Localization and Clustering in Nuclei

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Localization and clustering in nucleonic matter

…quantality parameter: $$\Lambda_{\mathrm{Mot}} \hat{=} \frac{\hbar^2}{m\bar{r}^2|V_0|}$$

inter-particle distance ($\bar{r}$); depth of the potential ($|V_0|$)

➠ ratio of the zero-point kinetic energy of the confined particle to its potential energy.

B. Mottelson ➠ the transition between a solid phase (small kinetic energy compared to the potential at equilibrium) and a liquid (relatively large kinetic energy in comparison to the depth of the potential) occurs for $\Lambda_{\mathrm{Mot}} \simeq 0.1$.

For nuclear matter: the inter-nucleon distance ~ 1 fm, the strength of the nucleon-nucleon interaction $|V_0| \simeq 100$ MeV, $mc^2 \simeq 940$ MeV ⇒ $\Lambda_{\mathrm{Mot}} \simeq 0.4$ is a characteristic value for the nuclear quantum liquid phase.

J. P. Ebran, E. Khan, T. Nikšić, and D. Vretenar, J. Phys. G **44**, 103001 (2017)

Liquid-cluster transition in finite nuclei

…the de Broglie wavelength for the motion of nucleons: $\lambda_{\rm dB} = 2\pi\hbar/\sqrt{2m(E-V)}$.

… for E ~ 0 and V = − V_0 ⇒ $\lambda_{\rm dB} = \pi\bar{r}\sqrt{2\Lambda_{\rm Mot}}$ … no nuclear mass or size dependence!

DEF. Localization parameter:

$$\alpha_{\rm loc} \hat{=} \frac{\Delta r}{\bar{r}}$$

…spatial dispersion of single-nucleon wave functions:

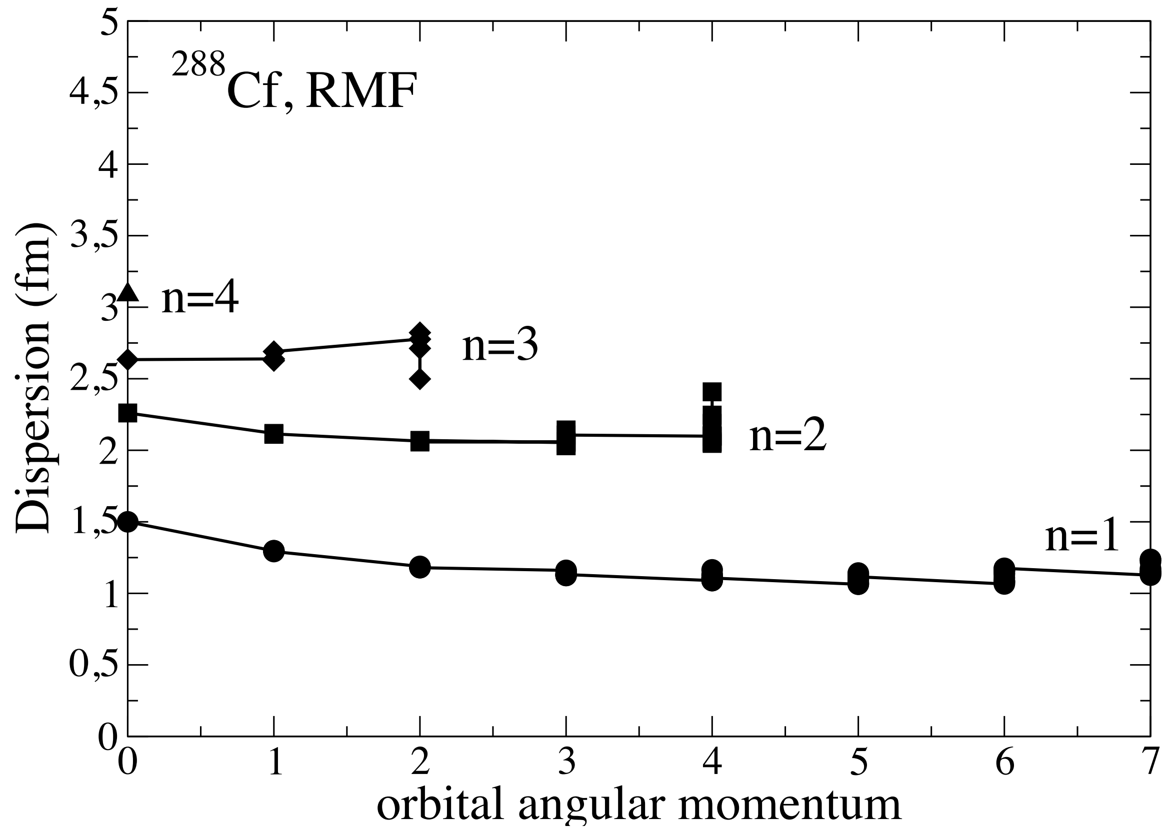
$$\Delta r = \sqrt{\langle r^2\rangle - \langle r\rangle^2}$$

For $\alpha_{\rm loc}$ >>1 ⇒ delocalised orbits of individual nucleons (Fermi liquid phase).

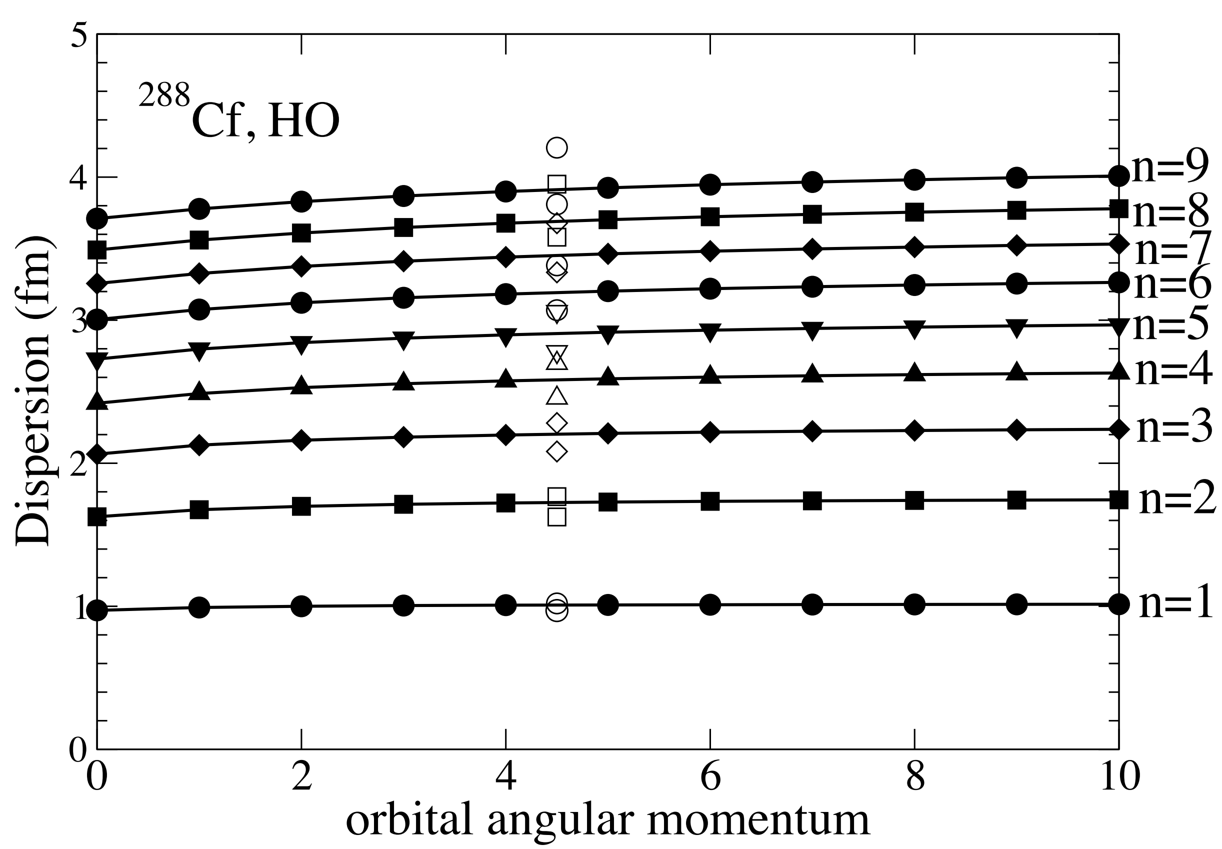
When $\alpha_{\rm loc}$ <<1 ⇒ localised nucleons (crystal-like structure).

For $\alpha_{\rm loc}$ ≈ 1 the spatial dispersion of the single-nucleon wave function ≈ inter-nucleon distance ⇒ transition from the quantum liquid phase to a hybrid phase of cluster states.

J.-P. EBRAN, E. KHAN, R.-D. LASSERI, AND D. VRETENAR
PHYSICAL REVIEW C **97**, 061301(R) (2018)



Radial dispersions *Δr* of the single-neutron wave functions of 288Cf, obtained in a self-consistent relativistic mean-field (RMF) calculation based on the energy density functional DD-ME2.



For a spherical three-dimensional harmonic oscillator (3D HO) potential:

$$\langle r^2 \rangle = b^2\left(N + \tfrac{3}{2}\right) = b^2\left(2n' + l + \tfrac{3}{2}\right),$$

$$N = 2(n-1) + l$$

$$\frac{\langle r \rangle}{b} = \sum_{q=0}^{n'} \frac{(-1)^q (l+q+1)!\,\Gamma\left(n' - q - \frac{1}{2}\right)}{q!\,(n'-q)!\,\Gamma\left(l+q+\frac{3}{2}\right)\Gamma\left(-q-\frac{1}{2}\right)},$$

