The impact of static deformation and fluctuations in collective degrees of freedom on separation energies around shell closures (in energy-density functional-based methods)

Michael Bender

Université Bordeaux 1; CNRS/IN2P3; Centre d'Etudes Nucléaires de Bordeaux Gradignan
UMR5797, Chemin du Solarium, BP120, 33175 Gradignan, France

Nuclear magic numbers : New features far from stability.
Confronting theoretical approaches and experiment
Espace de Structure Nucléaire Théorique, Saclay, France, May 4th 2010

particle-number restoration operator

$$\hat{P}_{N_0} = \frac{1}{2\pi} \int_0^{2\pi} d\phi_N \; e^{i\phi_N(\hat{N}-N_0)}$$

angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \; \sin(\beta) \int_0^{2\pi} d\gamma \; \mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma) \hat{R}(\alpha,\beta,\gamma)$$

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

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

$f_J(K)$ is the weight of the component K and determined variationally

Axial symmetry (with the z axis as symmetry axis) allows to perform the α and γ integrations analytically, whereas the sum over K collapses, $f_J(K) \sim \delta_{K0}$

see talk by L. Egido for further technical details

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

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

Angular-momentum projected GCM gives the

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

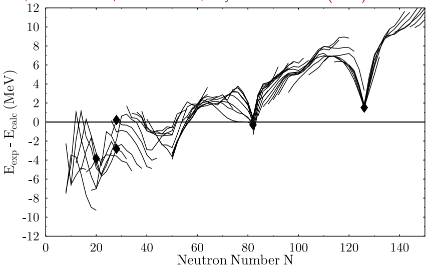
see talk by L. Egido for further technical details

Summary of technical details

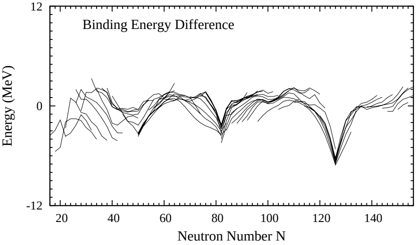
- even-even nuclei
- intrinsic shapes constrained to axial symmetry
- projection on particle number and angular momentum
- mixing of configurations with different intrinsic deformation
- Skyrme interaction SLy4 + density-dependent zero-range pairing interaction

Masses from self-consistent mean-field calculations

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

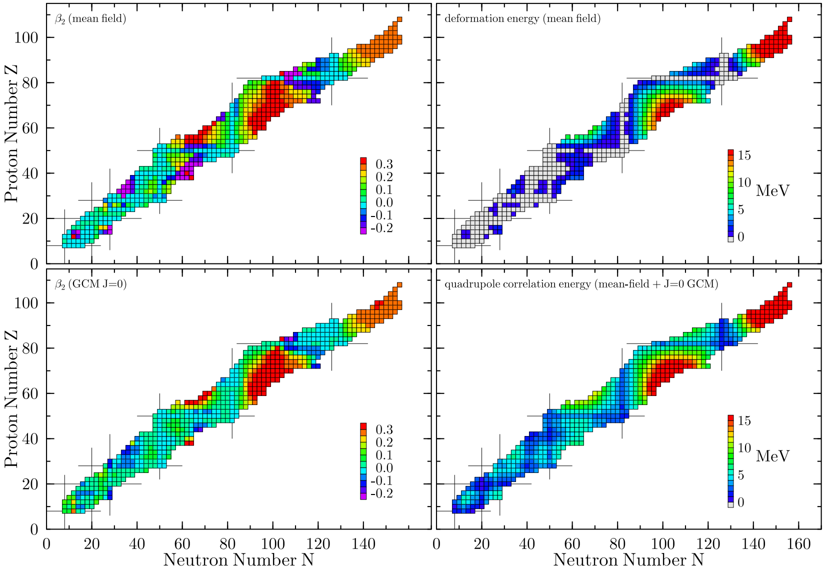


G. F. Bertsch, B. Sabbey, M. Uusnäkki, Phys. Rev. C 71 (2005) 054311.

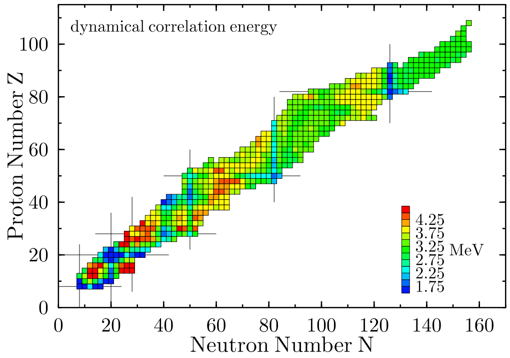


- Skyrme interaction SLy4 + density-dependent pairing interaction
- other parameterizations give qualitatively similar results
- Wrong trend with A
- overestimated shell effects visible at $N = 20$, 50, 82 and 126
- missing Wigner energy
- The slightly wrong trend with mass and isospin can be removed 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.
- But what about the arches?

