Shell structure of superheavy elements

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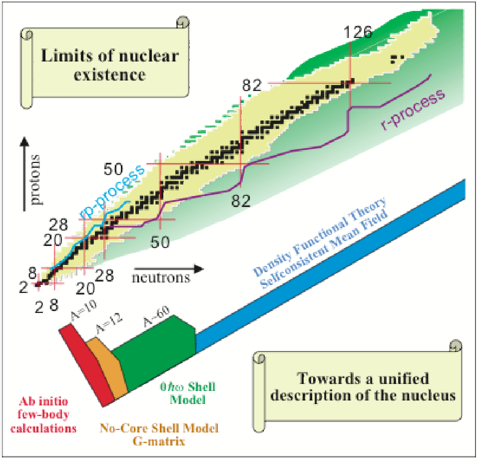
Workshop on the spectroscopy of transactinide nuclei
Espace de Structure Nucleéaire Théorique,
DAPNIA/SPhN, CEA Saclay, France, 29. January 2007

Setting the stage

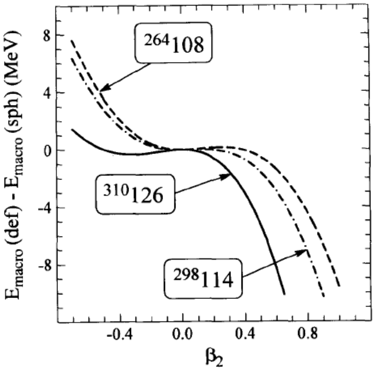


Definition

Superheavy elements (SHE) are nuclei with vanishing liquid-drop fission barrier

- Coulomb repulsion from large charge number Z stronger than the surface tension
- stabilized by quantum shell effects only
- almost all properties are determined by the variation of shell structure with N, Z and deformation

S. Ćwiok, J. Dobaczewski, P.–H. Heenen, P. Magierski, W. Nazarewicz, Nucl. Phys. A611 (1996) 211



macroscopic fission barrier

Single-particle energies – a word of caution

- Shell structure is usually discussed in terms of the spectrum of eigenvalues of the single-particle Hamiltonian ϵ_μ in even-even nuclei

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

which reflect the mean field in the nucleus.

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- Shell structure is usually discussed in terms of the spectrum of eigenvalues of the single-particle Hamiltonian ϵ_μ in even-even nuclei

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  which reflect the mean field in the nucleus.
- In spite of Koopman's theorem, the ϵ_μ provide at best a zeroth-order approximation to experimental single-particle energies, that are obtained as separation energies (i.e. differences of total binding energies), and should not be directly compared with them.
- The reason is that the two many-body states that have to be compared to determine the experimental single-particle energy are significantly different.
- Rearrangement effects of the mean field, the different structure of the mean-field state of an even-even and an odd-A nucleus (blocking, additional mean fields that originate from interactions involving currents and spin densities in the odd-A nucleus from broken time-reversal invariance, . . .) different correlations beyond the mean field in magic and non-magic nuclei add significant corrections to the observable single-particle energy.

Spherical shell structure: predictions for magic numbers

The challenges

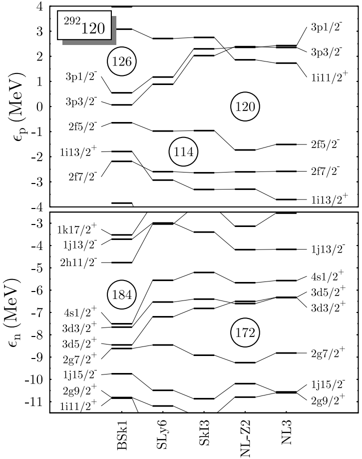
- large density of single-particle levels around the Fermi energy
- strong Coulomb fields try to polarize the nucleus

The results

- the traditional, sometimes dogmatic, prediction for spherical SHE by the canonical parameterizations of the standard single-particle potentials (Nilsson, Folded-Yukawa, Woods-Saxon) is $Z = 114$, $N = 184$
- some heretics got $Z = 126$ with different fit strategies of the same phenomenological potentials, but were first ignored and afterwards forgotten
- It was also noted that the size of the $Z = 114$ shell depends on the surface thickness of Woods-Saxon and Folded-Yukawa potentials.
- self-consistent models (nearly) consistently give different shell closures: $Z = 120$, 126 and $N = 172$, 184
- for reasons to be explained below, one does not get all combinations of those, though

Single-particle spectra. – A multitude of possible shell closures

K. Rutz, M. B., T. Bürvenich, T. Schilling, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 56 (1997) 238.
M. B., K. Rutz, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 60 (1999) 034304.