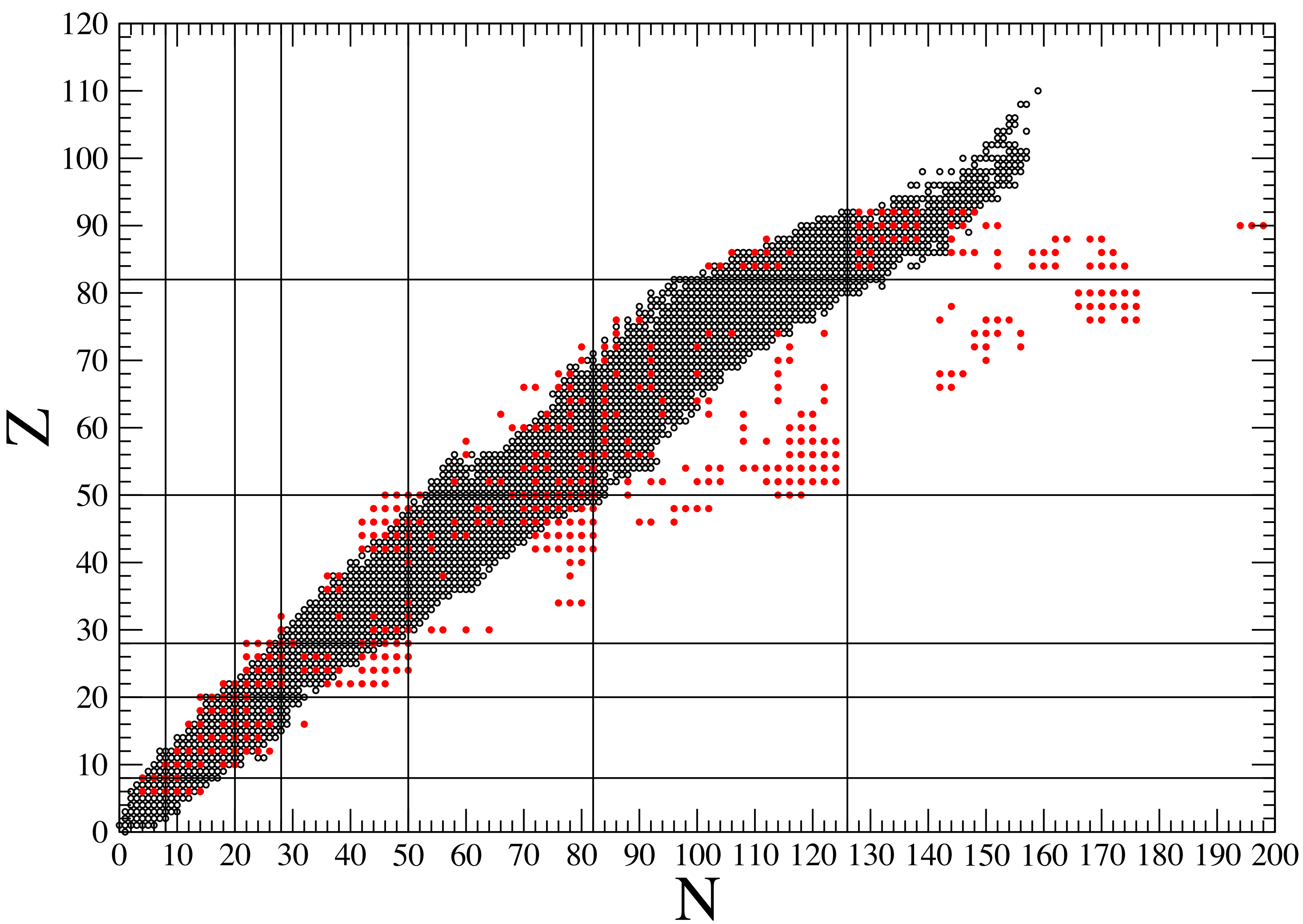
$$n' \equiv n - 1$$

For a spherical three-dimensional harmonic oscillator (3D HO) potential:

$$\alpha_{\rm loc} = \frac{2\Delta r}{r_0} \simeq \frac{b}{r_0}\sqrt{2n-1} = \frac{\sqrt{\hbar(2n-1)}}{\left(2mV_0 r_0^2\right)^{1/4}} A^{1/6}.$$

For relatively light nuclei with A ≤ 30 and n = 1 states occupied, $\alpha_{\rm loc} \leq 1 \Rightarrow$ formation of α-like clusters.

…formation of individual α-like clusters from valence nucleons in heavy nuclei:



Microscopic RHB prediction of nuclei that have small radial dispersion of the single-particle states of valence nucleons, plotted on the background of empirically known nuclides on the N-Z plane.

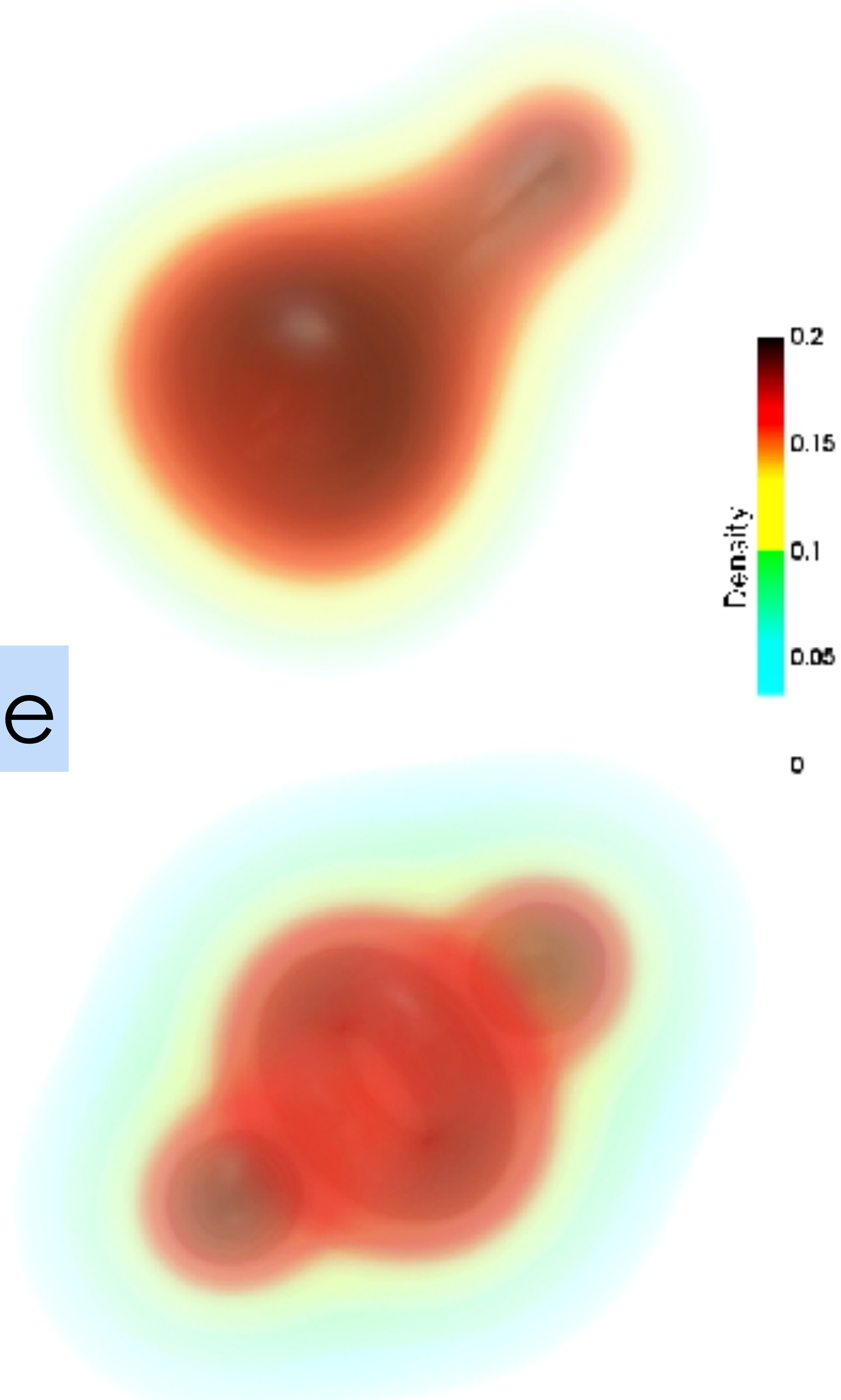
The single-nucleon dispersions are calculated for the functional DD-ME2 and separable pairing and assuming axial symmetry.

J.-P. EBRAN, E. KHAN, R.-D. LASSERI, AND D. VRETENAR

PHYSICAL REVIEW C **97**, 061301(R) (2018)

Clusters in light alpha-conjugate nuclei

Self-consistent mean-field calculations based on nuclear energy density functionals (EDFs), with constraints on mass multipole moments.



^{20}Ne

The confining potential determines the energy spacings between single-nucleon orbitals in deformed nuclei, the localization of the corresponding wave functions, and the degree of nucleonic density clustering.

Important role of nuclear shape deformation: removes the degeneracy of single- nucleon levels associated with spherical symmetry.

Cluster states cannot be isolated from the continuum of scattering states ⇒ open quantum systems.

How atomic nuclei cluster

J.-P. Ebran[1], E. Khan[2], T. Nikšić[3] & D. Vretenar[3]

19 JULY 2012 | VOL 487 | NATURE | 341

Nucleon localization functions:

kinetic energy density — density — current density

σ ($\uparrow$ or $\downarrow$)

q (n or p)

$$C_{q\sigma}(\vec{r}) = \left[1 + \left(\frac{\tau_{q\sigma}\rho_{q\sigma} - \frac{1}{4}|\vec{\nabla}\rho_{q\sigma}|^2 - \vec{j}^{\,2}_{q\sigma}}{\rho_{q\sigma}\tau^{\mathrm{TF}}_{q\sigma}}\right)^2\right]^{-1}$$

$$\tau^{\mathrm{TF}}_{q\sigma} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}_{q\sigma}$$

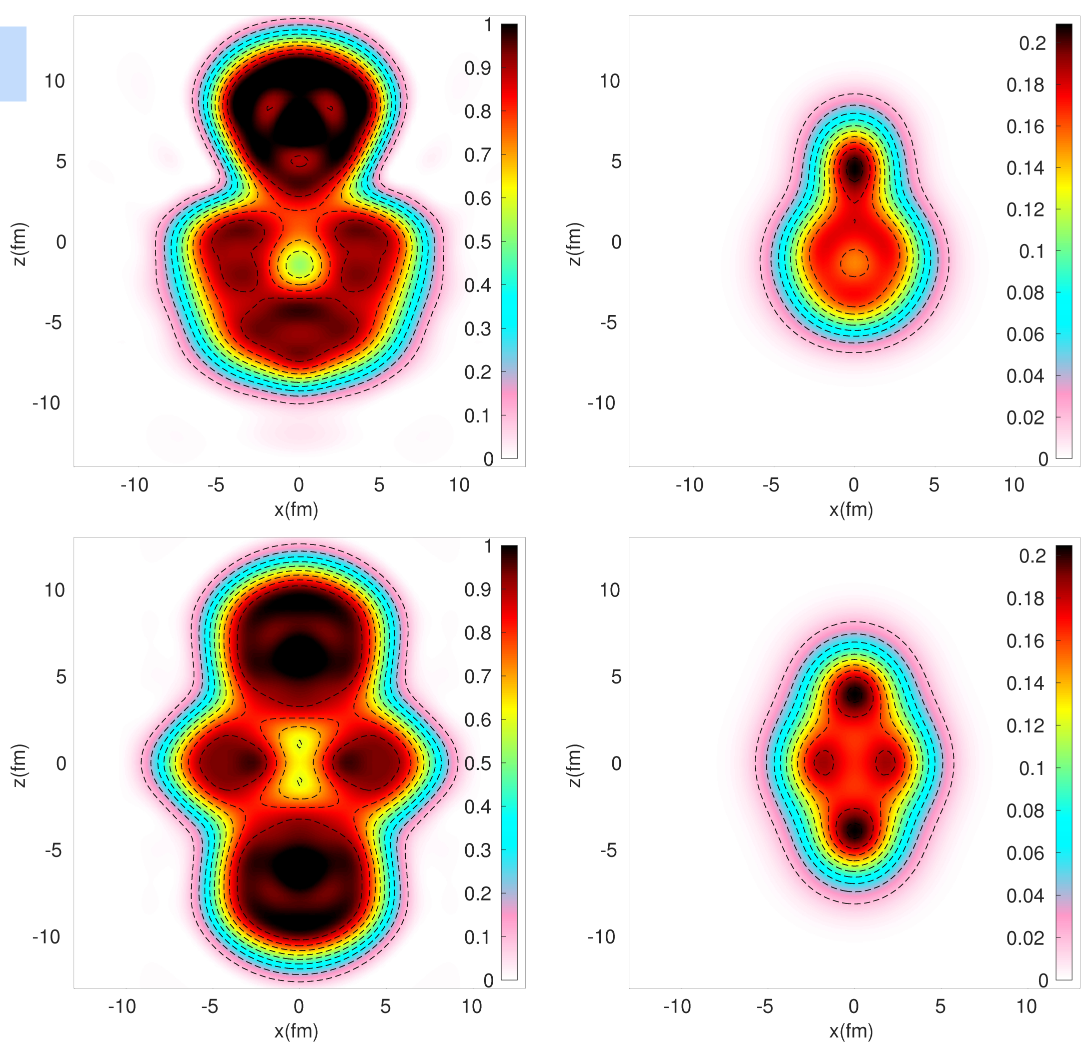
For homogeneous nuclear matter: $C_{q\sigma} = 1/2$

