Stability and properties of heavy and superheavy nuclei in mean-field model with Skyrme energy density functional

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The Segre chart of the SHN (A.D. 2013)



The Skyrme EDF

$$E_{Sk} = \sum_{t=0,1} \int \mathrm{d}^3 \boldsymbol{r} \left(\mathcal{H}_t^{even}(\boldsymbol{r}) + \mathcal{H}_t^{odd}(\boldsymbol{r}) \right),$$

time-even Skyrme EDF $(
ho_t,\, au_t,\,\mathbb{J}_t^{jk})$ even-even nuclei

$$\mathcal{H}_{t}^{even}(\boldsymbol{r}) = C_{t}^{\rho}[\rho_{0}]\rho_{t}^{2} + C_{t}^{\Delta\rho}\rho_{t}\Delta\rho_{t} + C_{t}^{\tau}\rho_{t}\tau_{t} + C_{t}^{J0}\mathcal{J}_{t}^{2} + C_{t}^{J1}\boldsymbol{J}_{t}^{2} + C_{t}^{J2}\mathfrak{J}_{t}^{2} + C_{t}^{\nabla J}\rho_{t}\boldsymbol{\nabla}\cdot\boldsymbol{J}_{t}, \qquad (\text{spin-orbit term})$$

time-odd Skyrme EDF $(m{s}_t,\,m{T}_t,\,m{j}_t,\,m{F}_t)$

$$\mathcal{H}_{t}^{odd}(\boldsymbol{r}) = C_{t}^{s}[\rho_{0}]\boldsymbol{s}_{t}^{2} + C_{t}^{\Delta s}\boldsymbol{s}_{t} \cdot \Delta\boldsymbol{s}_{t} + C_{t}^{T}\boldsymbol{s}_{t} \cdot \boldsymbol{T}_{t} + C_{t}^{j}\boldsymbol{j}_{t}^{2} + C_{t}^{\nabla j}\boldsymbol{s}_{t} \cdot (\boldsymbol{\nabla} \times \boldsymbol{j}_{t}) \qquad \text{(spin-orbit term)} + C_{t}^{\nabla s}(\boldsymbol{\nabla} \cdot \boldsymbol{s}_{t})^{2} + C_{t}^{F}\boldsymbol{s}_{t} \cdot \boldsymbol{F}_{t}, \qquad \text{(pure tensor terms)}$$

The total energy in the Skyrme-HF/HFB model

$$E^{tot} \equiv \langle \Phi_{HF} | \hat{H} | \Phi_{HF} \rangle \geqslant E_{g.s.}$$

=
$$\int d^3 \boldsymbol{r} \left[\mathcal{E}_{kin} + \mathcal{E}_{Sk} + \mathcal{E}_{Coul}^{dir} + \mathcal{E}_{Coul}^{ex} + \mathcal{E}_{pair} \right] + E_{corr},$$

$$\begin{split} \mathcal{E}_{kin} &= \frac{\hbar^2}{2m} \tau_0(\boldsymbol{r}), & \text{kinetic energy density} \\ \mathcal{E}_{Coul}^{dir} &= \frac{1}{2} e^2 \rho_p(\boldsymbol{r}) \int \mathrm{d}^3 \boldsymbol{r}' \frac{\rho_p(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}, & \text{direct Coulomb en. density} \\ \mathcal{E}_{Coul}^{ex} &= -\frac{3}{4} e^2 \left(\frac{3}{\pi}\right)^{1/3} \rho_p^{4/3}(\boldsymbol{r}) & \text{exchange Coulomb en. density} \\ \mathcal{E}_{pair}^{ex} &= \sum_{q=p,n} \frac{V_q^0}{4} \left[1 - V^1 \left(\frac{\rho_0(\boldsymbol{r})}{\rho_{st}}\right)^\beta \right] \tilde{\rho}_q^2(\boldsymbol{r}), \text{ Isovector pairing en. density} \\ V^1 &= 0, 1, \text{ or } 1/2 & \text{for volume-, surface-, or mix-type pairing} \\ \rho_{st} &= 0.16 \text{ fm}^{-3}, \tilde{\rho}_q(\boldsymbol{r}) \text{- pairing density for protons and neutrons.} \end{split}$$

