Advantages and limitations of multi-reference EDF calculations

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Workshop on "Cross-fertilization between

shell model and energy density functional methods"

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What is a multi-reference energy density functional method?

multi-reference (MR) EDF is the extension of single-reference (SR) EDF analogous to GCM being an extension of HFB

- HF/HFB: Slater determinant/HFB state as basic building block

$$E_q^{HFB} = \langle \mathrm{SR}_q | \hat{H} | \mathrm{SR}_q \rangle$$

- SR EDF: density matrices of a Slater determinant/HFB state as building blocks

$$\mathcal{E}_q^{\mathrm{SR}} = \mathcal{E}_q^{\mathrm{SR}}[\rho_{qq}, \kappa_{qq}, \kappa_{qq}^*], \quad \text{where} \quad \rho_{qq} = \langle \mathrm{SR}_q | \hat{\rho} | \mathrm{SR}_q \rangle \quad \text{etc}$$

- GCM: coherent superposition of Slater determinants/HFB states

$$\begin{aligned} |\mathrm{MR}_\mu\rangle &= \sum_q f_\mu(q) \, |\mathrm{SR}_q\rangle \\ \Rightarrow \quad E_\mu &= \langle \mathrm{MR}_\mu | \hat{H} | \mathrm{MR}_\mu \rangle = \sum_{q,q'} f_\mu^*(q) \, \langle \mathrm{SR}_q | \hat{H} | \mathrm{SR}_{q'} \rangle \, f_\mu(q') \end{aligned}$$

- MR EDF: transition density matrices between a Slater determinant/HFB states as building blocks

$$\mathcal{E}_\mu^{\mathrm{MR}} = \sum_{q,q'} f_\mu^*(q) \, \mathcal{E}_{qq'}^{\mathrm{MR}}[\rho_{qq'}, \kappa_{qq'}, \kappa_{qq'}^*] \, f_\mu(q') \quad \text{where} \quad \rho_{qq'} = \langle \mathrm{SR}_q | \hat{\rho} | \mathrm{SR}_{q'} \rangle$$

Multi-reference energy density functional methods

- Examples for MR EDF calculations are symmetry restoration and the superposition of states which differ in collective coordinates or single-particle degrees of freedom
- all other observables and transition matrix elements are (currently) calculated as operator matrix elements between MR states
- full model space of occupied states (for similar approaches using shell-model spaces and a shell-model Hamiltonian see the talk by A. Petrovici)
- universal energy density functional $\mathcal{E}$ (no agreement about a unique interaction yet, though: Skyrme, Gogny, Fayans, relativistic Lagrangians, ...; many parameterizations thereof)
- energy functionals used in nuclear physics are not entirely antisymmetric (at least through the density dependencies)
- MR calculations in atomic/molecular physics are (to the best of my knowledge) always done with the (perhaps rescaled) bare Coulomb interaction, not energy functionals
- MR EDF methods are what is customary called "beyond mean field"
- the set of reference states is usually (but not necessarily) determined through separate self-consistent calculations to optimize the description of static correlations (deformation, pairing, ...)

SR/MR energy density functional methods

Reasons for the popularity of this approach:

- Numerically feasible for all nuclei
- Intuitive interpretation of the ingredients in terms of shapes of a nuclear liquid and (deformed) shells of single-particle states in the SR states
- Universal energy functionals allow the straightforward calculation of nuclei far off the known region (the realiability of this extrapolation is a different question)

The nuclear single-reference energy density functional (SR-EDF) approach is widely known as self-consistent mean-field method and often abusively called Density Functional Theory, or classified as Hartree-Fock or Hartree-Fock-Bogoliubov, although from a purist's/pedant's point of view, nuclear SR-EDF does very rarely, if ever, meet the formal definition of any of these approaches

Why going "beyond the mean field"? I. Symmetry breaking

- nuclei are described in a body-fixed "intrinsic frame"
- In the laboratory frame, mean-field states might not be eigenstates of

momentum	for finite nuclei
angular momentum	for deformed nuclei
parity	for octupole-deformed nuclei
particle number	paired systems

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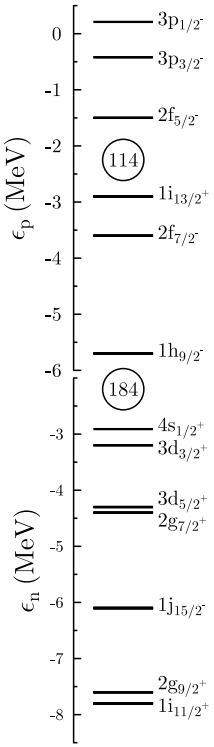
- but: missing correlations related to symmetry restoration, and difficult connection to the lab frame for spectroscopic observables, absence of selection rules for transitions
- Approximation schemes for projected observables based on a single symmetry-breaking mean-field state (Kamlah expansion etc) work well only in the limit of *large* symmetry breaking
- For many observables the restoration of broken symmetries has a much larger effect in the limit of small symmetry breaking

Symmetry breaking: Ground-state deformation driven by shell effects



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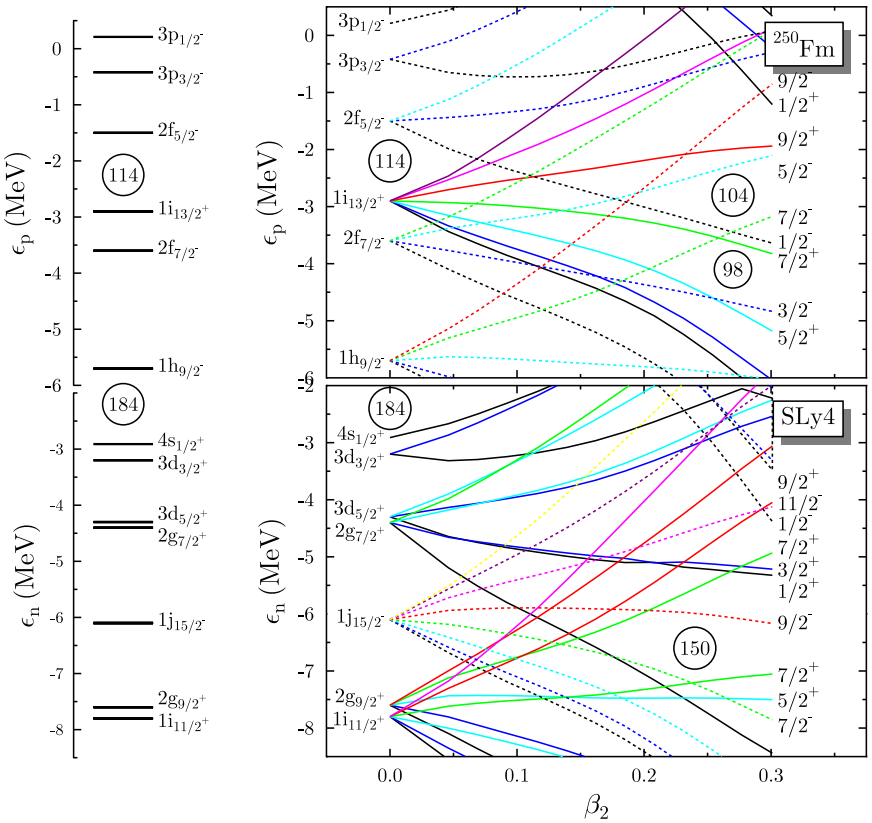

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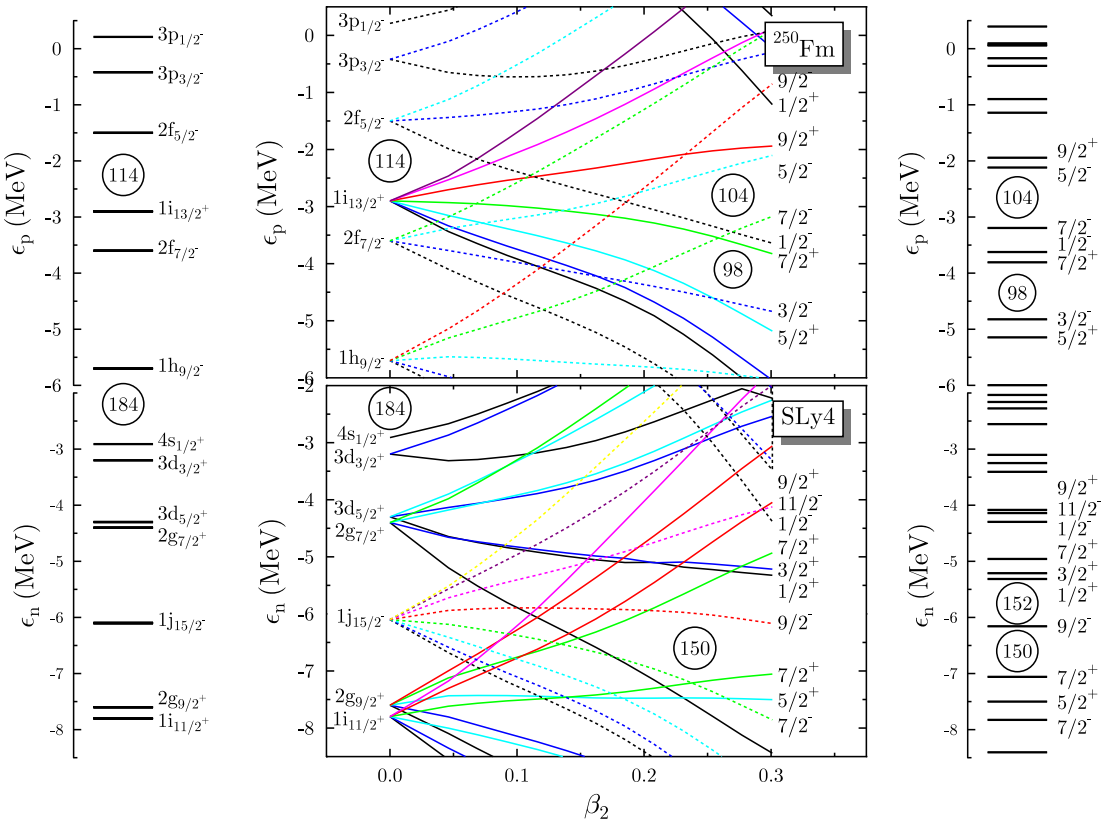

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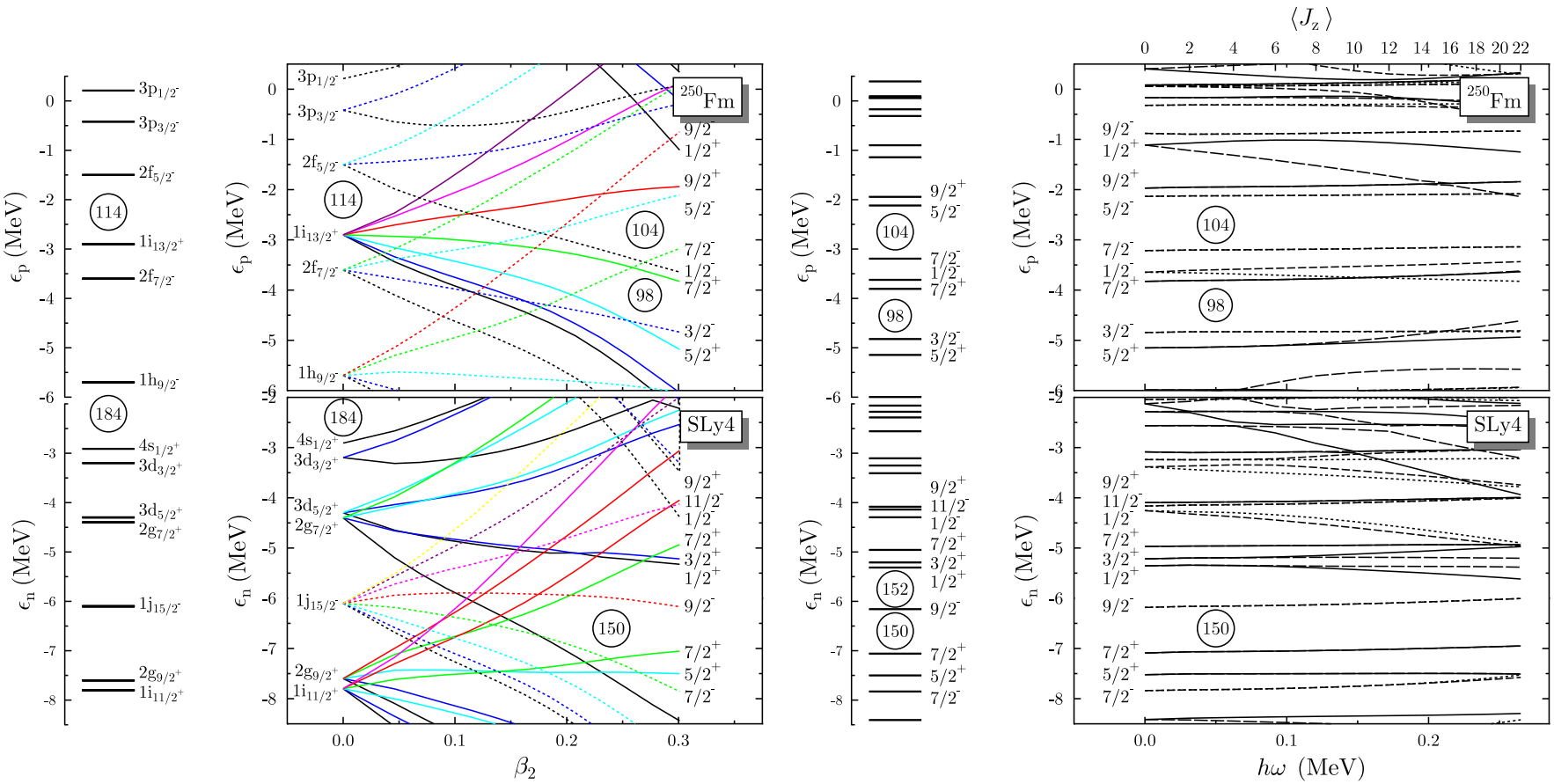
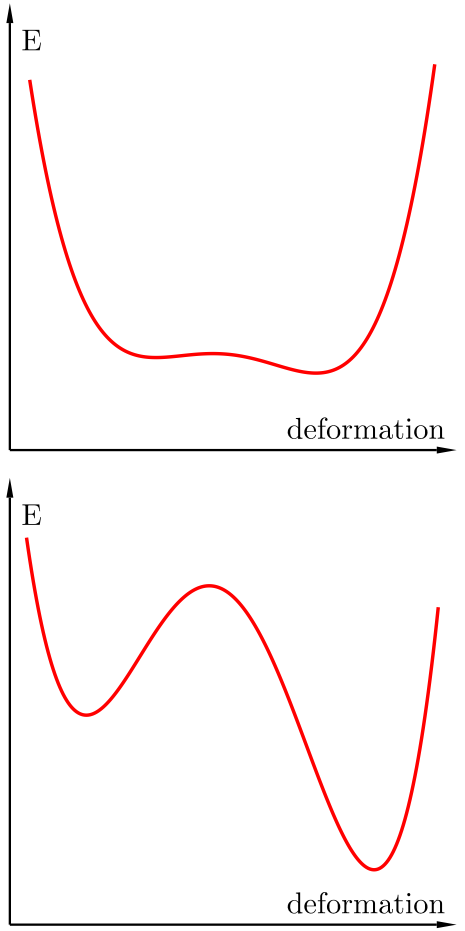


- the nucleus goes from a spherical configuration with high level density to a deformed configuration with low level density, which is more favorable (remember that at spherical shape the levels are $(2J+1)$-fold degenerate, at deformed shape they are two-fold degenerate)
- For ^{250}Fm, the energy gain from deformation (compared to the spherical mean-field state) is of the order of 25 MeV.