For the **α**-cluster (four particles): $C_{q\sigma}(\vec{r}) \approx 1$

Proton localization function

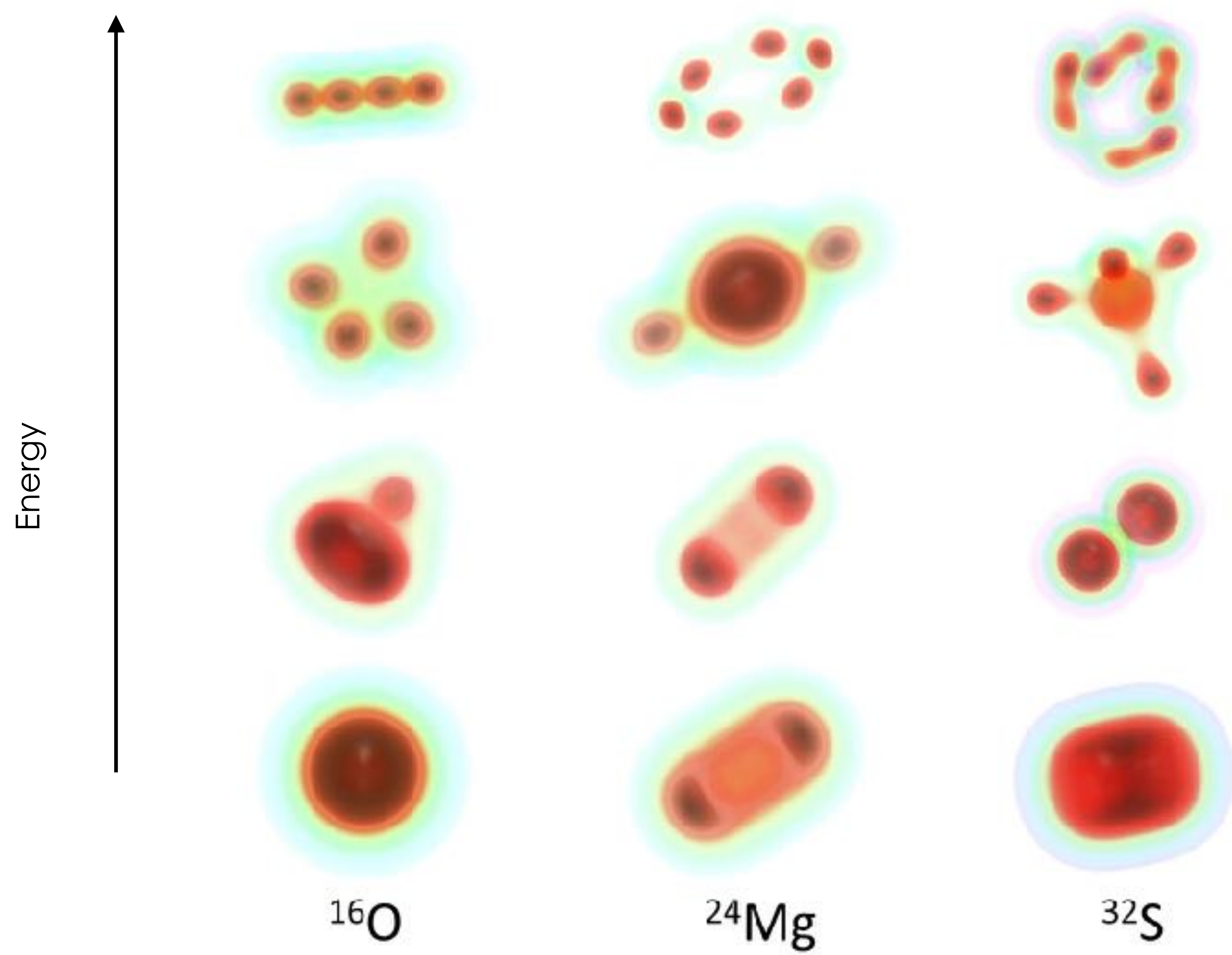
total density (in nucleon/fm^3)

^{20}Ne



J. Phys. G: Nucl. Part. Phys. **44** (2017) 103001

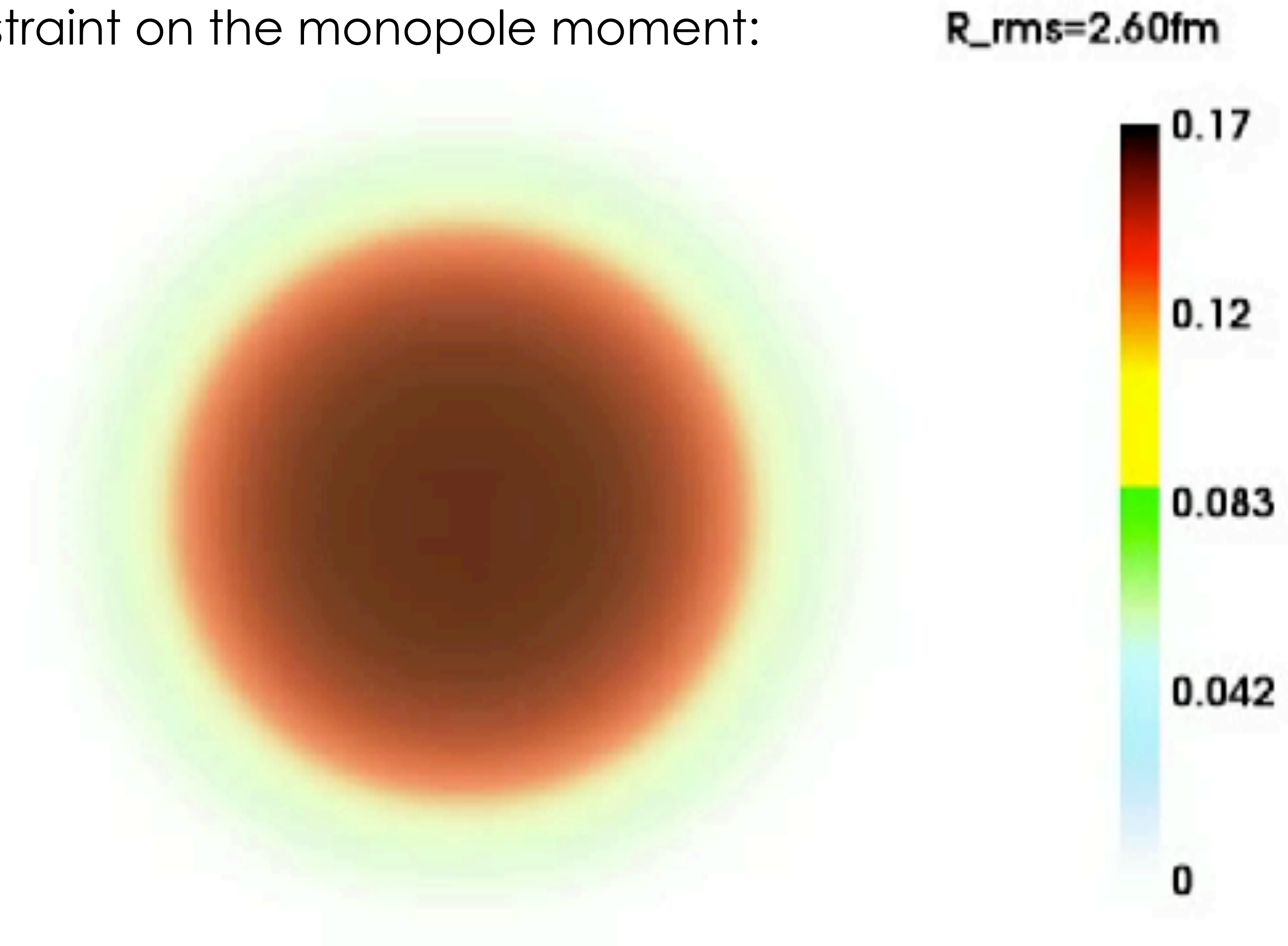
Intrinsic densities of deformation-constrained configurations in N = Z nuclei



Role of nuclear saturation ⇒ spontaneous alpha-clustering at low density

⇒ locally enhances the nucleonic density toward its saturation value, thus increasing the binding of the system.

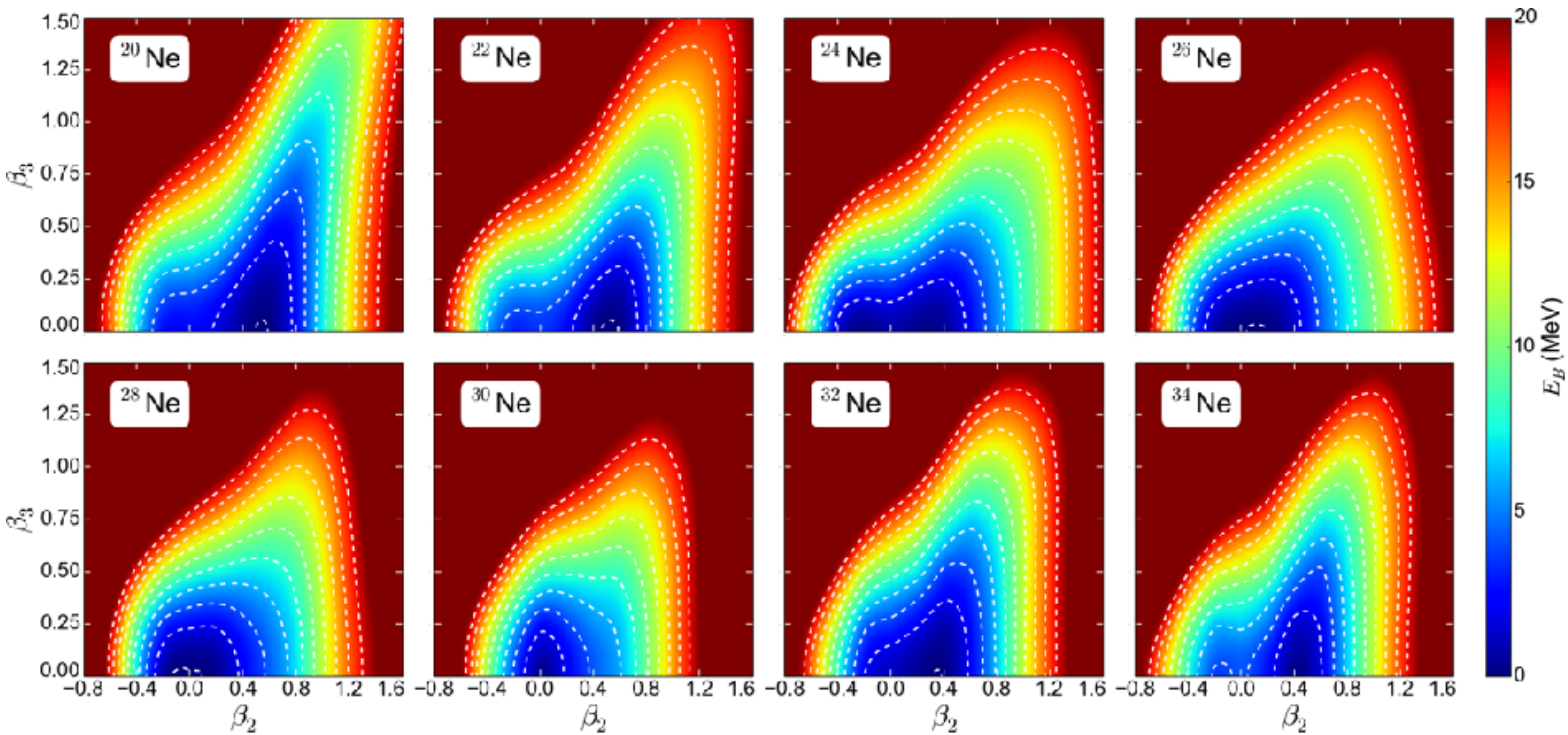
^{16}O - SCMF calculation with a constraint on the monopole moment:



EBRAN, KHAN, NIKŠIĆ, AND VRETENAR
PHYSICAL REVIEW C 89, 031303(R) (2014)

Beyond self-consistent mean field: collective correlations related to symmetry restoration and nuclear shape fluctuations

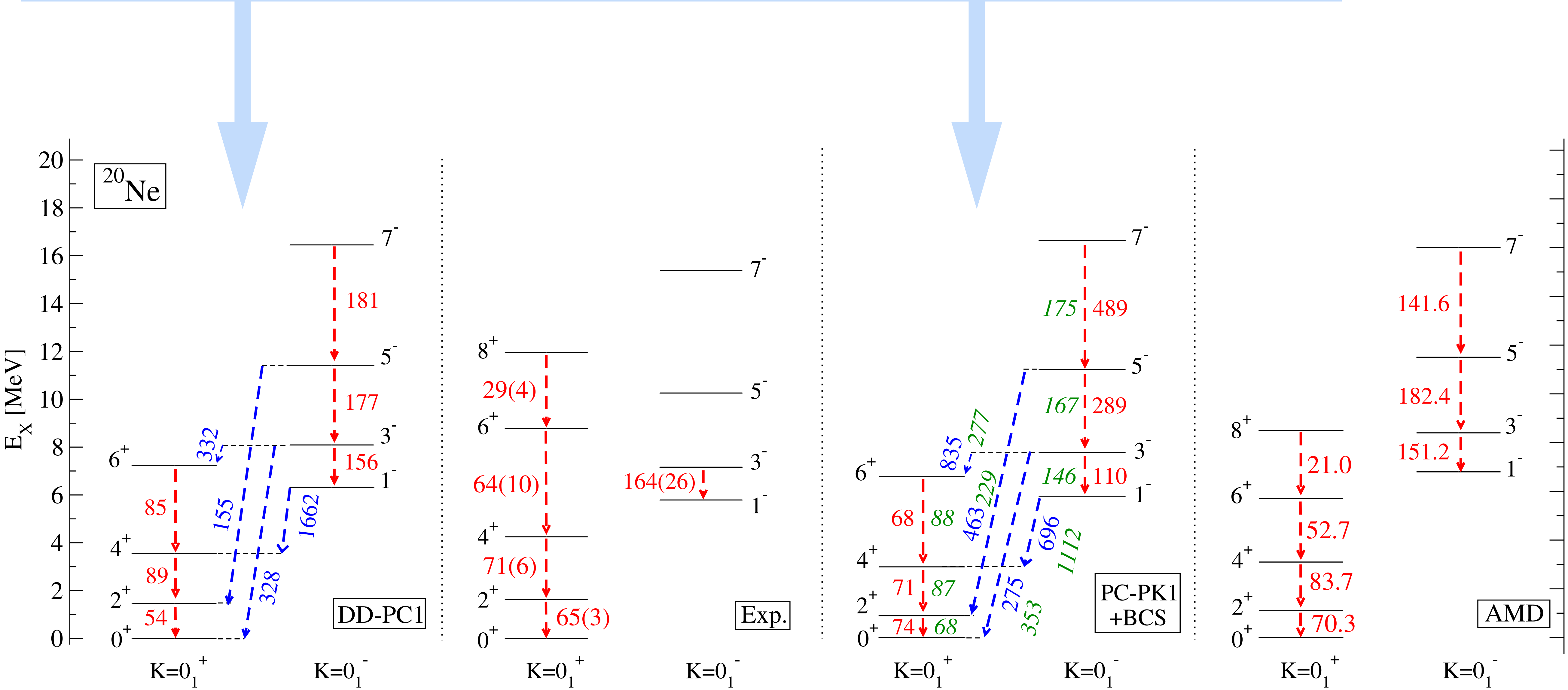
Quadrupole and octupole collectivity and cluster structures in neon isotopes



MAREVIĆ, EBRAN, KHAN, NIKŠIĆ, AND VRETENAR

PHYSICAL REVIEW C **97**, 024334 (2018)

GCM configuration mixing of angular-momentum and parity projected SCMF states



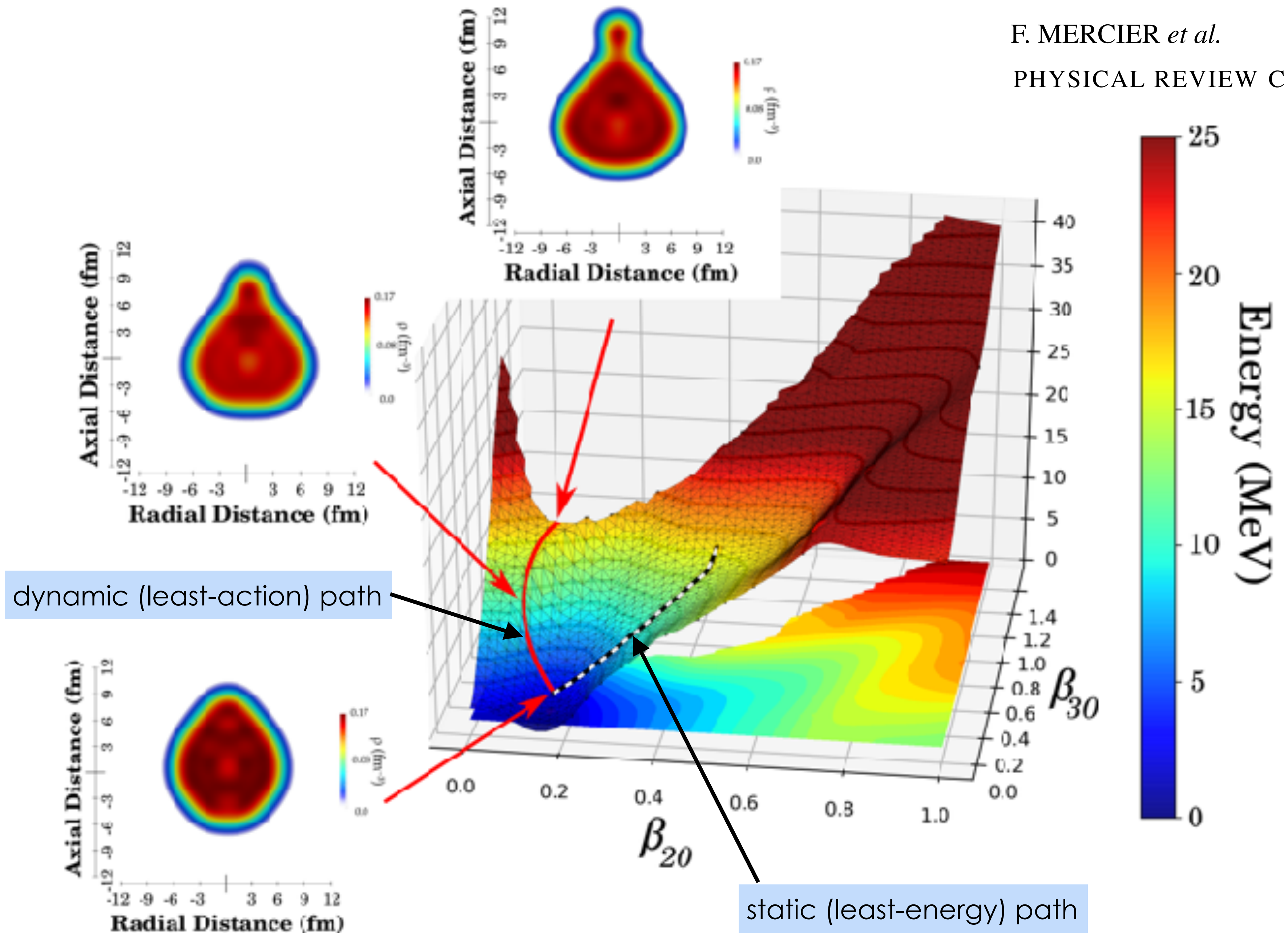
MAREVIĆ, EBRAN, KHAN, NIKŠIĆ, AND VRETENAR

PHYSICAL REVIEW C **97**, 024334 (2018)

^{108}Xe and ^{104}Te α-decay chain

➠ lightest region of the nuclear mass table in which a-particle emission has been identified.

F. MERCIER *et al.*
PHYSICAL REVIEW C **102**, 011301(R) (2020)



Deformation-energy surface of ^{104}Te in the quadrupole-octupole axially symmetric plane. RHB model based on the DD-PC1 functional.

… the action integral

$$S(L) = \int_{s_{\rm in}}^{s_{\rm out}} \frac{1}{\hbar}\sqrt{2\mathcal{M}_{\rm eff}(s)[V_{\rm eff}(s) - E_0]}ds$$

From s_{in} to the scission point: $V_{eff} = E_{RHB}(\beta_2, \beta_3) - E_{ZPE}$

$$\mathcal{M}_{\rm eff}(s) = \sum_{ij} \mathcal{M}_{ij} \frac{dq_i}{ds}\frac{dq_j}{ds}$$

➠ perturbative cranking collective inertia

From the scission point to s_{out}: Coulomb potential $V_{\rm eff}(\beta_3) = e^2\frac{Z_1Z_2}{R} - Q,$ Exp. Q-value

… effective collective mass $\mathcal{M}_{\rm eff} = \frac{\mu}{9Q_{30}^{4/3}f_3^{2/3}}$

… octupole moment $Q_{30} = f_3R^3$ $f_3 = \frac{A_1A_2}{A}\frac{(A_1 - A_2)}{A}$

