Beyond-mean-field models for the description of shape coexistence

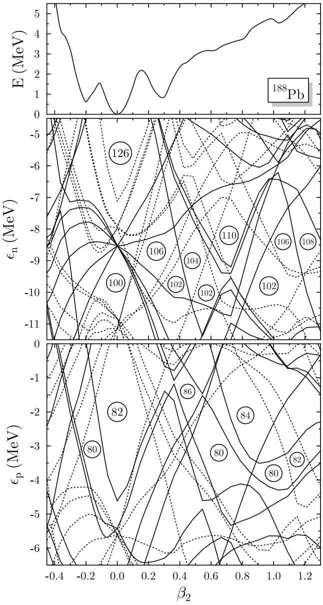
Michael Bender

Institut de Physique Nucléaire de Lyon
CNRS/IN2P3 & Université de Lyon & Université Lyon 1
69622 Villeurbanne, France

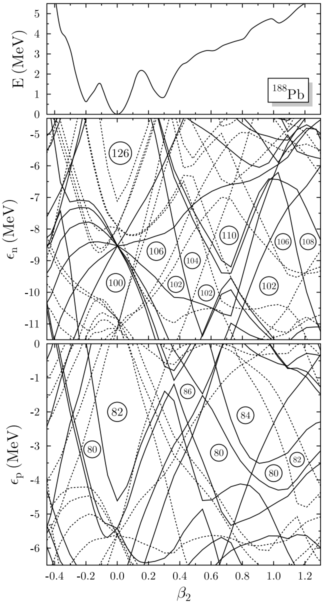
Workshop on
Shape coexistence and electric monopole transitions in atomic nuclei"

Espace de Structure et réactions Nucléaires Théorique (ESNT)

25 October 2017


E (MeV)
188Pb
ϵ_n (MeV)
126
110
106
108
106
104
100
102
102
102
ϵ_p (MeV)
82
86
84
80
80
80
82
β_2

Horizontal vs. vertical expansion of correlations



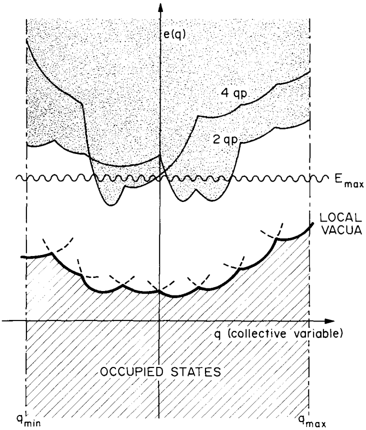
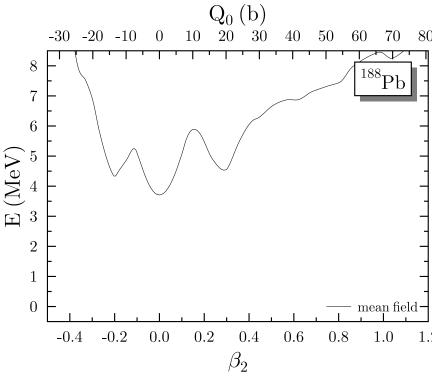


Fig. 1. Schematic plot of the energy versus the collective variable. The dark envelopes show the positions of the local vacua. The domain of the collective variable is defined by $q_{\min}$, $q_{\max}$ and the energy cut $E_{\max}$.

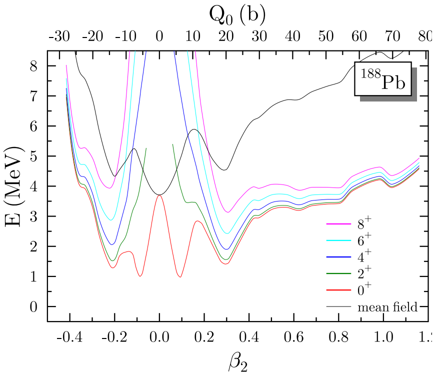
F. Dönau *et al*, NPA496 (1989) 333.

Our implementation(s)

- Coordinate space representation on a 3d mesh using Lagrange-mesh techniques in a box.
- "HF+BCS" or "HFB" solved with two-basis method
- full space of occupied single-particle states. There is no inert core; hence effective charges are not necessary to compensate for basis size and the bare charges are used. (There nevertheless might be effective charges for reasons related to mapping the NN interaction onto an EDF).
- Skyrme energy density functionals.
- "surface" pairing energy density functionals.



M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.



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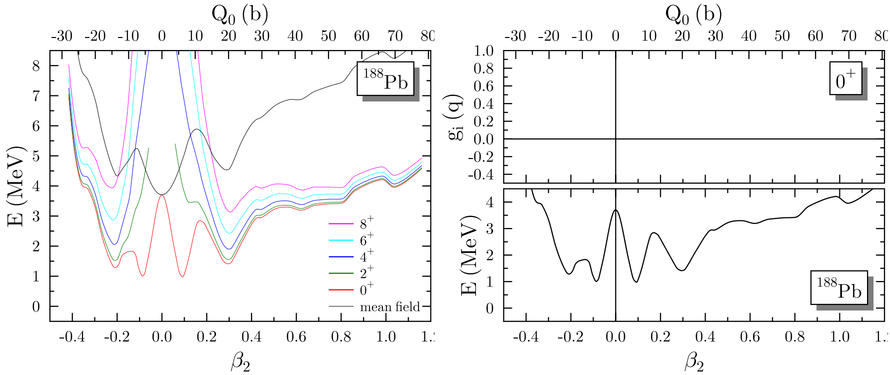

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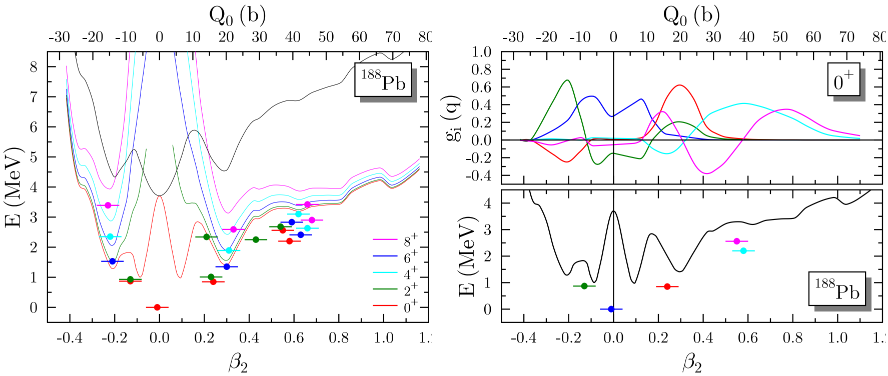
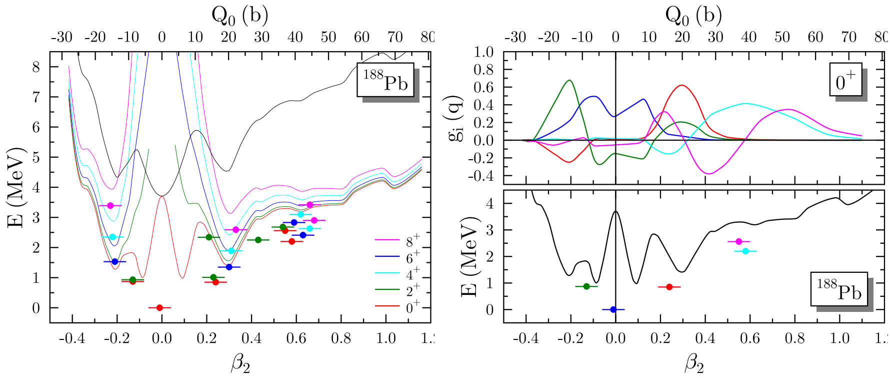


M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Attention: $g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation q in the collective state



