Fission properties of superheavy elements

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Outline

1. Formal framework
   - The Skyrme energy functional
   - Optimization by least-squares fits
   - Computation of fission barriers and lifetimes
2. Shell gap and magic numbers
3. Fission of SHE
   - Systematics of barriers
   - Fission lifetimes
   - Competing decay channels
4. Least-squares optimization and covariance (correlation) analysis

Formal framework

The Skyrme energy functional

$$E_{\text{tot}} = E_{\text{kin}} + \int d^3r\,\mathcal{E}_{\text{Skyrme}}(\rho, \tilde{\rho}, \tau, \tilde{\tau}, \mathbf{J}, \tilde{\mathbf{J}}, \ldots) + \int d^3r\,\mathcal{E}_{\text{pair}}(\chi_p, \chi_n, \rho) + E_{\text{Coul}} - E_{\text{corr}}$$

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kinetic energy

effective potential energy

pairing functional

Coulomb en. (exchange = Slater appr.)

correlations from low energy modes: c.m., rotation, vibrat.

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The Skyrme energy functional can be quantified in terms of the following parameters:

$\mathcal{E}_{\text{Skyrme}}$:

		isoscalar		isovector
bulk:	equilibrium	E/A, $\rho_{0,equil}$		
	incompressibility	K	, symmetry energy	a_{sym} , a'_{sym}
	surface energy	a_{surf}	, surf.symm. energy	$a_{\text{surf,sym}}$
	effective mass	m^*/m	, TRK sum rule	κ_{TRK}
s.p.:	spin-orbit	b_4	, isovect. spin orbit	b'_4

$\mathcal{E}_{\text{pair}}$:

proton and neutron pairing strenghts: $V_{\text{pair},p}$, $V_{\text{pair},n}$

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The parameters are adjusted to empirical data $\leftrightarrow$ least squares fits.
Fit to large pool of ground state properties of finite nuclei (= SV-min):
$\Longrightarrow$ well fixed parameters $\leftrightarrow$; loosely determined $\leftrightarrow$

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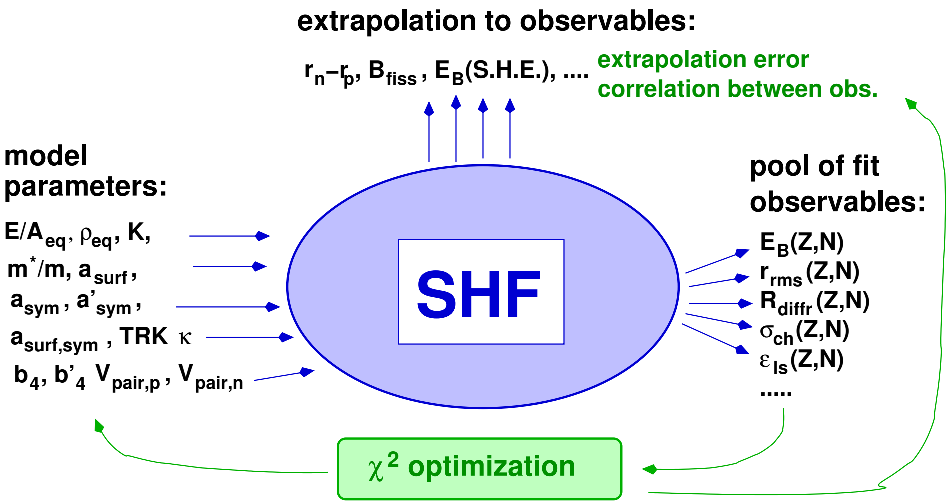
the can be turned to by fitting also giant resonances (= SV-bas)

Optimization by least-squares fits



Least-squares optimization

quality measure: $\chi^2(\mathbf{p}) = \sum_{\nu \in \{\text{data}\}} \frac{\mathcal{O}_\nu(\mathbf{p}) - \mathcal{O}_\nu^{(\text{exp})}}{\Delta \mathcal{O}_\nu}$, **p**=SHF-params., $\mathcal{O}_\nu$=observable

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minimization: $\chi^2(\mathbf{p}) \approx \chi^2(\mathbf{p}_0) + \frac{1}{2}(\mathbf{p}-\mathbf{p}_0)\hat{\mathcal{M}}(\mathbf{p}-\mathbf{p}_0)$, $\mathbf{p}_0$= optimal params.