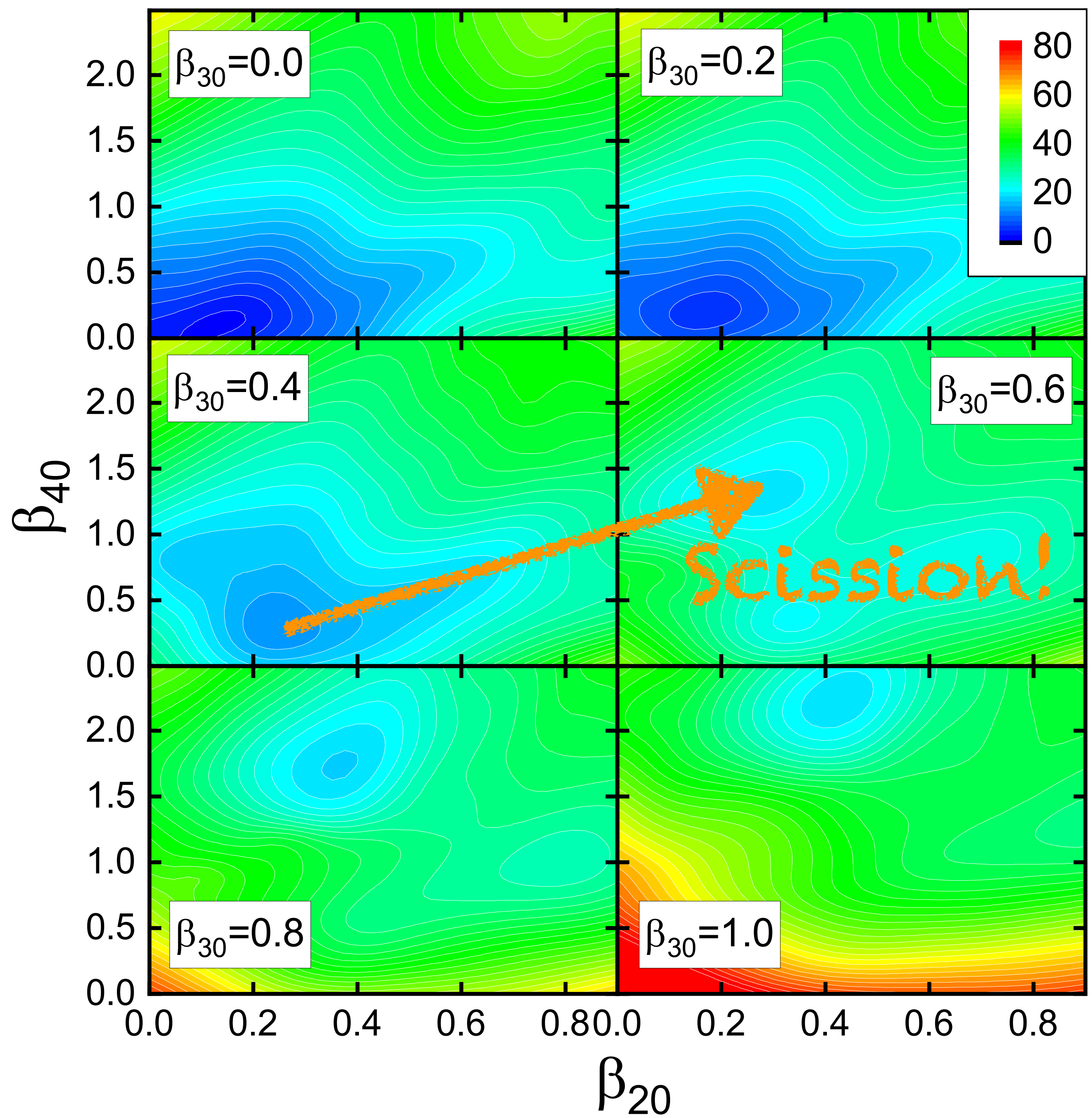
➠ … barrier penetration probability

$$P = \frac{1}{1 + \exp[2S(L)]}$$

$$T_{1/2} = \ln 2/(nP)$$

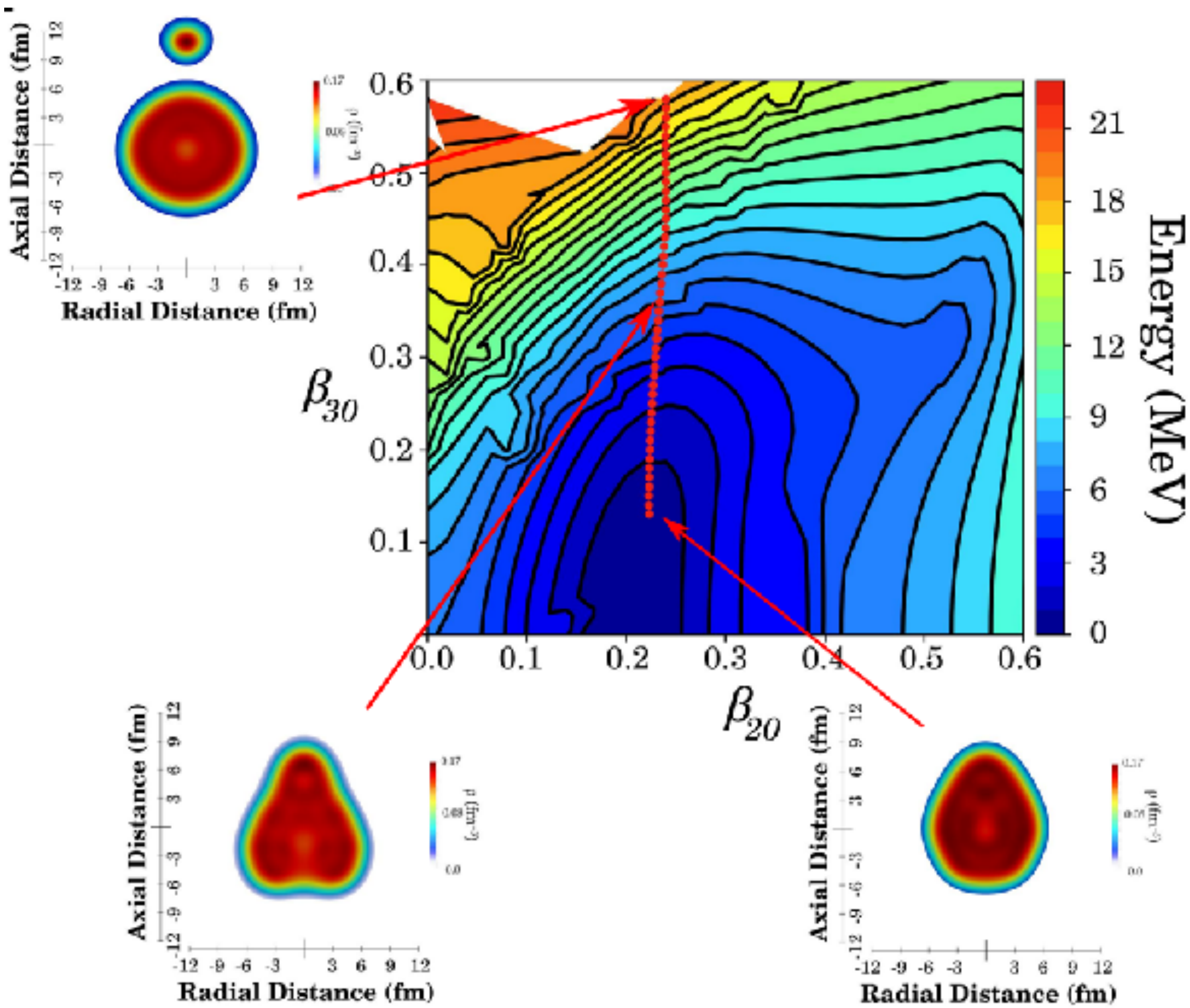
n → $10^{20.38}$ s^{-1}

The scission point is determined by a discontinuity in β40.



Deformation-energy surface of ^{104}Te in the quadrupole-hexadecupole axially symmetric plane for selected values of the octupole deformation β30.

Deformation-energy surface of ^{108}Xe in the quadrupole-octupole axially symmetric plane.



Experimental half-lives for superallowed a-decay of ^{104}Te: <18 ns, and ^{108}Xe: 58 ($^{+106}_{-23}$) μs.

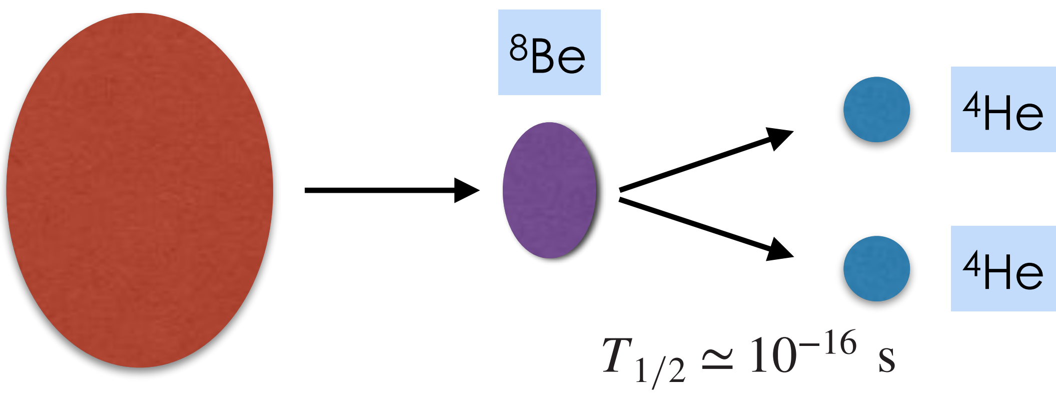
Calculated half-lives: 197 ns for ^{104}Te and 50 μs for ^{108}Xe.

PHYSICAL REVIEW C **102**, 011301(R) (2020)

Microscopic Description of 2α Decay in ^{212}Po and ^{224}Ra

F. MERCIER *et al.*

PHYSICAL REVIEW LETTERS **127**, 012501 (2021)



… not observed yet.

$T_{1/2} > 10^{33}$ years

Symmetric (back to back) 2α mode

… least action path

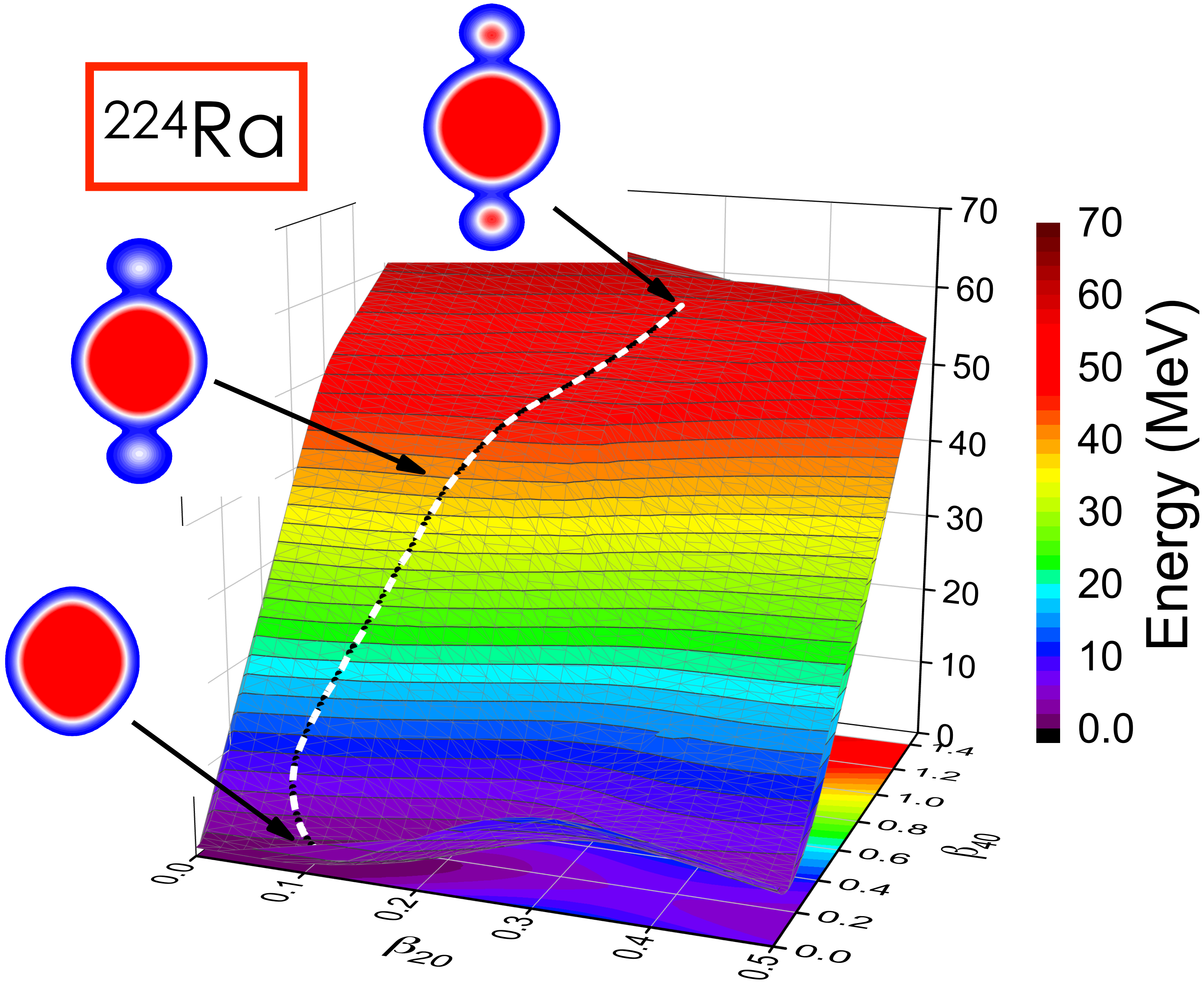
$$S(L) = \int_{s_{\rm in}}^{s_{\rm out}} \frac{1}{\hbar} \sqrt{2\mathcal{M}_{\rm eff}(s)[V_{\rm eff}(s) - E_0]}ds,$$

From s_{in} to the scission point:

$$V_{eff} = E_{RHB}(\beta_2, \beta_4) - E_{ZPE}$$

$$\mathcal{M}_{\rm eff}(s) = \sum_{ij} \mathcal{M}_{ij} \frac{dq_i}{ds} \frac{dq_j}{ds}$$

➠ perturbative cranking inertia in the β_2 and β_4 collective space



log $T_{2\alpha}$[s] = 14.24

For the ^{8}Be-mode: log $T_{2\alpha}$[s] = 27.87.