Why going "beyond the mean field"? II. Soft nuclei

- arbitrary when energy changes slowly with collective coordinate (transitional nuclei)
- ground-state correlations from vibrational motion
- interpretation of coexisting minima: mean-field states with different deformation are not orthogonal and are coupled by the interaction.



Why going "beyond the mean field"? III. Spectroscopy

1. The self-consistent mean field offers limited access to spectroscopy only
   - rotational bands and in-band transition moments from cranked SCMF
   - one-quasiparticle states in odd-A nuclei and bands on top of them
   - two-quasiparticle states in even-even nuclei
   - harmonic vibrations from linear response (QRPA)

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   - two-quasiparticle states in even-even nuclei
   - harmonic vibrations from linear response (QRPA)
2. What is missing are for example
   - rotational bands of not well deformed nuclei and out-of-band transition moments
   - vibrational excited states (and transition moments between them)
   - coupling of rotational and vibrational modes
   - mixing of bands

Correlations within and beyond the mean field – classification and semantics

One makes the hypothesis that there is a more-or-less clean and unique separation of correlations into three different classes

1. In-medium correlations (short-range repulsion, large tensor component of the bare nucleon-nucleon force) are integrated out into an an effective energy density functional (EDF)

Danger of double counting when adjusting the EDF phenomenologically in SR calculations and using it for MR EDF calculations afterwards
Danger of double counting (1) and (3) when the variational space for (3) includes states that describe in-medium correlations

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2. static correlations: deviation of a single deformed and paired mean-field state from a spherical Slater determinant as described by a deformed and paired self-consistent mean-field ground state $\Rightarrow$ SR EDF approach
   - Correlated observables: multipole moments of the density, pairing gaps
   - Correlated excitations: rotational bands of well-deformed nuclei, 1- and 2-quasiparticle energies

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   - Correlated observables: multipole moments of the density, pairing gaps
   - Correlated excitations: rotational bands of well-deformed nuclei, 1- and 2-quasiparticle energies
3. dynamical correlations: collective fluctuations around a given mean-field state described by a coherent superposition of many mean-field states $\Rightarrow$ MR EDF approach
   - Correlated observables: out-of-band transition moments
   - Correlated excitations: vibrational states, rotational bands of not well-deformed nuclei

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Multi-Reference EDF I: Symmetry restoration

particle-number projector

$$\hat{P}_{N_0} = \frac{1}{2\pi}\int_0^{2\pi} d\phi_N \underbrace{e^{-i\phi_N N_0}}_{\text{weight}} \overbrace{e^{i\phi_N \hat{N}}}^{\text{rotation in gauge space}}$$

angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2}\int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation in real space}}$$

K is the z components of angular momentum in the body-fixed frame.
Projected states are given by

$$|JMq\rangle = \frac{1}{\mathcal{N}_{Jq}} \sum_{K=-J}^{+J} f_J(K)\, \hat{P}^J_{MK}\, \hat{P}^Z\, \hat{P}^N\, |q\rangle = \frac{1}{\mathcal{N}_{Jq}} \sum_{K=-J}^{+J} f_J(K)\, |JMKq\rangle$$

axial symmetry (with the z axis as symmetry axis) allows to perform the α and γ integrations analytically, while the sum over K collapses, $f_J(K) = \delta_{K0}$
For triaxial states and even-even nuclei the integration interval can be reduced to 1/16 of the full $16\pi^2$

Multi-Reference EDF II: Symmetry restoration schemes

- projection after variation (PAV): project mean-field minimum.
  - Advantage: simple
  - Problem: not variational. always unreliable in case of absent/weak static correlations
- variation after projection (VAP): vary projected state to determine the Slater determinant/HFB state that gives optimum projected state
  - Advantage: variational
  - Problem: too expensive in the EDF context for angular-momentum projection that somebody dared to implement it; exists for particle number and parity projection
- minimization after projection (MAP): generate set of mean-field states that differ in a collective coordinate that measures the amount of symmetry breaking, project them and search for the minimum of this energy curve/surface
  - Advantage: simple (although more expensive than PAV)
  - Problem: not fully variational. Might fail if (projected) energy surface is soft in degrees of fredom that are not explicitely treated
- . . . or combine projection with a mixing of states that differ in a collective coordinate that measures the amount of symmetry breaking. This automatically includes the minimum of the projected energy curve/surface and additionally correlations not related to symmetry restoration

Multi-Reference EDF III: Configuration Mixing via the Generator Coordinate Method

Superposition of angular-momentum projected SCMF states

$$|JM\nu\rangle = \sum_q \sum_{K=-J}^{+J} f_{J\nu}(q,K)\,|JMqK\rangle \qquad \begin{cases} |JMqK\rangle & \text{projected mean-field state} \\ f_{J\nu}(q,K) & \text{weight function} \end{cases}$$

$$\frac{\delta}{\delta f^*_{J\nu}(q,K)} \frac{\langle JM\nu|\hat{H}|JM\nu\rangle}{\langle JM\nu|JM\nu\rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation}$$

$$\sum_{q'} \sum_{K'=-J}^{+J} \left[\mathcal{H}_J(qK,q'K') - E_{J,\nu}\,\mathcal{I}_J(qK,q'K')\right] f_{J,\nu}(q'K') = 0$$

with

$$\mathcal{H}_J(qK,q'K') = \langle JMqK|\hat{H}|JMq'K'\rangle \quad \text{energy kernel}$$
$$\mathcal{I}_J(qK,q'K') = \langle JMqK|JMq'K'\rangle \quad \text{norm kernel}$$

A Hamiltonian is used here for the transparent formulation of the principles of the multi-reference EDF method. The actual caculations use an energy density functional generalized to multi-reference calculations which will be discussed later

Going Beyond the Mean Field IV: Configuration Mixing via the Generator Coordinate Method

The angular-momentum projected GCM gives the

- correlated ground state for each value of J
- spectrum of excited states for each J

Furthermore

- the weight functions $f_{J,\nu}(q, K)$ are not orthonormal
- projection is a special case of the GCM, where the group structure determines the collective path and the weight function.
- angular momentum-projection is part of the "quadrupole correlations", as it mixes states with different orientations of the quadrupole tensor.
- particle-number restoration (exactly or on the average) is necessary as matrix elements between two mean field states with average particle number $\langle q|\hat{N}|q\rangle = \langle q'|\hat{N}|q'\rangle = N$ will not have the same average particle number $\langle q|\hat{N}|q'\rangle \neq N$

Physics goals of MR EDF calculations

- move focus of EDF methods away from ground-state properties
- description of characteristic collective excited states at low excitation energy, hopefully also of characteristic few-quasiparticle excitations (not yet tried in the EDF context)
- treat correlations *not* easily absorbed into the EDF. Usually these are related to the finite size and surface of the system, strongly depend on the structure of the nucleus, and fluctuate rapidly with N, Z, deformation, ...
- restore quantum numbers to have selection rules for transitions
- proper transition from vibrational to rotational nuclei
- description of shape coexistence phenomena

Currently existing implementations

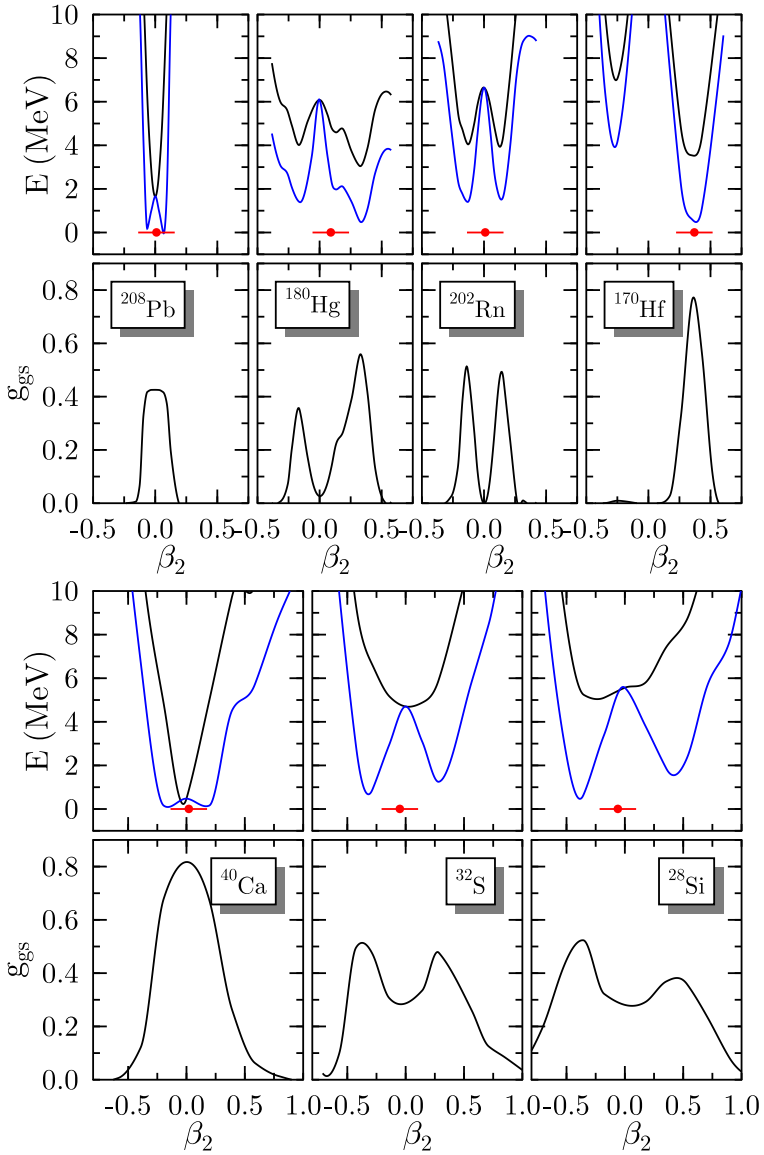
"Exact" MR EDF (solving the Hill-Wheeler-Griffin equation)

- Madrid (Gogny interaction): GCM of particle-number and angular-momentum projected axial reflection symmetric mean-field states, GCM of parity projected octupole deformed axial states, particle-number projection (VAP)
- Zagreb/Munich (relativistic point-coupling Lagrangian): GCM of particle-number and angular-momentum projected axial reflection symmetric mean- field states (see talk by P. Ring)
- Oak Ridge (Skyrme functional): particle-number projection of spherical and axial mean-field states (VAP and PAV)
- Warsaw (Skyrme interaction) angular-momentum projection of cranked triaxial Slater determinants (PAV)
- Tsukuba/Sendai (Skyrme interaction): mixing of parity and/or angular momentum projected slater determinants
- Bordeaux/Bruxelles/Lyon/Saclay (Skyrme functional): GCM of particle-number and angular-momentum projected axial and triaxial mean-field states, GCM of parity projected octupole deformed axial states

Approximate MR EDF (solving a collective Schrödinger equation)

- Bruyerès-le-châtel (Gogny interaction): 5D collective Bohr Hamiltonian
- Lublin/Bordeaux (Skyrme functional): 5D collective Bohr Hamiltonian
- Erlangen (Skyrme functional): Bohr-Hamiltonian of axial states

Typical Situations

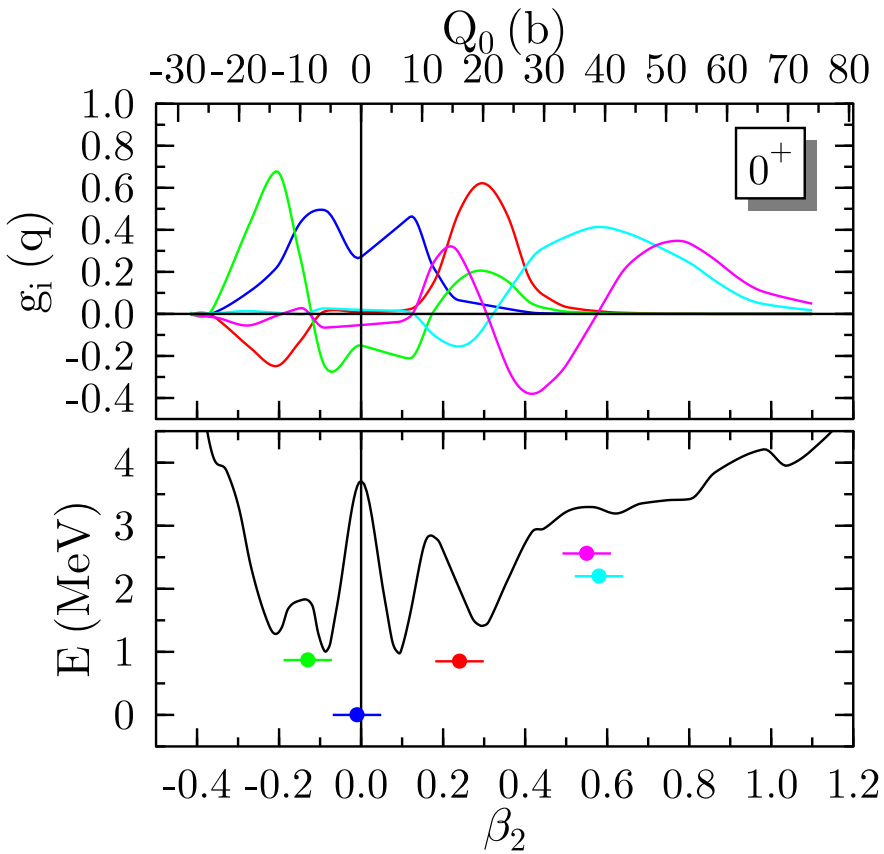


nucleus	E_{def}	$E_{J=0}$	E_{GCM}	E_{corr}
^{208}Pb	0.0	1.7	0.0	1.7
^{180}Hg	3.0	2.6	0.5	3.1
^{170}Hf	12.2	2.9	0.5	3.4
^{202}Rn	2.6	2.7	1.4	4.0
^{48}Ca	0.0	1.4	0.7	2.0
^{32}S	0.0	3.8	0.9	4.7
^{28}Si	0.7	4.2	0.6	4.9

- E_{def}: static deformation energy
- $E_{J=0}$: energy gain from projection
- E_{GCM}: energy gain from mixing projected states
- $E_{\text{corr}} = E_{J=0} + E_{\text{GCM}}$: total dynamical correlation energy

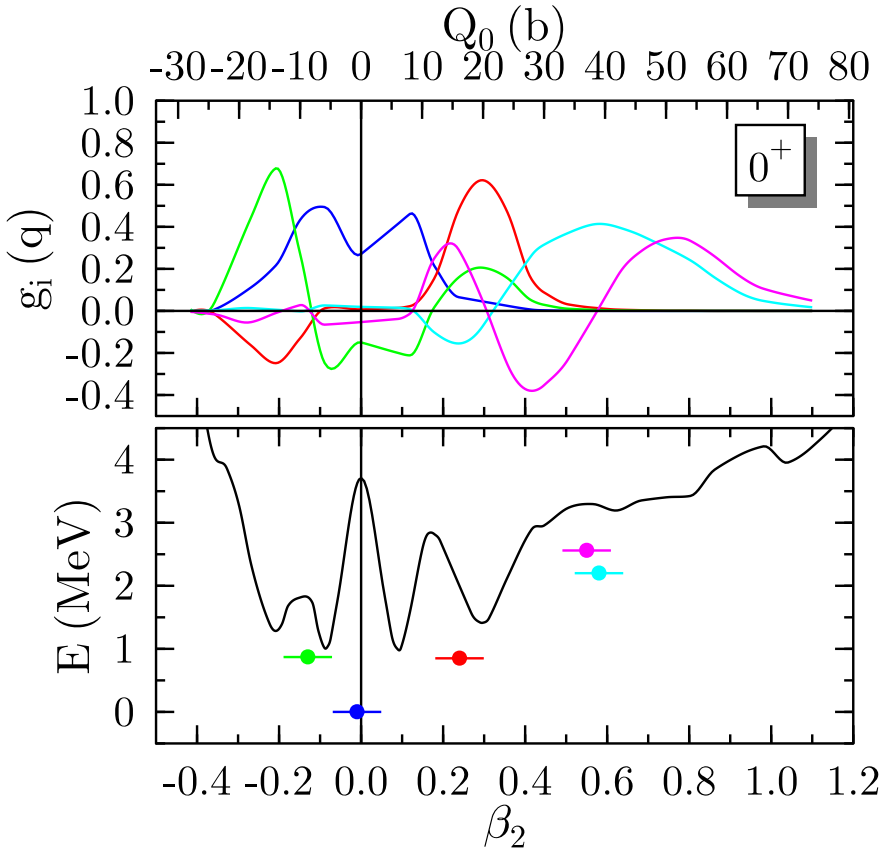
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