The equality-constrained prpblem (ECP)

$$\begin{cases} \min_{\bar{\rho}} E^{tot}[\bar{\rho}] \\ \text{subject to:} \quad \sum_{\substack{q=p,n \\ \sum_{\lambda\mu}} \langle \Phi(\bar{\rho}) | \hat{N}_q | \Phi(\bar{\rho}) \rangle = N_q, \\ \sum_{\lambda\mu} \langle \Phi(\bar{\rho}) | \hat{Q}_{\lambda\mu} | \Phi(\bar{\rho}) \rangle = Q_{\lambda\mu}, \end{cases}$$

$$E^{tot}[\bar{\boldsymbol{\rho}}] \equiv E^{tot}[\rho, \tau, \mathbb{J}; \boldsymbol{s}, \boldsymbol{T}, \boldsymbol{j}, \boldsymbol{F}; \tilde{\rho}] \qquad \text{objective function} \\ = \int d^3 \boldsymbol{r} \left(\mathcal{E}_{kin}(\boldsymbol{r}) + \mathcal{E}_{Sk}(\boldsymbol{r}) + \mathcal{E}_{Coul}^{dir}(\boldsymbol{r}) + \mathcal{E}_{Coul}^{ex}(\boldsymbol{r}) + \mathcal{E}_{pair}(\boldsymbol{r}) \right) + E_{corr}$$

$$\langle \hat{Q}_{10} \rangle = \sqrt{\frac{4\pi}{3}} \sum_{i=1}^{A} \langle r_i Y_{10}(\theta_i, \phi_i) \rangle = \sum_{i=1}^{A} \langle z_i \rangle = 0 \quad \begin{array}{l} \text{dipole moment condition} \\ \text{to avoid center of mass motion} \end{array}$$

$$\hat{Q}_{20} = \sqrt{\frac{16\pi}{5}} \sum_{i=1}^{A} r_i^2 Y_{20}(\theta_i, \phi_i) = \sum_{i=1}^{A} \left(2z_i^2 - x_i^2 - y_i^2 \right) \quad \begin{array}{l} \text{quadrupole moment} \\ \text{stretching/squeezing} \end{array}$$

$$\hat{Q}_{30} = \sqrt{\frac{4\pi}{7}} \sum_{i=1}^{A} r_i^3 Y_{30}(\theta_i, \phi_i) = \sum_{i=1}^{A} \left[z_i^3 - \frac{3}{2} z_i \left(x_i^2 + y_i^2 \right) \right] \quad \begin{array}{c} \text{octupole moment} \\ \text{mass-asymmetry} \end{array}$$

$$\hat{Q}_{40} = \sqrt{\frac{4\pi}{9}} \sum_{i=1}^{A} r_i^4 Y_{40}(\theta_i, \phi_i)$$

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hexadecapole moment necking

The augmented Lagrangian functional associated with ECP

$$\begin{split} E_{c}^{'}[\bar{\boldsymbol{\rho}},\boldsymbol{\lambda},\boldsymbol{\Lambda}] &= E^{tot}[\bar{\boldsymbol{\rho}}] - \sum_{q=p,n} \lambda_{q} \langle \Psi(\bar{\boldsymbol{\rho}}) | \hat{N}_{q} | \Psi(\bar{\boldsymbol{\rho}}) \rangle \\ &+ \sum_{\lambda\mu} C_{\lambda\mu} \Big(\langle \Psi(\bar{\boldsymbol{\rho}}) | \hat{Q}_{\lambda\mu} | \Psi(\bar{\boldsymbol{\rho}}) \rangle - Q_{\lambda\mu} \Big)^{2} & \text{quadratic penalty function} \\ & \left(QPM \right) \\ & \left[+ \sum_{\lambda\mu} \Lambda_{\lambda\mu} \Big(\langle \Psi(\bar{\boldsymbol{\rho}}) | \hat{Q}_{\lambda\mu} | \Psi(\bar{\boldsymbol{\rho}}) \rangle - Q_{\lambda\mu} \Big) \right] & \text{linear penalty function} \\ & (LCM) \end{split}$$

 $\lambda_p,\lambda_n,\Lambda_{\lambda\mu}$ Lagrange multipliers, $C_{\lambda\mu}>0$ penalty parameters

