, 4-A021 (2023);

K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt, Phys. Rev. C **107**, 054616 (2023).

Example of the potential energy surface

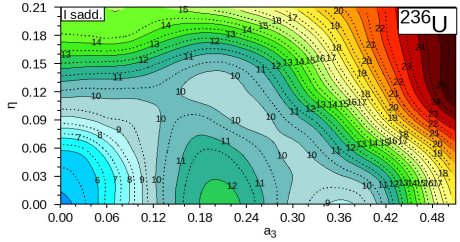


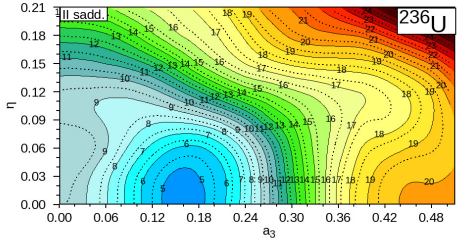
Here, c is elongation, η - non-axial, a_3 - left-right asymmetry, and a_4 - waist/neck parameter.

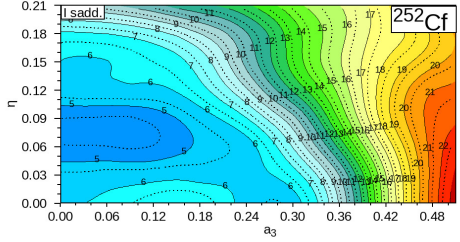
Role of non-axial and left-right asymmetries

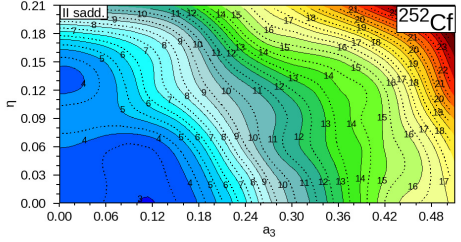
first saddle

second saddle

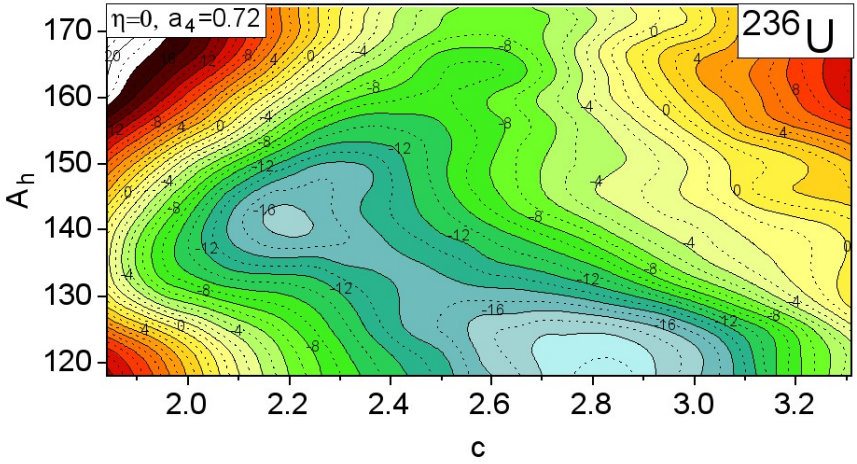








Example of the potential energy surface around scission



$$E_{\rm pot} = E_{\rm LSD} + E_{\rm shell} + E_{\rm pair}. \quad \text{Here, } A_{\rm h} \simeq \frac{A}{2}(1 + a_3) \quad \text{and} \quad T = 0$$

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Pairing energy and entropy of nucleus at finite temperature

$$E_{\rm BCS}(T) = 2\sum_{\nu>0} e_\nu n_\nu^{\Delta,T} - \frac{\Delta^2}{G}\ ; \qquad S_{\rm pair} - 2\sum_{\nu>0}[n_\nu^{\Delta,T}\ln n_\nu^{\Delta,T} + (1-n_\nu^{\Delta,T})\ln(1-n_\nu^{\Delta,T})]$$

where

$$n_\nu^{\Delta,T} = \frac{1}{2}\left(1 - \frac{e_\nu - \lambda}{E_\nu}\tanh\frac{E_\nu}{2T}\right)$$

is the temperature dependent occupation probability and $E_\nu = \sqrt{(e_\nu-\lambda)^2+\Delta^2}$.
The particle number and gap equations are:

$$N = 2\sum_{\nu>0} n_\nu^{\Delta,T} \quad \text{and} \quad \frac{2}{G} = 2\sum_{\nu>0}\frac{1}{E_\nu}\tanh\frac{E_\nu}{2T}$$