From the scission point to s_{out}: superposition of two alpha+nucleus Coulomb potentials

$$V_{\rm eff}(\beta_2) = 2e^2\frac{Z_1 Z_2}{R} - Q_{2\alpha}$$

... effective collective mass $$\mathcal{M}_{\rm eff} = \frac{\mu}{8A_2 q_{20}}$$

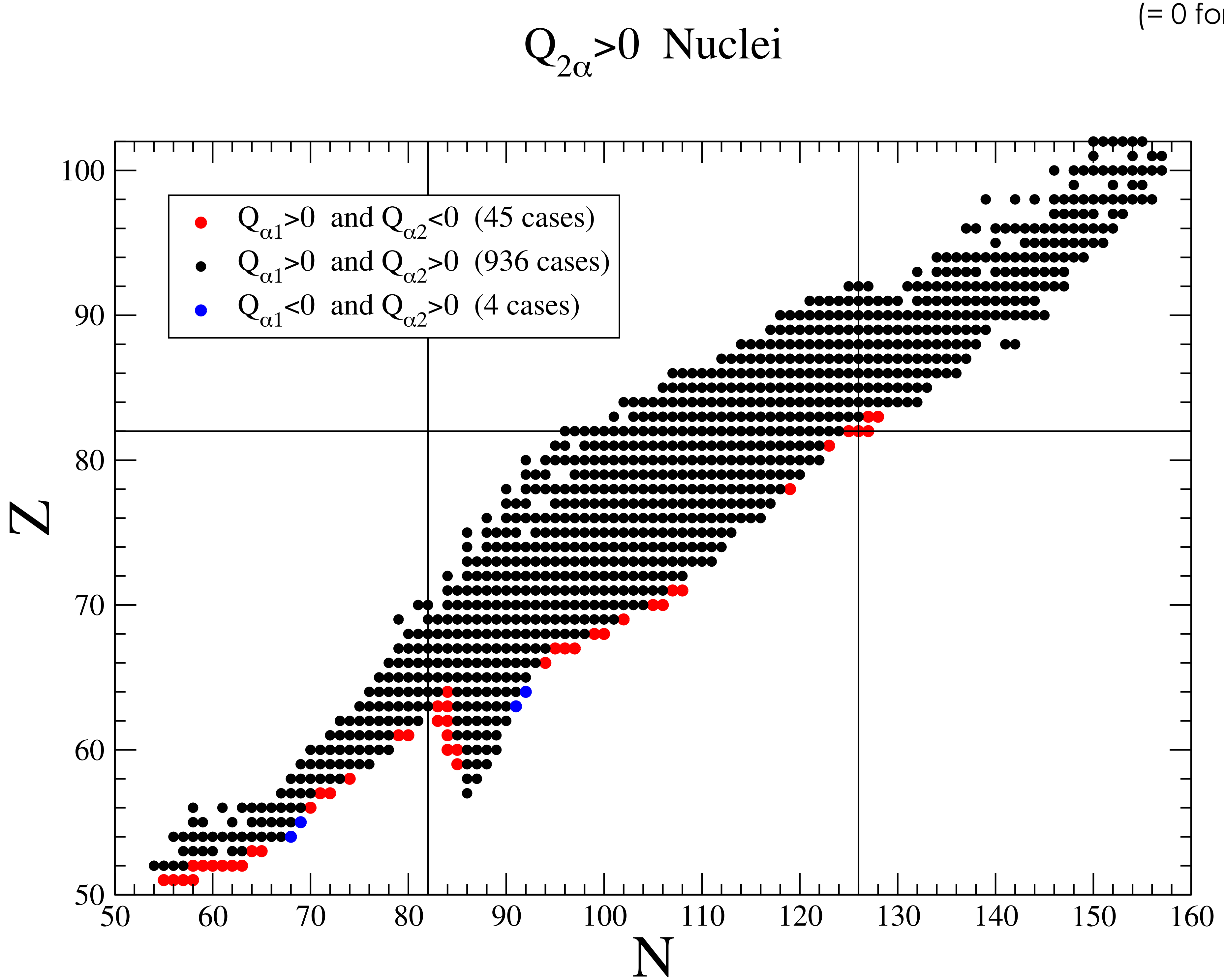
... quadrupole moment $$q_{20} = 2A_2 R.$$

F. MERCIER *et al.*

PHYSICAL REVIEW LETTERS **127,** 012501 (2021)

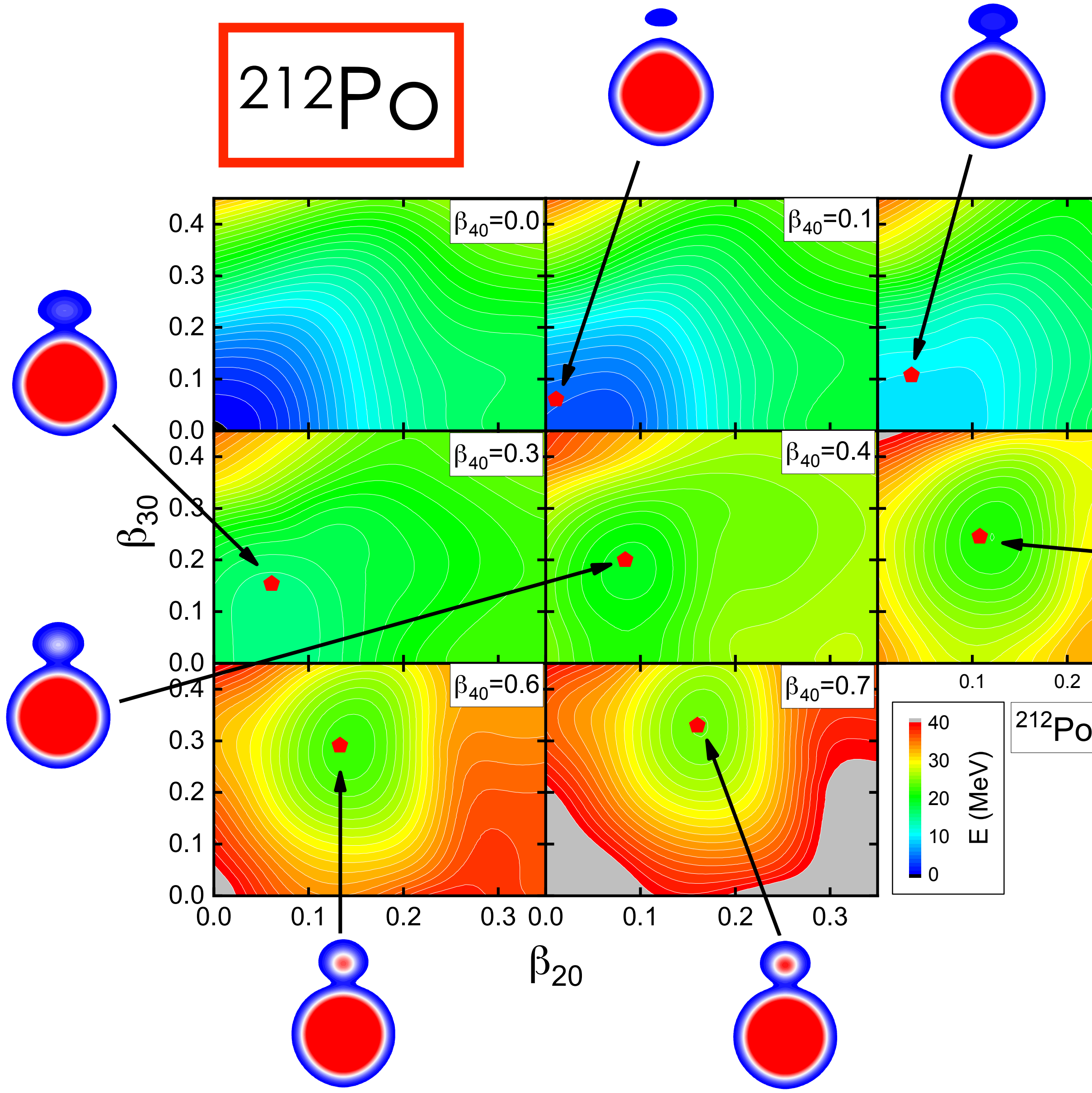
$$Q_{2\alpha} = Q_{\alpha 1} + Q_{\alpha 2} + \Delta E$$

Difference between excitation energies
(= 0 for transitions between ground states)