The augmented Lagrange method (ALM):

$$\Lambda_{\lambda\mu}^{k+1} = \Lambda_{\lambda\mu}^{k} + 2C_{\lambda\mu}^{k} \left(\langle \Psi(\bar{\boldsymbol{\rho}}^{k}) | \hat{Q}_{\lambda\mu} | \Psi(\bar{\boldsymbol{\rho}}^{k}) \rangle - Q_{\lambda\mu} \right)$$

The first-order (necessary) variational condition

$$\frac{\delta}{\delta \bar{\boldsymbol{\rho}}} E_c'[\bar{\boldsymbol{\rho}}^*, \boldsymbol{\lambda}^*, \boldsymbol{\Lambda}^*] = 0 \quad \Rightarrow \quad E^{tot}[\bar{\boldsymbol{\rho}}^*] = E_{HF}^{tot}$$

and $\sum_{q=p,n} \langle \Psi(\bar{\rho}^*) | \hat{N}_q | \Psi(\bar{\rho}^*) \rangle = N_q$, $\sum_{\lambda\mu} \langle \Psi(\bar{\rho}^*) | \hat{Q}_{\lambda\mu} | \Psi(\bar{\rho}^*) \rangle = Q_{\lambda\mu}$

The augmented Lagrangian method (ALM)



HFODD: the self-consistent symmetries

- time-reversal \hat{T}
- parity \hat{P}
- x-, y-, z-signature $\hat{R}_{x,y,z} = \exp(-i\pi \hat{J}_{x,y,z})$
- x-, y-, z-simplex $\hat{S}_{x,y,z} = \hat{P}\hat{R}_{x,y,z}$
- x-, y-, z-simplex*T $\hat{S}_{x,y,z}^T = \hat{T}\hat{S}_{x,y,z}$



\hat{T}	\hat{S}_y	$\hat{S}_y^{\scriptscriptstyle T}$
\hat{P}	\hat{S}_y	\hat{R}_{y}
\hat{R}_{y}	$\hat{S}_x^{ \mathrm{\scriptscriptstyle T}}$	$\hat{S}_z^{\scriptscriptstyle T}$
1	1	1
1	0	0
0	1	0
0	0	1
0	0	0

$$\hat{S}_{y} = 1 \Longrightarrow Q_{\lambda\mu} = \left\langle \hat{Q}_{\lambda\mu} \right\rangle \in \mathbb{R}$$
$$Q_{\lambda-odd,\mu} \neq 0 \quad only \ for \ \hat{P} = 0$$

HFODD: all allowed symmetries (for T=1)



HFODD: all allowed symmetries (for T=0)



Model

The symmetry unrestricted code HFODD [1] and an augmented Lagrangian method [2] were used to solve constrained HFB equations with SkM* Skyrme force [3] in the p-h channel and a density dependent mixed pairing [4, 5] interaction in the p-p channel.

The stretched harmonic oscillator basis of HFODD was composed of states having not more than $N_0 = 26$ quanta in either of the Cartesian directions, and not more than 1140 states in total.

The collective mass tensor of the fissioning superfluid nucleus was computed by means of the perturbative cranking approximation to the adiabatic time-dependent Hartree-Fock-Bogoliubov approach [6].

	SkM*	SLy4	Units/Comments
t_0	-2645.0	-2488.913	$MeV fm^3$
t_1	410.0	486.818	$MeV fm^5$
t_2	-135.0	-546.395	$MeV fm^5$
t_3	15595.0	13777.0	MeV fm ^{3+α}
x_0	0.09	0.834	-
x_1	0.0	-0.344	-
x_2	0.0	-1.000	-
x_3	0.0	1.354	-
1/lpha	6.0	6.0	-
W_0	120.0	123.0	$MeV fm^5$
C_t^J	0.0	0.0	(spin-orbit tensor term, \mathbb{J}^2)
$ ho_{st}$	0.16	0.16	${\rm fm}^{-3}$
eta	1.0	1.0	-
E_{cut}	60	-	MeV (HFB)
E_{cut}	-	N or Z	(no. of s.p. states, BCS)
V^1	0.5	1	(0.5-mixed, 1-surface pairing)
V_n^0	-268.9	-842.0	$MeV fm^3$
V_p^0	-332.5	-1020.0	$MeV fm^3$

[1] N. Schunck *et al.*, **183**, 166 (2012).

