Nuclear octupole shapes in Actinides with Fayans functionals

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4) At the heart of nuclei • Density Functional Theory -> iterative self-consistent operations -> stable solution

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- Energy Density Functional

$$\begin{aligned} \epsilon_t^{even} &= \left(C_{t0}^{\rho} + \rho_0^{\gamma} C_{tD}^{\rho} \right) \rho_t^2 + C_t^{\tau} \rho_t \tau_t + C_t^{\Delta \rho} \rho_t \Delta \rho_t + C_t^{\nabla J} \rho_t \nabla J_t + C_t^J J_t^2 \\ \epsilon_t^{odd} &= \left(C_{t0}^s + \rho_0^{\gamma} C_{tD}^s \right) s_t^2 + \cdots \quad t = 0, 1 \end{aligned}$$

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- Octupole deformation [2], lower impact in current gen EDFs
- Fayans Pairing Term [3] -> adjusted Next-gen Fayans Functionals [4] [5] [6]

1) At the heart of nuclei Skyrme and

$$\mathcal{E}_{\text{pair},q} = \frac{1}{4} V_{\text{pair},q} \left(1 - \frac{\rho_0}{\rho_{\text{pair}}} \right) \breve{\rho}_q^2 \qquad (q = p, n)$$

$$\begin{split} \mathcal{E}_{\mathrm{Sk},t} &= C_t^{\rho\rho}(\rho_0)\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\rho\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t + C_t^{J^2}\boldsymbol{J}_t^2\\ E_{\mathrm{C}} &= e^2\int d^3r\,d^3r'\rho_p(\boldsymbol{r})\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\rho_p(\boldsymbol{r}')\\ \mathcal{E}_{\mathrm{C,ex}} &= -\frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{4/3}. \end{split}$$

Fayans EDFs

$$\mathcal{E}_{\mathrm{Fy},q}^{\mathrm{pair}} = \frac{2\varepsilon_F}{3\rho_{\mathrm{sat}}} \breve{\rho}_q^2 \left[f_{\mathrm{ex}}^{\xi} + h_+^{\xi} x_{\mathrm{pair}}^{\gamma} + h_{\nabla}^{\xi} r_s^2 (\nabla x_{\mathrm{pair}})^2 \right]$$

$$\begin{split} x_{t} &= \frac{\rho_{t}}{\rho_{\text{sat}}}, \quad x_{\text{pair}} = \frac{\rho_{0}}{\rho_{\text{pair}}} \\ \mathcal{E}_{\text{Fy}}^{\text{v}} &= \frac{1}{3} \varepsilon_{F} \rho_{\text{sat}} \left[a_{+}^{\text{v}} \frac{1 - h_{1+}^{\text{v}} x_{0}^{\sigma}}{1 + h_{2+}^{\text{v}} x_{0}^{\sigma}} x_{0}^{2} + a_{-}^{\text{v}} \frac{1 - h_{1-}^{\text{v}} x_{0}}{1 + h_{2-}^{\text{v}} x_{0}} x_{1}^{2} \right] \\ \mathcal{E}_{\text{Fy}}^{\text{s}} &= \frac{1}{3} \varepsilon_{F} \rho_{\text{sat}} \frac{a_{+}^{\text{s}} r_{s}^{2} (\nabla x_{0})^{2}}{1 + h_{+}^{\text{s}} x_{0}^{\sigma} + h_{\nabla}^{\text{s}} r_{s}^{2} (\nabla x_{0})^{2}} \\ \mathcal{E}_{\text{Fy}}^{\text{ls}} &= \frac{4 \varepsilon_{F} r_{s}^{2}}{3 \rho_{\text{sat}}} \left(\kappa \rho_{0} \nabla \cdot J_{0} + \kappa' \rho_{1} \nabla \cdot J_{1} + g J_{0}^{2} + g' J_{1}^{2} \right) \\ \mathcal{E}_{\text{C,ex}}^{\text{c}} &= -\frac{3}{4} e^{2} \left(\frac{3}{\pi} \right)^{1/3} \rho_{p}^{4/3} (1 - h_{\text{C}} x_{0}^{\sigma}) \end{split}$$

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- Actinides and superheavy clusters expected to present β_3 [7] [8]





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- Systematic survey





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• Ground state energy, β_2 , β_3 , $\Delta_{1;2n}$, rms radii, etc.