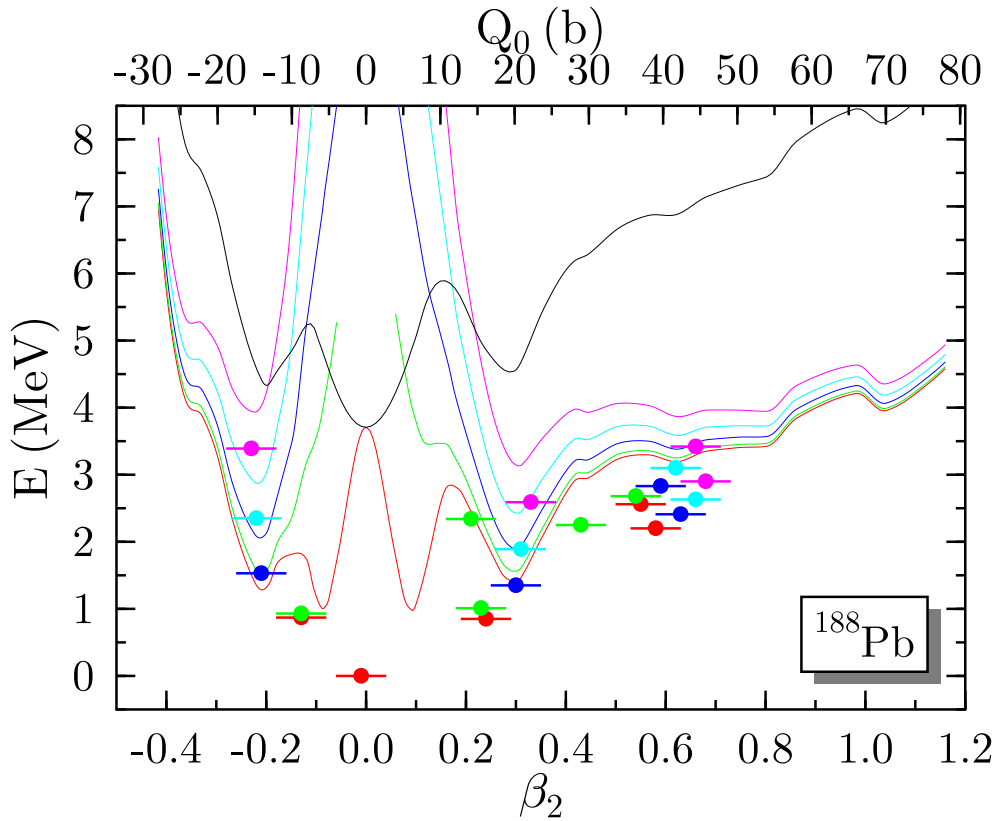
Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method



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

Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method



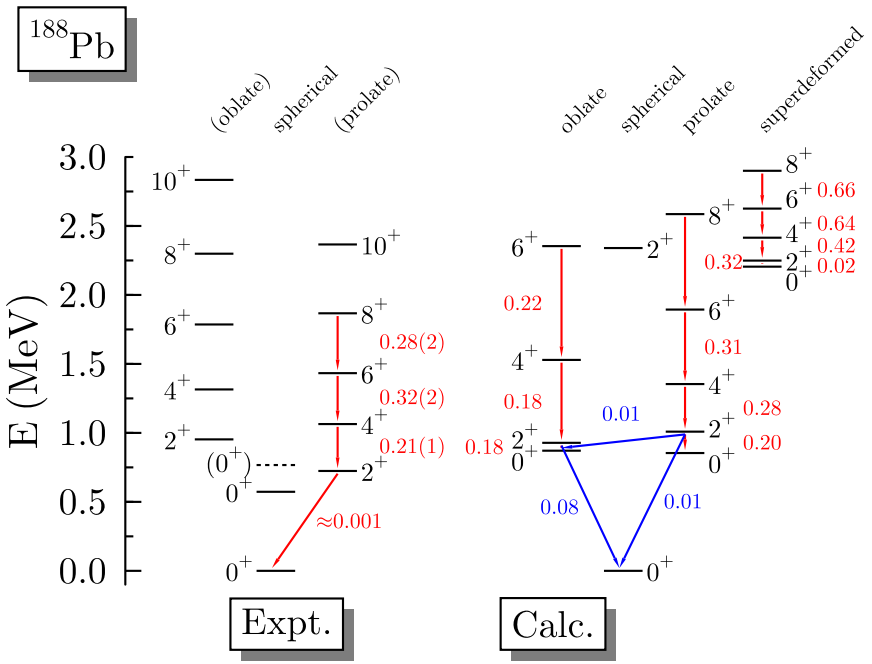


M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Particle-number and angular-momentum projected GCM: ^{188}Pb

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

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

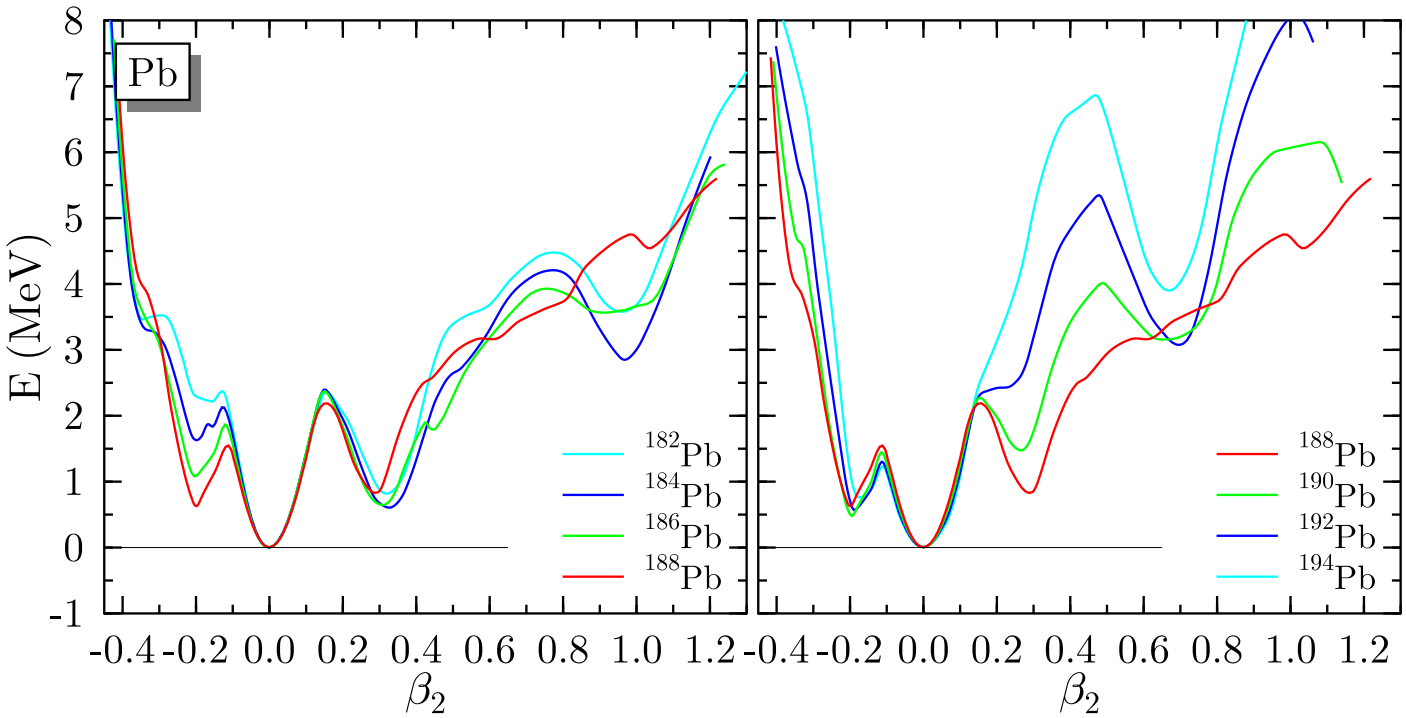


- in-band and out-of-band $E2$ transition moments directly in the lab frame
- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion") $\Rightarrow$ no effective charges necessary
- no adjustable parameters

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

$$\beta_2^{(t)}(J_\nu) = \frac{4\pi}{3R^2A}\sqrt{\frac{B(E2; J_\nu \rightarrow J-2_{\nu'})}{(J\,0\,2\,0\,|(J-2)\,0)^2 e^2}} \quad \text{with} \quad R = 1.2\,A^{1/3}$$

Shape coexistence in the neutron-deficient Pb region



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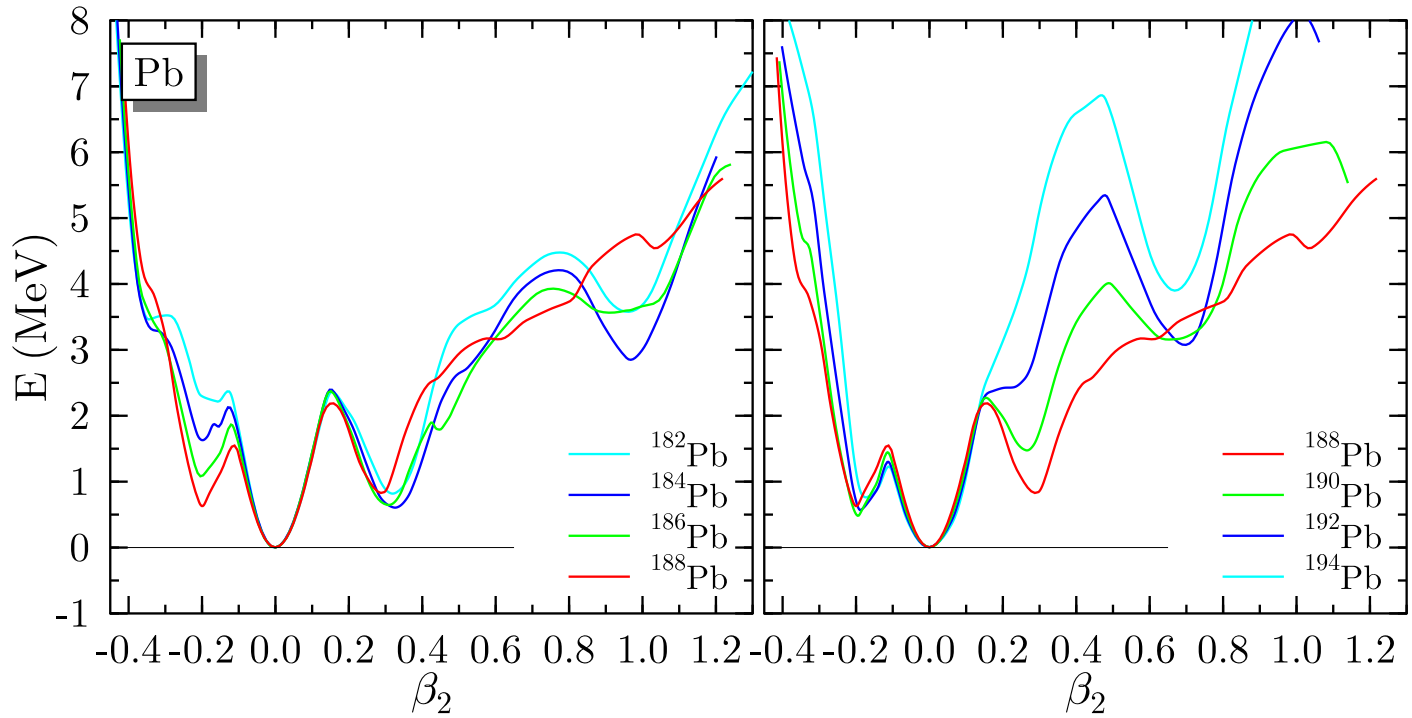