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reasonable range: minimum $\chi_0^2 = \chi^2(\mathbf{p}_0) \leftrightarrow$ optimal

vicinity $\chi^2(\mathbf{p}) \leq \chi_0^2 + 1 \leftrightarrow$ area of “reasonable” model parameters

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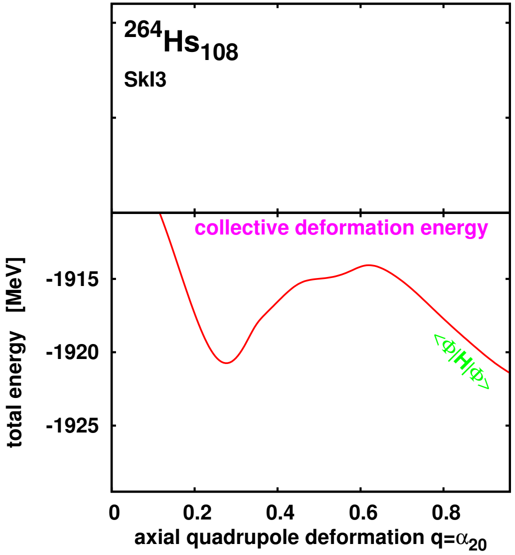
extrapolation: value $= A_0 = A(\mathbf{p}_0)$, error $= \Delta A = \sqrt{\frac{\partial A}{\partial \mathbf{p}}\hat{\mathcal{M}}^{-1}\frac{\partial A}{\partial \mathbf{p}}}$

Computation of fission barriers and lifetimes

Computation of fission life-times



1) Deformation path $|\Phi_q\rangle$ (CHF):

$$\delta_{\langle\Phi_q|}\langle\Phi_q|\hat{H}-\lambda\hat{Q}_{20}|\Phi_q\rangle = 0$$

2) Deformation energy $\mathcal{V}$:

$$\mathcal{V}(q) = \langle\Phi_q|\hat{H}|\Phi_q\rangle$$

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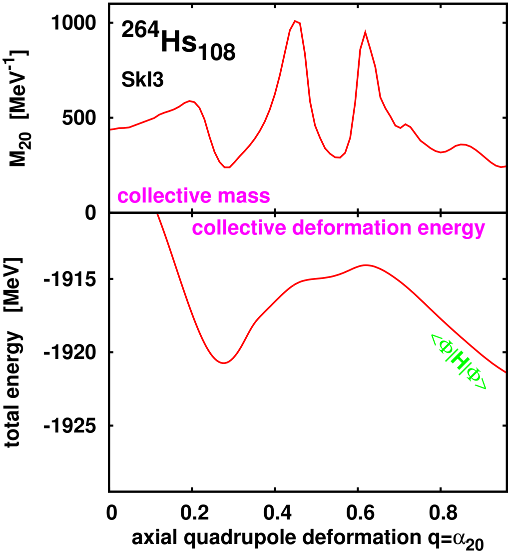

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$$[\hat{H},\hat{R}]|\Phi_q\rangle = \mathrm{i}\partial_q|\Phi_q\rangle$$

$$\mathcal{M}^{-1} = \langle\Phi_q|[\hat{R},[\hat{H},\hat{R}]]|\Phi_q\rangle$$

4) Momentum of inertia $\Theta \leftrightarrow$ as $\mathcal{M}$

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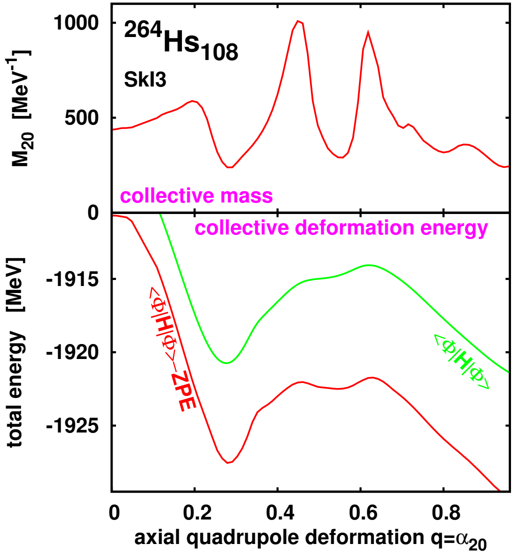

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($\mathcal{Z}\equiv$ zero-point energy)