2) Actinides and octupoles

- Actinides and superheavy clusters expected to present β_3 [7] [8]
- Systematic survey



- Spanned whole cluster 84 < Z < 108; 120 < N < 150
- Ground state energy, β_2 , β_3 , $\Delta_{1;2n}$, rms radii, etc.
- Comparison to current-gen EDFs and studies on pear-shaped nuclei [9]

3) Fayans results in Actinides (FYdrHFB)

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1) Even-even computation around expected Q2-Q3 for min(E) of odd nucleus

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- 2) Select reasonable blocking orbitals candidates

90_Th_210_FYdrHFB neutron blocking

num=	1 block=	1 state=	1	1 Eqp=	0.98849777	(1-2N)E=	-0.43803999	Ovlp=	0.48581159	1-[5,3,0]
num=	2 block=	1 state=	2	2 Eqp=	1.03132448	(1-2N)E=	-0.79448565	Ovlp=	0.50056312	1+[6, 2, 0]
num=	3 block=	2 state=	1	154 Eqp=	1.03849441	(1-2N)E=	0.59329136	Ovlp=	0.66069727	3-[5,4,1]
num=	4 block=	1 state=	3	3 Eqp=	1.09072859	(1-2N)E=	0.31649926	Ovlp=	0.61462786	1-[5,4,1]
num=	5 block=	2 state=	2	155 Eqp=	1.12867326	(1-2N)E=	-0.92131424	Ovlp=	0.53585210	3+[6, 3, 1]
num=	6 block=	3 state=	1	290 Eqp=	1.33024372	(1-2N)E=	-1.16652448	Ovlp=	0.60205808	5+[6, 2, 2]
num=	7 block=	2 state=	3	156 Eqp=	1.33143102	(1-2N)E=	-1.08108058	Ovlp=	0.51947902	3-[5,3,2]
num=	8 block=	3 state=	2	291 Eqp=	1.36263221	(1-2N)E=	-1.21421565	Ovlp=	0.57512942	5-[5,3,2]
num=	9 block=	4 state=	1	410 Eqp=	1.65087848	(1-2N)E=	-1.53015780	Ovlp=	0.58929986	7+[6, 3, 3]
num=	10 block=	5 state=	1	515 Eqp=	2.11694535	(1-2N)E=	-2.00442036	Ovlp=	0.76908035	9+[6, 2, 4]
num=	11 block=	5 state=	2	516 Eqp=	2.62695340	(1-2N)E=	2.52311239	Ovlp=	0.83796064	9+[6, 0, 4]
num=	12 block=	1 state=	4	4 Eqp=	2.63183142	(1-2N)E=	1.52769455	Ovlp=	0.76577608	1-[5, 5, 0]
num=	13 block=	1 state=	5	5 Eqp=	2.67050206	(1-2N)E=	-1.69863083	Ovlp=	0.62843667	1-[5, 1, 0]
num=	14 block=	2 state=	4	157 Eqp=	2.74809493	(1-2N)E=	-2.68508005	Ovlp=	0.71099017	3-[5,1,2]
num=	15 block=	6 state=	1	606 Eqp=	2.76648130	(1-2N)E=	-2.57569794	Ovlp=	0.90042656	11+[6, 1, 5]
num=	16 block=	1 state=	6	6 Eqp=	2.78133078	(1-2N)E=	-2.70752540	Ovlp=	0.69568921	1-[5, 0, 1]
num=	17 block=	6 state=	2	607 Eqp=	2.95067683	(1-2N)E=	2.77257885	Ovlp=	0.91231534	11+[6, 0, 6]

- 1) Even-even computation around expected Q2-Q3 for min(E) of odd nucleus
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num=	6 block=	3 state=	1	290 Eqp=	1.33024372	(1-2N)E=	-1.16652448	Ovlp=	0.60205808	5+[6, 2, 2]
num=	7 block=	2 state=	3	156 Eqp=	1.33143102	(1-2N)E=	-1.08108058	Ovlp=	0.51947902	3-[5,3,2]
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num=	11 block=	5 state=	2	516 Eqp=	2.62695340	(1-2N)E=	2.52311239	Ovlp=	0.83796064	9+[6, 0, 4]
num=	12 block=	1 state=	4	4 Eqp=	2.63183142	(1-2N)E=	1.52769455	Ovlp=	0.76577608	1-[5, 5, 0]
num=	13 block=	1 state=	5	5 Eqp=	2.67050206	(1-2N)E=	-1.69863083	Ovlp=	0.62843667	1-[5, 1, 0]
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3) Unconstrained calculation for each possible configuration