- BSk1, SLy6; SkI3: Skyrme
- NL-Z2, NL3: RMF

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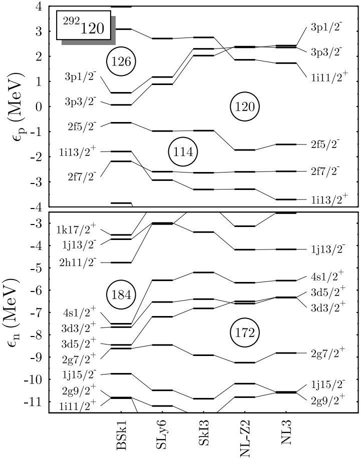
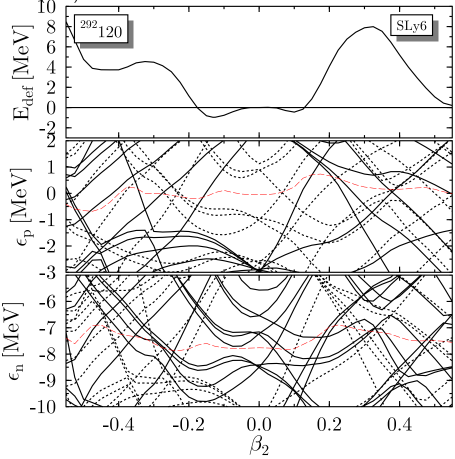


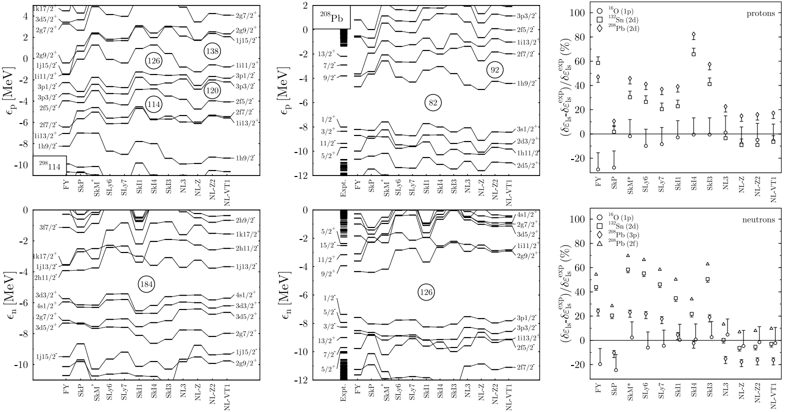


- BSk1, SLy6; SkI3: Skyrme
- NL-Z2, NL3: RMF

- large gaps at sphericity do not necessarily imply a spherical ground state

How realistic are the predictions for spherical shell structure?

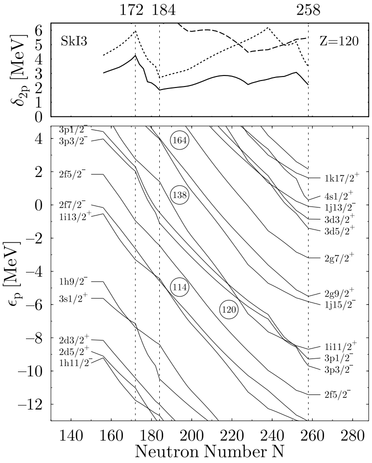
M. B., K. Rutz, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 60 (1999) 034304.

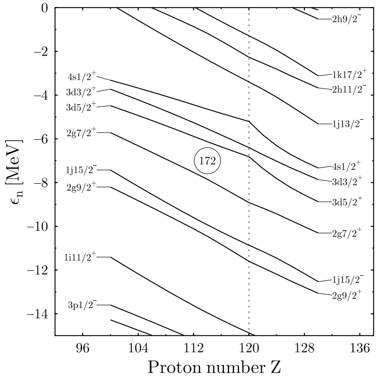


$\Rightarrow$ benchmark shell structure for "lighter" nuclei

- $Z = 114$ requires large spin-orbit splitting of the $2f$ state
- models which give a pronounced $Z = 114$ shell closure overestimate the known spin-orbit splittings in heavy nuclei

Evolution of spherical single-particle spectra – shell quenching



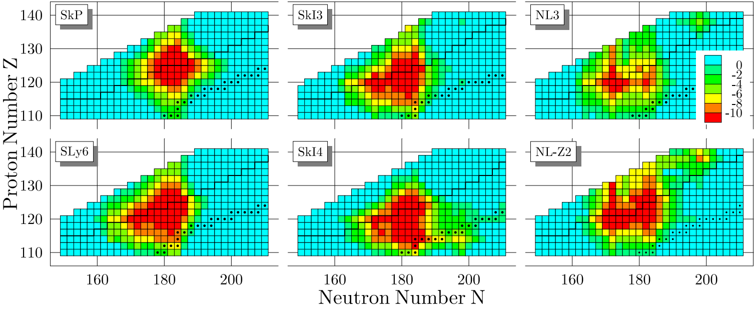


M. B., K. Rutz, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 60 (1999) 034304.

- Shell closures for one nucleon species depend strongly on the number of the other species
- The effect predicted by existing mean-field interactions is much stronger for SHE than for light elements – where the observed shell quenching is almost always underestimated

How important are the actual shell closures?