Intrinsic Deformation and Quadrupole Correlation Energy

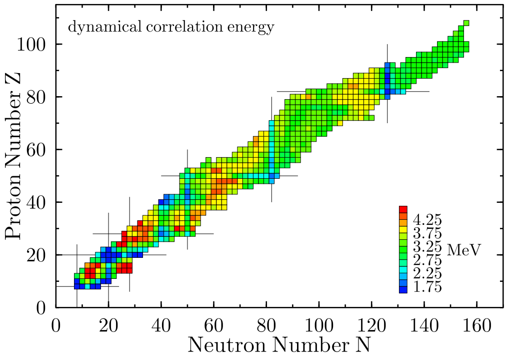


M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

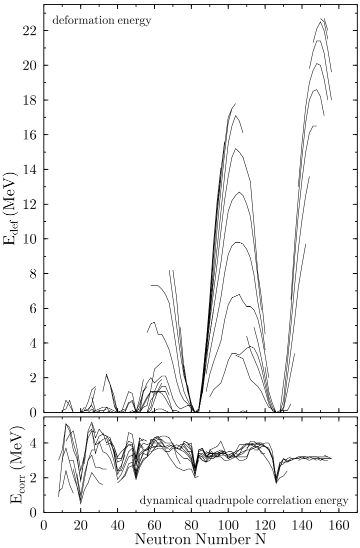


M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

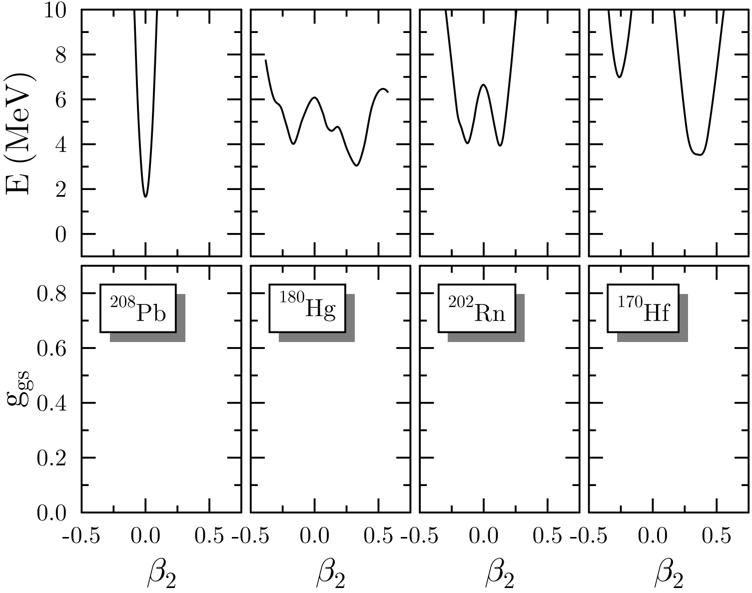
Static and Dynamic Quadrupole Correlation Energies



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

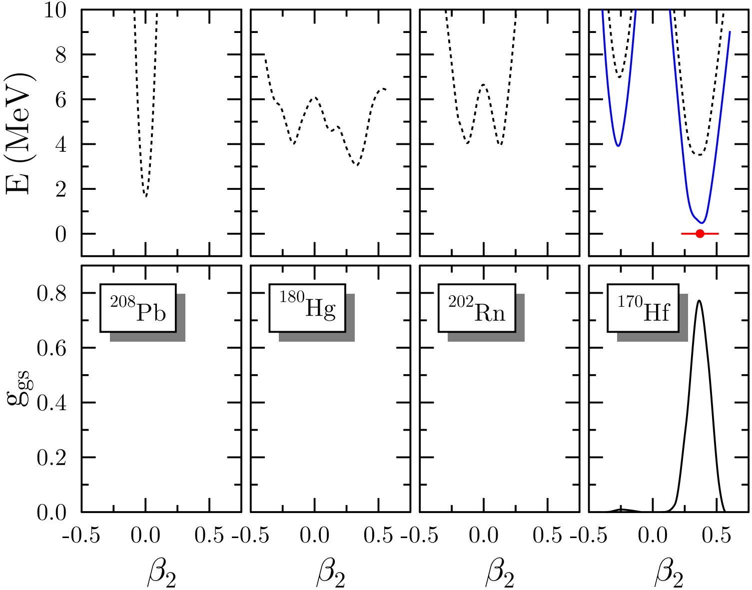


Typical situations



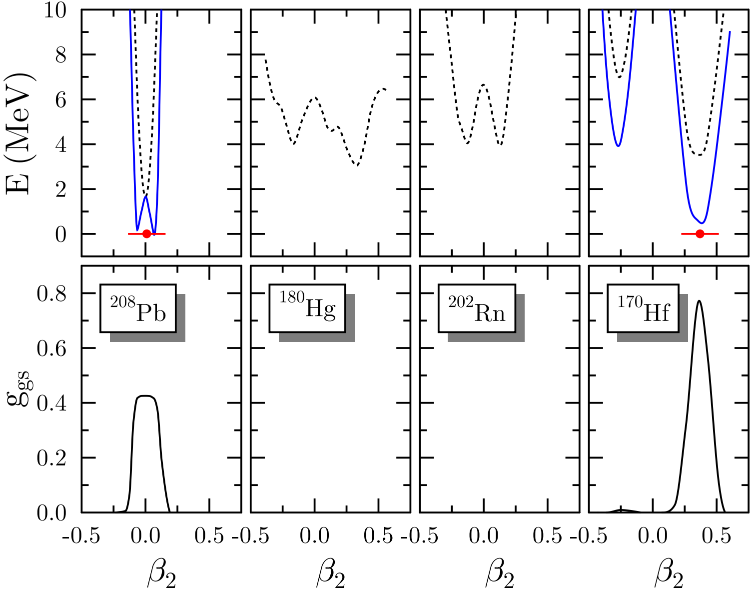
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Typical situations