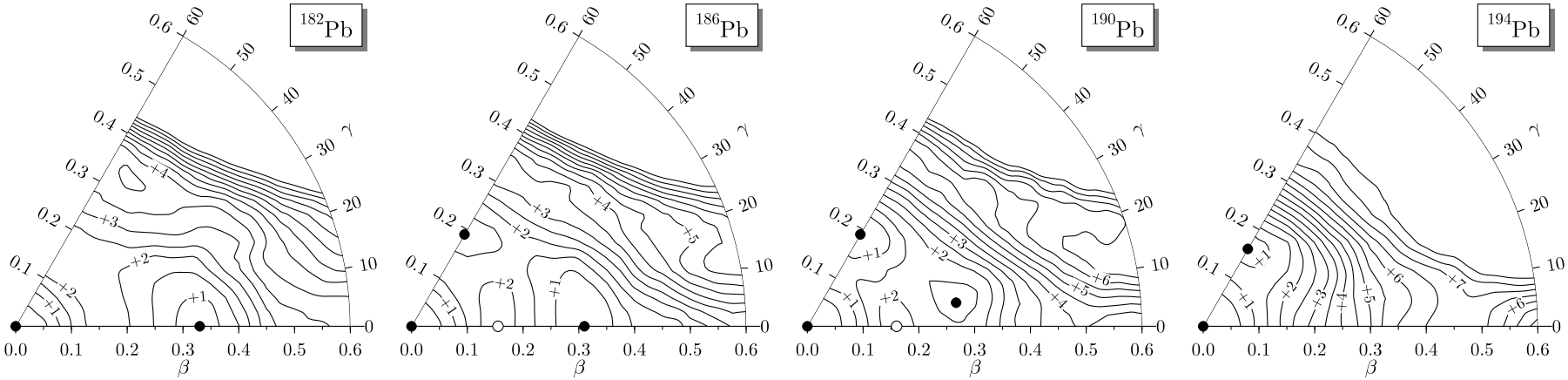

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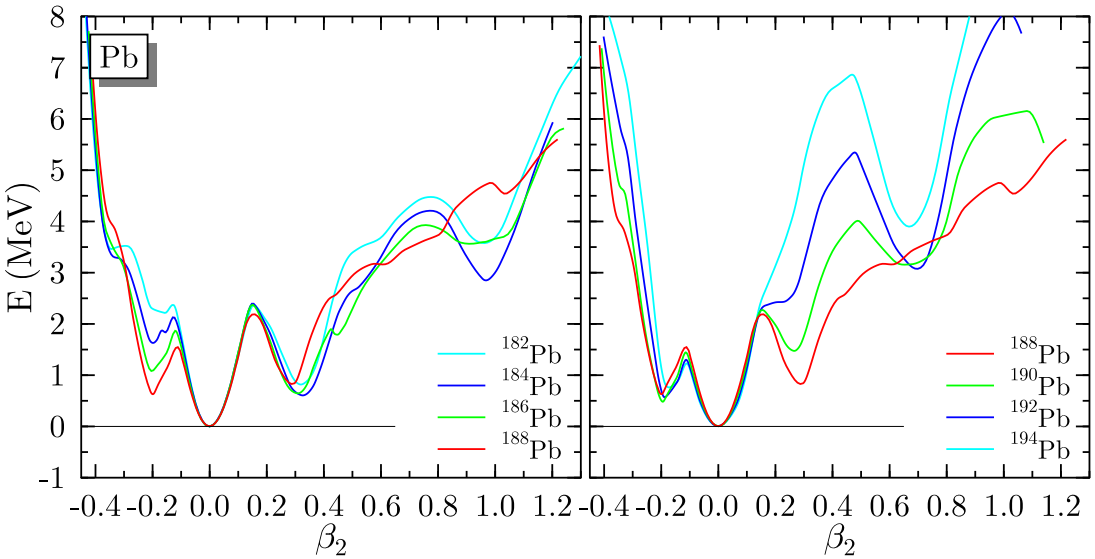
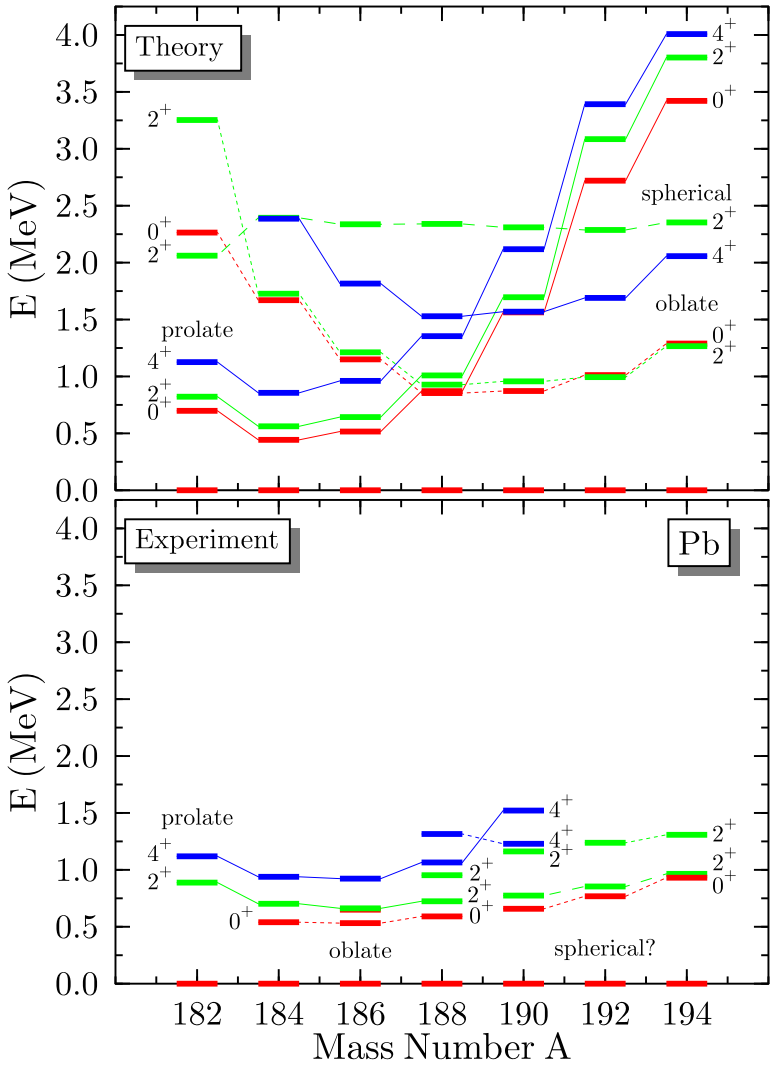


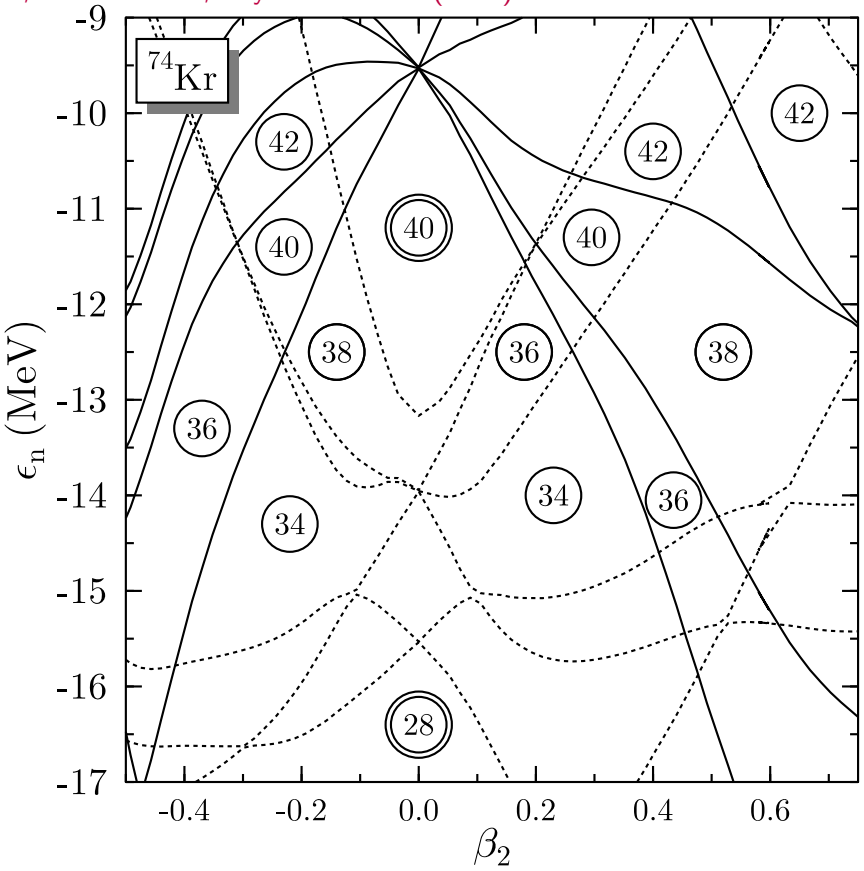


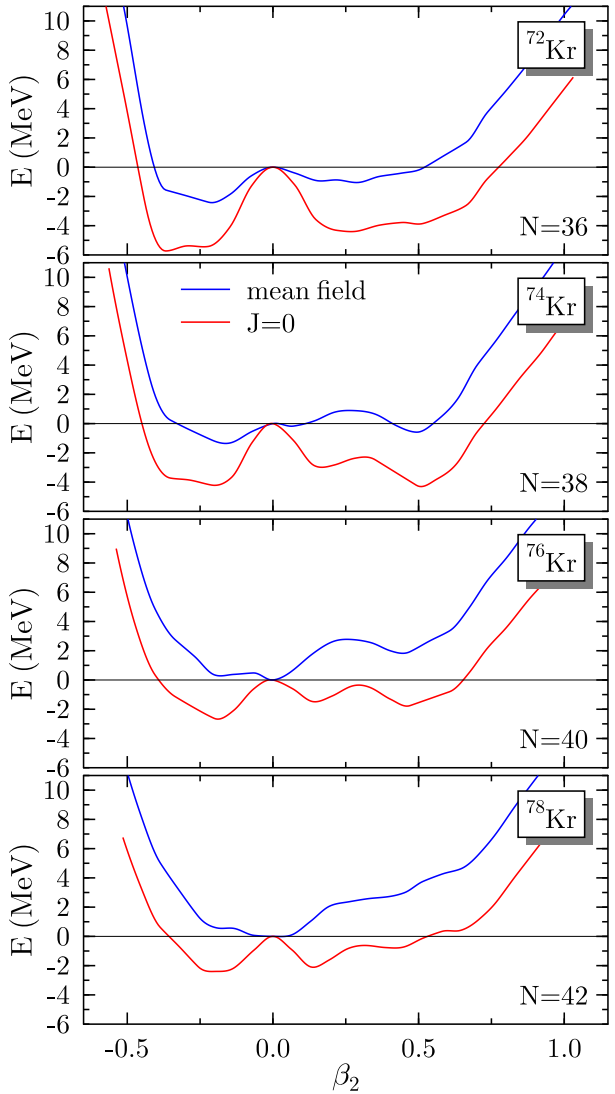
- SLy6+density-dependent pairing
- There are no adjustable parameters!
- excitation energy of the projected GCM bandheads is different from that of the mean-field minima.
- projected GCM gives prolate (oblate) bands also in nuclei without prolate (oblate) mean-field minimum
- calculated spectra are too spread out

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

Shape coexistence in the neutron-deficient Kr region I

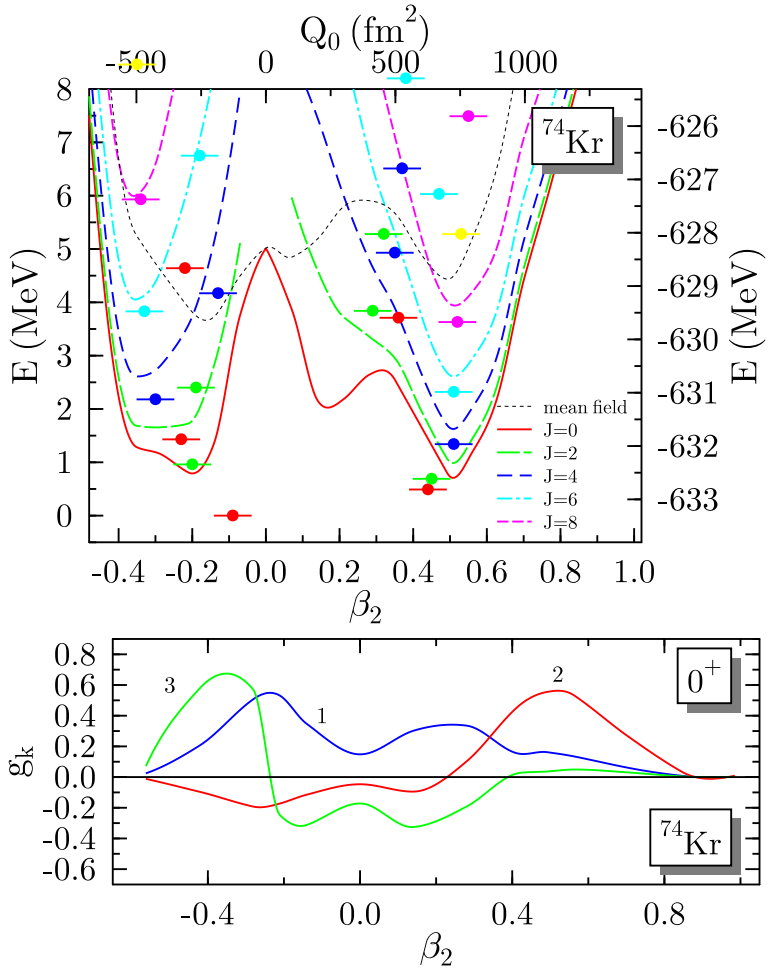
M. B., P. Bonche, P.-H. Heenen, Phys. Rev. C 74 (2006) 024312

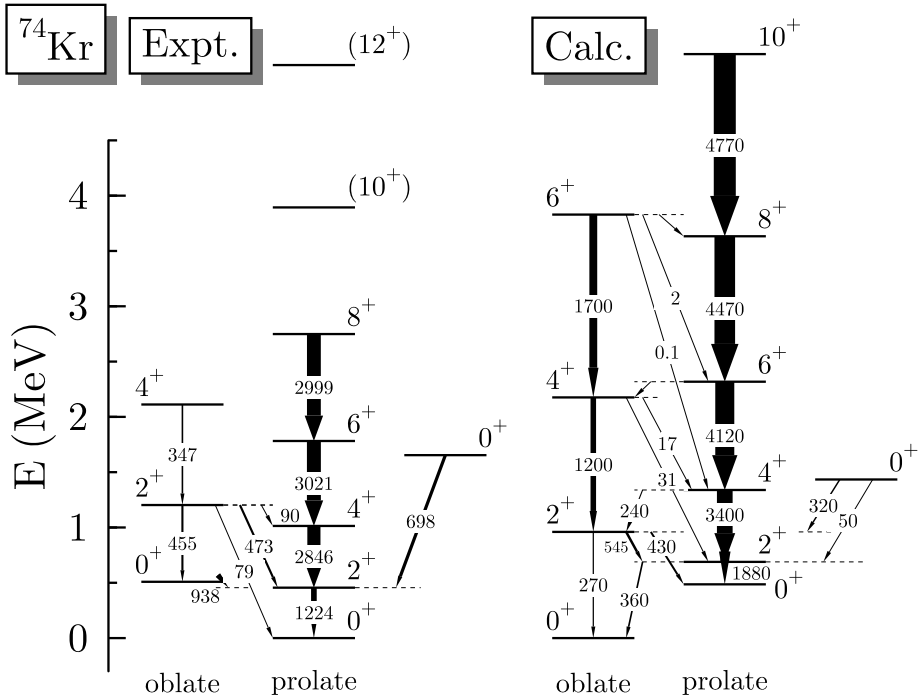




- Nearly each minimum or plateau in the mean-field energy curve can be directly linked to a gap in the Nilsson diagram

Shape coexistence in the neutron-deficient Kr region. II. ^{74}Kr





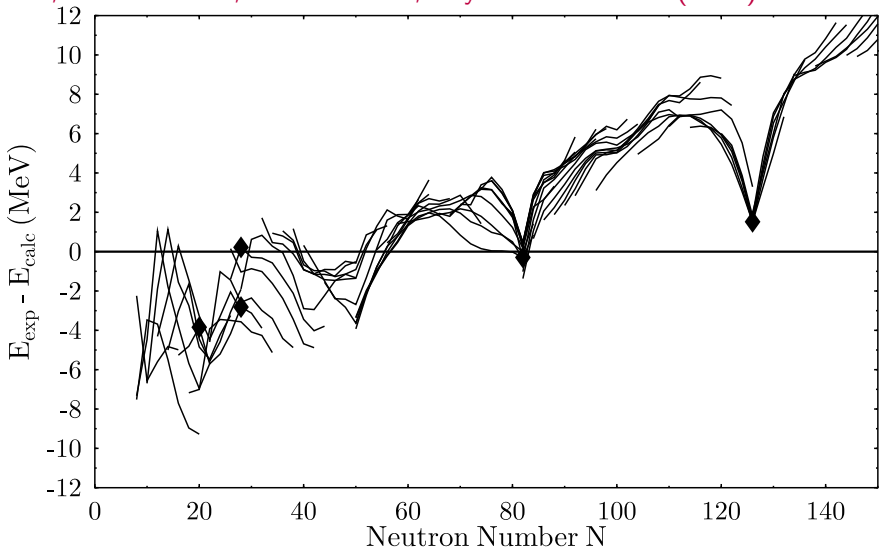
- SLy6+density-dependent pairing
- There are no adjustable parameters...

Experiment: E. Clément *et al.* Phys. Rev. C75 (2007) 054313, A. Görgen *et al.* Eur. Phys. J. A26 (2005) 153

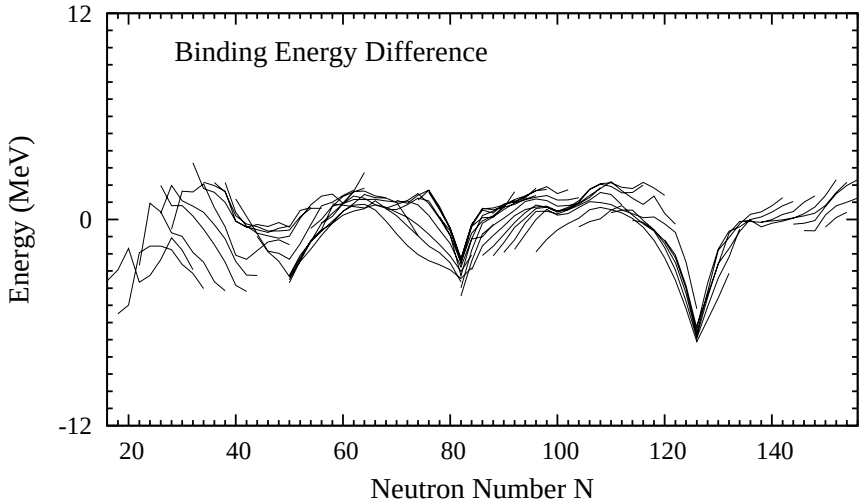
M. B., P. Bonche, P.-H. Heenen, Phys. Rev. C 74 (2006) 024312.