M. B., W. Nazarewicz, P.-G. Reinhard, Phys. Lett. B515 (2001) 42.



- Total shell correction energy extracted from fully self-consistent calculations assuming spherically symmetric shapes
- Shell correction at deformed shapes might be even larger, which will lead to deformed ground states as there is no liquid drop barrier.
- This is the case for the island of deformed SHE around ^{270}Hs, which is not visible on the plot
- Very extended region of shell stabilization of spherical shapes that is in most cases spread over *all* predicted spherical shell closures.

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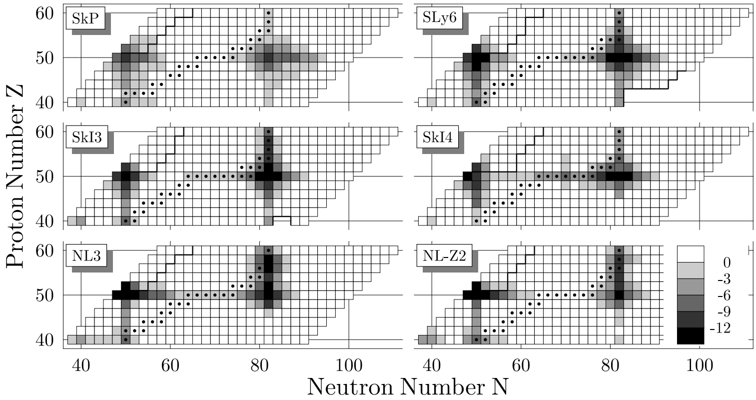
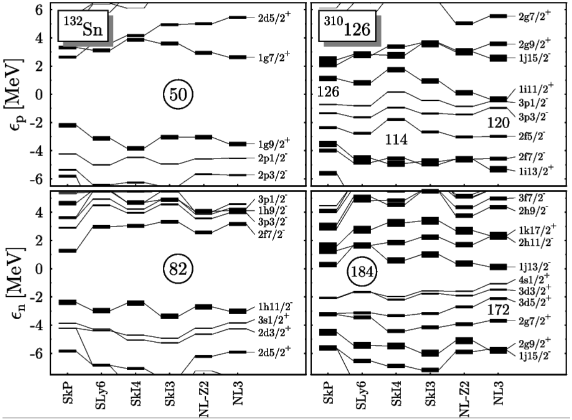


- Extra binding from shell effects is much more localized in light nuclei

Why are the actual shell closures less important in SHE?

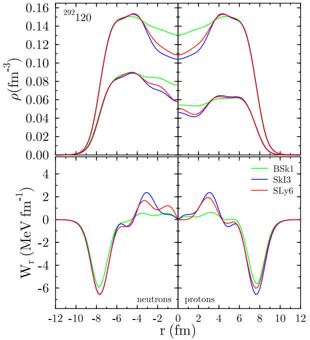
M. B., W. Nazarewicz, P.-G. Reinhard, Phys. Lett. B515 (2001) 42.



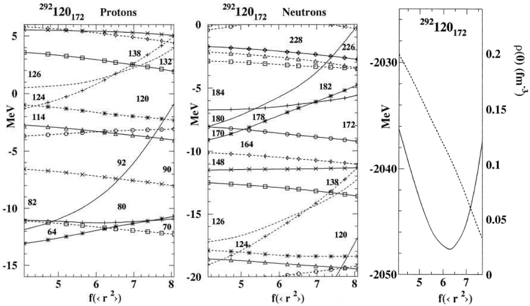
- All possible shell closures are in a region of low-j levels amidst a vast sea of highly degenerated high-j levels
- The extra binding from shell effects ("shell correction energy") is not very sensitive to the actual position of the low-j levels

Polarization effects at spherical shape

M. B., K. Rutz, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 60 (1999) 034304.



J. Dechargé, J.-F. Berger, K. Dietrich, M. S. Weiss, Phys. Lett. B451 (1999) 275

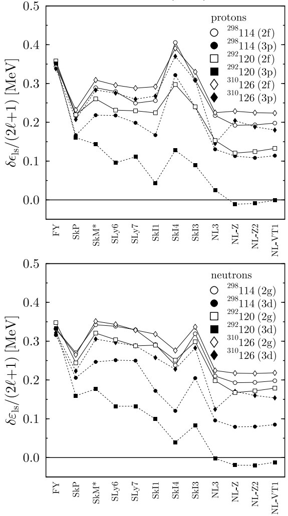


- calculation with Skyrme interactions in spherical symmetry
- semi-bubble density profile leads to anomalies of the spin-orbit splittings (they may disappear or even reverse for certain levels)