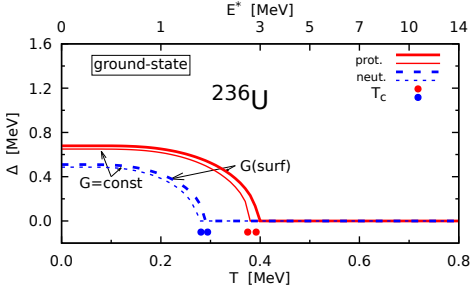
Solid-state estimate of the critical temperature T_c at which Δ vanishes*:

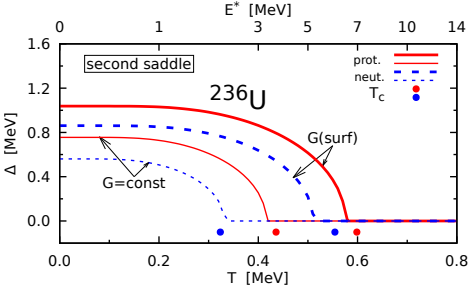
$$T_c = \left(\frac{e^C}{\pi}\right)\Delta(T=0) \approx 0.57\Delta(T=0)\ ,$$

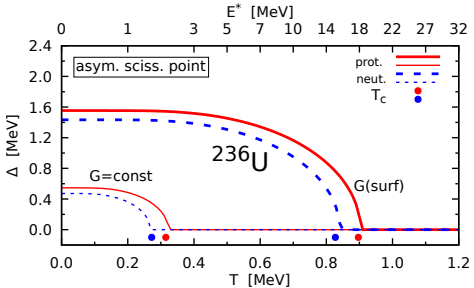
where C is the Euler constant.

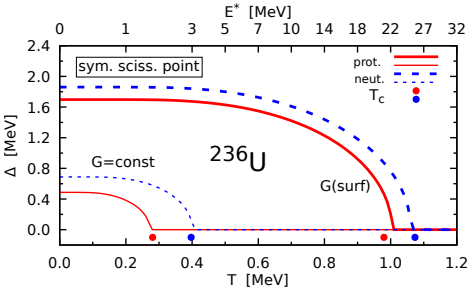
* E.M. Lifshitz and L.P. Pitaevskii, *Statistical Physics*, Part 2.

Pairing Δ as a function of temperature for G=const and G ∼ S



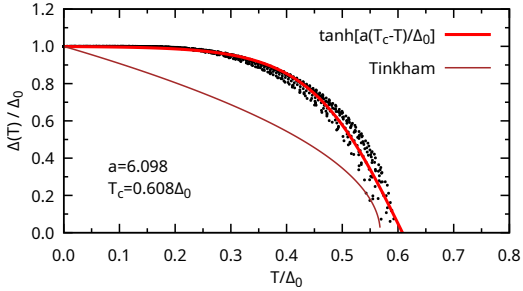






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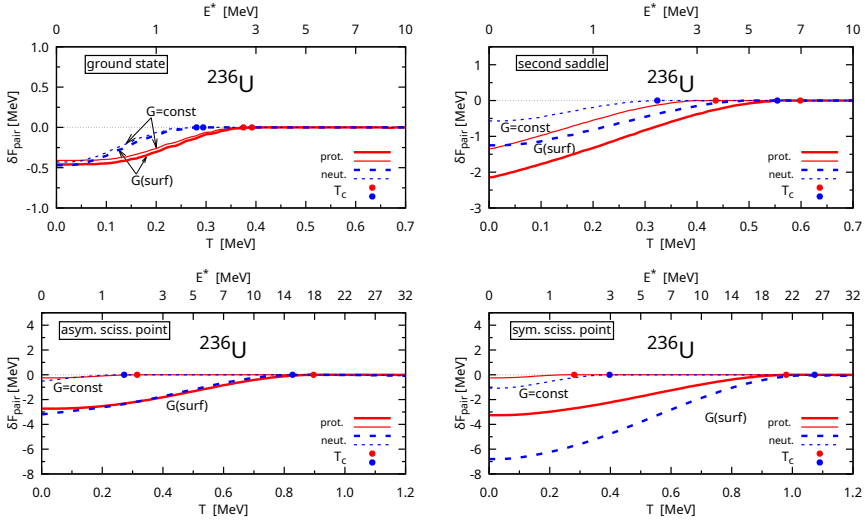
Scalling law for the Δ temperature dependence



$$\Delta(T) = \Delta_0 \tanh\left(a\frac{T_c - T}{\Delta_0}\right) \quad \text{with} \quad T_c = 0.609\Delta_0,\ a = 6.044,\ \text{and}\ \Delta_0 = \Delta(T=0).$$

Here all $\Delta(T)$ points both for G=const and G$\sim$ S, proton and neutron in the ground-state, the second saddle, the asymmetric and symmetric scission points are taken into account.
The thin brown line corresponds to expression $\Delta(T) = \Delta_0\sqrt{1 - 1.76\,T/\Delta_0}$ used in the solid state physics and valid around T_c only.