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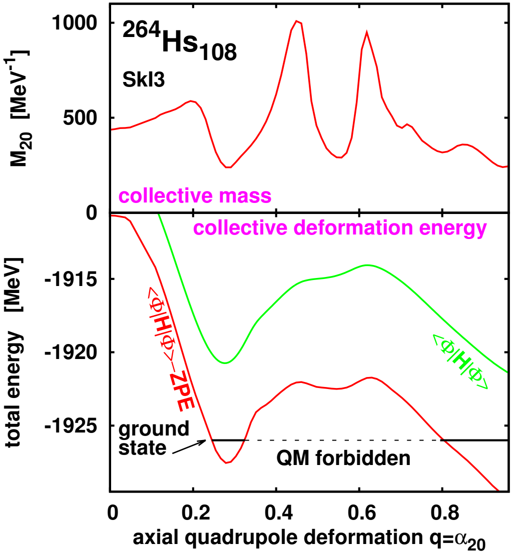

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($\mathcal{Z} \equiv$ zero-point energy)

6) Ground state energy $E_{\rm gs}$:
solve Schr.eq. with V and $\mathcal{M}$

7) Tunneling probability $P \leftrightarrow$ WKB

8) Repetition time $T_{\rm rep} \leftrightarrow$ WKB

$\Longrightarrow$ fission lifetime $\tau_{\rm fis} = T_{\rm rep}/P$

"ab initio" – no free parameters

Computation of barriers and lifetimes – strengths and weaknesses

$\rightarrow$ model assumptions: 1D fission path
can be spanned by quadrupole constraint

+ self-consistent computation of dynamical response (coll. mass, inertia,ZPE)

+ Skyrme force the only “model parameter” – determined from g.s. properties

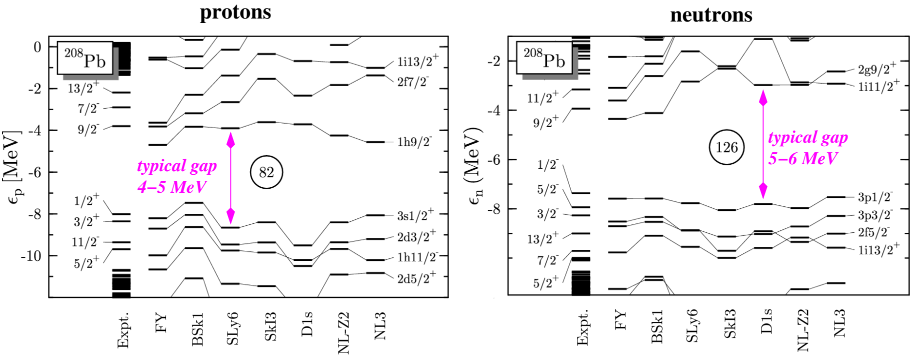
? do we need mutiple fission paths (in vicinity as well as topologically different)

- ignoring triaxial side-walks near prolate fission barrier
($\leftrightarrow$ possibly up to 2 MeV lower barriers)

Shell gap and shell correction

Well developed shell gaps – example ^{208}Pb

single nucleon spectra near the Fermi energy for ^{208}Pb for a variety of models

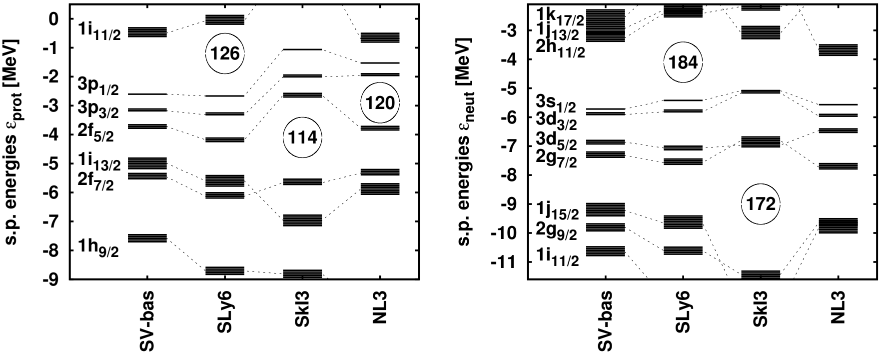


proton and neutron shell gaps are well developed for all models and forces

$\Longrightarrow$ the "magic numbers" $Z = 82$ and $N = 126$ well visible

Single nucleon spectra and shell gaps in SHE

single nucleon spectra near the Fermi energy for SHE Z=114/N=184
computed for a variety of mean-field models
plotted with multiplicity of states to indicate density of states (d.o.s)