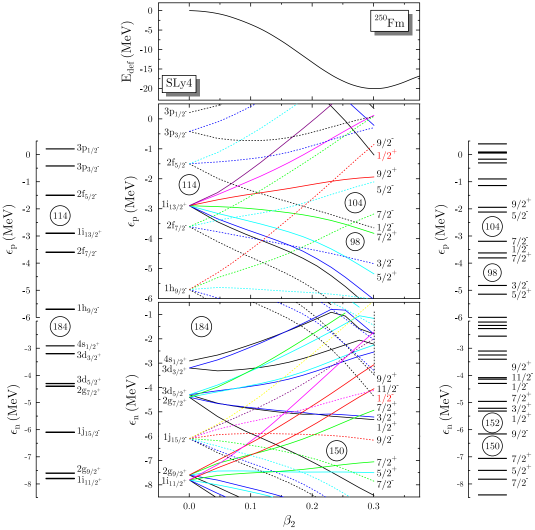
- calculations with the Gogny force D1s and a constraint on the density profile
- the single-particle spectra are very sensitive to the density profile
- the effect is triggered by the non-occupation of low-j states located inside the nucleus, and amplified by the Coulomb interaction

Polarization effects at spherical shape: consequences for spin-orbit splittings

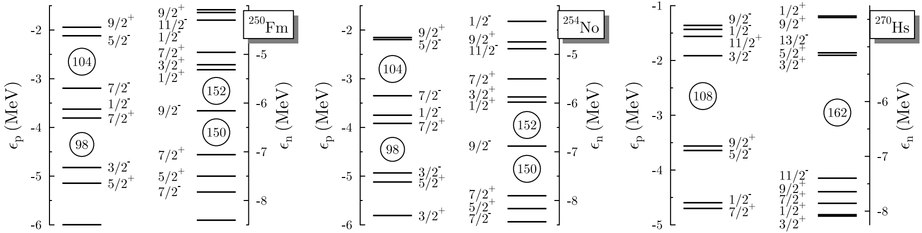
M. B., K. Rutz, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 60 (1999) 034304.



- As a consequence of the large polarisation of the density distribution, the spin-orbit splittings become strongly state dependent, and even might revert for some small-j levels.



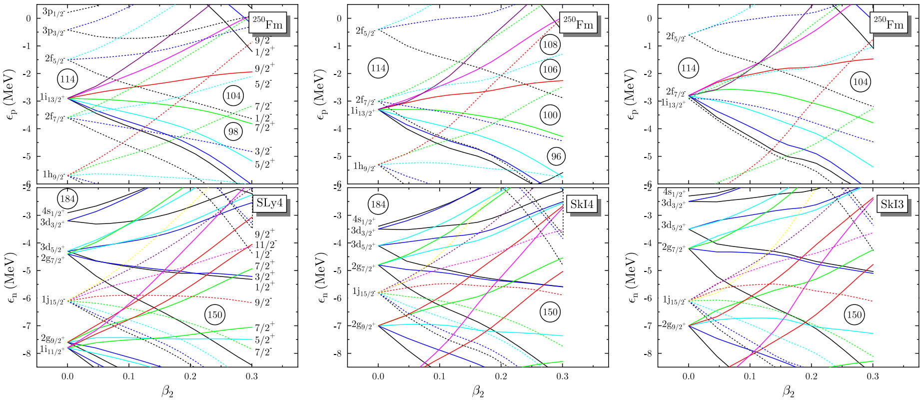
- the nucleus goes from a spherical configuration with high level density to a deformed configuration with low level density.
- As the "liquid-drop" energy surface is more or less flat, the actual deformation is determined entirely by the favorable shell structure.
- The deformation energy reflects the change in "shell correction" energy.



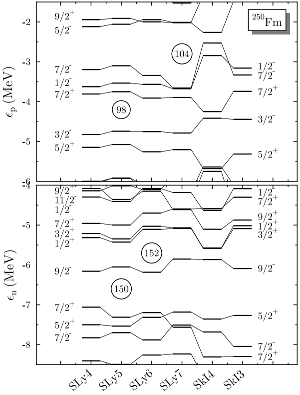
Adding nucleons shifts the deformed shell structure as

- the spherical shell structure changes
- the ground-state deformation slightly changes. The nucleus rearranges itself for the maximal gain in binding energy that is possible for a given number of occupied levels.

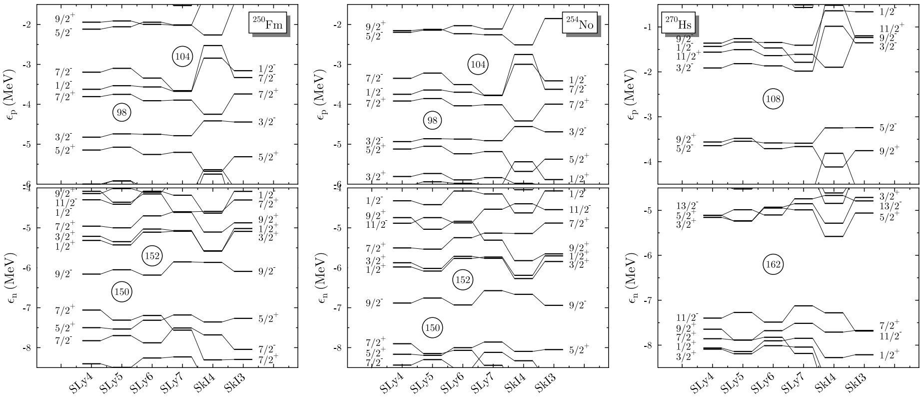
Ground-state deformation: dependence on the effective interaction