Masses from self-consistent mean-field calculations

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.

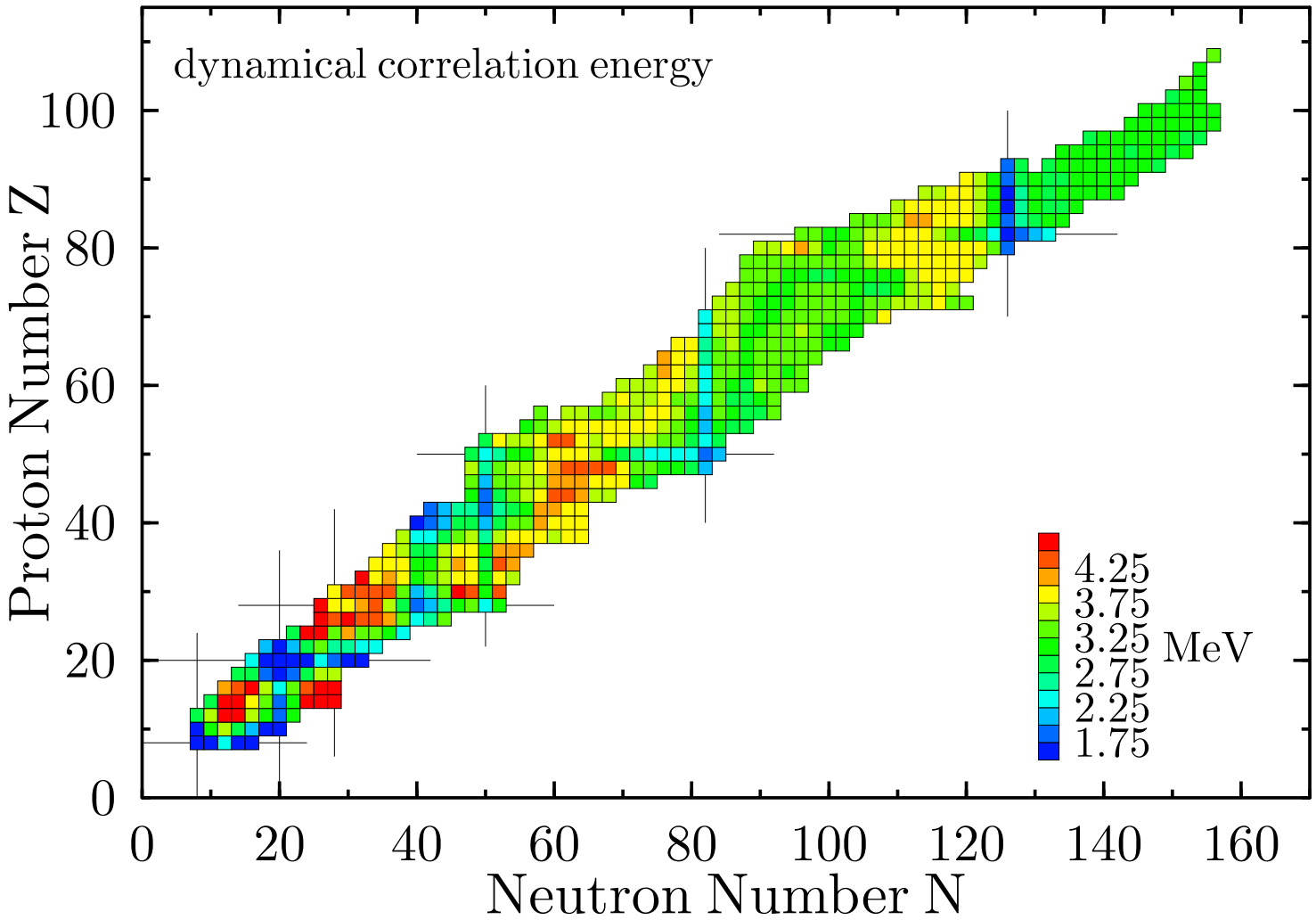


G. F. Bertsch, B. Sabbey, M. Uusnäkki, Phys. Rev. C 71 (2005) 054311.



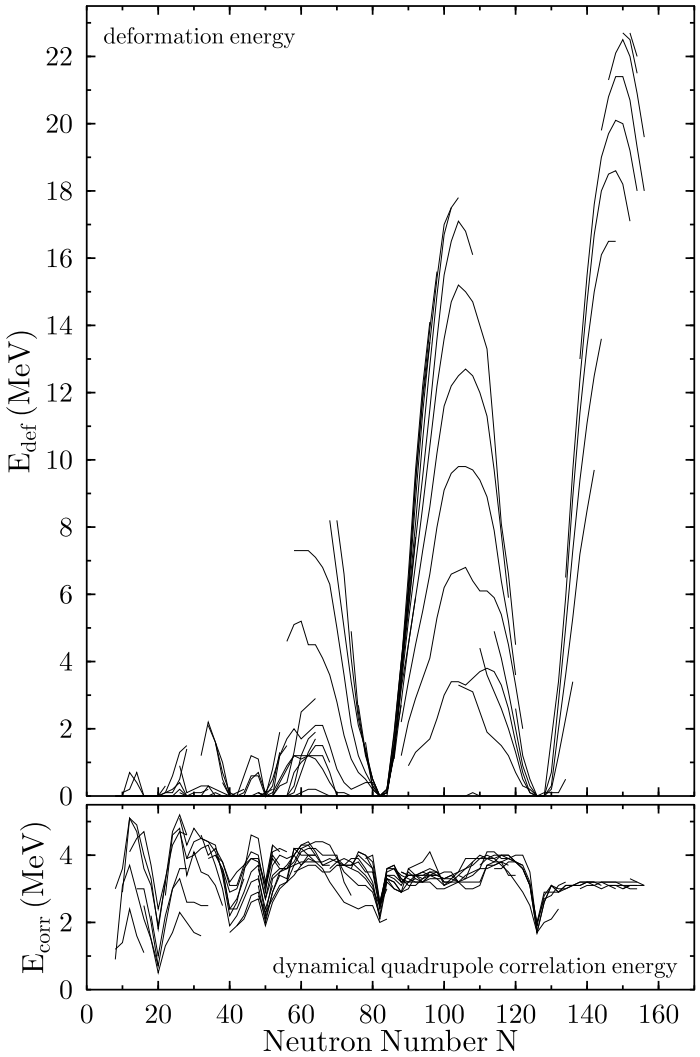
- Skyrme interaction SLy4 + density-dependent pairing interaction
- other parameterizations give qualitatively similar results
- Wrong trend with A
- overestimated shell effects visible at $N = 20$, 50, 82 and 126
- missing Wigner energy
- The slightly wrong trend with mass and isospin can be removed by a slight (a few permille) perturbative readjustment of the parameters of SLy4. The major change is a reduction of the volume energy coefficient by 0.09 MeV.
- And what about the arches?

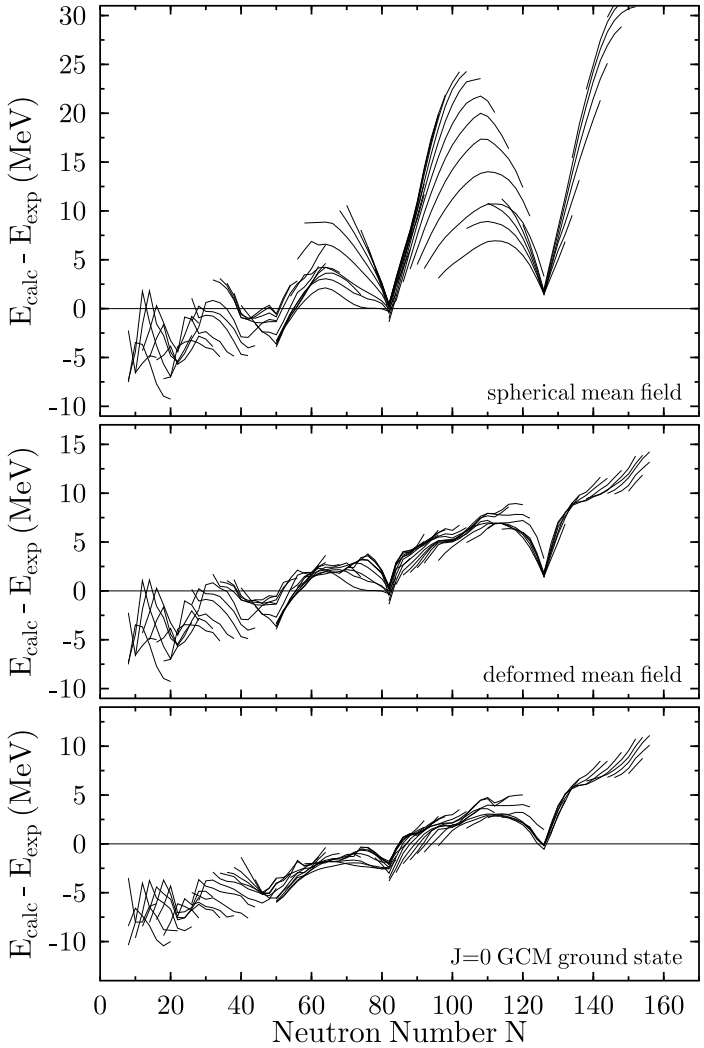
Quadrupole Correlation Energy from Projection and Configuration Mixing



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

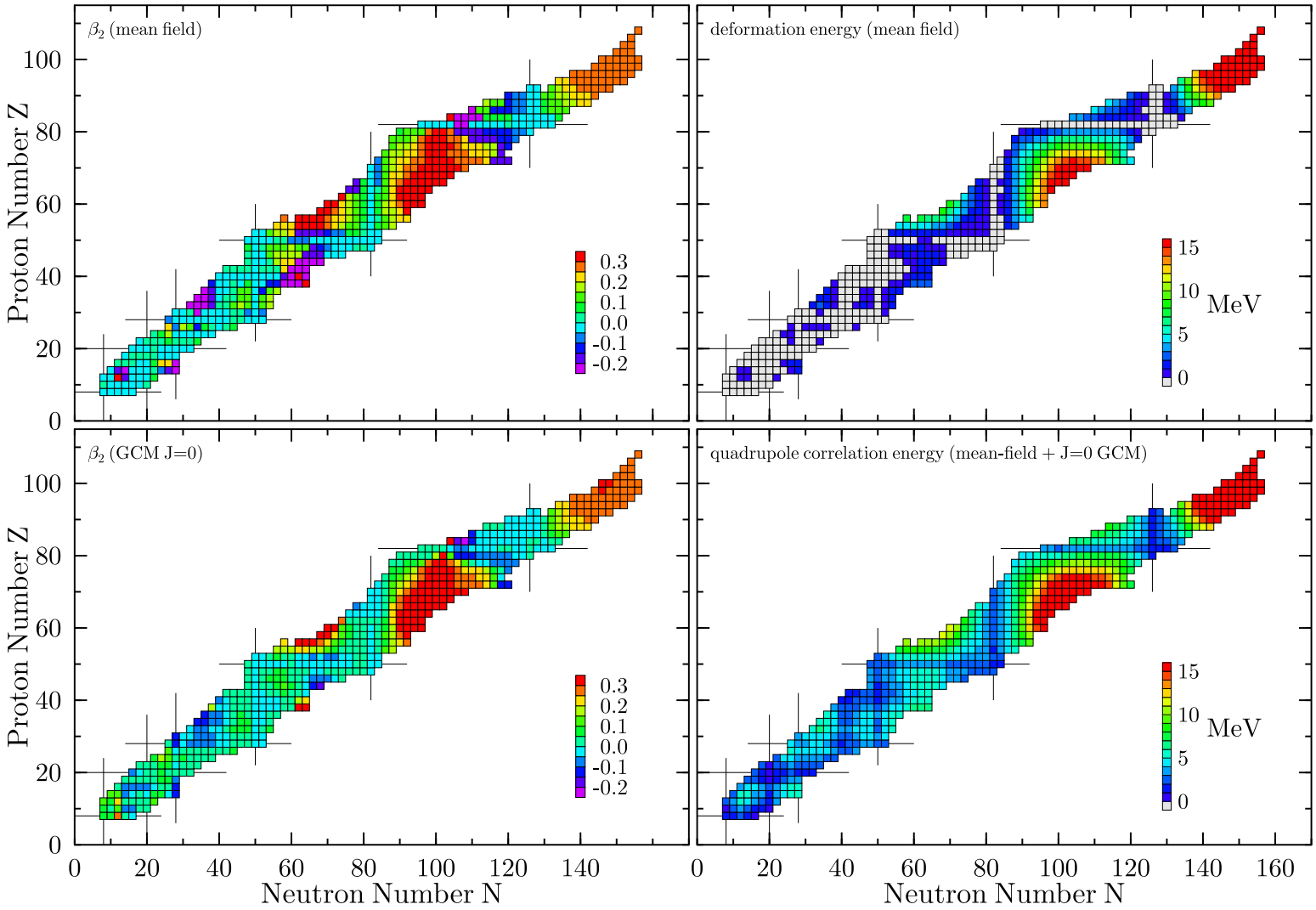
Static and Dynamic Quadrupole Correlation Energies





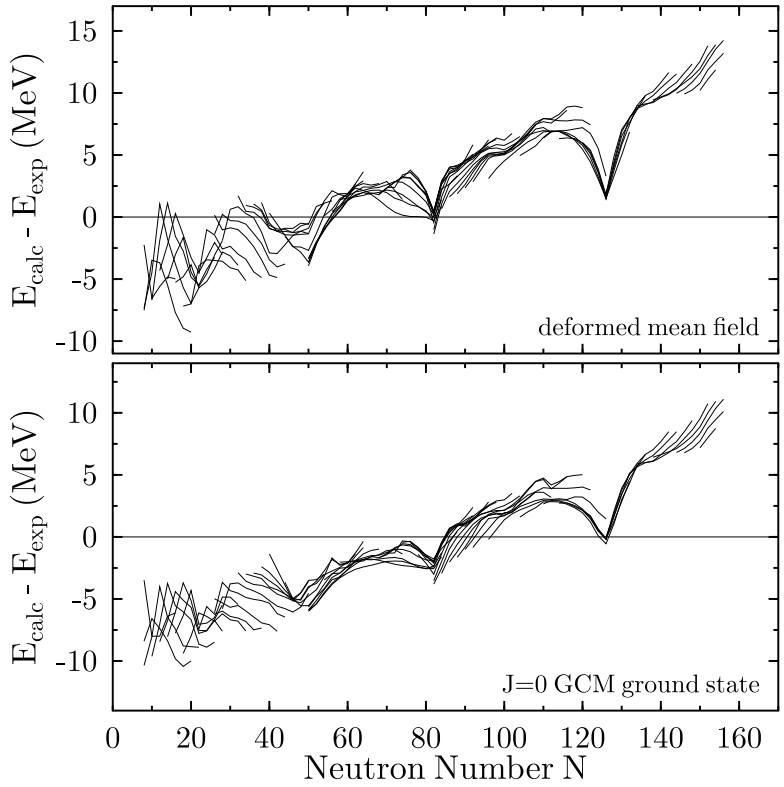
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Intrinsic Deformation and Quadrupole Correlation Energy