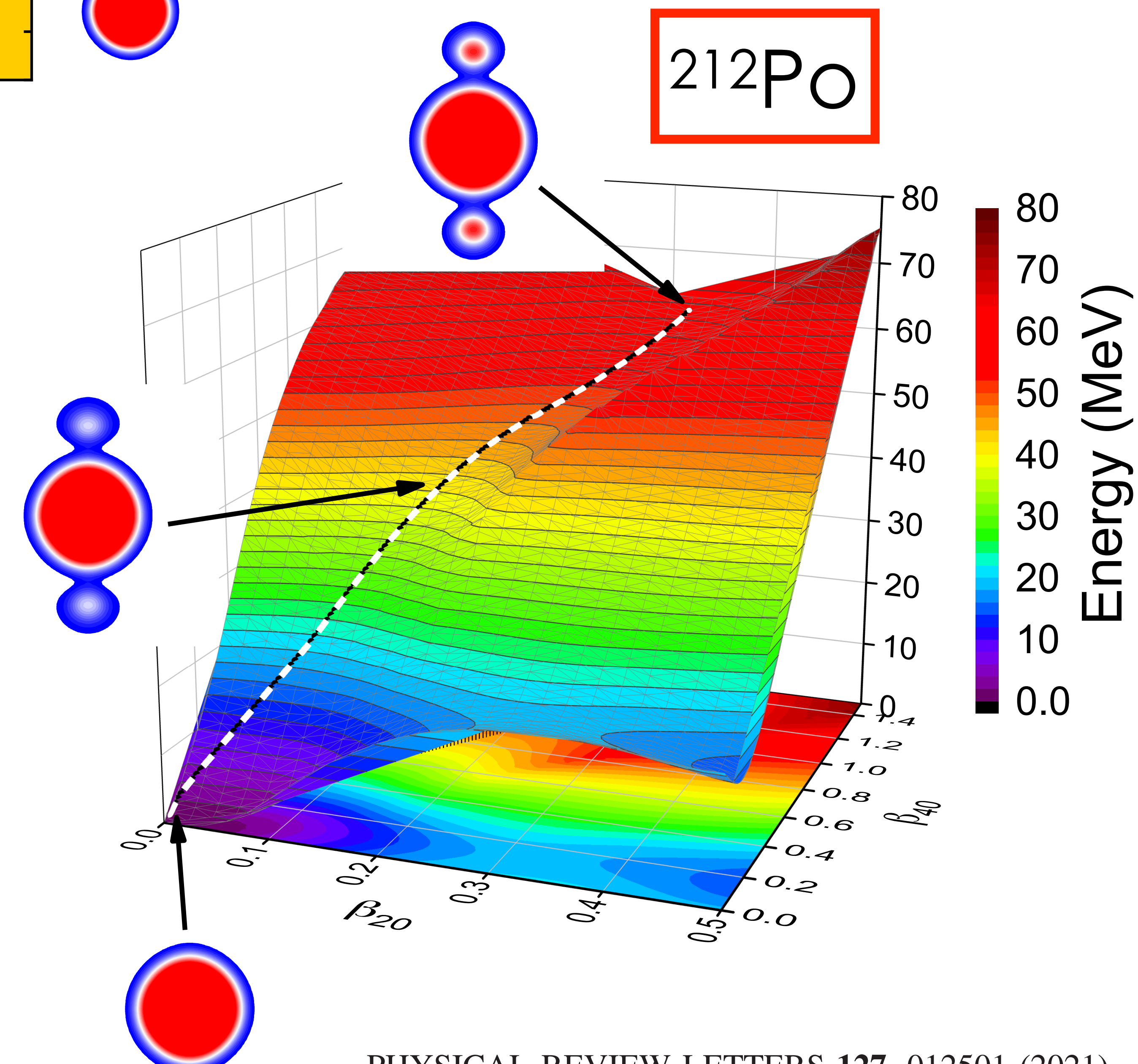
… extremely low probability!

nuclei for which one of the sequential single-a decays is energetically forbidden!



$(\beta_{20}, \beta_{30}, \beta_{40})$ collective space

Single alpha-decay: T_α = 0.6 μs (exp. 0.3 μs)



Double alpha-decay:

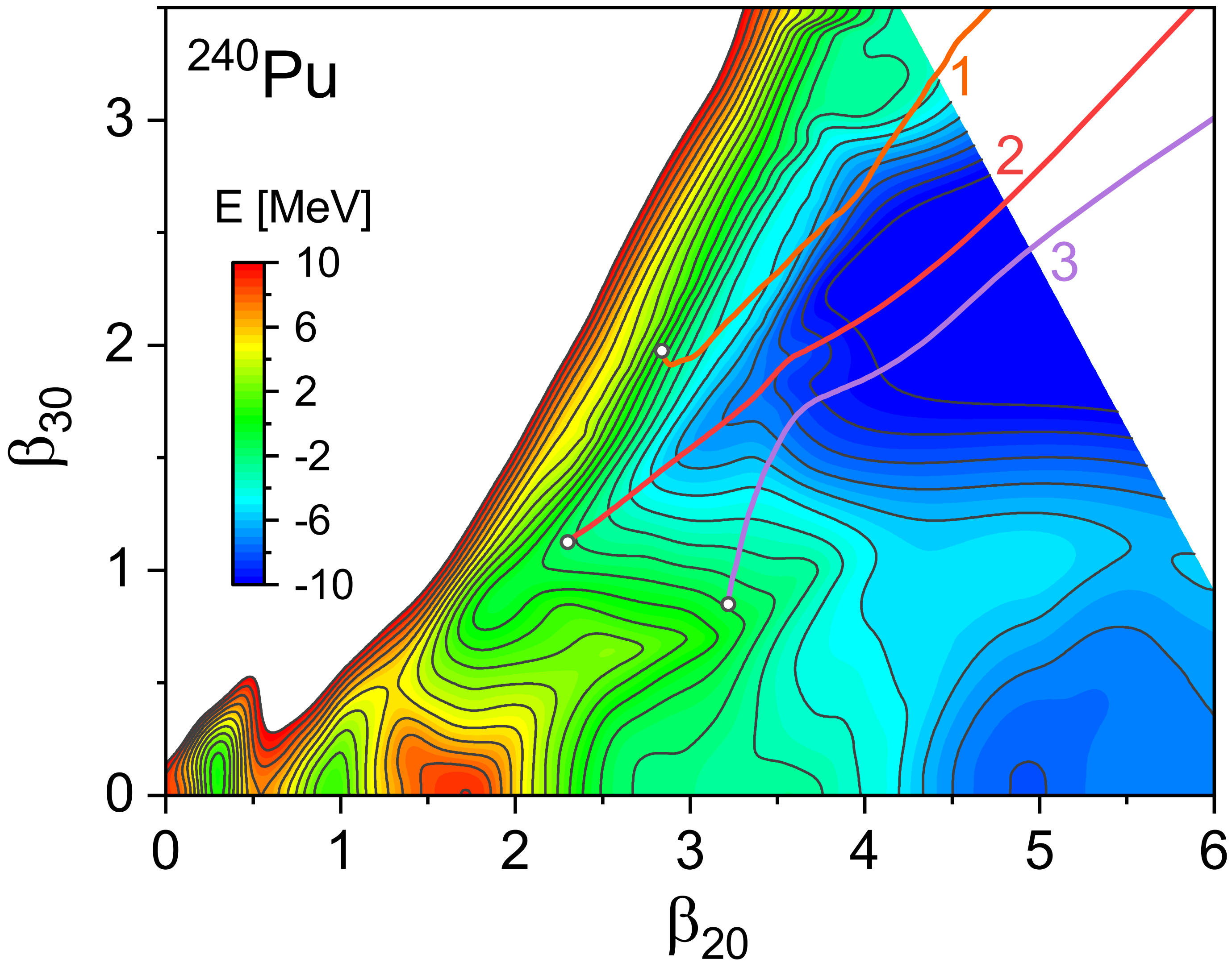
log $T_{2\alpha}$[s] = 18.36

For the ^{8}Be decay channel: log $T_{2\alpha}$[s] = 38.82.

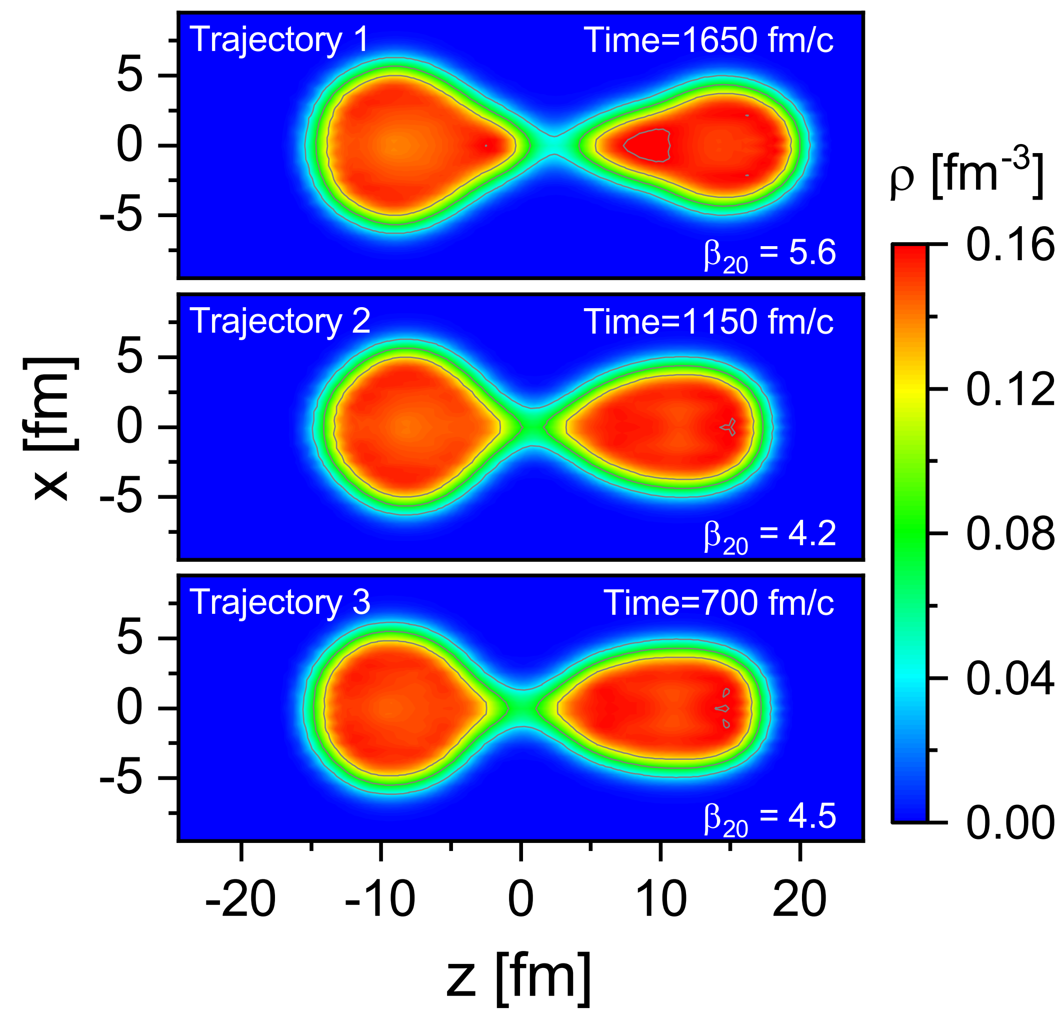
PHYSICAL REVIEW LETTERS **127,** 012501 (2021)

Dynamical synthesis of ^4He in the scission phase of nuclear fission

TDDFT fission trajectories



Density profiles at times immediately prior to the scission event.



Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022)

Nucleon localization functions:

kinetic energy density — density — current density

σ ($\uparrow$ or $\downarrow$)

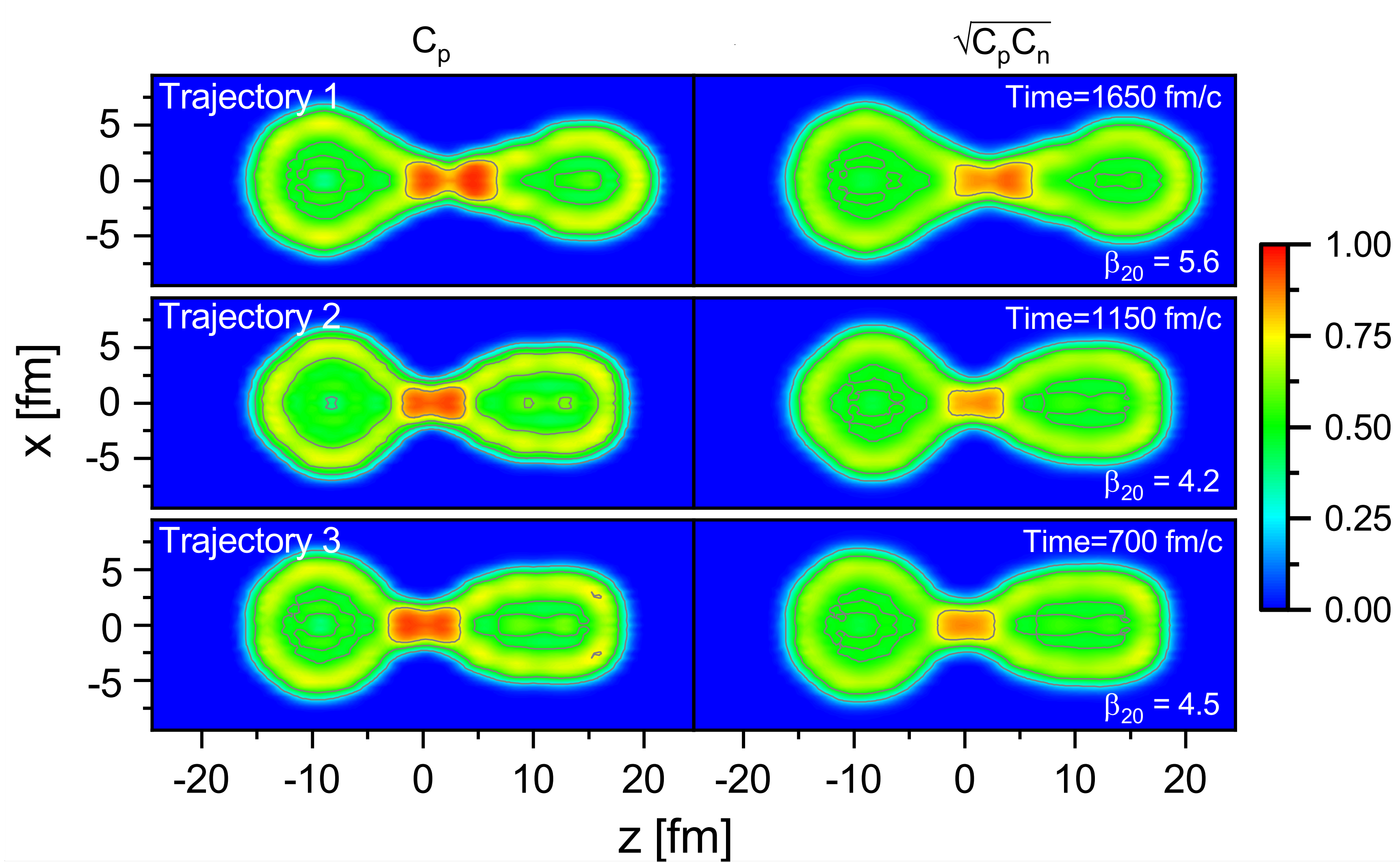
q (n or p)

$$C_{q\sigma}(\vec{r}) = \left[1 + \left(\frac{\tau_{q\sigma}\rho_{q\sigma} - \frac{1}{4}|\vec{\nabla}\rho_{q\sigma}|^2 - \vec{j}^{\,2}_{q\sigma}}{\rho_{q\sigma}\tau^{\mathrm{TF}}_{q\sigma}}\right)^2\right]^{-1}$$

$$\tau^{\mathrm{TF}}_{q\sigma} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}_{q\sigma}$$

For homogeneous nuclear matter: $C_{q\sigma} = 1/2$

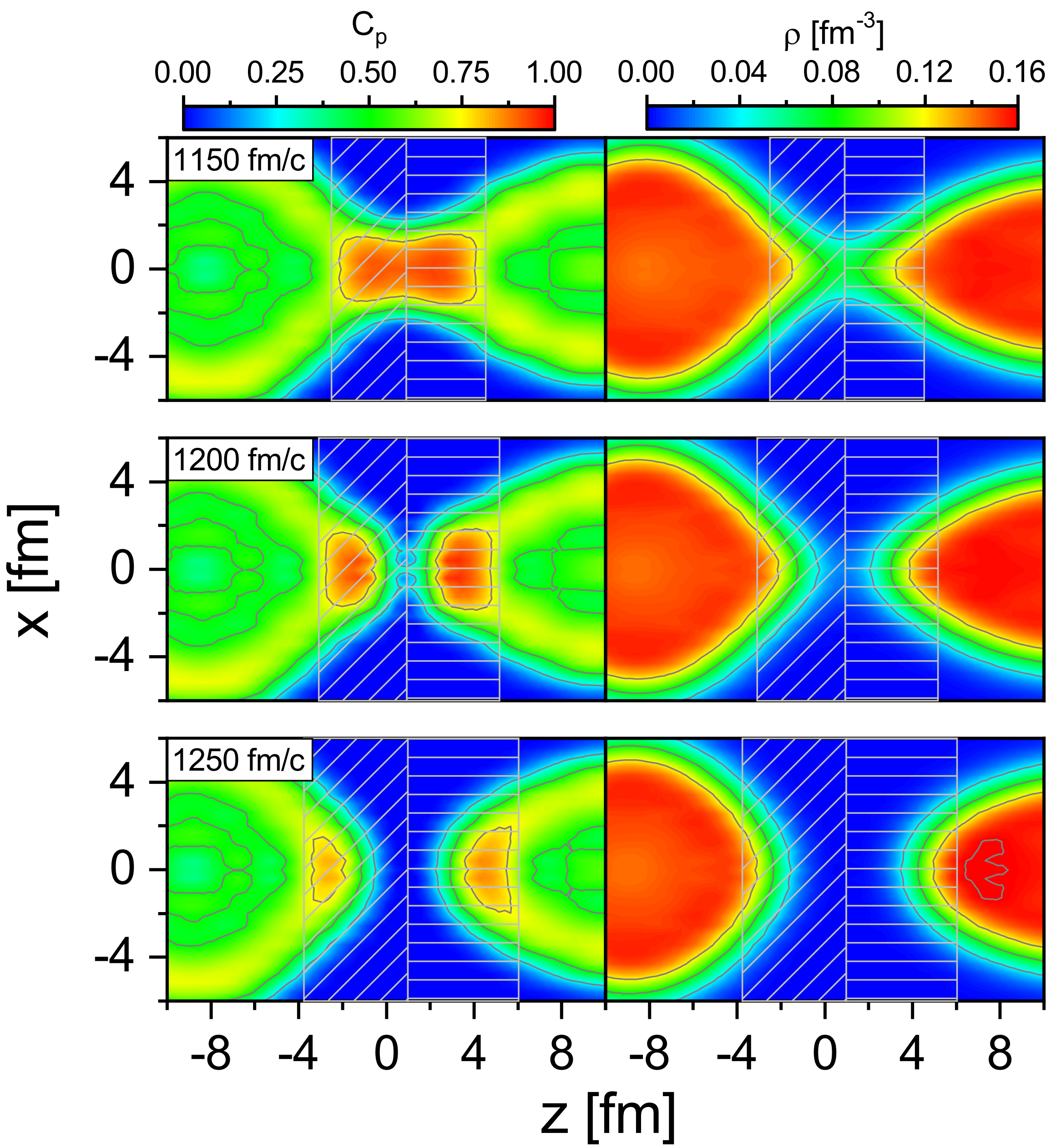
For the a-cluster of four particles: $C_{q\sigma}(\vec{r}) \approx 1$



Trajectory 2

Proton localization

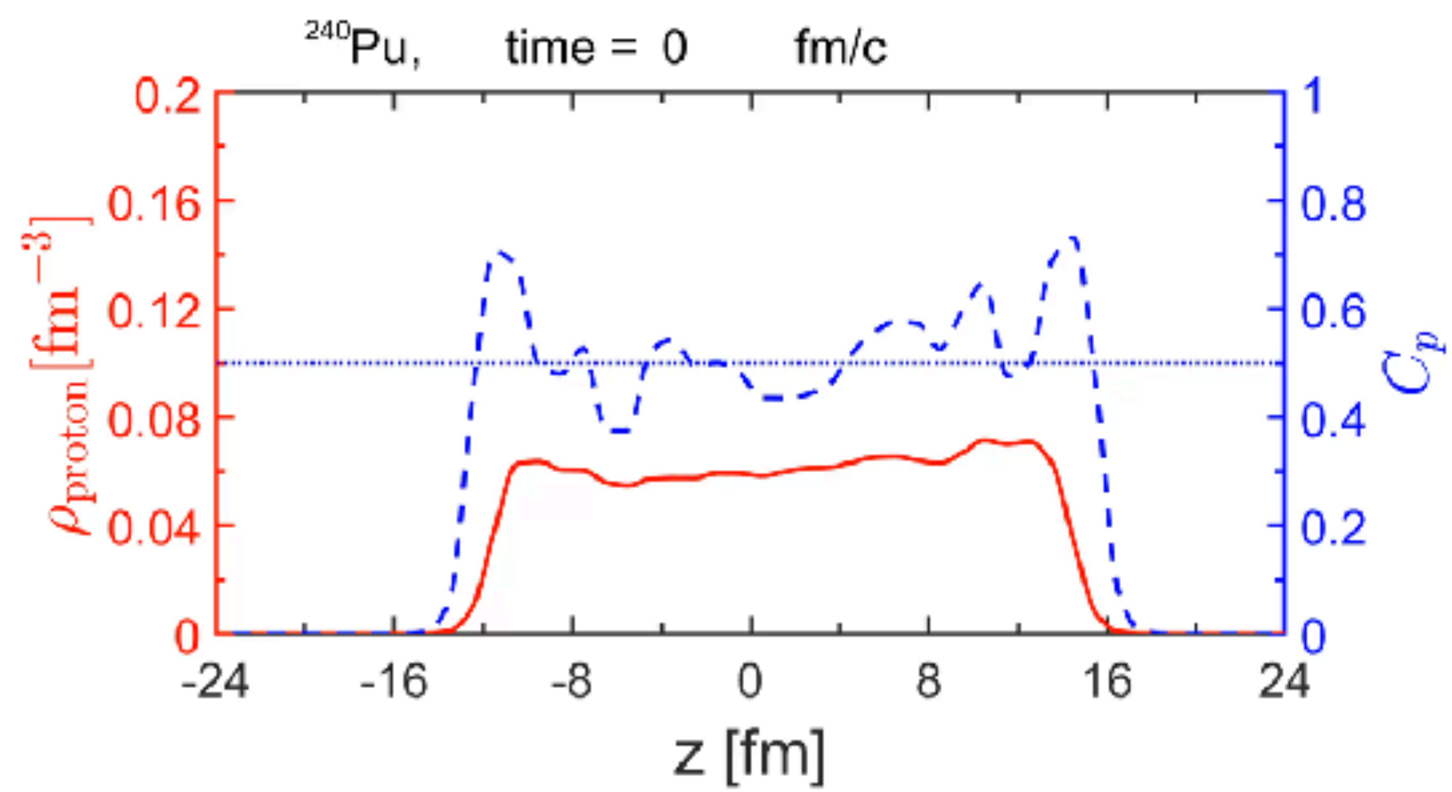
Density



When are these light clusters formed?

What is their structure?

What is their role in the scission mechanism?



Ren, Vretenar, Nikšić, Zhao, Zhao, Meng, Phys. Rev. Lett. **128**, 172501 (2022)

Methods based on the framework of Energy Density Functionals

✔ …accurate microscopic description of universal collective phenomena that reflect the organisation of nucleonic matter in finite nuclei.

✔ … nucleon localization and formation of light clusters at sub-saturation densities.

✔ … cluster structure and dynamics in light N=Z and neutron-rich nuclei (quasi-molecular structures).

✔ … alpha-decay in medium-heavy and heavy nuclei.

✔ … nuclear fission dynamics ➠ cluster formation in the neck during the scission phase ⇒ ternary fission.