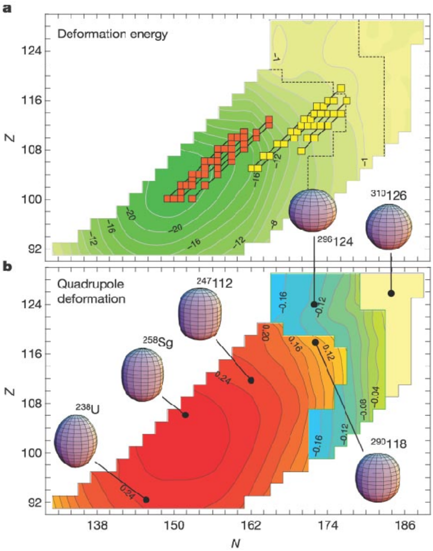
Shell structure at the deformed ground state



Shell structure at the deformed ground state



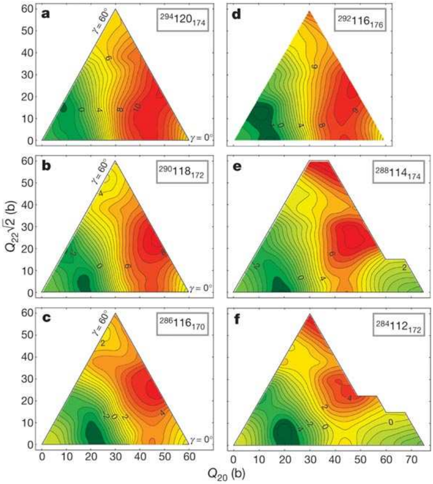
S. Ćwiok, P.-H. Heenen, W. Nazarewicz, Nature 433 (2005) 709



- predictions with the Skyrme interaction SLy4
- most other interactions give qualitatively similar results for the systematics, alyjough the predictions for a particular nucleus in the transitional region might be very different.
- the α-decay chains of SHE produced in cold-fusion reactions (GSI, RIKEN) are located in a region of strong deformation
- the α-decay chains of SHE produced in hot-fusion reactions (FLNR) start to explore a region of transitional nuclei

Deformation – transitional region

S. Ćwiok, P.-H. Heenen, W. Nazarewicz, Nature 433 (2005) 709



predictions with the Skyrme functional SLy4

- nuclei in the transitional region are often γ soft
- the (static) fission barrier is also through triaxial shapes

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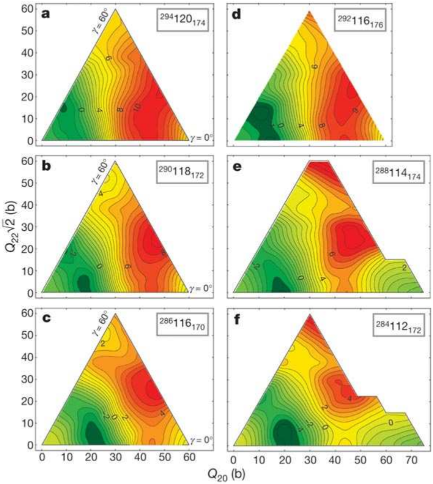
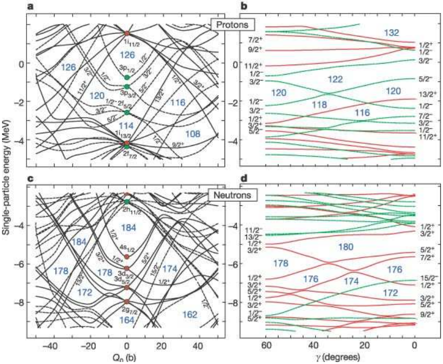
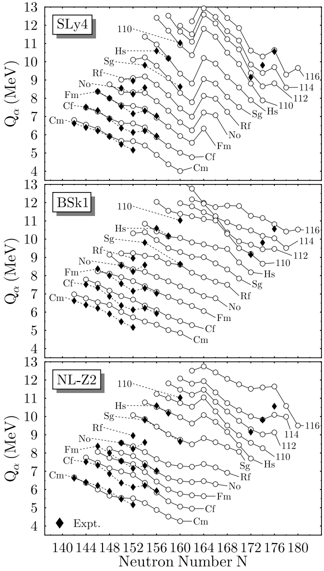


predictions with the Skyrme functional SLy4

- nuclei in the transitional region are often γ soft
- the (static) fission barrier is also through triaxial shapes
- the low density of single-particle levels persists for triaxial shapes



Shell effects in the nuclear masses of SHE: Q_α values of even-even nuclei



- Skyrme interactions SLy4 and BSk1 and finite-range relativistic Hartree Lagrangian NL-Z2
- nobody is perfect
- the global mass fit BSk1 performs less well for superheavy elements than the traditional energy functionals SLy4 and NL-Z2
- deformed shell closure predicted for $N = 150$, but experiment says $N = 152$