spectrum much more diffuse than in ^{208}Pb

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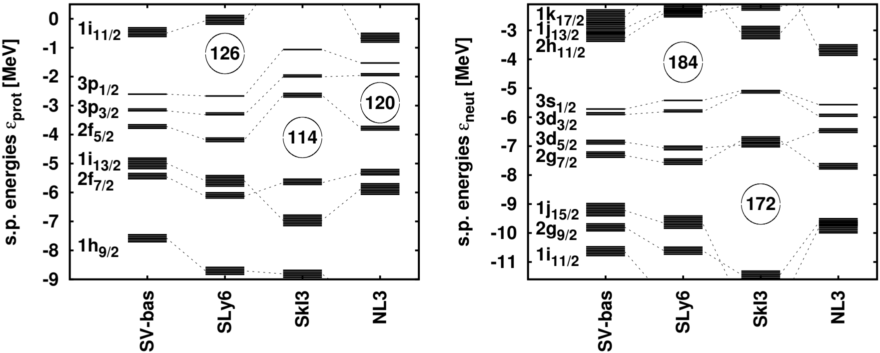


protons: high d.o.s. $Z \lessapprox 114$ & $Z \gtrapprox 126$, loosely filled $114 < Z < 126$
$\Longrightarrow$ floating & weak shell closures, broad region of shell stabilization

Shell correction energies in SHE

(super−)heavy elements exist only due to shell effects

- fission−stabilization through shell effects
- estimate of shell−stabilization by the shell−correction energy

$$E_{corr} = \sum \varepsilon_\alpha - \int d\varepsilon\, g(\varepsilon)$$

$$g(\varepsilon) \propto \sum \exp\left(-\frac{(\varepsilon-\varepsilon_\alpha)^2}{\sigma^2}\right)$$

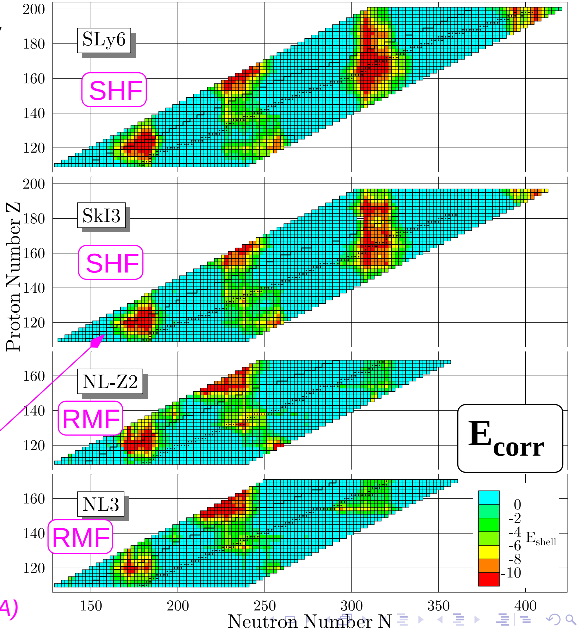
= difference of

quantized sum of s.p.e. and

smoothed distribution (LDM)

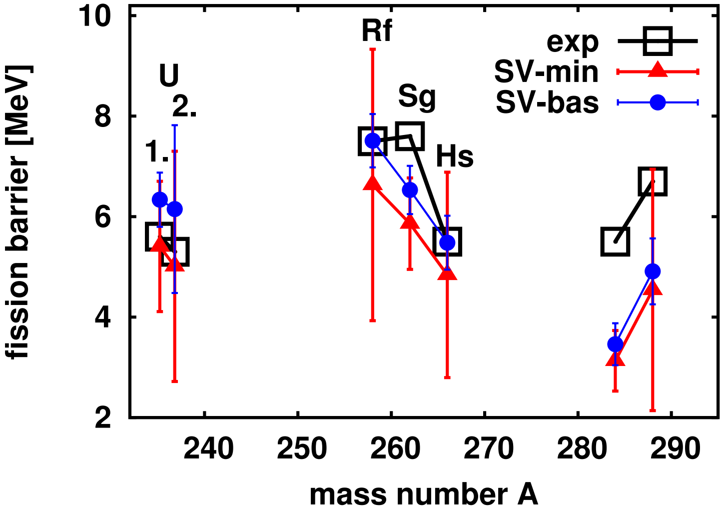
magic numbers obsolete replaced by broad islands of shell stabilization

RMF models produce systematically less E_{corr} (trend develops with increasing A)