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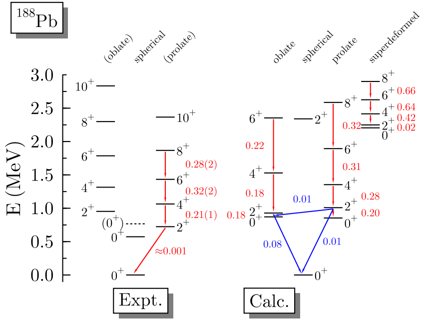
M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Experiment: T. Grahn *et al*, Phys. Rev. Lett. **97** (2006) 062501

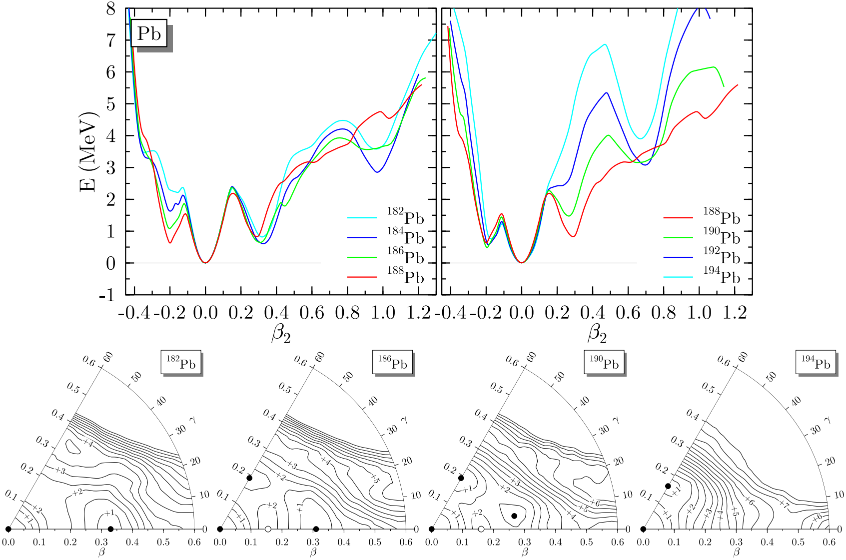


- in-band and out-of-band $E2$ transition moments directly in the laboratory frame with correct selection rules
- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion")
- $\Rightarrow$ *no effective charges necessary*
- *no adjustable parameters*

$$B(E2; J'_{\nu'} \to J_\nu) = \frac{e^2}{2J'+1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} |\langle J M \nu | \hat{Q}_{2\mu} | J' M' \nu' \rangle|^2$$

$$\beta_2^{(t)} = \frac{4\pi}{3R^2 A} \sqrt{\frac{B(E2; J \to J-2)}{(J\,0\,2\,0\,|(J-2)\,0)^2 e^2}} \quad \text{with} \quad R = 1.2\,A^{1/3}$$

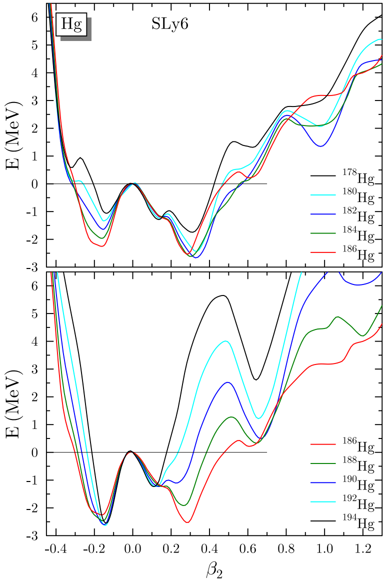
Mean-field deformation energy: Pb isotopes (SLy6)

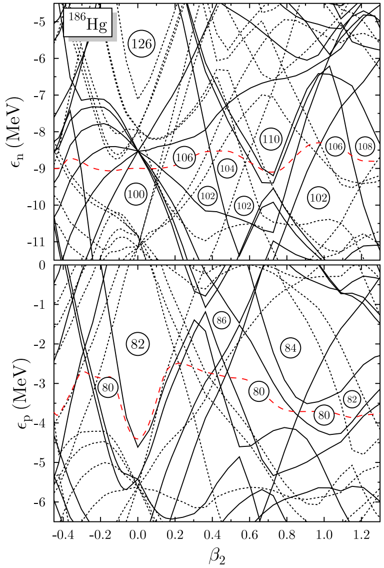


M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Mean-field deformation energy: Hg isotopes (SLy6)

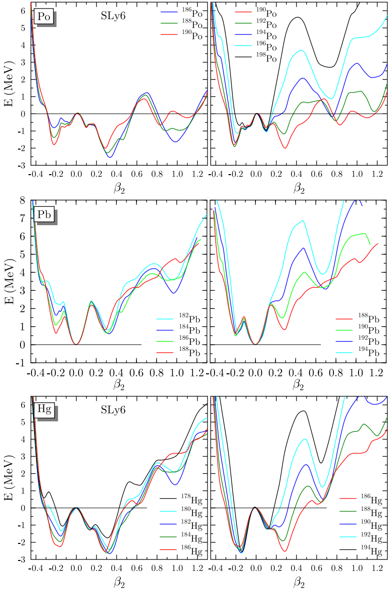
data used in J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322

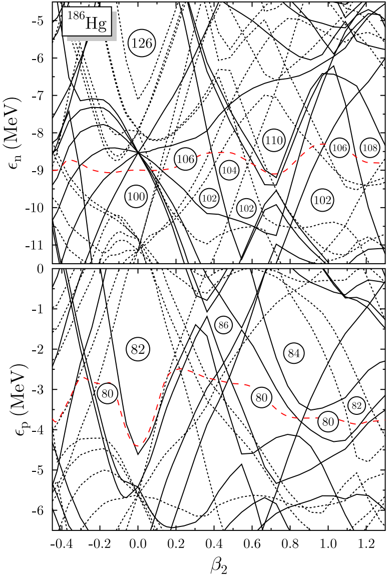




Mean-field deformation energy: Hg, Pb, and Po (SLy6)