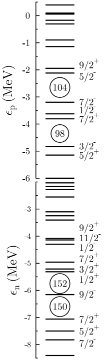
plot: M. B., P.-H. Heenen, P.-G. Reinhard, Rev. Mod. Phys. 75 (2003) 121.

data SLy4: S. Ćwiok, W. Nazarewicz, and P. H. Heenen, Phys. Rev. Lett. 83, (1999) 1108.

data BSk1: M. Samyn, S. Goriely, P. -H. Heenen, J. M. Pearson, F. Tondeur, Nucl. Phys. A700 (2002) 142

data NL-Z2: M. B., Phys. Rev. C 61 (2000) 031302(R)

How to use spectroscopy of deformed nuclei to learn about spherical shell structure



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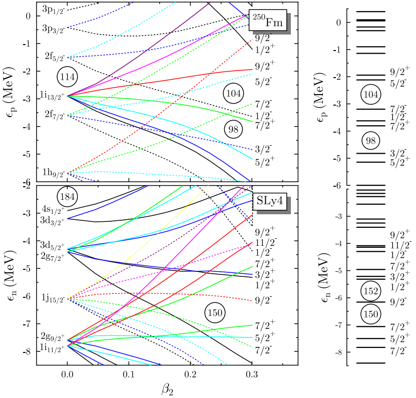

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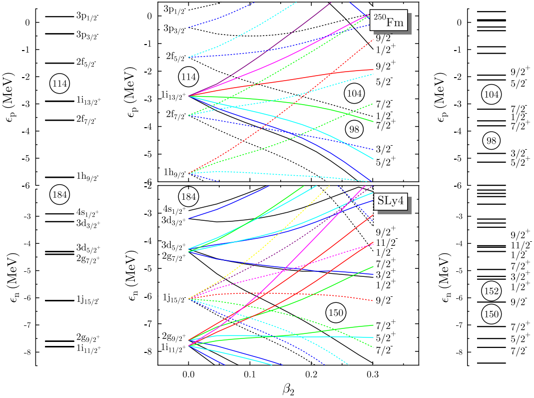
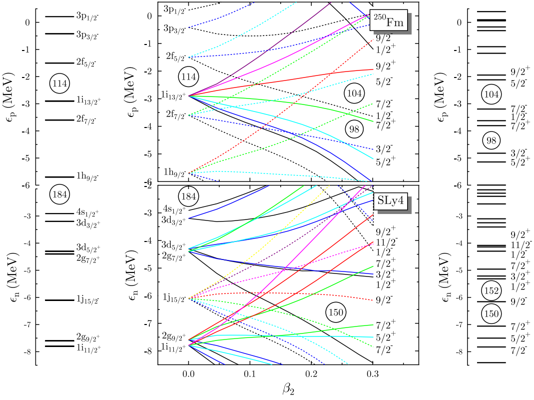
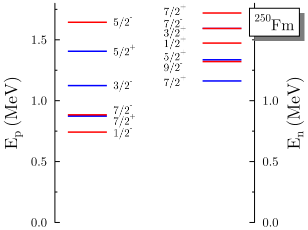


How to use spectroscopy of deformed nuclei to learn about spherical shell structure



- Single-particle states originating from levels above and below the potential spherical $Z = 114$ (sub-)shell closure are close to the Fermi energy for the deformed ground states of SHE in the $Z \approx 100$, $N \approx 150$ region. The low-j levels that will determine the size of the predicted shell gaps at $Z = 120$ and $Z = 126$ are out of reach as they are pushed up with deformation.

. . . but these will be one-quasiparticle states in odd-A nuclei



Perturbative approach: look at one-quasiparticle energies that are eigenvalues of the HFB Hamiltonian

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E_\mu \begin{pmatrix} U \\ V \end{pmatrix}$$

red (blue) levels correspond to single-particle states above (below) the Fermi surface

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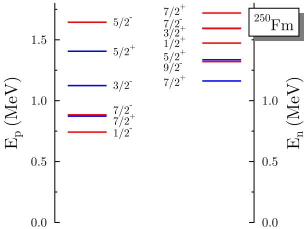

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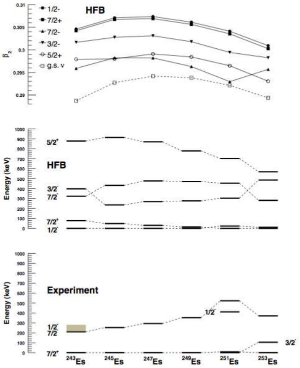
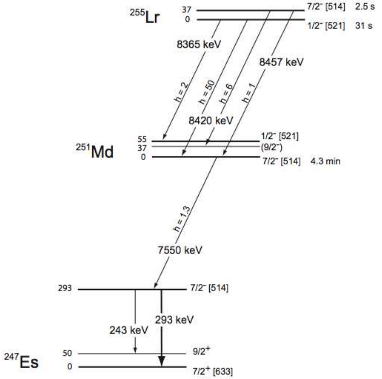
A. Chatillon, Ch. Theisen, ..., Eur. Phys. J. A **30** (2006)