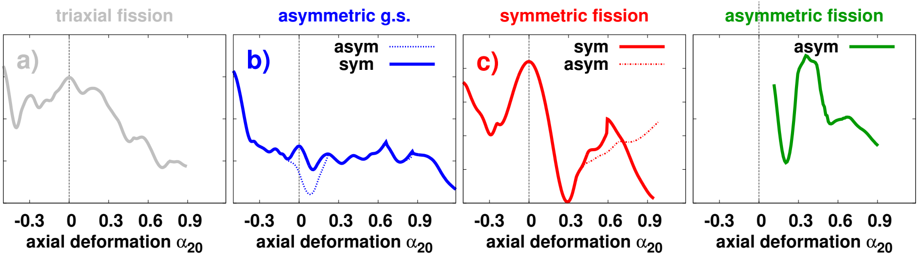
Fission of super-heavy elements (SHE)

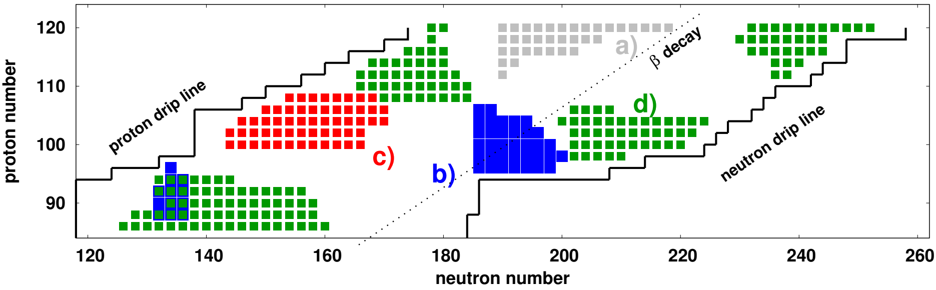
Trends of extrapolation uncertainties: fission barriers



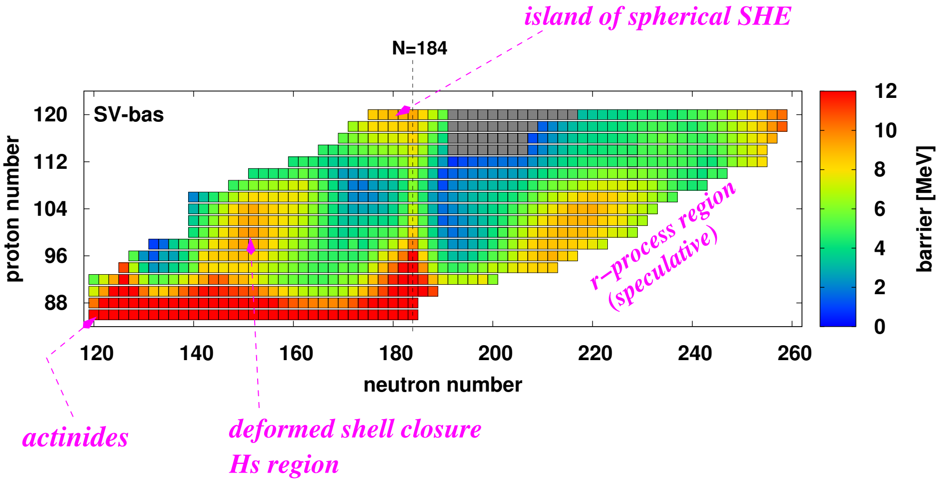
extrapolation uncertainties surprisingly small, no growth towards SHE
SV-min = fit to g.s. only; SV-bas = g.s. & giant resonances ↔ much smaller uncert.
experimental values for upper SHE outside error bars ↔ modeling ?