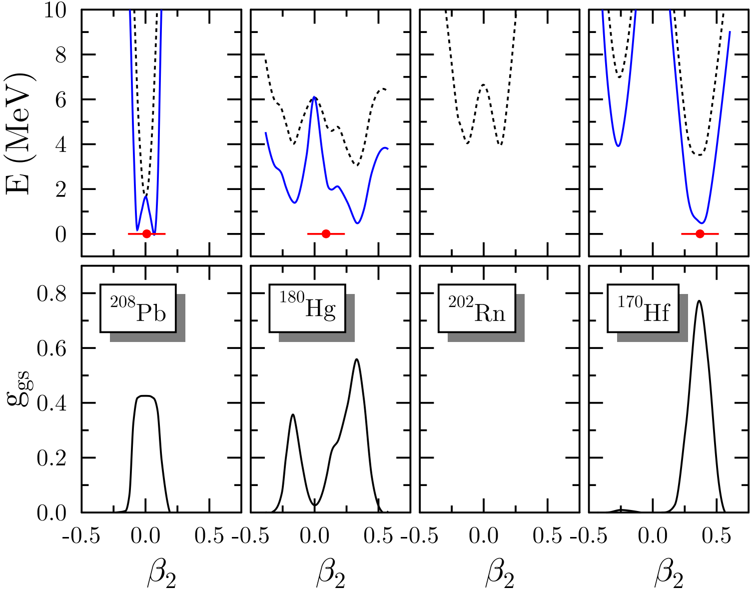
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Typical situations

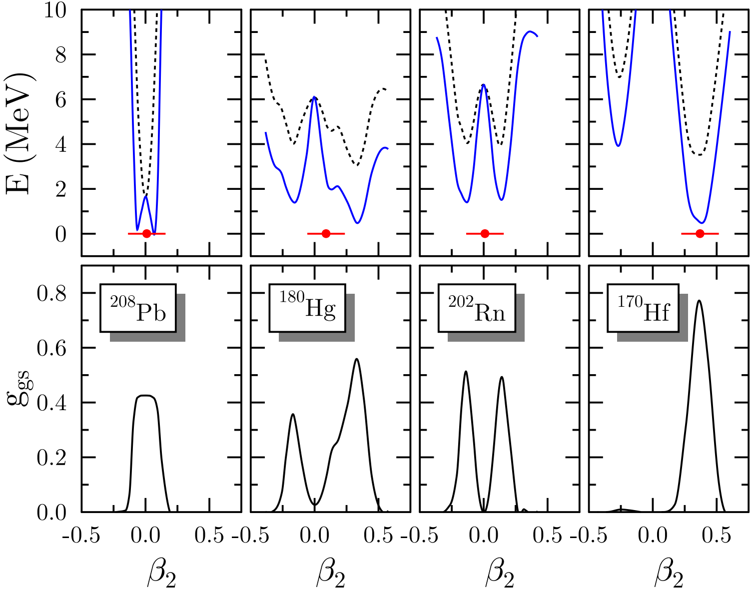


M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Typical situations

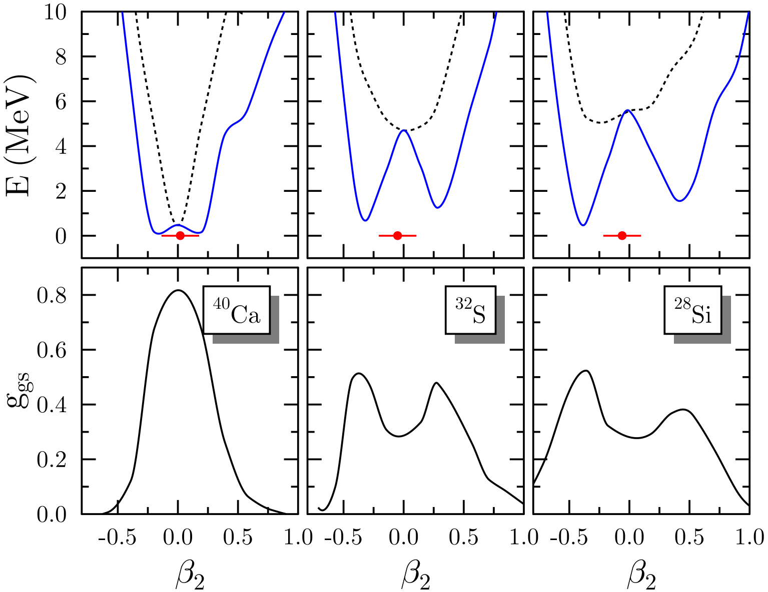


M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322



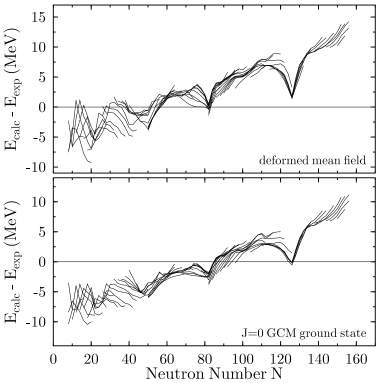
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Other typical situations