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Mass residuals



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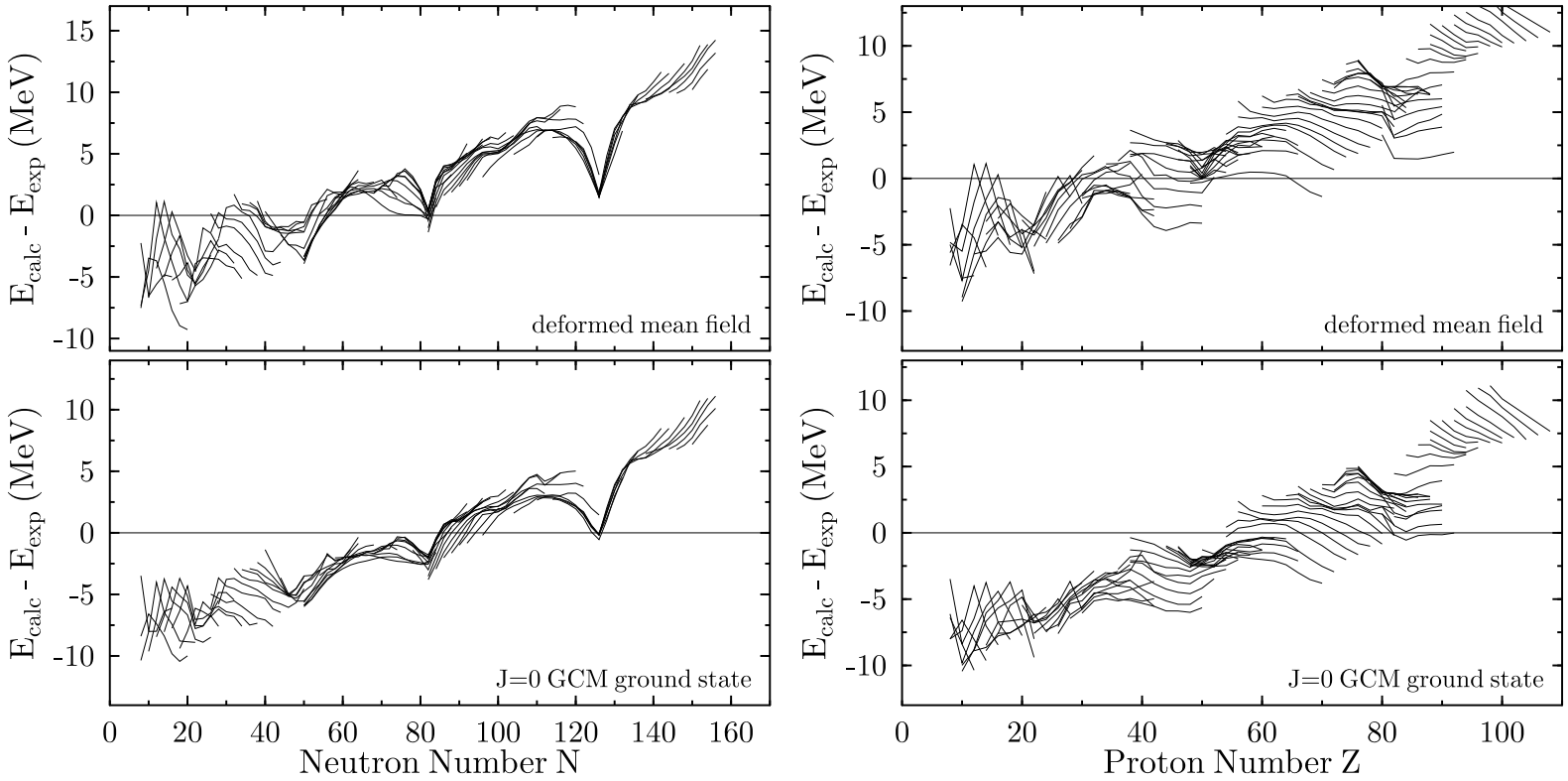
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Mass residuals

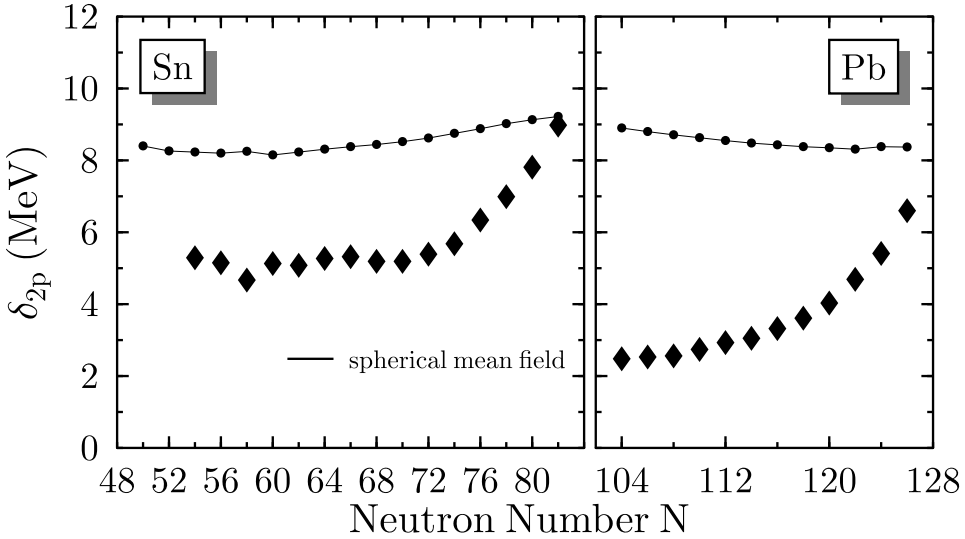


- Shell effects are not overestimated in general, they are overestimated for neutrons
- This might well be a problem with the effective interaction, not so much with large missing correlations

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Systematics of mass differences

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102505
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322



- The two-nucleon gap

$$\delta_{2p}(N,Z) = E(N,Z-2) - 2E(N,Z) + E(N,Z+2)$$
$$\delta_{2n}(N,Z) = E(N-2,Z) - 2E(N,Z) + E(N+2,Z)$$

approximates twice the gap in the single-particle spectrum at shell closures *if the structure of the nuclei involved is the same*

-
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Systematics of mass differences

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102505
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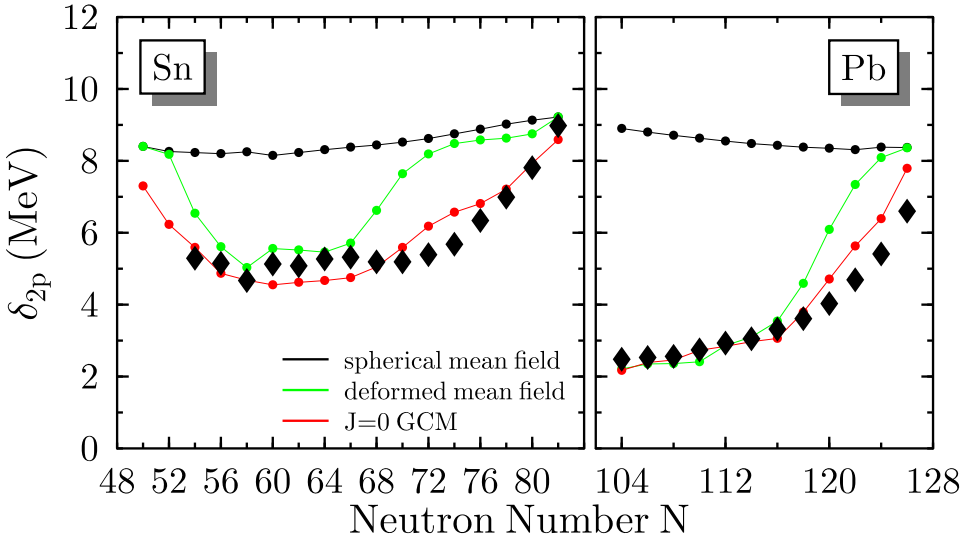

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$$\delta_{2p}(N,Z) = E(N,Z-2) - 2E(N,Z) + E(N,Z+2)$$
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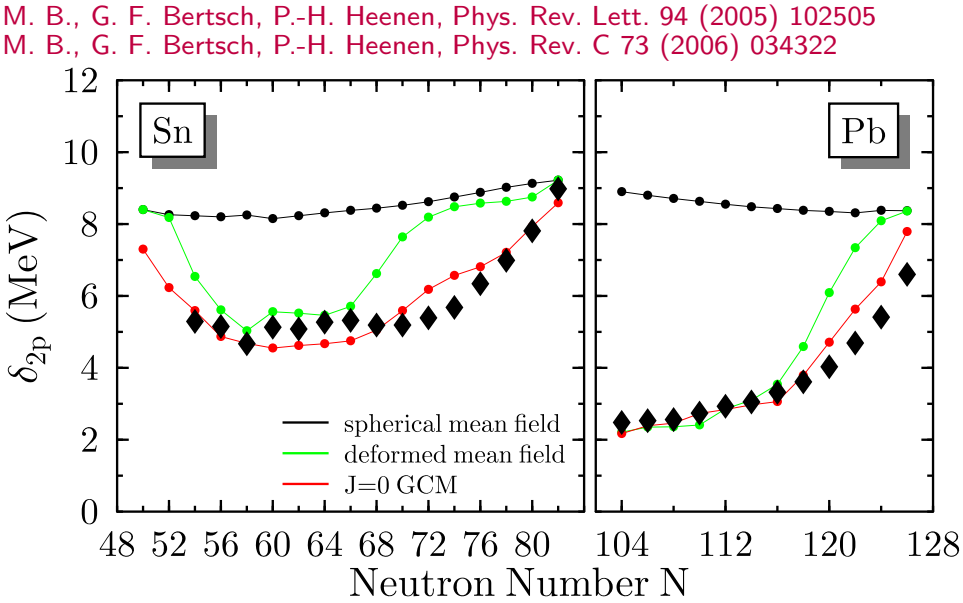
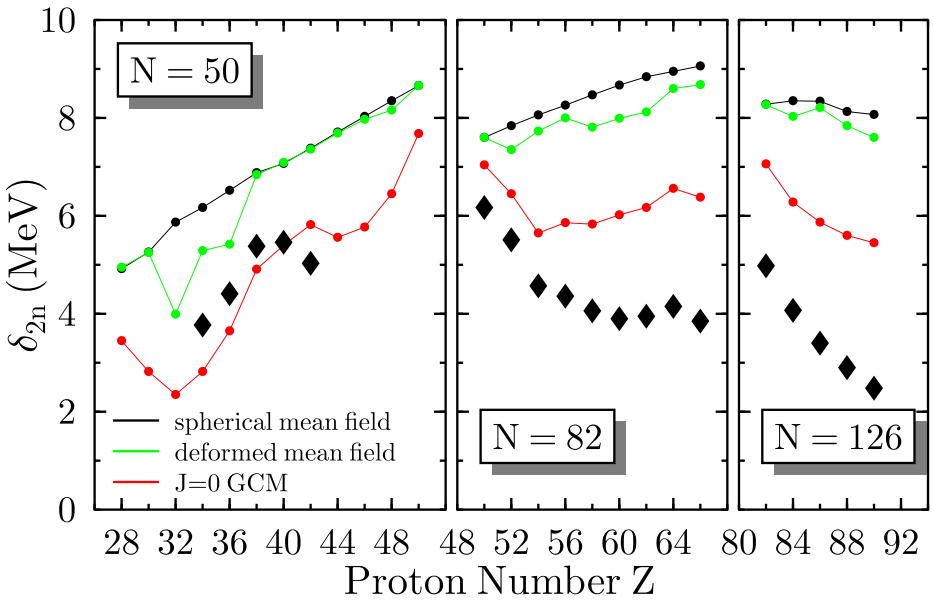
  approximates twice the gap in the single-particle spectrum at shell closures if the intrinsic structure of the nuclei involved is the same

- often invalid assumption as adjacent nuclei are softer or even deformed.

Systematics of mass differences

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102505
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322





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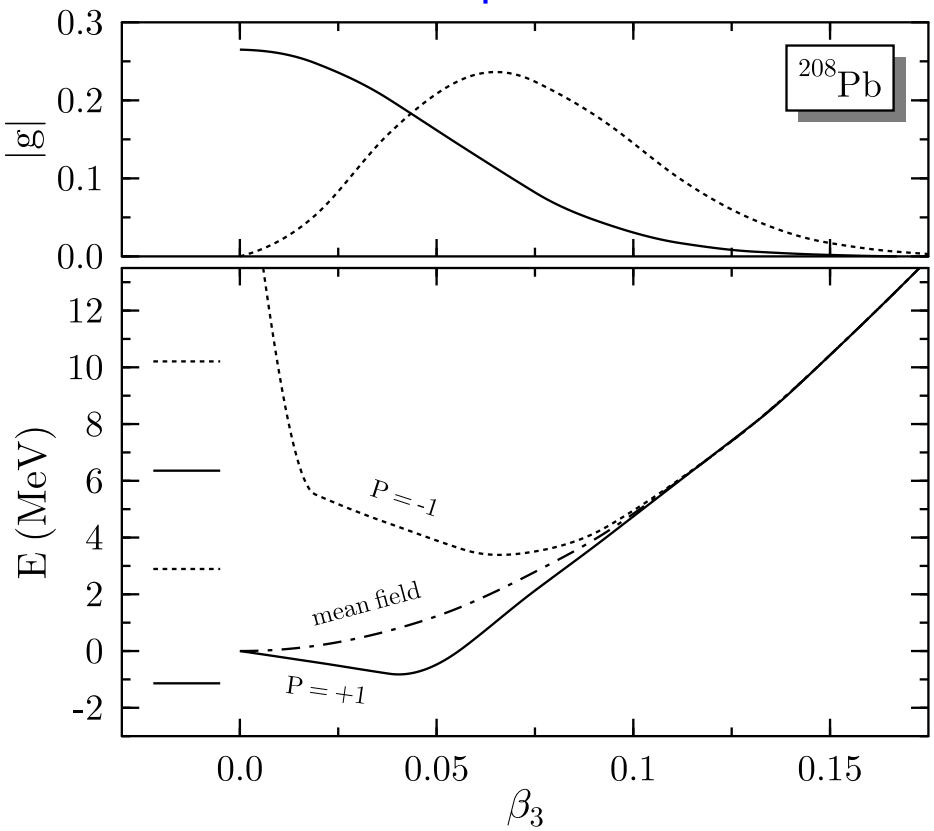
  approximates twice the gap in the single-particle spectrum at shell closures *if the structure of the nuclei involved is the same*

- often invalid assumption as adjacent nuclei are softer or even deformed.
- good (mediocre) results for protons (neutrons) reflect the mass residuals

Other collective degres of freedom

Octupole

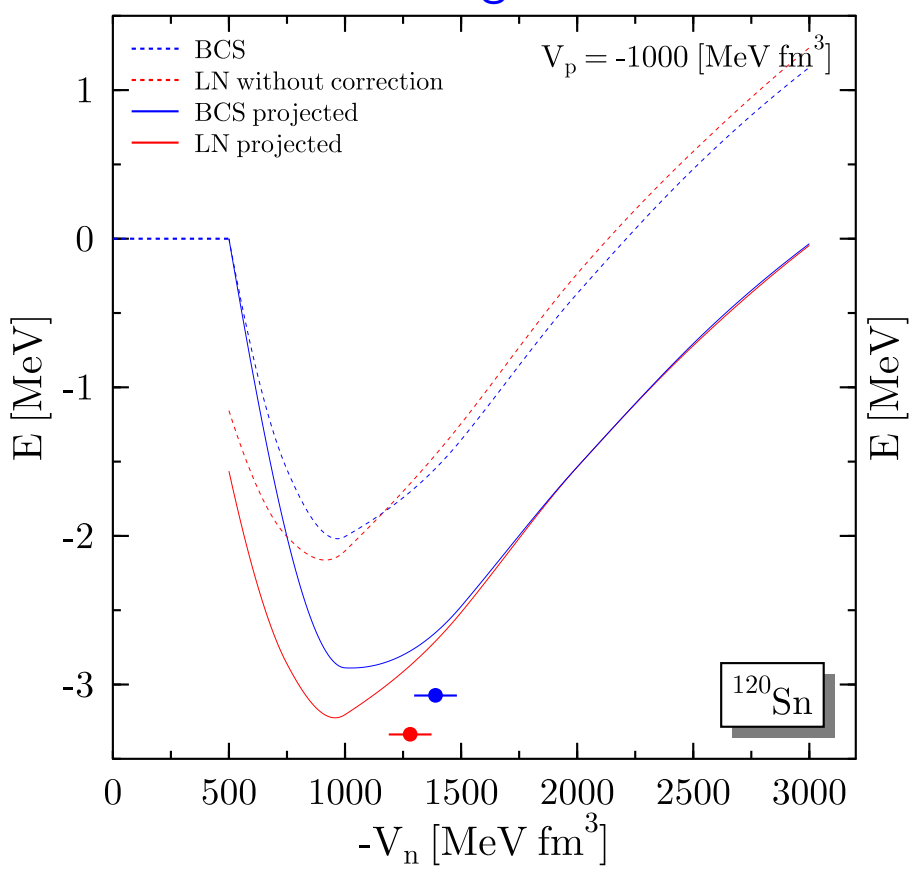


Mixing of parity and particle-number projection of octupole-deformed states in ^{208}Pb (at finite β_3 these are quadrupole deformed as well!)