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num=	2 DIOCK=	1 state=	2	2 Eqp=	1.03132448	(1-2N)E=	-0.79448565	ovib=	0.50056312	1+[6,	2,	0]
num=	3 block=	2 state=	1	154 Eqp=	1.03849441	(1-2N)E=	0.59329136	Ovlp=	0.66069727	3-[5,	4,	1]
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- Unconstrained calculation for each possible configuration 3)
- Lowest E -> Ground state 4)

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- 3) Unconstrained calculation for each possible configuration
- 4) Lowest E -> Ground state

Whole Q2-Q3 landscape unreasonable for non-ee nuclei; but isotopic chains can be built

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90_Th_120-150_FYdrHFB



90_Th_120-150_FYstd





• Current-gen widely used EDFs: UNEDF(0;1;2), SLY4, etc

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• Survey of pear-shaped landscapes with Skyrme-based EDFs [9]



$$0.00$$
 0.05 0.10 0.15 ≥ 0.20
 $β_3$

[9] Y. Cao, S.E. Agbemava, A.V. Afanasjev et al., Phys. Rev. C, 102, 12 (2020)



• Survey of pear-shaped landscapes with Skyrme-based EDFs [9]



et al., Phys. Rev. C, 102, 12 (2020)







FYdrHFB 84_108 - 120_150 beta_3

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Difference in ground state energy gained from the inclusion of octupole deformation



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FYdrHFB 84_108 - 120_150 Ediff

Difference in ground state energy gained from the inclusion of octupole deformation



Ν

FYdrHFB 84_108 - 120_150 Ediff: E(q2,q3)-E(q2,q3=0)

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108 Hs 0.035 Sg 106 Rf 104 0.030 No 102 0.025 Fm 100 Cf 98 0.020 Ζ 96 Cm β_3 Pu 94 0.015 92 U 90 Th 0.010 Ra 88 0.005 86 Rn Ро 84 0.000 120 122 124 126 128 130 132 134 136 138 140 142 144 146 148 150

Ν

FYstd 84_108 - 120_150 beta_3

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Difference in ground state energy gained from the inclusion of octupole deformation



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Difference in ground state energy gained from the inclusion of octupole deformation







• Given minor revisions -> as good as current state-of-the art Skyrme EDFs



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- Coherent results regarding E, r_{rms} , Δ_n , β_2 , odd-even effects, etc.



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- Returned predicted octupole clusters in Actinides with stronger β_3



- Given minor revisions -> as good as current state-of-the art Skyrme EDFs
- Coherent results regarding *E*, r_{rms} , Δ_n , β_2 , odd-even effects, etc.
- Returned predicted octupole clusters in Actinides with stronger β_3
- Strong step towards better understanding of heavily-deformed nuclei complex processes s.a. systematics, spectra, nuclear Schiff moment, fission, etc.



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FYdrHFB 54_64 - 84_100 beta_2

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FYdrHFB 54_64 - 84_100 beta_3

Cesium-centered cluster





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0.35 64 - 0.30 62 0.25 60 - 0.20 Ζ β_2 0.15 58 0.10 56 0.05 54 0.00 . 86 . 88 . 90 . 94 96 84 92 98 100 **/06/2024 G. Danneaux Ν

59

FYstd 54_64 - 84_100 beta_2



64 - 0.0200 - 0.0175 62 - 0.0150 60 0.0125 Ζ β₃ - 0.0100 58 0.0075 56 - 0.0050 - 0.0025 54 0.0000 . 86 84 88 90 92 94 96 98 100 G. Danneaux **/06/2024 Ν

60

FYstd 54_64 - 84_100 beta_3





FYstd 54_64 - 84_100 Ediff: E(q2,q3)-E(q2,q3=0)







FYstd 84_108 - 120_150 beta_2



FYdrHFB 84_108 - 120_150 beta_2