data used in J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322

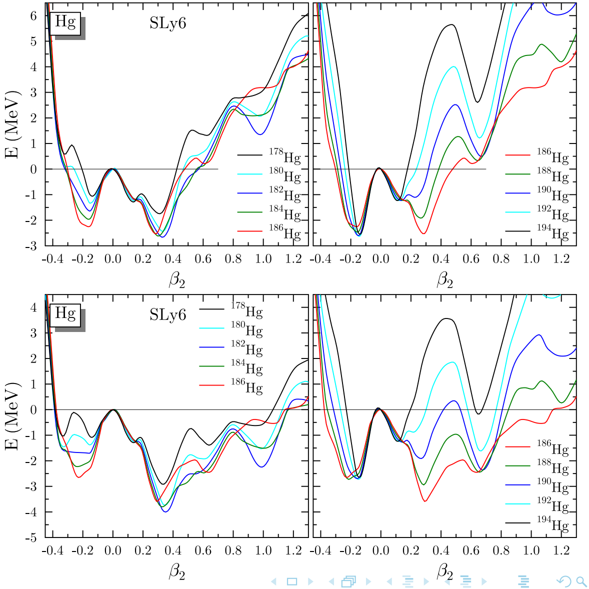




data used in J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322

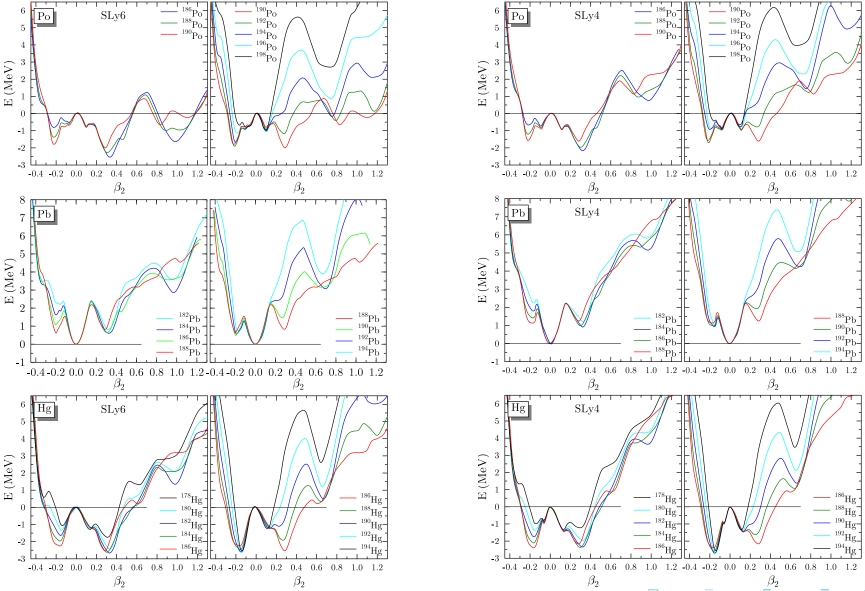
N and *Z* restoration

N, *Z* and $J = 0$ restoration

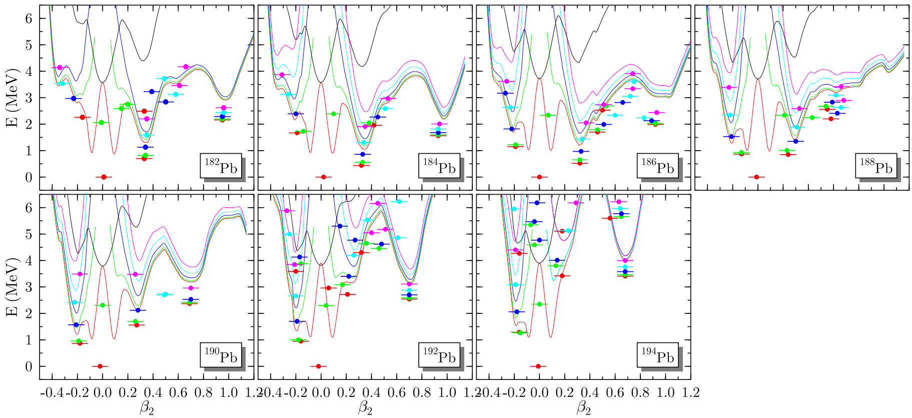


SLy6 ($a_{surf} = 17.74$ MeV) vs. SLy4 ($a_{surf} = 18.37$ MeV)

M. Bender, P.-H. Heenen, unpublished

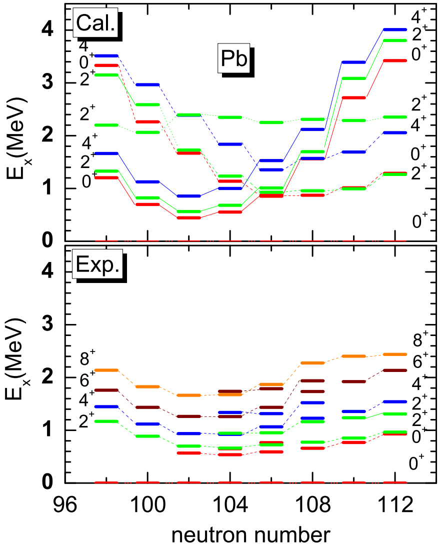


Shape coexistence in the neutron-deficient Pb isotopes



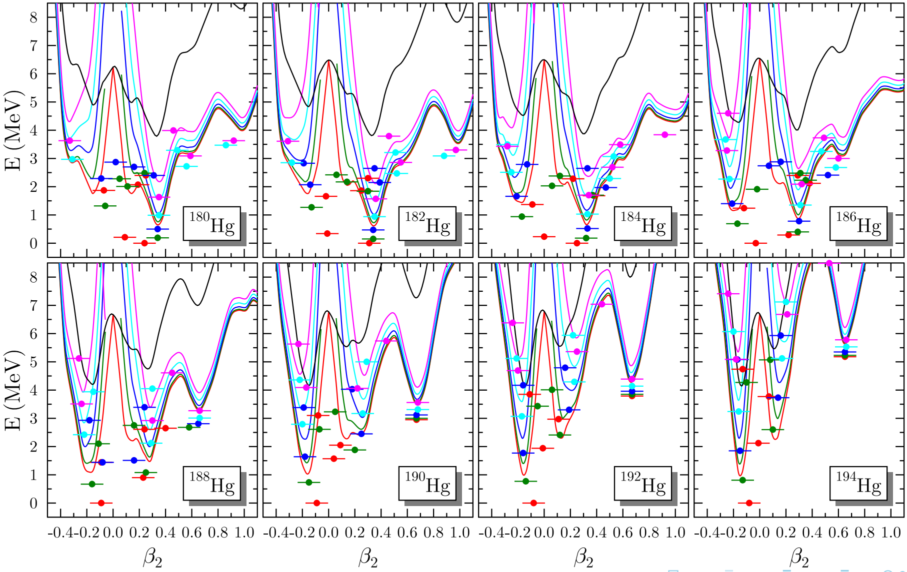
M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

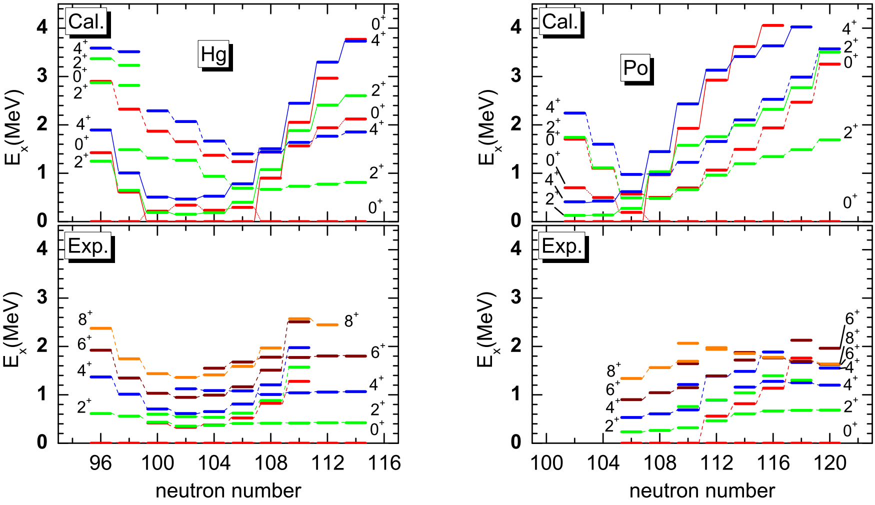
- overall structure of bands and crossing between prolate and oblate bands is well described.
- excitation energy of the projected GCM bandheads is different from that of the mean-field minima.
- projected GCM gives prolate (oblate) bands also in nuclei without prolate (oblate) mean-field minimum
- calculated spectra are too spread out (the variational space used here is too small for fine details of the binding energy that are on the order of < 1 MeV out of 1500 MeV; "Peierls-Yoccoz" instead of "Thouless-Valatin" moments of inertia)



J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322.