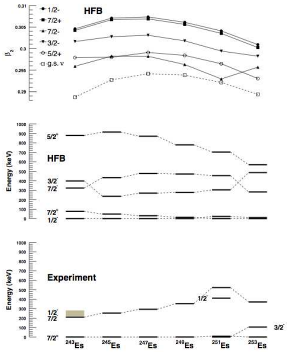


Better you do the real thing: calculate the one-quasiparticle states self-consistently solving the HFB equations for all possible (and reasonable) blocked configurations and use the differences of their total binding energies

Deformed shell structure I. Quasiparticle states in odd-A nuclei

A. Chatillon, Ch. Theisen, . . . , P. Bonche, P.-H. Heenen, M. B., . . . , Eur. Phys. J. A **30** (2006)

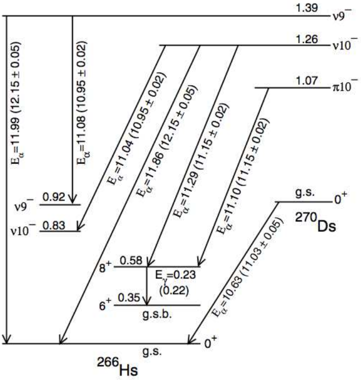




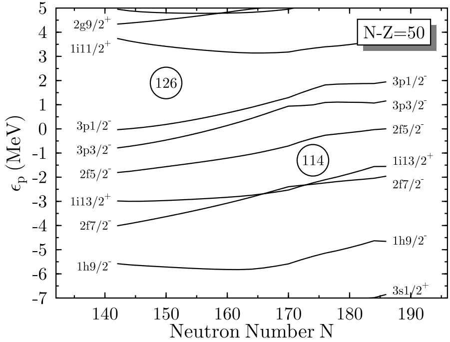
- available data in the $A \approx 250$ region are incompatible with a major spherical shell closure at $Z = 114$
- the data suggest that relative shifts of spherical single-particle levels of several 100 keV are necessary

Deformed shell structure II. High-K isomers

- two-quasiparticle excitations on top of the deformed ground state of an even-even superheavy nucleus might lead to long living high-K isomers
- Like one-quasiparticle states in odd-A isotopes they provide information about the relative distance of single-particle levels
- some cases are known from experiment: ^{254}No, ^{266}Hs, ^{270}Ds
- F. R. Xu, E. G. Zhao, R. Wyss, P. M. Walker, Phys. Rev. Lett. 92 (2004) 252501 point out that high-K isomers might have much longer lifetimes than the (zero-quasiparticle) "ground state".

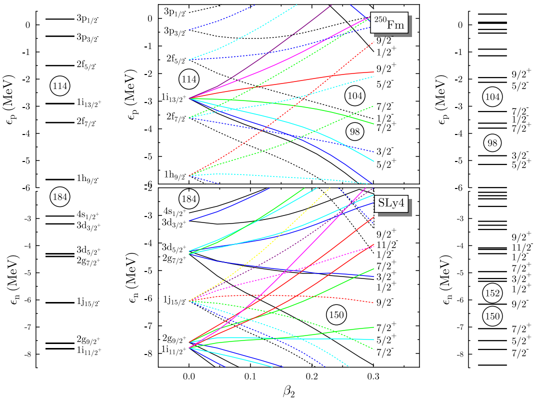


A word of caution.



- Plot: Spherical single-particle energies of protons at spherical shape along the $N - Z = 50$ α-decay chain
- Single-particle energies predicted by self-consistent mean-field models evolve rapidly in SHE, correlated to changes in the density profiles, so what we learn about the magic numbers in the spherical single-particle spectrum in a non-magic nucleus might not be valid anymore for nuclei that actually have this magic number.

Deformed shell structure at finite angular momentum: rotational bands



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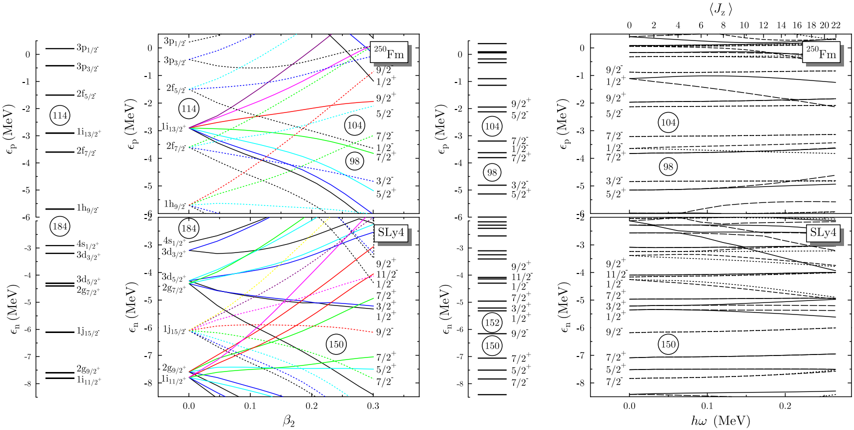
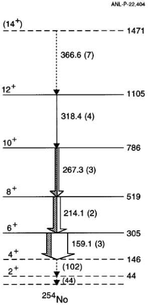