- [3] J. Bartel et al., Nucl. Phys. A **386**, 79 (1982).
- [4] J. Dobaczewski, W. Nazarewicz, and M. V. Stoitsov, Eur. J. Phys. A 15, 21 (2002).
- [5] A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz, Phys. Rev. C 80, 014309 (2009).
- [6] A. Baran, J. A. Sheikh, J. Dobaczewski, W. Nazarewicz, and A. Staszczak, Phys. Rev. C 84, 054321 (2011).

^[2] A. Staszczak, M. Stoitsov, A. Baran, and W. Nazarewicz, Eur. J. Phys. A 46, 85 (2010).

Model

The Skyrme EDF in the case of even-even nuclei (time-reversal symmetry)



Ground state pairing properties of e-e SHN



Proton *drip line*: Fermi energy $\lambda^{p} \leq 2$ MeV.

Geometric sizes



Groud state deformations



The e-e SHN form three regions:

- 1) a prolate-deformed (for N < 172),
- 2) spherical (N>180),
- 3) the transitional region (between the former two).

Shape phase transitions and critical-point phenomena in atomic nuclei

R.F. Casten, Nature Physics 2, 811 - 820 (2006)

Geometric collective model (GCM) - A. Bohr (1952)

$V(\beta,\gamma) = A\beta^2 + B\beta^3 \cos 3\gamma + C\beta^4, \quad (C>0)$



Interacting boson approximation (IBA-1) – Arima, lachello

 $U(6) \supset U(5) \supset O(5) \supset O(3)$ $U(6) \supset SU(3) \supset O(3)$ $U(6) \supset O(6) \supset O(5) \supset O(3)$

 $U(6) \supset \overline{SU(3)} \supset O(3)$ $U(6) \supset \overline{O(6)} \supset O(5) \supset O(3)$

Dynamical symmetries:

 $\begin{array}{ll} U(5) & (vibrational) \\ \overline{SU(3)}, \overline{SU(3)} & (rotational) \\ O(6), \overline{O(6)} & (\gamma \text{-soft}) \end{array} \end{array}$

Critical-point solutions:

$$V(\beta, \gamma) = A\beta^{2} + B\beta^{3} \cos 3\gamma + C\beta^{4}$$

$$V(\beta, \gamma) \approx V_{1}(\beta) + V_{2}(\gamma)$$

$$X(5): \quad V_{1} = V_{well}(\beta), \quad V_{2} = c(\gamma - \gamma_{o})^{2}, (c > 0)$$

$$E(5): \quad V_{1} = V_{well}(\beta), \quad V_{2} \equiv 0$$

F. lachello, PRL **85**, 3580 (2000); **87**, 052502 (2001).



(Fig. Casten)



Nuclear shape phase transitions















Critical (triple) point E(5)











Superdeformed oblate (SDO) SHN?



Superdeformed oblate (SDO) SHN?



Superdeformed oblate (SDO*) SHN



*P. Jachimowicz, Ml. Kowal, J. Skalski, Phys. Rev. C 83, 054302 (2011) Próchniak, A. S., Acta Phys. Polonica B 44, 287 (2013)

Superdeformed oblate (SDO) SHN



Superdeformed oblate (SDO) SHN



Superdeformed oblate (SDO) SHN



SHN phase diagram (Natura non facit saltus)



G.s. properties of SHN - Conclusions

- The e-e SHN form three regions: the prolate-deformed SU(3) (for N < 172), spherical U(5) (for N>180), and transitional region (γ-soft) O(6) between the former two.
- ✓ On the border between the O(6) and U(5) regions (for N = 180) nuclei exhibit a rather flat potential bottom and acquire the triple-point solutions E(5).
- ✓ The existence of superdeformed oblate (SDO) nuclei $\overline{SU(3)}$ for N ≤ 166 and Z ≥ 120 was validated.
- ✓ The heaviest even-even nuclei produced by ⁴⁸Ca induced reactions on actinide targets fall into the class of O(6) γ -soft nuclei.