data used in J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322

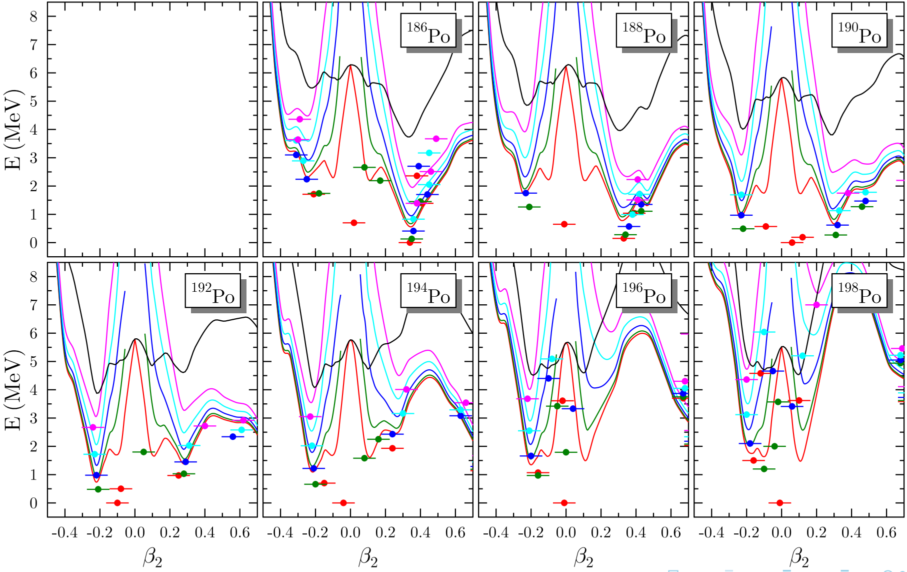


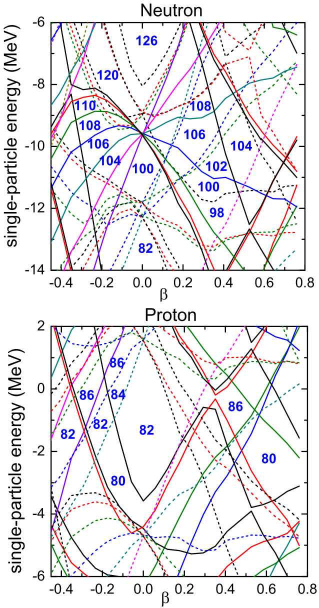


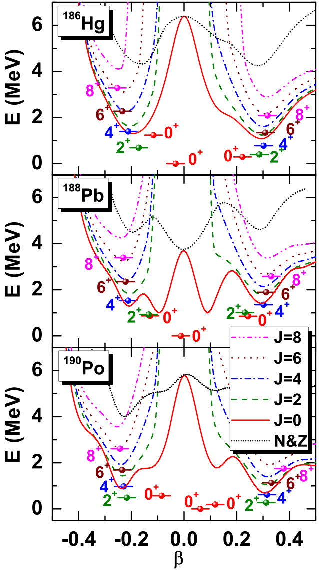
J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322

Shape coexistence in the neutron-deficient Po isotopes

data used in J. Yao, M. Bender, P.-H. Heenen, PRC 87 (2013) 034322







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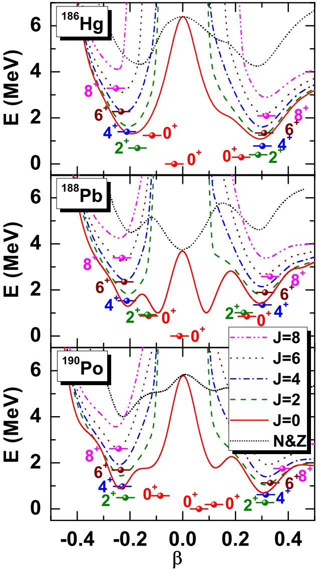
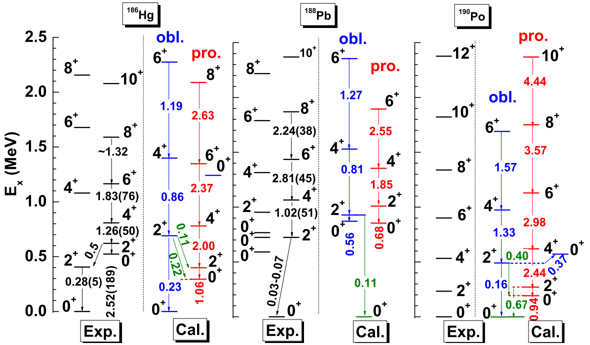
Shape coexistence in $N = 106$ isotones





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$E2$ strength

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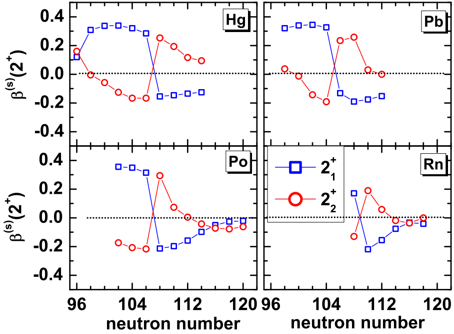

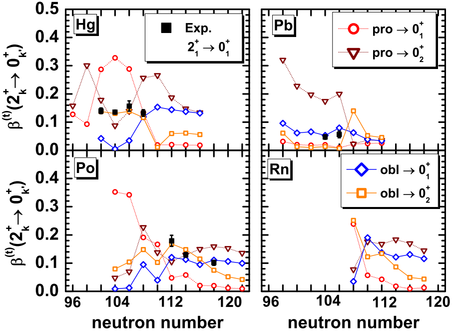

$$\beta^{(s)}(J_k) = \sqrt{\frac{5}{16\pi}} \frac{4\pi}{3ZR^2} \left(- \frac{2J+3}{J} \right) Q_s(J_k)$$

$$\beta^{(t)}(J_i, k_i \to J_f, k_f) = \frac{4\pi}{3ZR^2} \sqrt{\frac{B(E2; J_i, k_i \to J_f, k_f)}{e^2 \langle J_i 020 | J_f 0 \rangle^2}}$$

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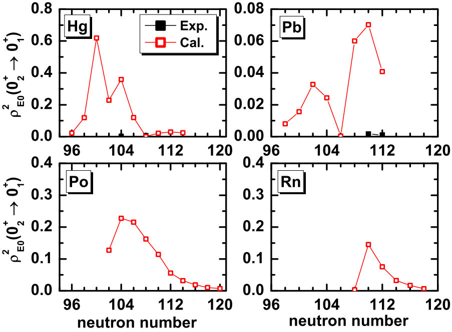

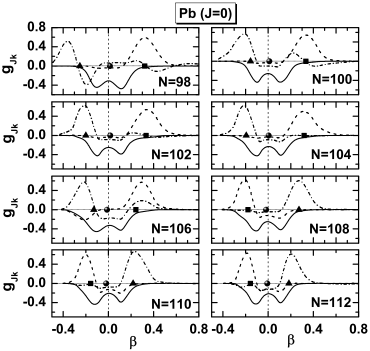

$$\rho^2_{E0}(J_k \to J_{k'}) = \left| \frac{\langle JM; k' | e \sum_p r_p^2 | JM; k \rangle}{eR^2} \right|^2$$