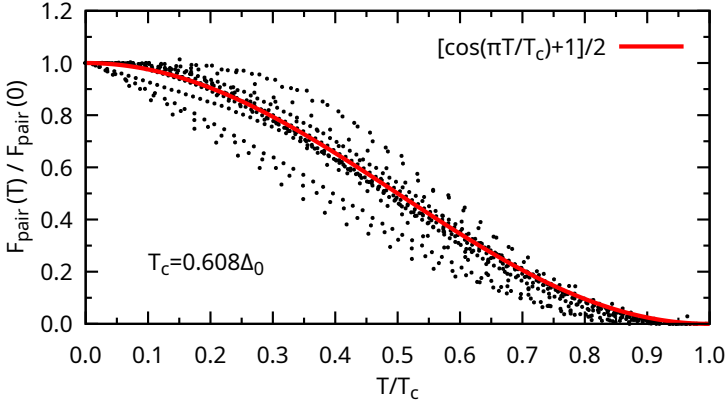
Pairing free energy as a function of temperature



$$\delta F_{\mathrm{pair}} = [E_{\mathrm{BCS}}(T) - TS_{\mathrm{pair}}(T)] - [E(T) - TS(T)]$$

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Scalling law for the temperature dependence of the free energy

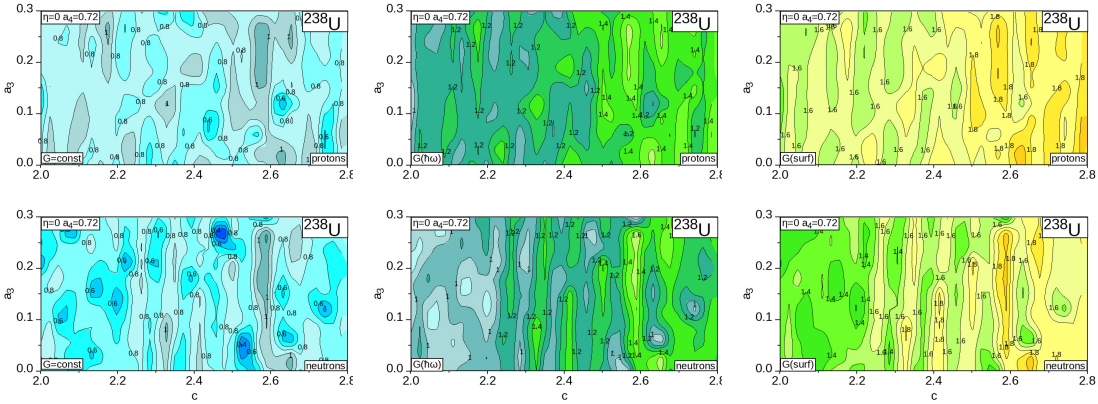


For $T \leq T_c$ $\quad F_{\rm pair}(T) = F_{pair}(0)\dfrac{\cos(\pi T/T_c)+1}{2}$, where $\quad F_{\rm pair} = F_{\rm BCS} - F_{\rm s.p.}$

All $\Delta(T)$ points both for G=const and G$\sim$ S, proton and neutron in the ground-state, the second saddle, the asymmetric and symmetric scission points (16 lines!) are taken into account.

Pairing gaps at scission for T=0 and three pairing strengths

$GN^{2/3} = 0.29\,\hbar\mathring{\omega}_0$ $GN^{2/3} = 0.29\,\hbar\omega_0(\mathrm{def})$ $GN^{2/3} = 0.29\,\hbar\mathring{\omega}_0 S(\mathrm{def})/S_{\mathrm{sph}}$



Here, $2\sqrt{15N}$ levels closest to the Fermi surface are taken when solving the BCS equations.

Average pairing gap of a cold fission fragment is around $\Delta \approx 12/\sqrt{A_f} \approx 1.1$ MeV.