SHN: alpha emission



SHN: Q $_{\alpha}$ - values



The spontaneous-fission half-life is inversely proportional to the probability of penetration through the barrier

$$T_{\frac{1}{2}}^{sf} = \frac{\ln 2}{n} \frac{1}{P}, \quad n \approx 10^{20.38} \, s^{-1}, \quad \frac{\ln 2}{n} = 10^{-20.54} \, s.$$

In the WKB semi-classical approximation for the probability P

$$T_{\frac{1}{2}}^{sf}[s] = \frac{10^{-20.54}}{\hbar\omega_0} \Big[1 + \exp(2S(L)) \Big],$$

where the action-integral calculated along a fission path L(s) in the multi-dimensional deformation space $\left\{q^{\lambda}\right\}$ is

$$S(L) = \int_{s_1}^{s_2} \left\{ \frac{2}{\hbar^2} B_{eff}(s) \left[V(s) - E \right] \right\}^{\frac{1}{2}} ds$$

The effective inertia associated with the fission motion along the path L(s) is

$$B_{eff}(s) = \sum_{k,l} B_{q^k q^l} \frac{dq^k}{ds} \frac{dq^l}{ds},$$

Barriers of even-even Fm isotopes





SF half-lives of even-even Fm isotopes



Experimental fission half-lives from:

•E. Holden and D.C. Hoffman, Pure Appl. Chem. 72, 1525 (2000).

•J. Khuyagbaatar et al., Eur. Phys. J. A 37, 177 (2008).

E^{tot} and $B_{20\,20}$ along sEF and aEF fission paths in ³⁰⁶122



PES with the sEF and aEF fission paths in ³⁰⁴120



PES with the sEF and aEF fission paths in ³⁰⁴120



³⁰⁶122₁₈₄ – sEF path



$^{306}122_{184} - aEF path$



sEF and aEF SF modes in even-even SHN



The contours show the predicted SF half-lives in logarithmic scale in s.







SF half-lives of even-even Fm isotopes (II)



Empty circles – (like before) the constrained HFB-SkM* calculations along Q_{20} coordinate with left-right asymmetry and non-axiality included; the mass parameters were obtained in the perturbative cranking approx. Energy of fissoning nucleus (bottom panel) was assumed to be equal $E_0 = 0.7 \text{ ZPE}(Q_{gs})$, where $\text{ZPE}(Q_{gs})$ is zero point energy (GCM+GOA model) at the ground state deformation.

Filled circles – the same as above, but the mass parameters were scaled by a factor 1.3 and E_0 energy was determined from the WKB quantization condition

$$\int_{a}^{b} \sqrt{2M(q)(E_{n}-V(q))} \, dq = \pi \left(n+\frac{1}{2}\right)\hbar, \quad n = 0, 1, 2, \dots$$

HFB-SkM* results for even-even SHN (II)



HFB-SkM* results for even-even SHN (II)



The circle radii are proportional to the decimal logarithms of total half-lives in s. max $T_{sf+\alpha+\beta} \approx 10^4 s$ for ²⁹⁴⁻²⁹⁶Cn

SHN with the extreme oblate deformation



SHN with the extreme oblate deformation



$^{306}122_{184}$ – toroidal shapes



The three-fragment valley in LDM



Fig. 2. The fission valley (the three-fragment valley) and the two-fragment valley. The associated shapes are sketched in a rough way.

Fig. 3. Schematic energy contour diagrams of the two-fragment valley and the fission valley, including (side view and plan view) the spherical minimum, caused by shell effects.

SHN by 3-body cold fusion ???





$${}^{132}\text{Sn}_{82} + {}^{132}\text{Sn}_{82} + {}^{40}\text{Ca}_{20} \rightarrow {}^{304}\text{120}_{184}$$
$${}^{48}\text{Ca}_{28} + {}^{48}\text{Ca}_{28} + {}^{208}\text{Pb}_{126} \rightarrow {}^{304}\text{122}_{182}$$



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Thank you!

¹⁹⁸Hg: the heteromodal fission



¹⁸⁰Hg: asymmetric fission!



²³²Th and ²³²U : the third minima?



²³²Th and ²³²U : the third minima?