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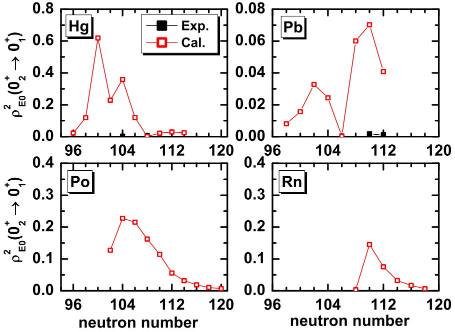
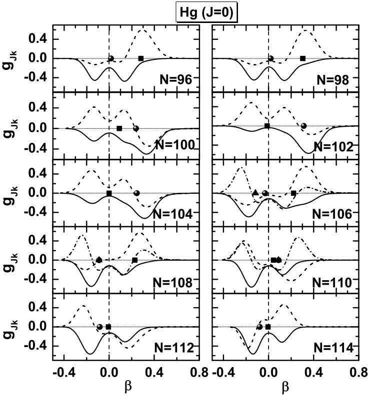
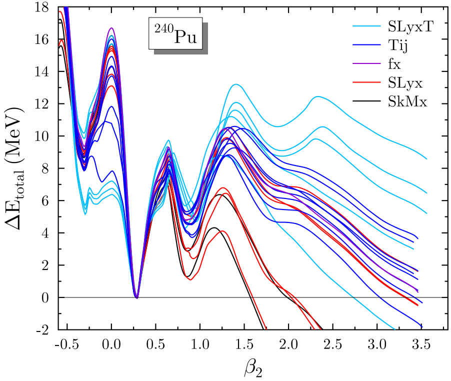
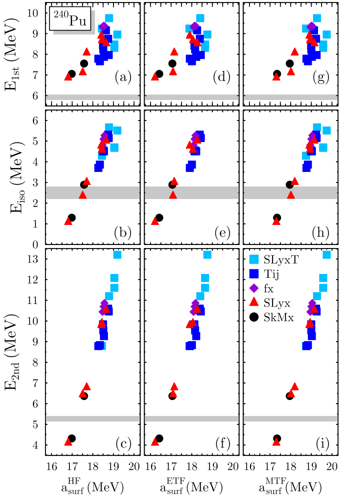




$$\rho^2_{E0}(J_k \to J_{k'}) = \left| \frac{\langle JM; k' | e \sum_p r_p^2 | JM; k \rangle}{eR^2} \right|^2$$

Construction of better parameterizations: control of surface properties

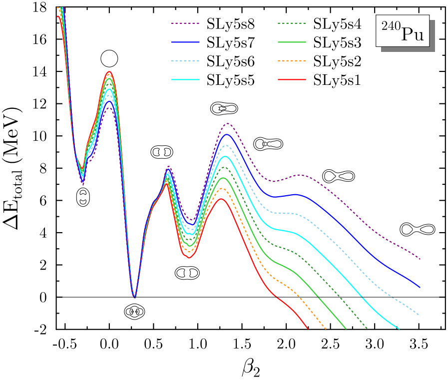




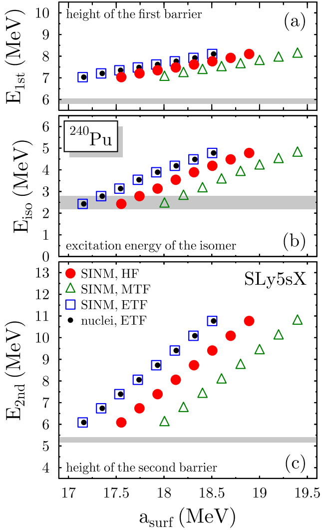
Jodon, Bennaceur, Meyer, Bender, PRC94 (2016) 024355

- most Skyrme parameterizations overestimate fission barriers ...
- ... although a few do well ...
- and a very few even systematically underestimate them.

Construction of better parameterizations: control of surface properties

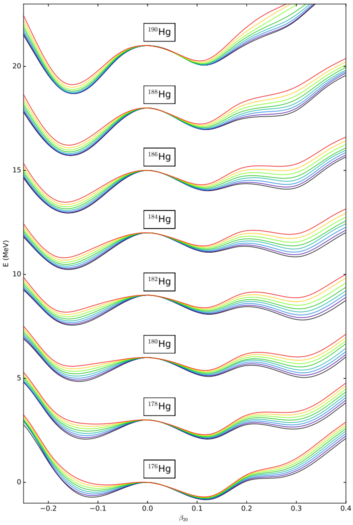


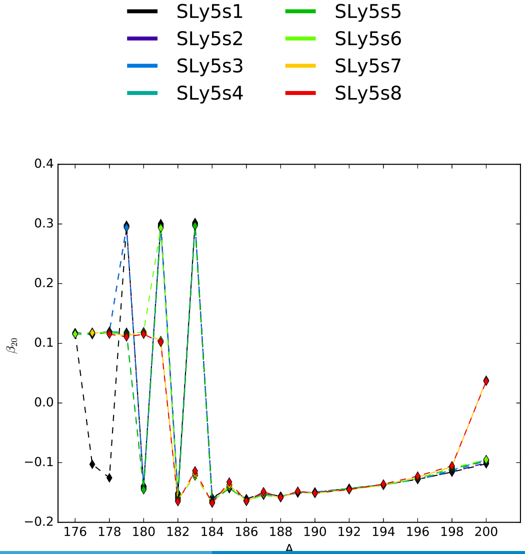
- add constraint on surface tension to the fit protocol
- (which requires understanding of the ambiguities of its determination)
- fit of SLy5s1, SLy5s2, . . . SLy5s8 as proof of principle.



Jodon, Bennaceur, Meyer, Bender, PRC94 (2016) 024355

W. Ryssens, M. Bender, P.-H. Heenen, in preparation





Construction of better parameterizations: control of surface properties

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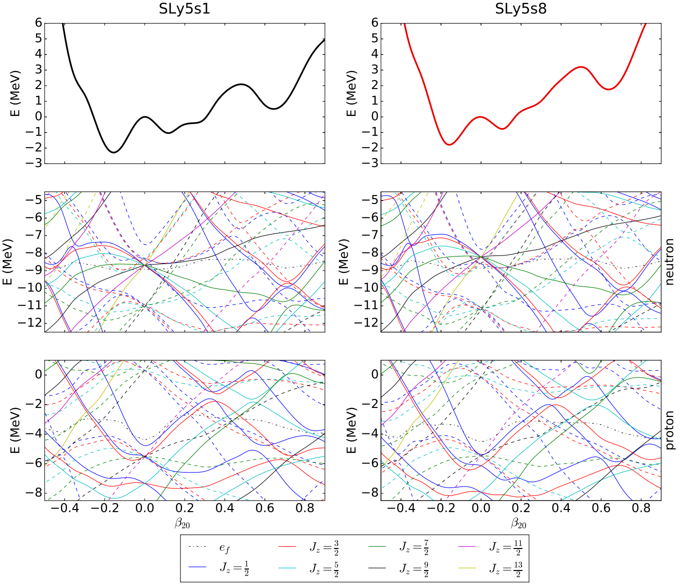
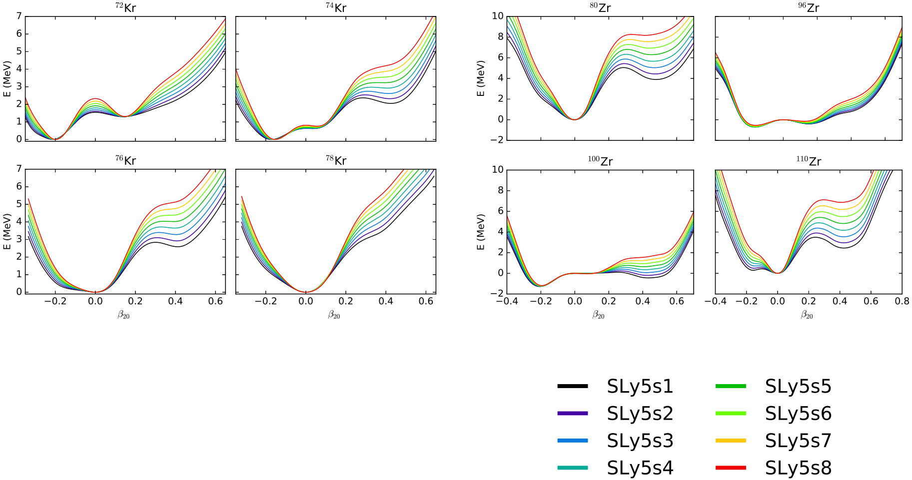
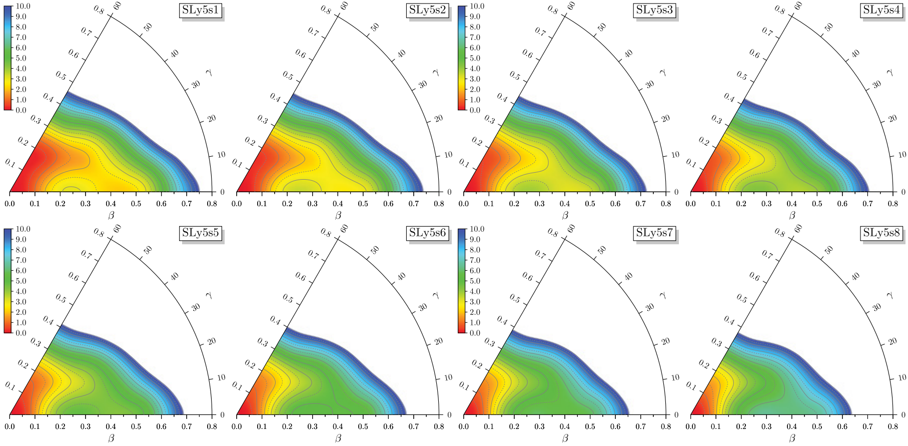