P.-H. Heenen, A. Valor, M. B., P. Bonche, H. Flocard, EPJA11 (2001) 393

plot: M. B., P.-H. Heenen, P.-G. Reinhard, RMP75 (2003) 121

Pairing

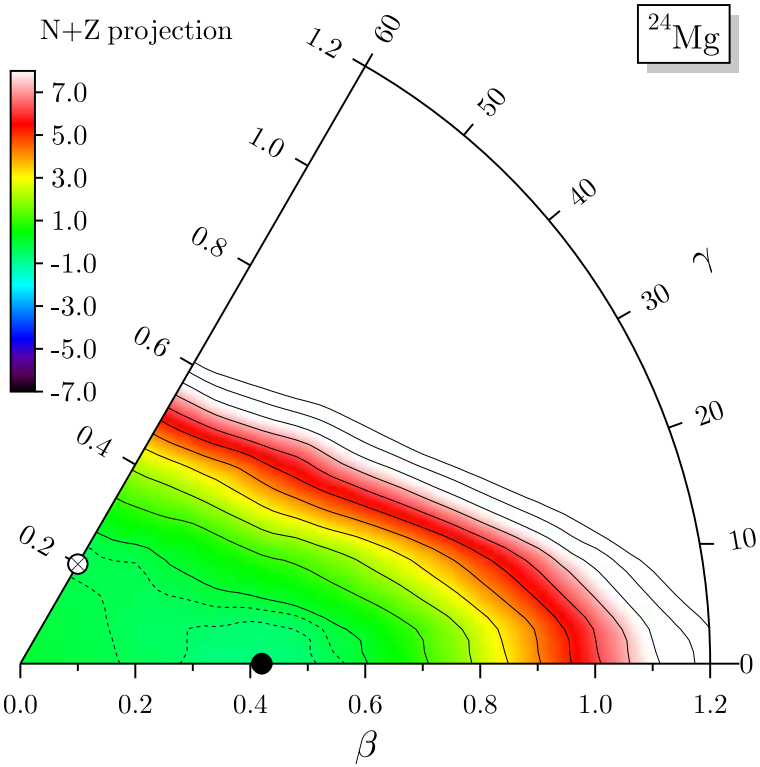


Mixing of particle number projected spherical states in ^{120}Sn with different amount of neutron pairing correlations

M. B., T. Duguet, Int. J. Mod. Phys. E16 (2007) 222

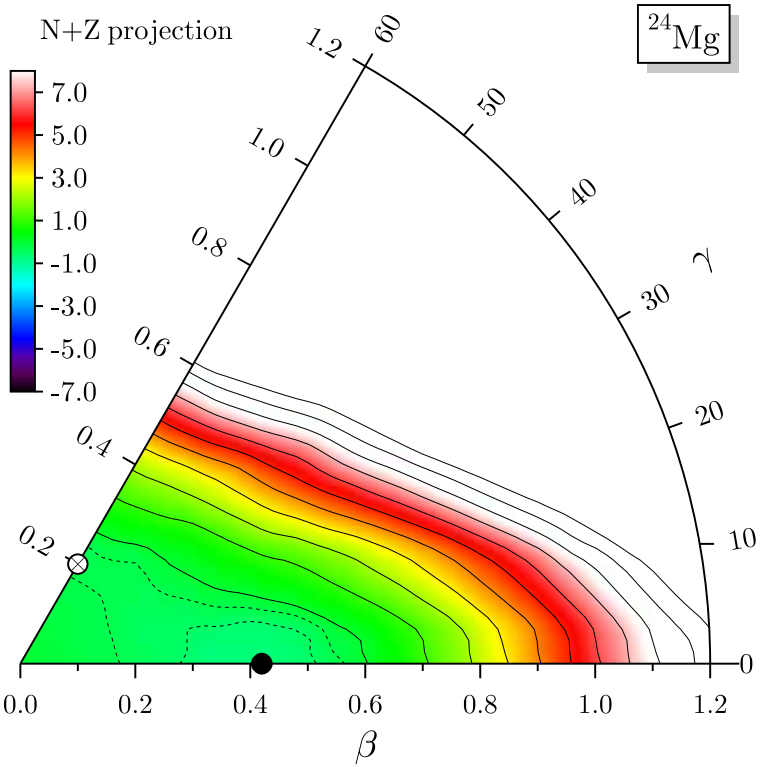
Mixing of angular-momentum projected triaxial states

mean-field deformation energy surface



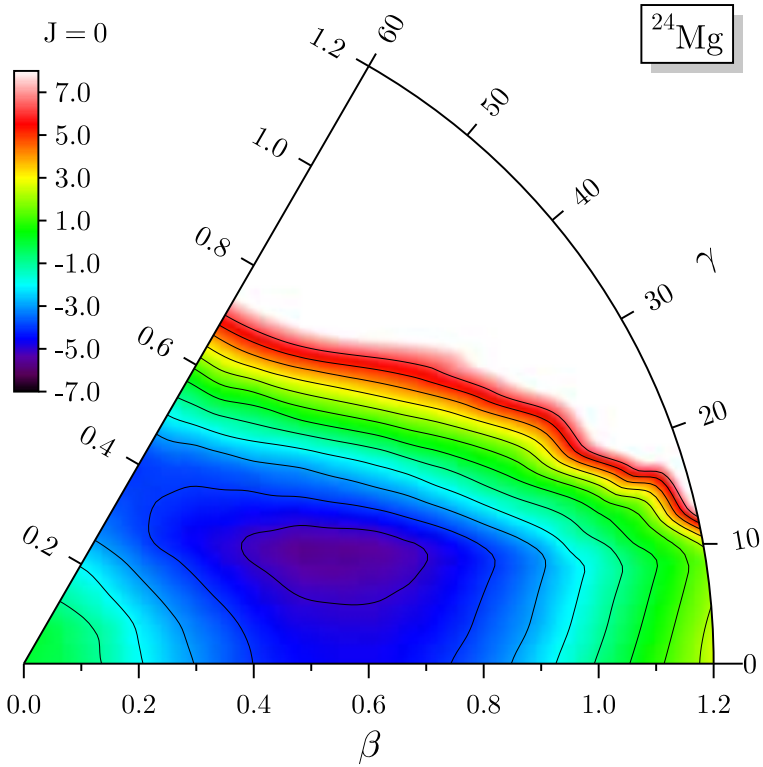
Mixing of angular-momentum projected triaxial states

mean-field deformation energy surface

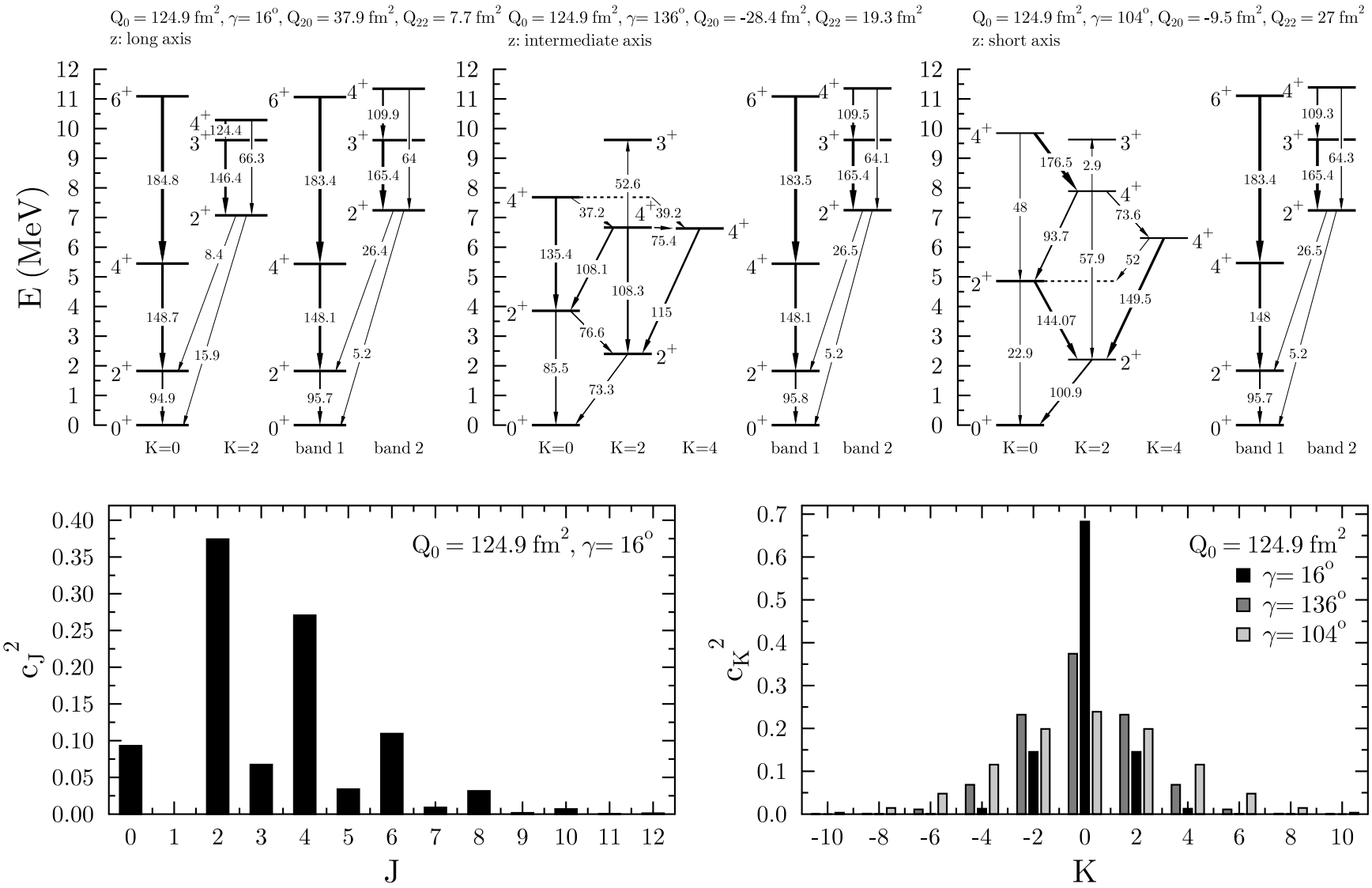


M. B. and P.-H. Heenen, in preparation

$J = 0$ projected deformation energy surface

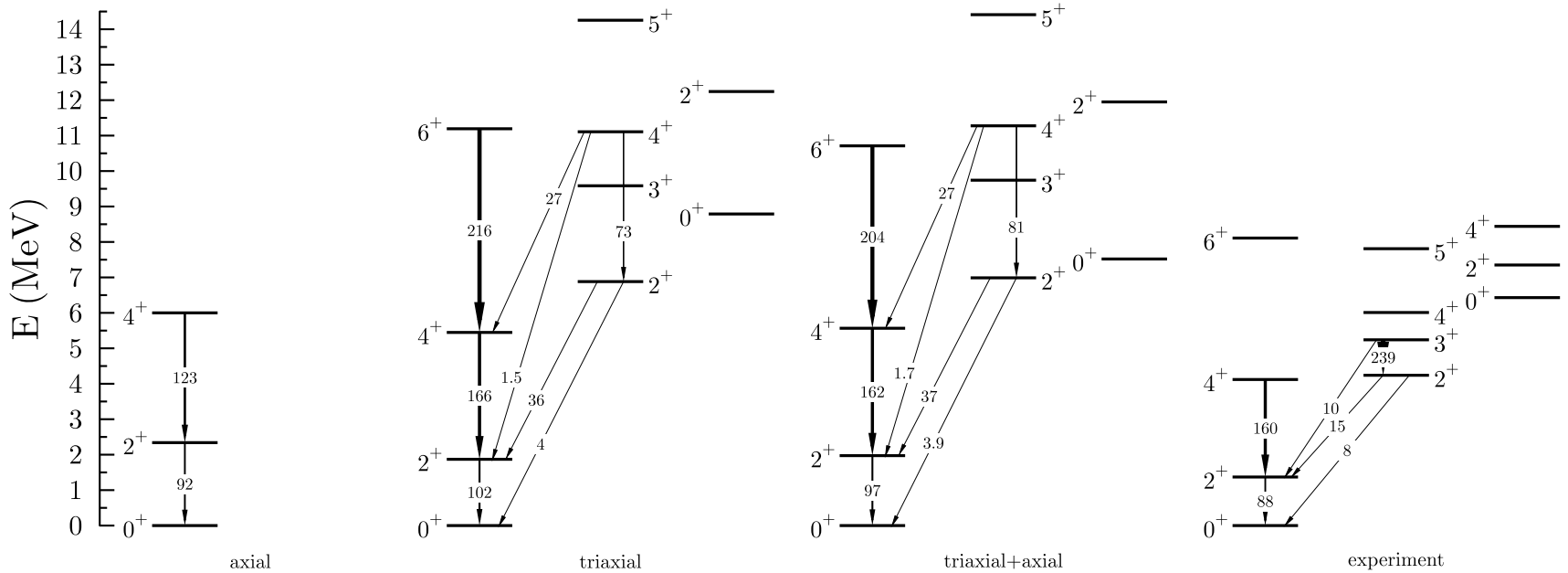


Mixing of angular-momentum projected triaxial states



M. B. and P.-H. Heenen, in preparation

Mixing of angular-momentum projected triaxial states (Preliminary results)



M. B. and P.-H. Heenen, in preliminary results

How to evaluate the MR energy density kernels?

- Any projected GCM calculation (symmetry restoration or GCM) requires the evaluation of non-diagonal kernels between a "left" and a "right" product state using the generalized Wick theorem which works very well for operators, but ...
- ...a MR EDF does not correspond to an operator matrix element!
- Standard recipe: Use analogy with Hamiltonian case. Replace the mean-field densities in the energy density functional with transition densities.