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

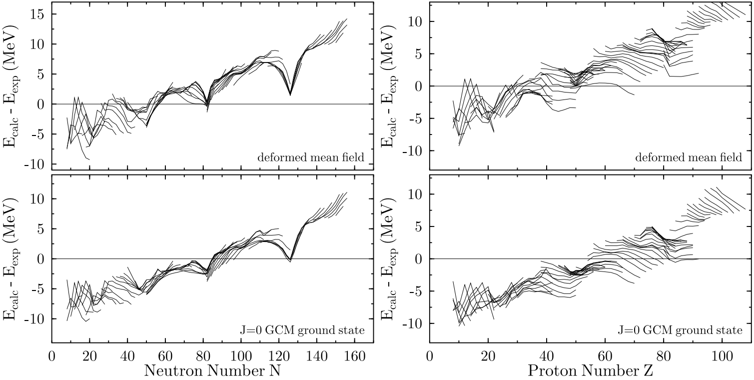
Mass residuals



-
-

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

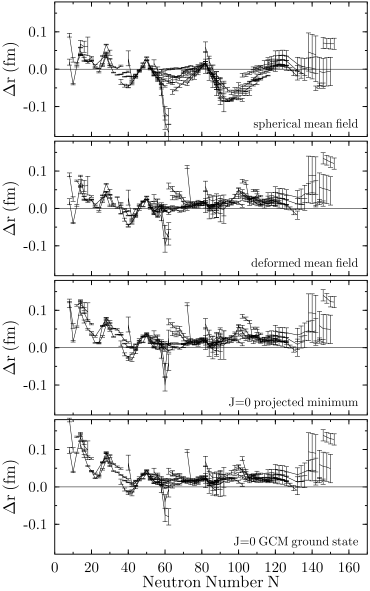
Mass residuals



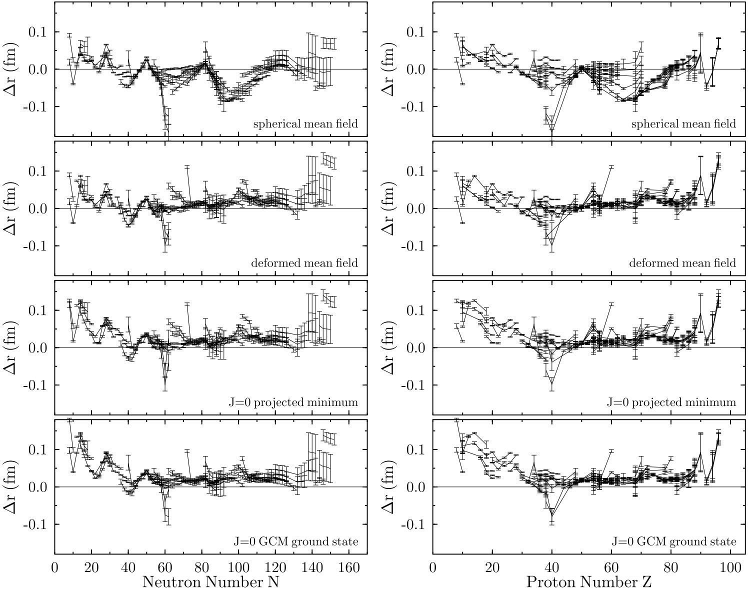
- Shell effects are not overestimated in general, they are overestimated for neutrons
- This might well be a problem with the effective interaction, not so much with large missing correlations

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

Consistency check: rms charge radii



Consistency check: rms charge radii



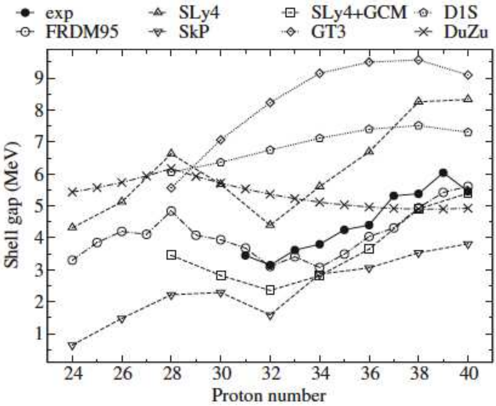
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

How is the evolution of shell structure related to systematics of masses?