W. Ryssens, M. Bender, P.-H. Heenen, in preparation

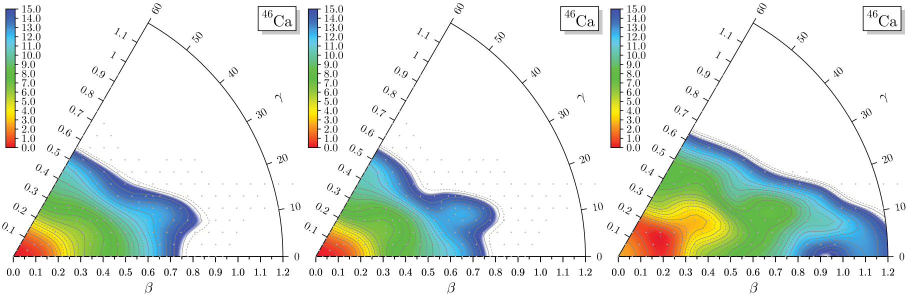


Construction of better parameterizations: control of surface properties

Full β-γ plane of ^{110}Zr for the parameterization SLy5s1 – SLy5s8



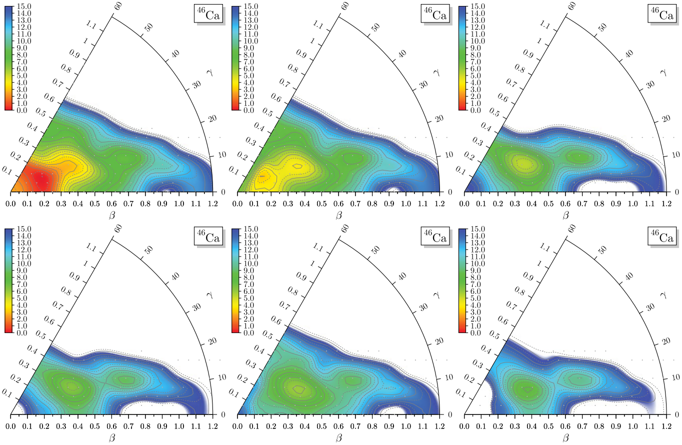
W. Ryssens, M. Bender, P.-H. Heenen, in preparation



Left: Non-projected total energy of the HFB vacua (without LN correction) relative to the spherical configuration. Middle: $N = 26$, $Z = 20$ projected total energy of the HFB vacua relative to the spherical configuration. Right: Energy of the projected $N = 26$, $Z = 20$, $J = 0$ HFB vacua.

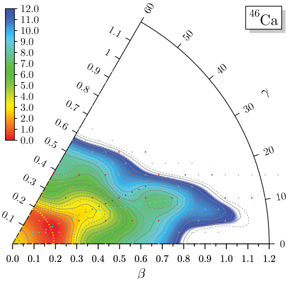
Bender & Heenen, to be published

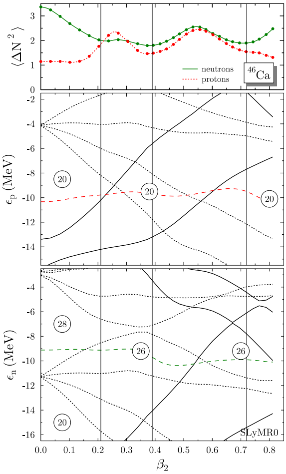
Low-lying states in ^{46}Ca

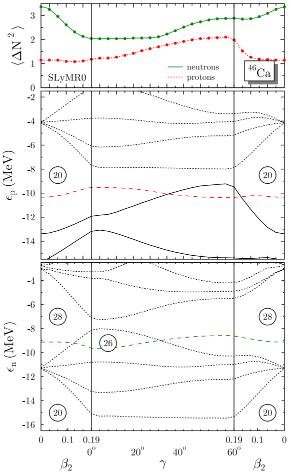


Top row: Right: Energy of the $J = 0$ HFB vacua. Middle: Energy of the lowest K-mixed $J = 2$ projected state . Right: Energy of the second K-mixed $J = 2$ state . Bottom row: Right: Energy of the $J = 3$ state. Middle: Energy of the lowest K-mixed $J = 4$ projected state. Right: Energy of the second K-mixed $J = 4$ state. The total energy is relative to the minimum of the $J = 0$ energy surface. All states are projected on $N = 26$, $Z = 20$,

Bender & Heenen, to be published





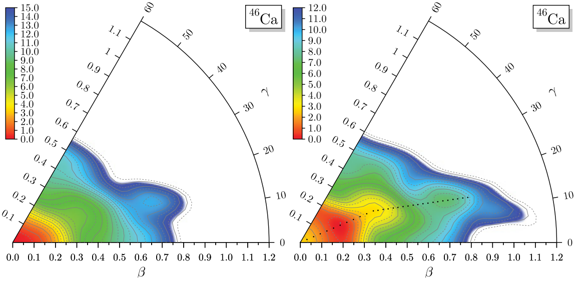


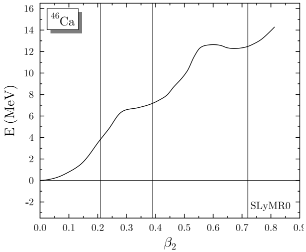
Nilsson diagram along the path indicated by cyan dots. Vertical bars indicate the deformation of the minima.

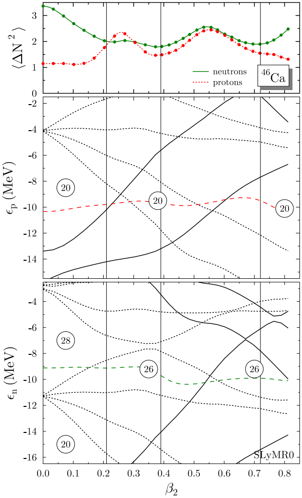
Nilsson diagram for a closed path through indicated by yellow dots.