Pathologies in the evaluation of the MR energy density kernels

- transition densities have a pole for orthogonal states
- the summations in the Wick theorem contains terms which are explicitely zero due to the properties of the matrix elements of two-body (or *n*-body) operators. These terms are not zero anymore for an EDF
- The overlap between two reference states might be zero. For operators this is not a problem, as all dangerous denominators cancel with combinations of terms in the nominator. For an EDF this is not the case anymore [Tajima, Flocard, Bonche, Dobaczewski and Heenen, NPA542 (1992) 355, Dönau, PRC58 (1998) 872, Anguiano, Egido, Robledo NPA696 (2001) 467, Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315]
- Transition densities are complex. The MR EDF built from transition densities is complex as well. In case of density dependent terms using non-integer powers of the density, the only seemingly consistent choice to construct the MR EDF [Robledo, Int. J. Mod. Phys. E16 (2007) 337] leads to a multi-valued functional [Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315]

Pathologies: further reading

This talk is not the appropriate place to discuss the pathologies contained in a MR EDF in great detail. This subject was covered in the following talks during the recent ESNT workshop on "Fondements de la theorie de la fonctionelle d'energie en physique nucléaire", November 6-7 2007

http://irfu.cea.fr/Sphn/Espace_Theorie/Nov2007/talks/Dobaczewski.ppt

http://irfu.cea.fr/Sphn/Espace_Theorie/Nov2007/talks/Robledo.pdf

http://irfu.cea.fr/Sphn/Espace_Theorie/Nov2007/talks/Lacroix.ppt

http://irfu.cea.fr/Sphn/Espace_Theorie/Nov2007/talks/Bender.pdf

Please note that what was said by myself about sum rules during this workshop is wrong. Their (hopefully) correct discussion will be given in the paper on the subject appearing anytime soon.

Pathologies: key ideas

a EDF contains spurious energies

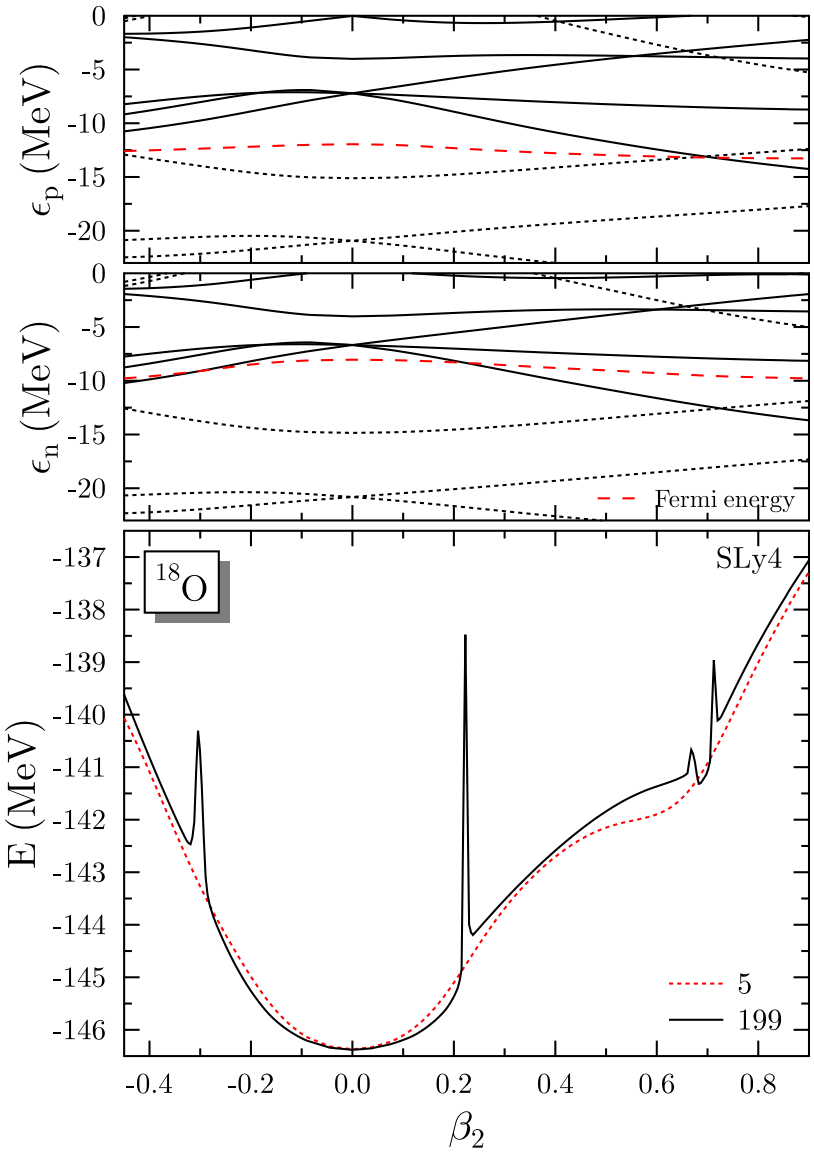
1. related to the incomplete antisymmetry of the SR/MR EDF (self interaction, self pairing)
2. due to the Generalized Wick Theorem (GWT) multiplying self interaction and self pairing contributions to the MR EDF with potentially divergent weights. Evaluating the same kernels with the Standard Wick Theorem (SWT) (which requires the construction of a very particular basis separately for each kernel) gives a different, *not* divergent, weight of these contributions.
3. due to the use of non-integer density dependencies, which become multivalued functions when plugging in complex transition densities (which is required by the consistency criteria of Robledo, Int. J. Mod. Phys. E16 (2007) 337)

The really dangerous pieces are (2) and (3). The second can be isolated comparing SWT and GWT, and removed afterwards

D. Lacroix, T. Duguet, M. B., in preparation
M. B., T. Duguet, D. Lacroix, in preparation
T. Duguet, M. B., K. Bennaceur, D. Lacroix, T. Lesinski, in preparation

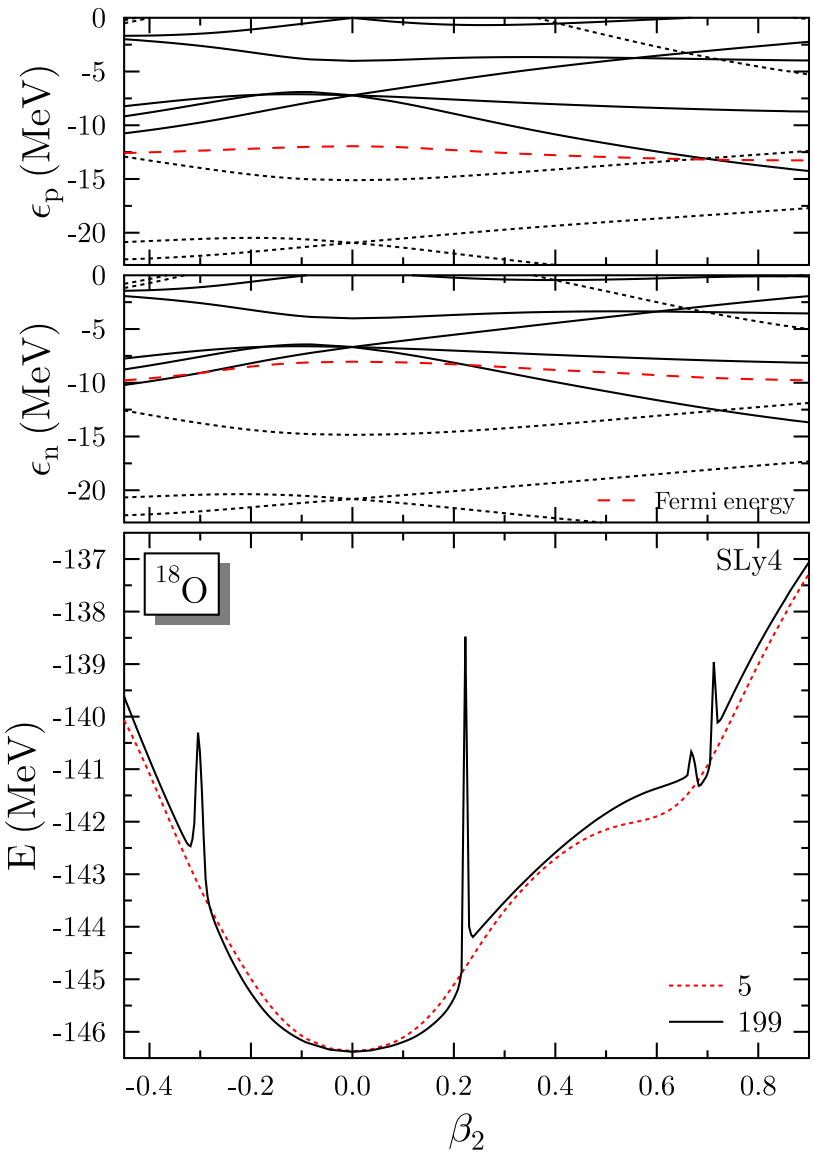
Particle-number restoration in ^{18}O. I. problems from GWT

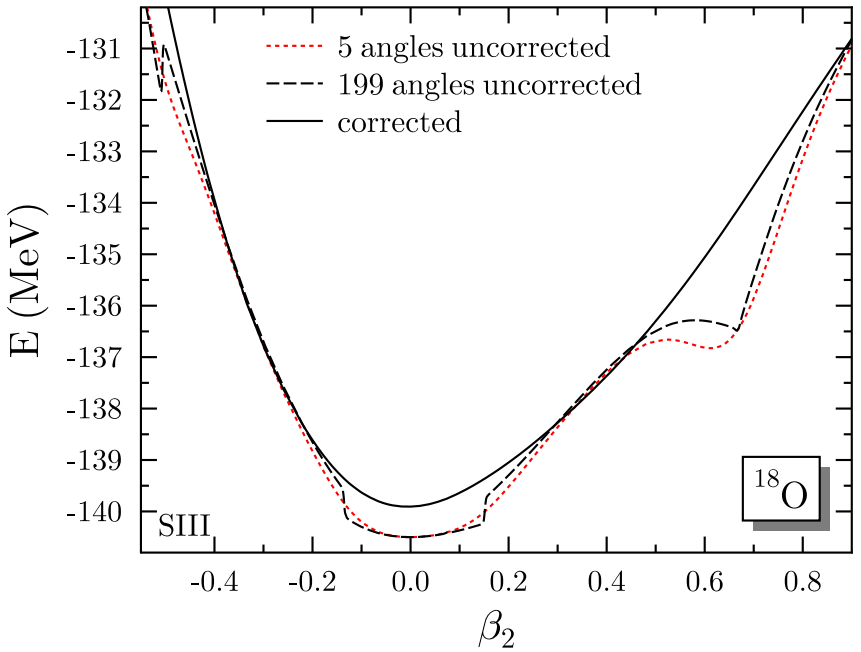
M. B., T. Duguet, D. Lacroix, in preparation



Particle-number restoration in ^{18}O. I. problems from GWT

M. B., T. Duguet, D. Lacroix, in preparation

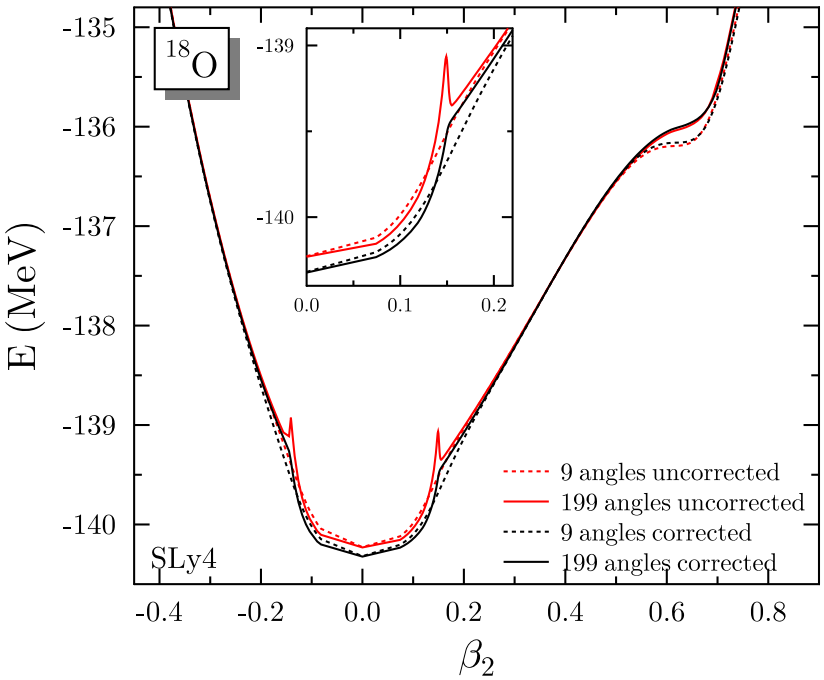




- left: SLy4 used as usual (but provoking the divergences). Results depend on the discretization of the integral over gauge angles.
- above: SIII with a correction for spurious terms. Corrected results are independent on the discretization.

Particle-number restoration in ^{18}O. II. non-integer density dependence

T. Duguet, M. B., K. Bennaceur, D. Lacroix, T. Lesinski, in preparation



- no regularization scheme available/ envisionable for non-integer density dependencies
- constraint on functional form of pathology free MR energy functionals
- source of the problem: replacing k_F dependencies by density dependencies identifying $k_F = (3\pi/2)^{1/3}\rho^{1/3}$ in the EDF when resumming the in-medium correlations into the functional, and identifying ρ with the transition density in MR EDF calculations

Achievements and open questions

SR and MR EDF methods are a powerful tool . . .
. . . but there is still a lot of work to be done.

- There is an urgent need for energy density functionals that give better single-particle spectra. Which are the relevant terms in the functional, how to adjust them to which observables?
- How to define a suitable and exhaustive collective space for MR-EDF calculations? Which symmetries to break, which to restore, how many collective degrees of freedom to take into account, how to optimize the collective path/surface, how to take single-particle degrees into account in an efficient manner, without sacrificing the applicability of the method to all nuclei (with computers available at the time this has all been worked out and the codes are written)?
- A formal framework for MR-EDF calculations has be be established, to avoid surprises as unexpected divergences
- construction of energy density functionals for SR and MR calculations based on first principles. How far can this be pushed?

Advantages of MR EDF

- keeps many widely appreciated features of SR EDF and resolves many of its limitations
- computational cost scales moderately with the number of (occupied) single-particle states and number of collective degrees of freedom
- moderate storage needed (compared to the shell model)
- Extrapolability thanks to the use of a universal energy density functional
- treating several collective degrees of freedom at the same time does not pose a (known) conceptual problem (in contrast to QRPA)

Limitations of current implementations of the method that can be overcome investing man and CPU hours

Missing pieces in the MR space (remaining symmetries, unexplored degrees of freedom)

- time-reversal breaking (cranked states, optimized for each J)
- 1-quasiparticle states (odd-A nuclei)
- 2-quasiparticle states (some with $K = 0$ and all with $K \neq 0$ cannot be generated by deformation)
- like-particle pairing vibrations (to complement particle-number projection)
- octupole/non-triaxial deformation and mixing, parity restoration (in addition to quadrupole dynamics)
- ATDHF motivated (time-reversal breaking) double constraints?
- proton-neutron mixing, isospin restoration, proton-neutron pairing vibrations
- restoration of Galilean invariance

Missing pieces in the construction of the EDF

- performance for "single-particle spectra"
- functional form of the EDF from first principles
- evaluation of the MR EDF from first principles

Limitations of the method as such according to the state of the art

- energy functionals should not be "too complicated"
- not every possible EDF usable in SR EDF can be used safely in MR EDF
- limitation to low-lying levels (for practical and conceptual reasons)
- limitation to to small (but larger than 7) number of collective degrees of freedom
- limitation to small number of explicit single-particle degrees of freedom in the reference states (cannot replace the shell model for those)
- limitation to (mainly) one-body observables (for conceptual reasons: functional constructed from one-body density matrices)
- limitation to observables explicitely probing small momentum transfer only (for conceptual reasons)

Acknowledgements

The work presented here would have been impossible without my collaborators on the various subjects touched upon during this talk

Karim Bennaceur	IPN Lyon, France
George F. Bertsch	INT Seattle, USA
Paul Bonche	SPhT, CEA Saclay, France
Thomas Duguet	SPhN, CEA Saclay, France
Hubert Flocard	CSNSM Orsay, France
Paul-Henri Heenen	PNTPM, Université Libre de Bruxelles, Belgium
Denis Lacroix	GANIL, France
Thomas Lesinski	IPN Lyon, France
Jacques Meyer	IPN Lyon, France