Shell correction and Strutinsky averaging at finite temperature

The Strutinsky average density is given by:

$$\tilde{g}(e) = \frac{2}{\gamma} \sum_{\nu} f\left(\frac{e_\nu - e}{\gamma}\right) \quad \text{with} \quad f(x) = \frac{e^{-x^2}}{\sqrt{\pi}} \sum_{n=0,2,..}^{M} a_n H_n(x)$$

The energy and entropy of the independent proton, or neutron, system are:

$$E(T) = 2\sum_{\nu} e_\nu n_\nu \ , \quad S(T) = -2\sum_{\nu} [n_\nu \ln n_\nu + (1-n_\nu)\ln(1-n_\nu)] \ ,$$

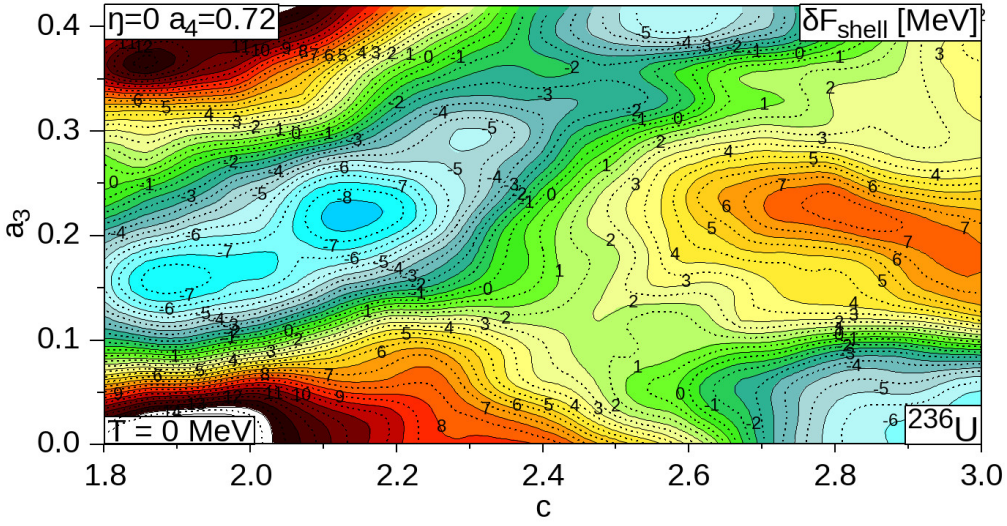
where $n_\nu = 1/\{1+\exp[(e_\nu - \lambda)/T]\}$ and λ is obtained from the condition $N = 2\sum_\nu n_\nu$.
Analogously the Strutinsky average energy and entropy are:

$$\tilde{E}(T) = \int_{-\infty}^{\infty} e\,\tilde{g}(e) n(e) de \ , \quad \tilde{S}(T) = -2\int_{-\infty}^{\infty} \{n(e)\ln n(e) + [1-n(e)]\ln[1-n(e)]\}\,\tilde{g}(e) de$$

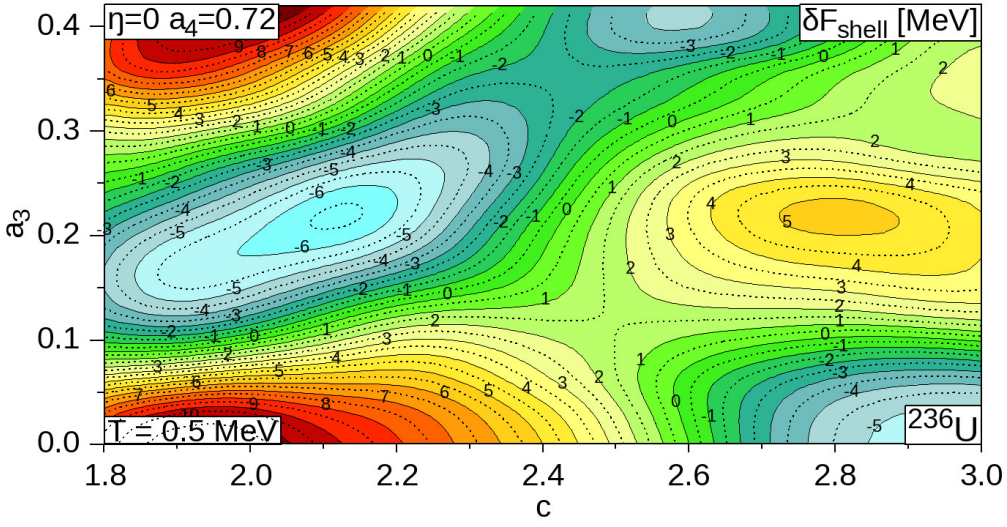
where $N = \int_{-\infty}^{\infty} \tilde{g}(e) n(e) de$ and $n(e) = 1/\{1+\exp[(e-\tilde{\lambda})/T]\}$.
Shell corrections to the total and free energies are:

$$\delta E_{\rm shell} = E(T) - \tilde{E}(T) \ , \qquad \delta F_{\rm shell}(T) = [E(T) - T\cdot S(T)] - [\tilde{E}(T) - T\cdot \tilde{S}(T)] \ .$$