Bender & Heenen to be published

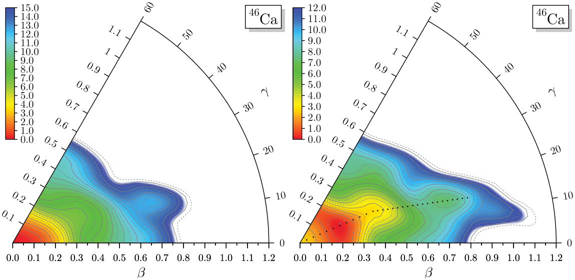
Low-lying states in ^{46}Ca

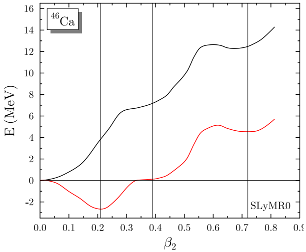


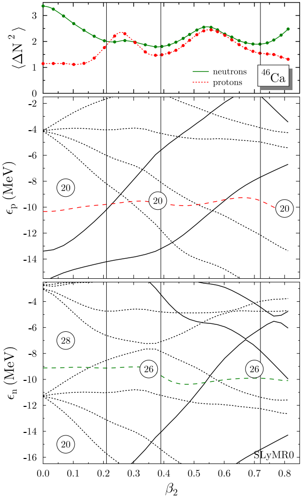




Bender, Bally, Heenen, to be published







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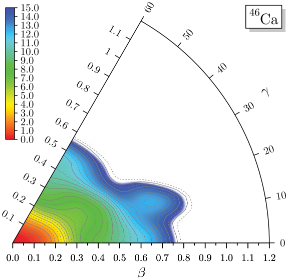
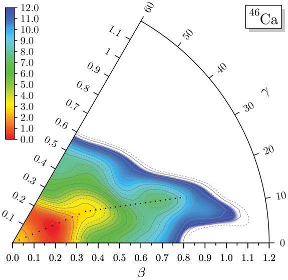
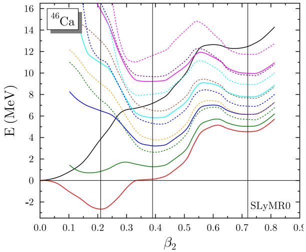
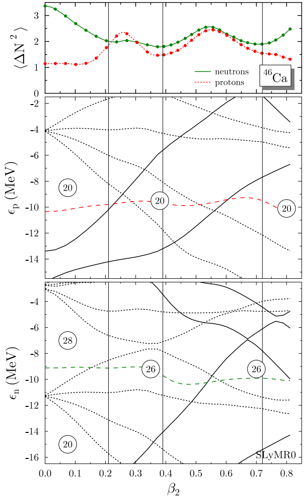
Low-lying states in ^{46}Ca









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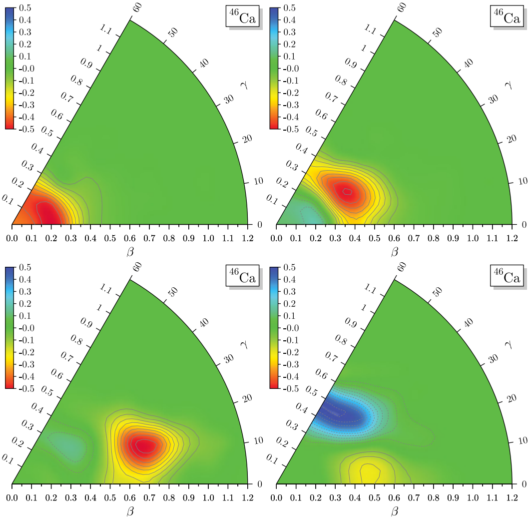
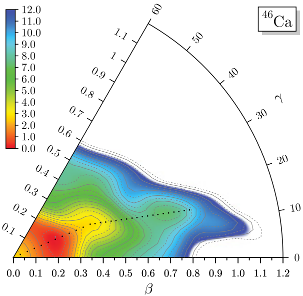
collective wave function of the four lowest 0^+ states





Bender, Bally, Heenen, to be published

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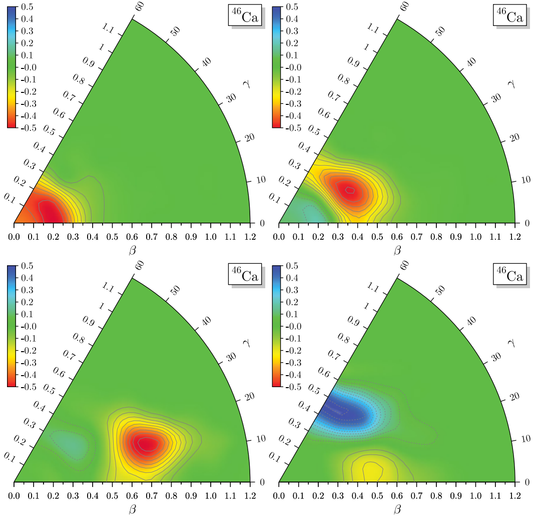

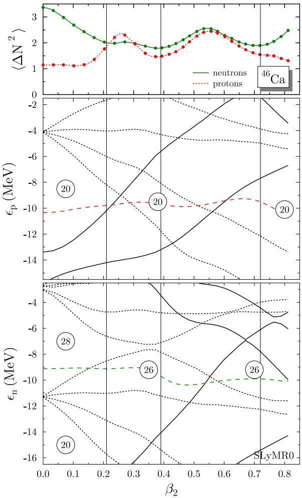

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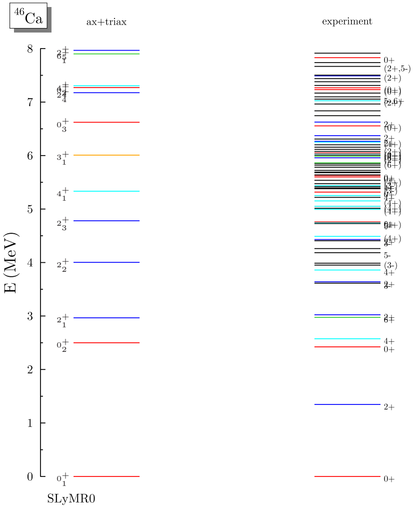
Low-lying states in ^{46}Ca



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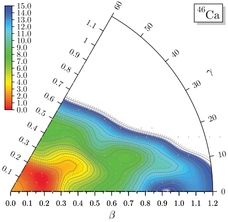
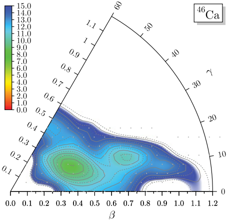
- There is a sequence of "seniority-2" states with $J^\pi = 2^+, 4^+, 6^+$ that in the shell-model is easily obtained by coupling two neutron holes in the $1f_{7/2}-$shell to these angular momenta.
- These are non-collective; hence, cannot be described by "traditional" GCM.

seniority 0

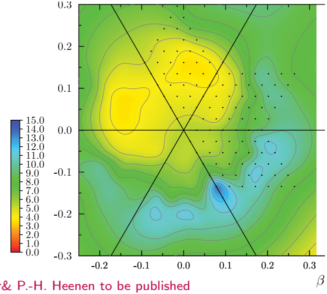
N, Z, $J = 0$ projected



N, Z, $J = 6$ projected



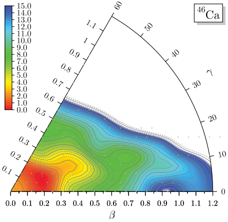
seniority 2, lowest N, Z, $J = 6$ projected