PRL 101, 052502 (2008) PHYSICAL REVIEW LETTERS week ending 1 AUGUST 2008

Evolution of the $N = 50$ Shell Gap Energy towards ^{78}Ni

J. Hakala, S. Rahaman, V.-V. Elomaa, T. Eronen, U. Hager,* A. Jokinen, A. Kankainen, I. D. Moore, H. Penttilä, S. Rinta-Antila,† J. Rissanen, A. Saastamoinen, T. Sonoda,‡ C. Weber, and J. Äystö§
Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland
(Received 20 March 2008; published 31 July 2008)



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

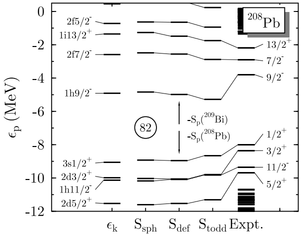
Empirical single-particle energies vs. eigenvalues of the single-particle Hamiltonian

- It is customary to discuss shell structure in terms of the spectrum of eigenvalues of the single-particle Hamiltonian ϵ_μ in even-even nuclei

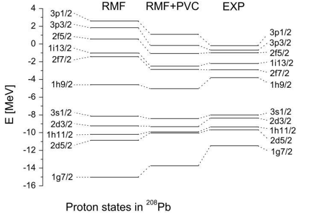
$$\hat{h}\,\psi_\mu = \epsilon_\mu\,\psi_\mu$$

  Koopman's theorem states that ϵ_μ is equal to the one-nucleon separation energy if
  - The nucleus is perfectly described by a HF state (i.e. that there are no correlations of any kind whatsoever)
  - rearrangement and polarization effects changing the single-particle wave functions when adding or removing a particle are negligible
- The structure of the mean-field state of an even- even and an odd-A nucleus is different (blocking, additional mean fields that originate from interactions involving currents and spin densities in the odd-A nucleus, ...), there always are correlations and they will give a different contribution to the binding in even-even and odd-A nuclei, etc.

K. Rutz, M. B., P.-G. Reinhard, J. A. Maruhn and W. Greiner, Nucl. Phys. A634 (1998) 67



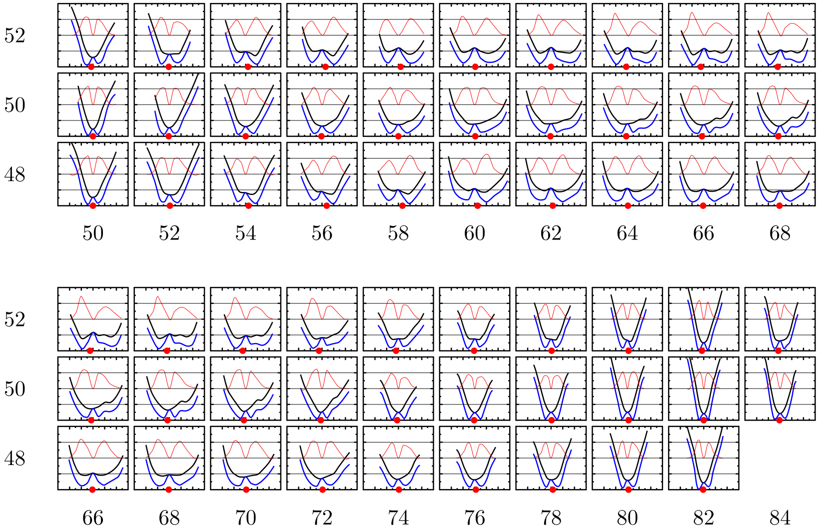
E. Litvinova, P. Ring, Phys. Rev. C 73 (2006) 044328



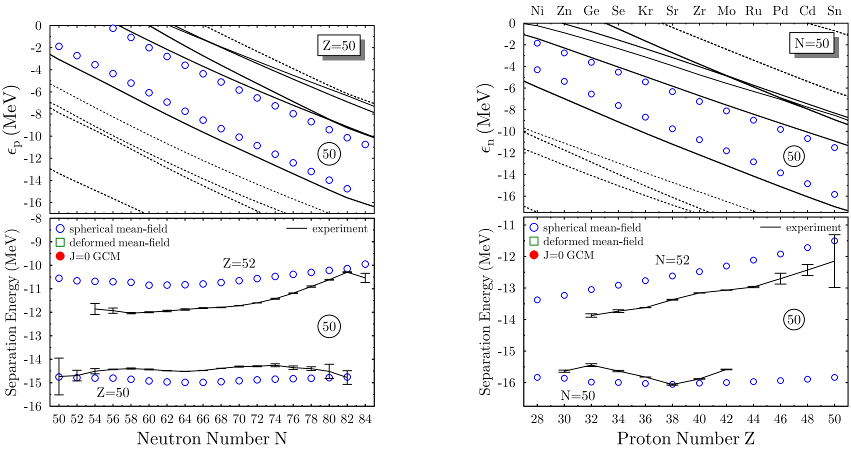
both calculations use a relativistic mean-field model