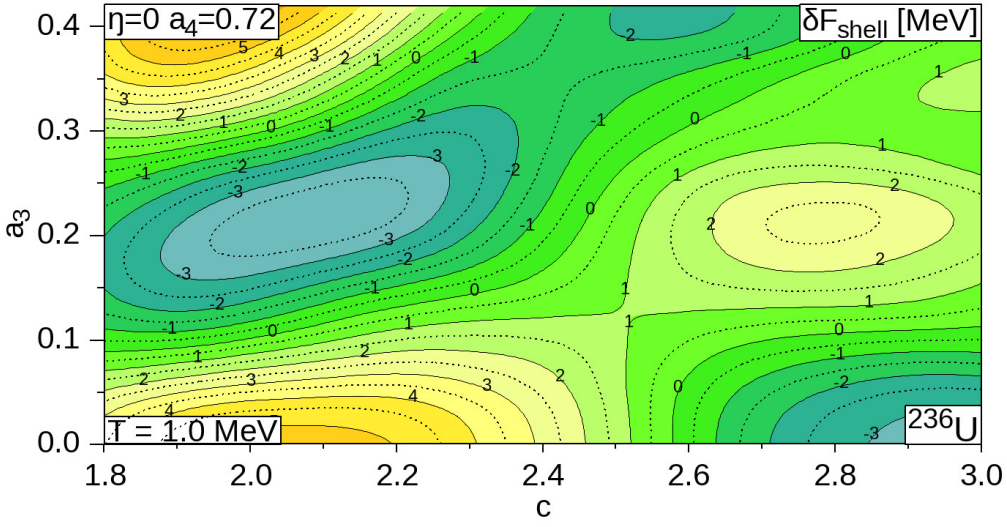
Free energy shell correction around scission for T=0



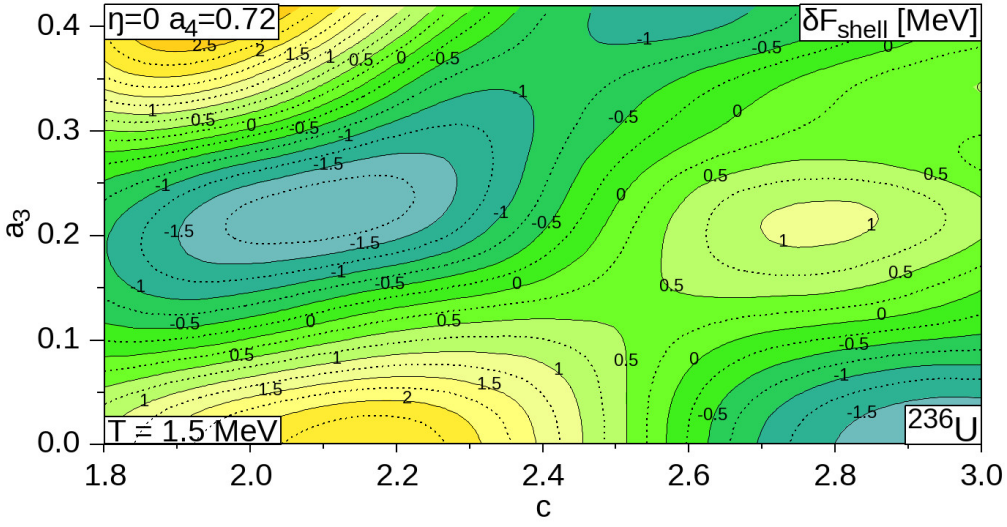
Free energy shell correction around scission for T=0.5 MeV



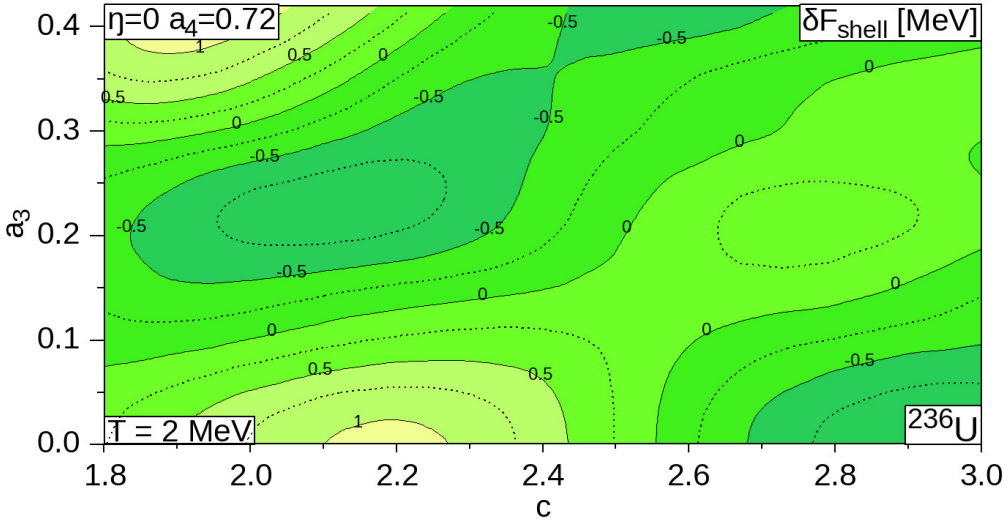
Free energy shell correction around scission for T=1 MeV