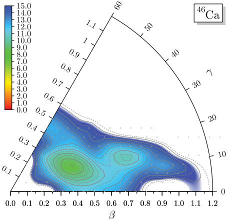
M. Bender& P.-H. Heenen to be published

seniority 0

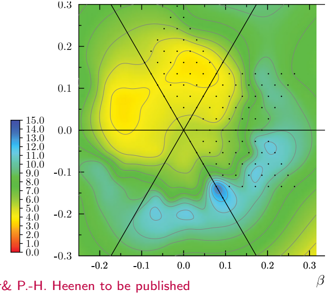
N, Z, $J = 0$ projected

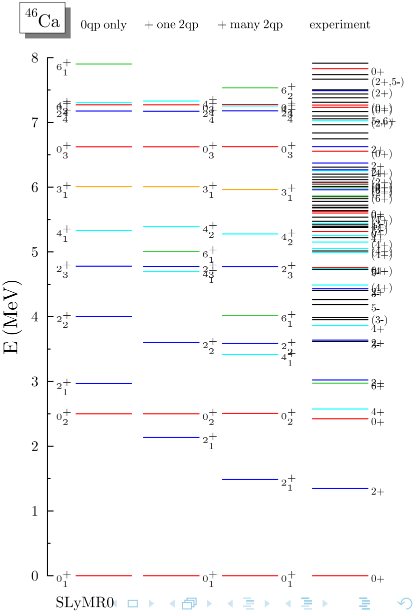


N, Z, $J = 6$ projected



seniority 2, lowest N, Z, $J = 6$ projected





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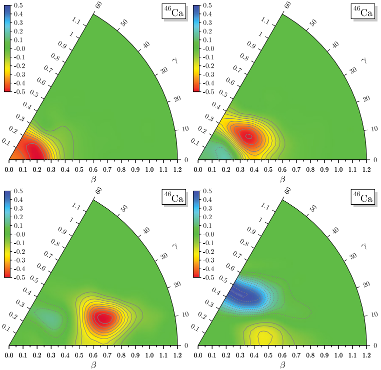
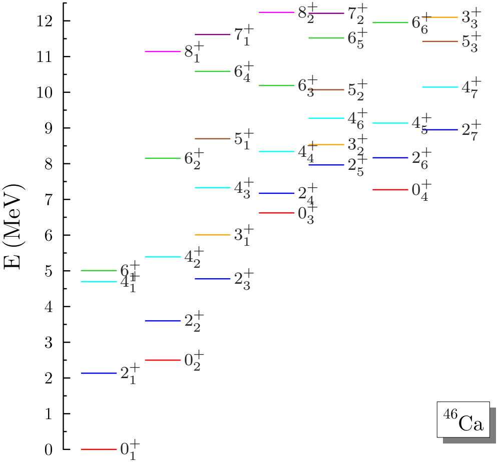
Low-lying states in ^{46}Ca

collective wave function of the four lowest 0^+ states





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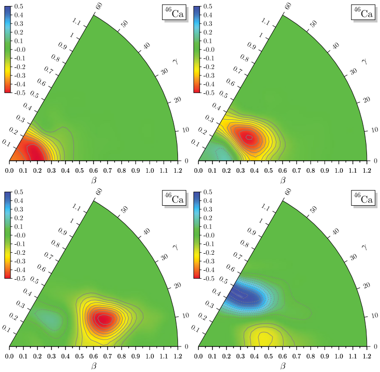
Low-lying states in ^{46}Ca



i1	i2	Ei	Ef	DeltaE	m(E0)	rho(E0)
		MeV	MeV	MeV	e fm^2	e
J_i =	0 ->	J_f =	0			
1	1	0.000	0.000	0.000	226.856	12.271
2	1	2.500	0.000	2.500	3.109	0.168
3	1	6.622	0.000	6.622	0.251	0.014
4	1	7.271	0.000	7.271	0.278	0.015
2	2	2.500	2.500	0.000	240.720	13.021
3	2	6.622	2.500	4.122	3.150	0.170
4	2	7.271	2.500	4.771	-0.481	-0.026
3	3	6.622	6.622	0.000	266.516	14.416
4	3	7.271	6.622	0.649	-1.629	-0.088

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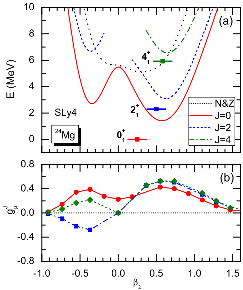
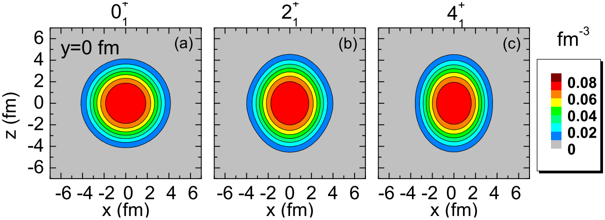
Laboratory densities



J. M. Yao, M. Bender, P.-H. Heenen, PRC 91 (2015) 024301



Contour plots of the 3D proton densities (in fm^{-3}) in the $y = 0$ plane for the 0^+_1 (a), 2^+_1 (b), 4^+_1 (c) states (with $M = 0$) in ^{24}Mg.

Transition density in the laboratory between GCM states $|J_i M_i \mu_i\rangle$ and $|J_f M_f \mu_f\rangle$ assuming axial HFB states

$$\rho^{J_f M_f \mu_f}_{J_i M_i \mu_i}(\mathbf{r}) = \sum_{q_f, q_i} f^{J_f *}_{\mu_f, q'} \langle q' | \hat P^{J_f}_{0M_f} \, \hat\rho(\mathbf{r}) \, \hat P^{J_i \dagger}_{0M_i} \, \hat P^N \, \hat P^Z | q\rangle \, f^{J_i 0}_{\mu_i, q}$$

with

$$\langle q'|\hat P^{J_f}_{0M_f}\,\hat\rho(\mathbf r)\,\hat P^{J_i\dagger}_{0M_i}\,\hat P^N\,\hat P^Z|q\rangle$$

$$= \frac{\hat J_i^2 \hat J_f^2}{(8\pi^2)^2}\int d\Omega' \, D^{J_f*}_{0M_f}(\Omega')\sum_K D^{J_i}_{K0}(\Omega')\int d\Omega'' \, D^{J_i}_{0K}(\Omega'')\langle q'|\hat\rho(\tilde{\mathbf r}_{\Omega'})\,\hat P^N\,\hat P^Z\,\hat R^\dagger(\Omega'')|q\rangle$$

$$\equiv \frac{\hat J_f^2}{8\pi^2}\int d\Omega' \, D^{J_f*}_{0M_f}(\Omega')\sum_K D^{J_i}_{KM_i}(\Omega')\,\hat R^\dagger(\Omega')\,\rho^{J_f J_i K0}_{q'q}(\mathbf r)$$

For the density of the GCM state $|JM\mu\rangle$ one obtains

$$\rho^{JM\mu}_{JM\mu}(\mathbf r) = \sum_{q_f,q_i} f^{J*}_{\mu,q'} \, f^{J0}_{\mu,q}\sum_\lambda Y_{\lambda 0}(\hat{\mathbf r})\,\langle JM\lambda 0|JM\rangle\sum_K\langle J0\lambda K|JK\rangle\int d\hat{\mathbf r}' \, \rho^{JJK0}_{q'q}(r,\hat{\mathbf r}')\,Y^*_{\lambda K}(\hat{\mathbf r}')$$

Summary

- Projected GCM is a versatile model enabling the description of many different situations (fluctuations in shape, shape coexistence, shape mixing) on the same footing.
- The mixing of shape coexisting states depends on many subtle details of the modeling.
- New generation of effective interactions is on its way.

The work presented here would have been impossible without my collaborators

founding fathers

Paul Bonche	SPhT, CEA Saclay
Hubert Flocard	CSNSM Orsay
Paul-Henri Heenen	Université Libre de Bruxelles

formal aspects of the big picture

Thomas Duguet	Irfu/CEA Saclay & KU Leuven & NSCL/MSU
Denis Lacroix	IPN Orsay

design and implementation of code extensions

Benoît Avez	CEN Bordeaux Gradignan
Benjamin Bally	CEN Bordeaux Gradignan, now SPhN, CEA Saclay
Veerle Hellemans	Université Libre de Bruxelles
Jiangming Yao	Université Libre de Bruxelles
Wouter Ryssens	IPN Lyon

development and benchmarking of new functionals

Karim Bennaceur	IPN Lyon & Jyväskylä
Dany Davesne	IPN Lyon
Robin Jodon	IPN Lyon
Jacques Meyer	IPN Lyon
Alessandro Pastore	formerly IPN Lyon, now University of York
Jeremy Sadoudi	Irfu/CEA Saclay first, then CEN Bordeaux Gradignan

color code: active (past) member of the collaboration