Collectivity-enhanced quenching of signatures of shell closures

M. B., G. F. Bertsch, P.-H. Heenen, unpublished



Eigenvalues of the single-particle Hamiltonian vs. S_{2q}

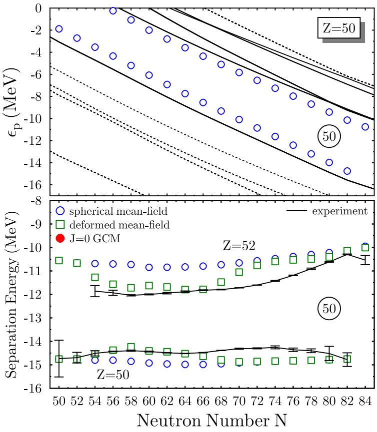


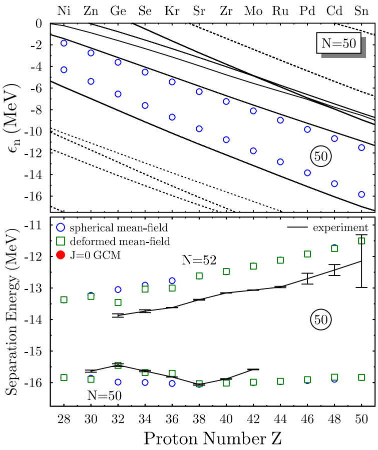
lower panel: $-S_{2p}(Z=50, N)/2$
The global linear trend is taken out subtracting
$\frac{N-82}{2}\,[S_{2p}(Z{=}50, N{=}50) - S_{2p}(Z{=}50, N{=}82)]$
using the spherical mean-field S_{2p}

lower panel: $-S_{2n}(Z, N=50)/2$
The global linear trend is taken out subtracting
$\frac{N-50}{2}\,[S_{2n}(Z{=}28, N{=}50) - S_{2n}(Z{=}50, N{=}50)]$
using the spherical mean-field S_{2n}

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

Eigenvalues of the single-particle Hamiltonian vs. S_{2q}



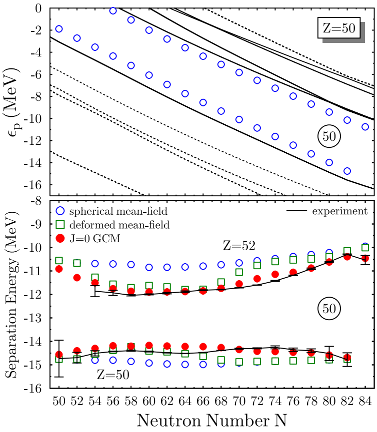


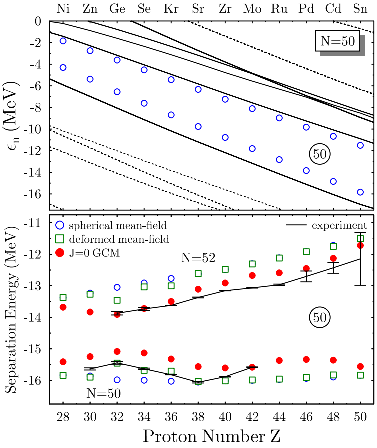
lower panel: $-S_{2p}(Z=50, N)/2$
The global linear trend is taken out subtracting
$\frac{N-82}{2}\,[S_{2p}(Z{=}50, N{=}50) - S_{2p}(Z{=}50, N{=}82)]$
using the spherical mean-field S_{2p}

lower panel: $-S_{2n}(Z, N=50)/2$
The global linear trend is taken out subtracting
$\frac{N-50}{2}\,[S_{2n}(Z{=}28, N{=}50) - S_{2n}(Z{=}50, N{=}50)]$
using the spherical mean-field S_{2n}

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

Eigenvalues of the single-particle Hamiltonian vs. S_{2q}





lower panel: $-S_{2p}(Z=50,N)/2$
The global linear trend is taken out subtracting
$\frac{N-82}{2}\,[S_{2p}(Z{=}50,N{=}50)-S_{2p}(Z{=}50,N{=}82)]$
using the spherical mean-field S_{2p}

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

lower panel: $-S_{2n}(Z,N=50)/2$
The global linear trend is taken out subtracting
$\frac{N-50}{2}\,[S_{2n}(Z{=}28,N{=}50)-S_{2n}(Z{=}50,N{=}50)]$
using the spherical mean-field S_{2n}

2.N:5 Nuclear Physics A318 (1979) 253–268; © North-Holland Publishing Co., Amsterdam

ALPHA DECAY PROPERTIES OF NEW PROTACTINIUM ISOTOPES

K.-H. SCHMIDT, W. FAUST and G. MÜNZENBERG
Gesellschaft für Schwerionenforschung, GSI, Darmstadt Germany

H.-G. CLERC, W. LANG, K. PIELENZ, D. VERMEULEN and H. WOHLFARTH
Institut für Kernphysik, Technische Hochschule Darmstadt, Germany

and

H. EWALD and K. GÜTTNER
II. Physikalisches Institut, Universität Giessen, Germany

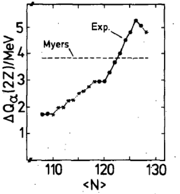


Fig. 12. Differences $\Delta Q_\alpha(2Z)$ of the Q_α values of the 84- and the 82-proton isotopes for different neutron numbers ($\langle N\rangle \doteq N_{\text{mother}}-1$). The prediction of Myers [16]) is compared with the experimental data. If no experimental values are known, the systematic of Viola *et al.* [18]) is used (stars).

Fig. 12 demonstrates the analogous influence of the 126-neutron shell on the 82-proton shell strength. In this case, the differences of the Q_α values of the polonium and lead isotopes are shown as a function of the mean neutron number $\langle N\rangle$.