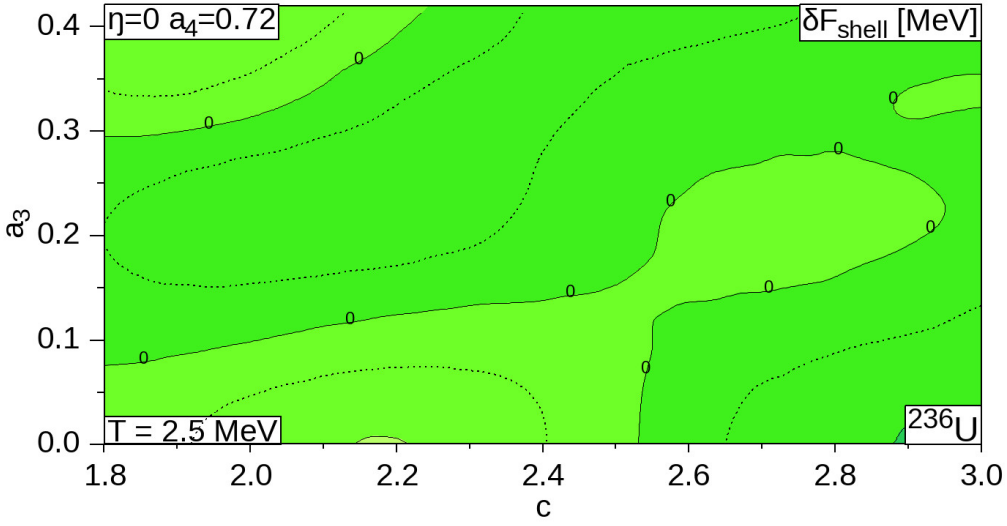
Free energy shell correction around scission for T=1.5 MeV



Free energy shell correction around scission for T=2 MeV

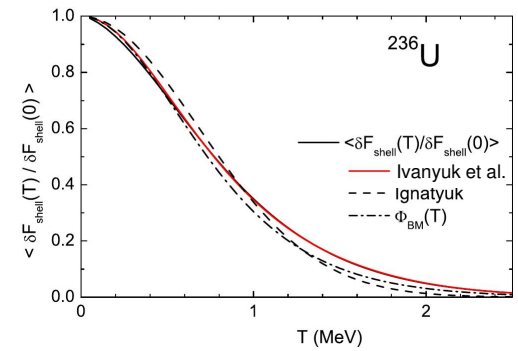


Free energy shell correction around scission for T=2.5 MeV



Shell correction temperature dependence in different models

Ivanyuk et al., PHYSICAL REVIEW C **97**, 054331 (2018)



A.V. Ignatyuk et al., Sov. J. Nucl. Phys. 21, 255 (1975):

$$\delta F_{\rm shell}(E^*) = \delta F_{\rm shell}(0)\exp(-E^*/E_d)\ ,$$

where $E_d = 20$ MeV and $E^* = aT^2$.

A. Bohr and B. Mottelson, Nuclear Structure, Vol. 2 (Benjamin, New York, 1975), p. 607.:

$$\delta F_{\rm shell}(T) = \delta F_{\rm shell}(0)\frac{\tau}{\sinh\tau}\ ,$$

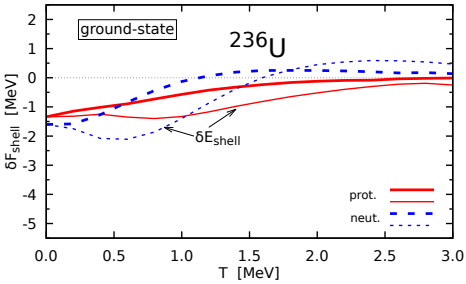
where $\tau = 2\pi^2 T/\hbar\omega_0$ with $\hbar\omega_0 = 41/A^{1/3}$ MeV. This BM formula was derived for the closed shell nuclei.