P. Reiter *et al.*, Phys. Rev. Lett. 82 (1999) 509



- The pioneering band seen for ^{254}No triggered instant calculations by everyone having a cranked mean-field code

Rotational bands

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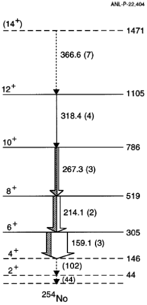
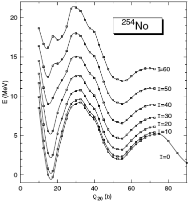
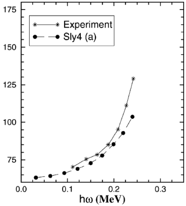


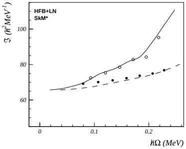
J. L. Egido, J. L. Robledo, Phys. Rev. Lett. 85 (2000) 1198



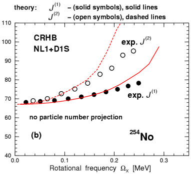
T. Duguet, P. Bonche, P.-H. Heenen, Nucl. Phys. A 679 (2001) 427



H. Laftchiev, D. Samsœn, P. Quentin, J. Piperova, Eur. Phys. J. A 12 (2001) 155



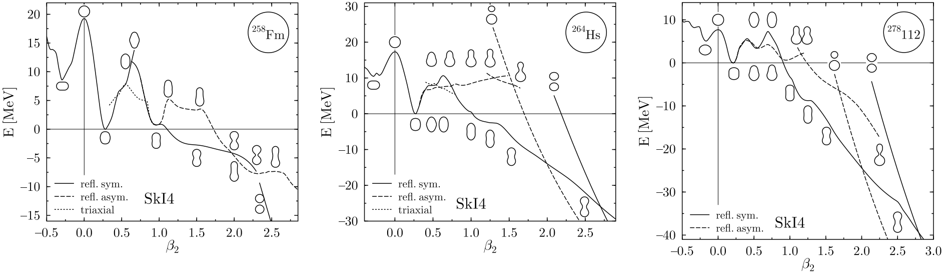
A. V. Afanasjev, T. L. Khoo, S. Frauendorf, G. A. Lalazissis, I. Ahmad, Phys. Rev. C 67 (2003) 024309



- The pioneering band seen for ^{254}No triggered instant calculations by everyone having a cranked mean-field code
- Rotational band in ^{254}No can be seen up to high spin
  $\Rightarrow$ the fission barrier persists to high spin
- Estimates for the $B(E2)$ values agree rather well with models.
- Many bands in adjacent nuclei (even-even and odd-A) have been seen since.

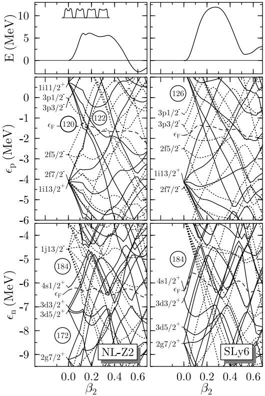
Shell structure at very large deformation: fission barriers

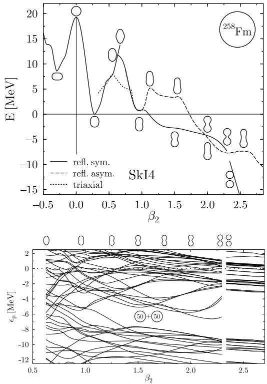
M. B., K. Rutz, P.-G. Reinhard, J. A. Maruhn, W. Greiner, Phys. Rev. C 58 (1998) 2126



- needed to predict stability and for calculations of fusion cross sections
- in most cases one-humped
- fission point are rather small deformation
- triaxiality may lower the barrier by several MeV
- reflection asymmetry does rarely play a role up to the fission point
- but: reflection asymmetry leads to the disapperance of the second barrier

Shell structure at very large deformation: fission barriers





- As the liquid-drop fission barrier vanishes for superheavy elements, such that it just falls off with increasing (prolate) deformation, the existence, height and width of the fission barrier reflects the variation of the "shell energy" with deformation.
- The variation of the "shell energy" reflects the evolution of the level density around the Fermi surface, which in turn is fixed by the spherical shell structure.

Summary

- Superheavy elements probe the physics of atomic nuclei at the extreme of high charge number
- Their features are determined by the evolution of shell structure with deformation, N and Z.
- For superheavy elements, "shell effects" in the total binding energy are qualitatively different from those in lighter nuclei. They are correlated to the low degeneracy of levels close to the Fermi energy, not to the actual shell closures.

The work presented here would have been impossible without my collaborators on this subject, most notably and in chronological order:

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