The observed mutual influence of the two shells is qualitatively expected from theoretical considerations [19]). For both protons and neutrons in the doubly magic ^{208}Pb the Fermi surface separates low-spin and high-spin single-particle states. The different spacial distributions of the appropriate wave functions may cause a coupling of the neutron and the proton levels by means of the total nuclear potential.

Nuclear Physics A399 (1983) 11–50

MUTUAL SUPPORT OF MAGICITIES AND RESIDUAL EFFECTIVE INTERACTIONS NEAR ^{208}Pb

N. ZELDES†, T. S. DUMITRESCU†† and H. S. KÖHLER†††
Niels Bohr Institute and Nordita, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

Received 1 November 1982

Abstract: We summarize experimental evidence in the lead region on the increased stability associated with neutron magic number when the proton number is magic, and vice versa. The effect is interpreted in the framework of the nuclear shell model with empirical effective interactions. Its relation to spherical Hartree-Fock calculations is pointed out and used to test Skyrme-type forces. None of the considered Skyrme interactions reproduce the effect.

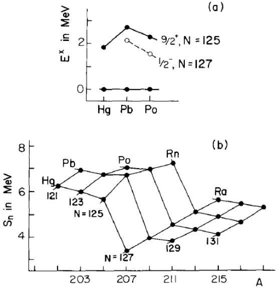
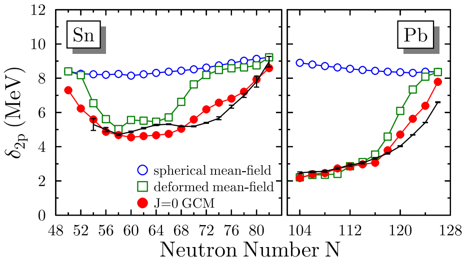
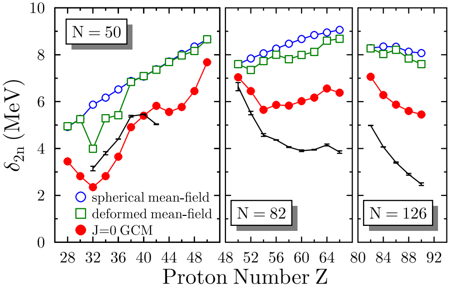


Fig. 1. (a) Excitation energies of single-neutron $\frac{9}{2}^+$ levels in $N = 125$ nuclei and of single neutron-hole $\frac{1}{2}^-$ levels in $N = 127$ nuclei. Data from Table of Isotopes [4]) and more recent literature [^{211}Po, ref. [5])]. (b) S_n systematics of odd-N nuclei near ^{208}Pb. Data from The 1977 Atomic Mass Evaluation [6]) and more recent literature [^{207}Hg, ref. [7])].

Two-nucleon gaps





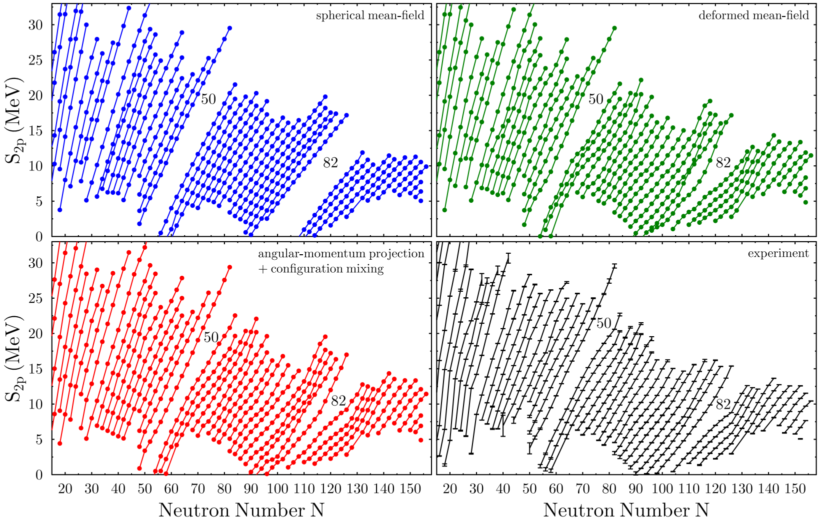
$$\delta_{2p}(N,Z) = S_{2p}(Z,N) - S_{2p}(Z-2,N)$$
$$\delta_{2n}(N,Z) = S_{2n}(Z,N) - S_{2n}(Z,N-2)$$

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

experimental values shown here include more recent data than the plots in the papers