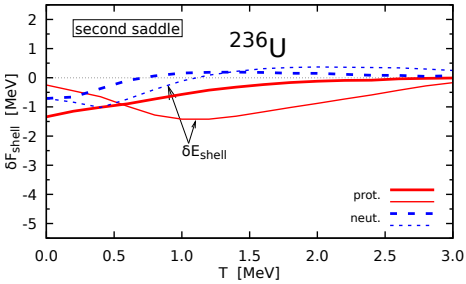
F.A. Ivanyuk et al., Phys. Rev. C **97**, 0.54331 (2018):

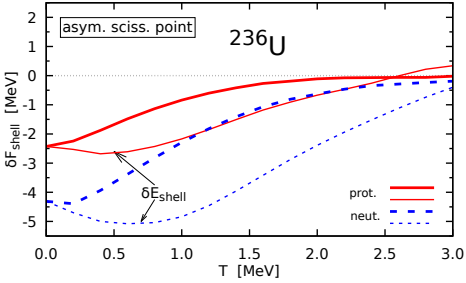
$$\delta F_{\rm shell}(E^*) = \delta F_{\rm shell}(0) = (e^{-E1/E_0}-1)/(e^{(E^*-E_1)/E_0}-1)\ , \quad \text{where}$$

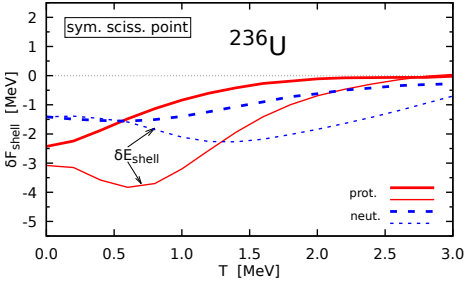
$E_0 \approx (-457 + 236A^{1/3} - 38.6A^{2/3} + 2.24A)$ MeV and $E_1 \approx (-391 + 230A^{1/3} - 43.6A^{2/3} + 2.62A)$ MeV.

Strutinsky shell correction to the free and total energies





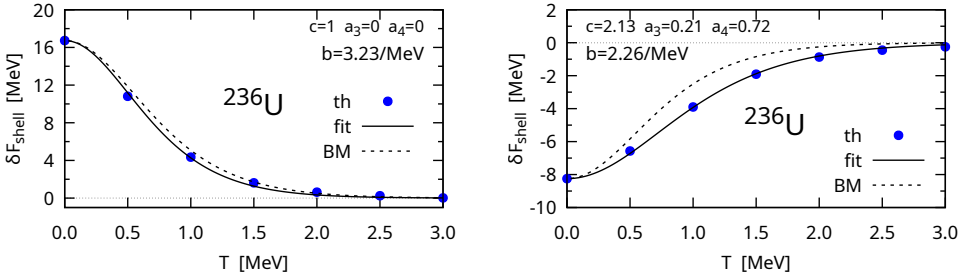




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Free energy shell correction as function of temperature

. spherical nucleus around the asymmetric scission point



Blue points corresponds to the evaluated free energy at different temperatures while the solid line shows the fit obtained with a similar function as proposed by Bohr and Mottelson:

$$\delta F_{\rm shell}(T) = \delta F_{\rm shell}(0)\frac{bT}{\sinh(bT)} \ ,$$

The BM formula gives $b = 2\pi^2/(\hbar\omega_0)$=2.98/MeV for spherical ^{236}U nucleus, which is close to our fitted value: 3.23, seen in the l.h.s. figure, while around scission b is much smaller then the BM estimate. It suggests that one has to take deformation dependence of $\hbar\omega_0$ in the BM formula.

Free energy shell correction as function of temperature

The above results suggest that one has to take the deformation dependence of the $\hbar\omega_0$ parameter in the BM formula. The deformation dependence of $\hbar\omega_0(\mathrm{def})$ is given by formula:

$$\frac{\hbar\omega_0(c)}{\hbar\overset{\circ}{\omega}_0} = \left(\frac{2\sqrt{c}+1/c}{3}\right)^3 ,$$

where c is nucleus elongation and $\hbar\overset{\circ}{\omega}_0 = 41/A^{1/3}$ MeV is the spherical harmonic oscillator frequency. The most probable elongation at the asymmetric scission is $c = 2.13$, so:

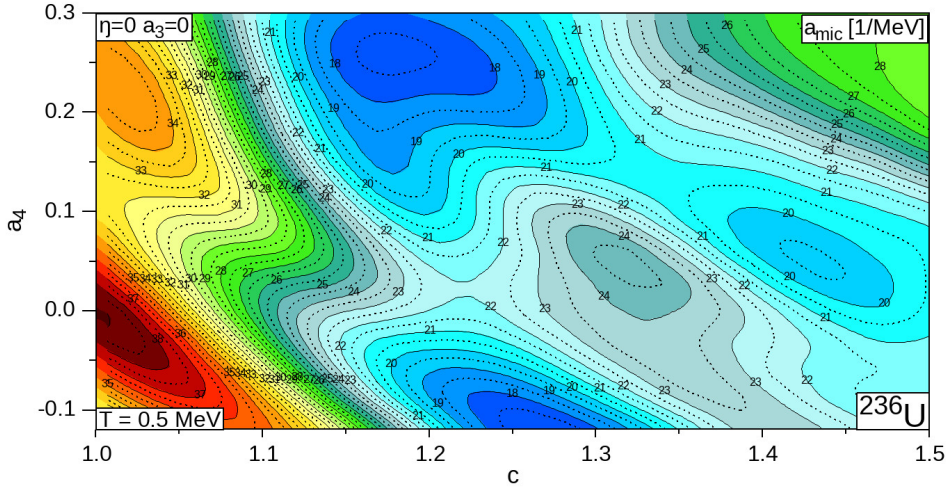
$$\frac{\hbar\omega_0(2.13)}{\hbar\overset{\circ}{\omega}_0} \cong 1.45 , \qquad \text{while} \qquad \frac{b(2.13)}{b(\mathrm{sph})} = \frac{3.23}{2.26} \cong 1.44 .$$

Taking the above relations into account, we modify the BM formula as follows:

$$\delta F_{\mathrm{shell}}(T,\mathrm{def}) = \delta F_{\mathrm{shell}}(0,\mathrm{def})\frac{\tau}{\sinh\tau} , \qquad \text{where} \qquad \tau = \frac{BT}{\hbar\omega_0(\mathrm{def})} .$$

Fit to all grid points of above maps gives $B \approx 21$ what is close to the BM constant $2\pi^2 \cong 19.74$.

Single particle level density parameter



We have used the relation $S = 2aT$ to evaluate the a parameter.

Summary:

- Fourier over Spheroid shape parametrization and the Yukawa-folded single-particle potential were used in our analysis.
- The macroscopic LSD energy with the temperature dependent shell and pairing free energy corrections were used to determine the potential energy surfaces in the 4D (c, a_3, a_4, η) space.
- Temperature dependence of the free-energy shell-correction around the scission configuration was studied in details.
- It was shown that the free energy shell correction scales with temperature according to the Bohr-Mottelson formula in which the H.O. frequency depends on the nucleus deformation.
- Universal scaling laws of the temperature dependence of the pairing gap and free energies was found.

An extended Langevin and Random-Walk types calculations of the fission fragment mass and charge yields corresponding to different excitation energies of Th-Fm nuclei are planned.

More details are in Ref. [K. Pomorski, A. Augustyn, T. Cap, Y.J. Chen, M. Kowal, M. Warda, Z.G. Xiao, Phys. Rev. C **114**, 024336 (2026)].

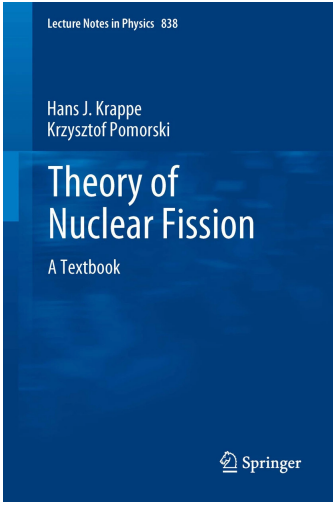
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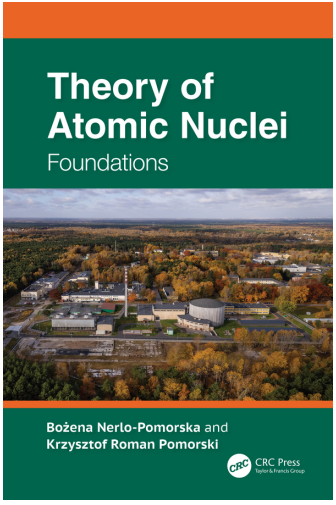
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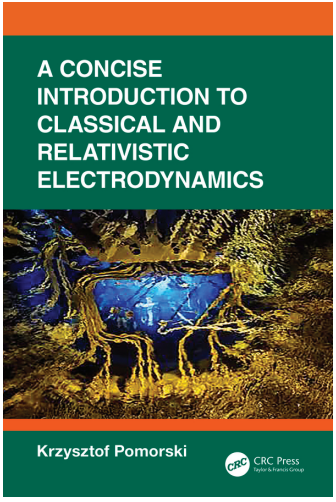
More details can be found in the books:



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