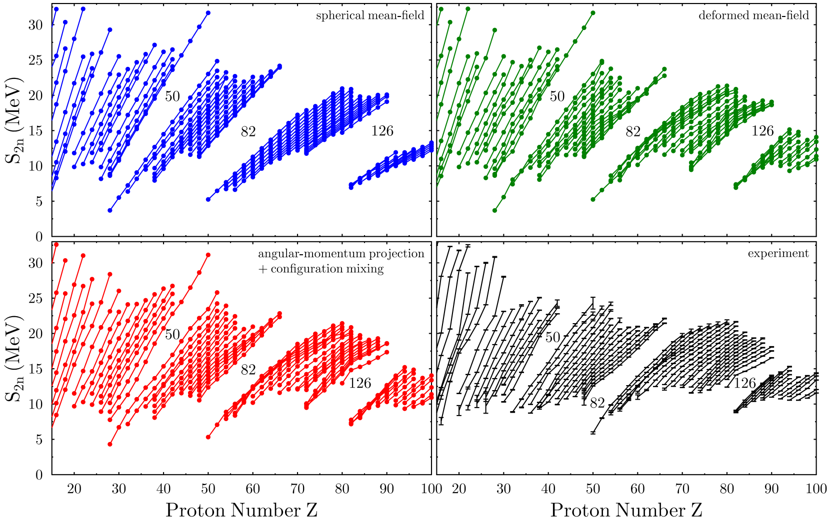
Collectivity-enhanced quenching of signatures of shell closures

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312



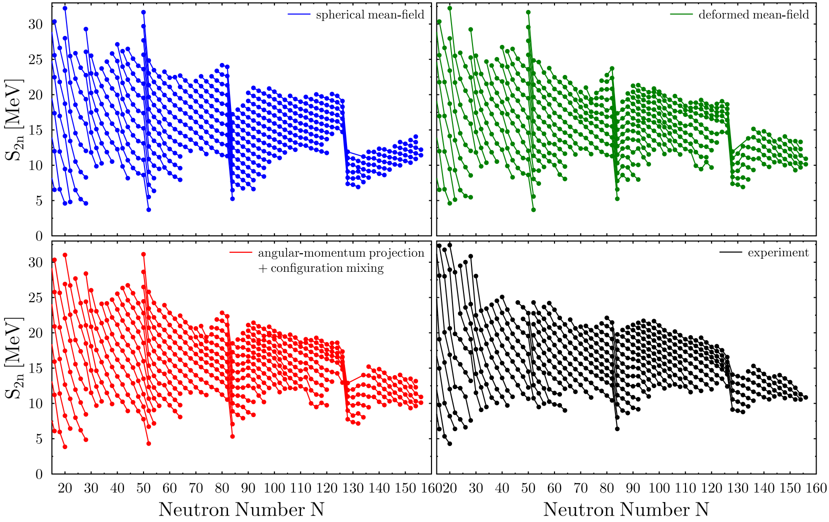
Collectivity-enhanced quenching of signatures of shell closures

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312



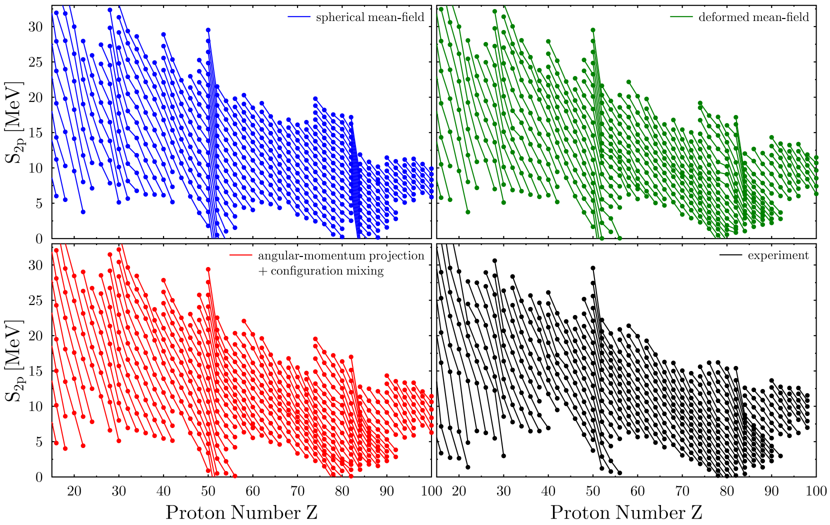
Collectivity-enhanced quenching of signatures of shell closures

M. B., G. F. Bertsch, P.-H. Heenen, unpublished



Collectivity-enhanced quenching of signatures of shell closures

M. B., G. F. Bertsch, P.-H. Heenen, unpublished



Summary and outlook

Nuclei are complex systems, oversimplistic models are prone to fail:

- Do not expect the conditions for the validity of Koopman's theorem to be fulfilled in nuclei.
- There is no Koopman's theorem for two-nuclon separation, but even when trying to approximate two-nuclon separation by two times the eigenvalues of the single-particle Hamiltonian, they are not comparable.
- Collectivity enhanced quenching of the separation energies has to be distinguished from real quenching of the spherical shells

Homework:

- improve energy functional (central and spin-orbit parts first, then tensor (cf. P.-H. Heenen's talk)
- improve modeling of pairing
- improve methodology to calculate odd-A nuclei on the mean-field level and beyond by projected GCM
- test other correlation modes [pairing (cf. L. Egido's talk); octupole, ...]
- look into other observables to establish internal consistency

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

Benoît Avez	CEN Bordeaux Gradignan, France
Benjamin Bally	CEN Bordeaux Gradignan, France
Karim Bennaceur	IPN Lyon, France
George F. Bertsch	INT Seattle, USA
Thomas Duguet	Irfu, CEA Saclay, France
Paul-Henri Heenen	Université Libre de Bruxelles, Belgium