Different types of fission paths and their regimes





Systematics of barriers in SHE – for the parameterization SV-bas



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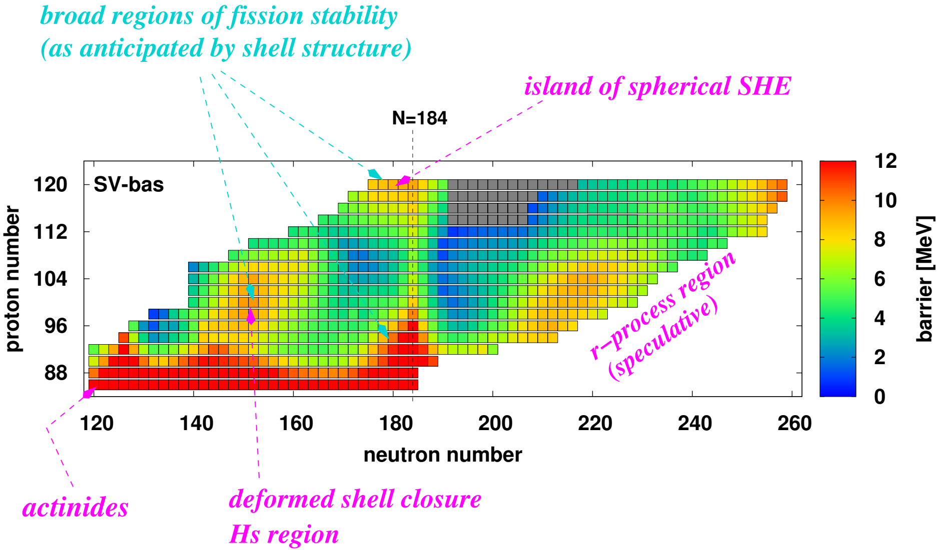

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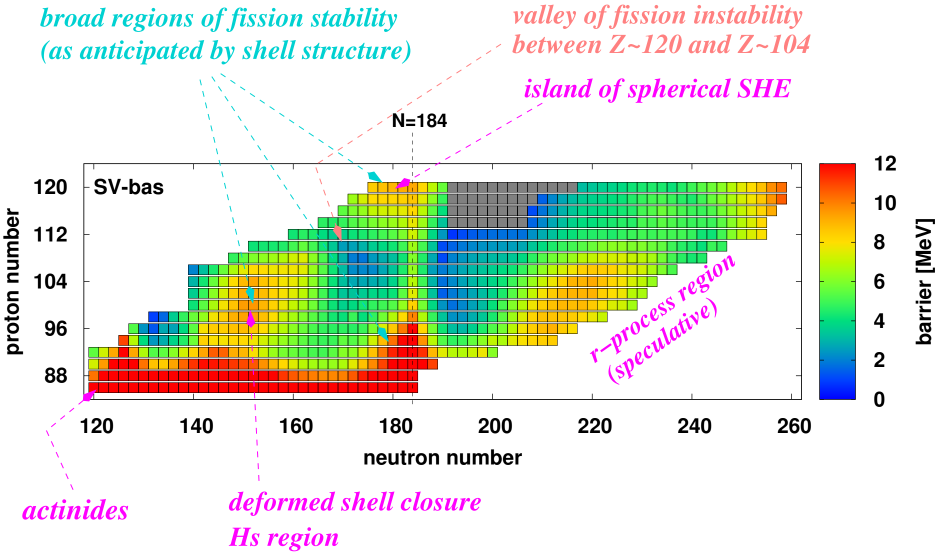
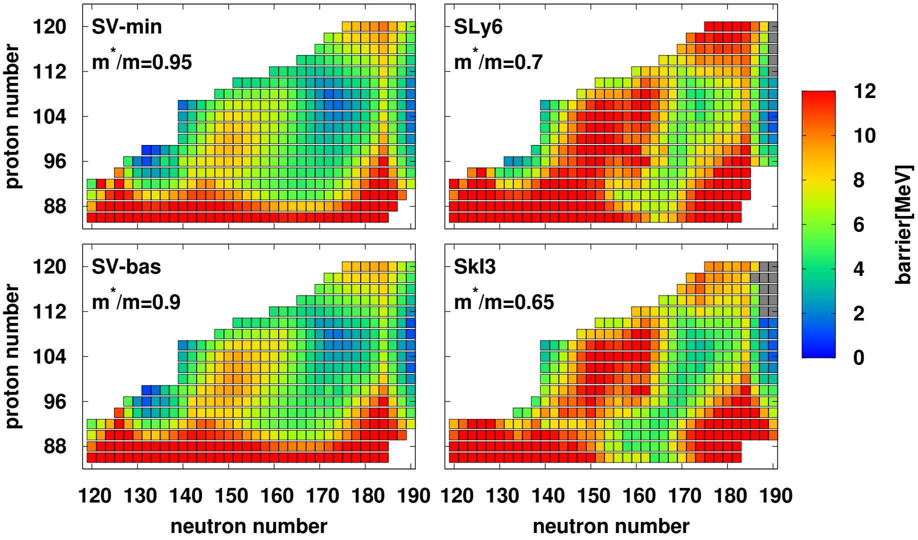


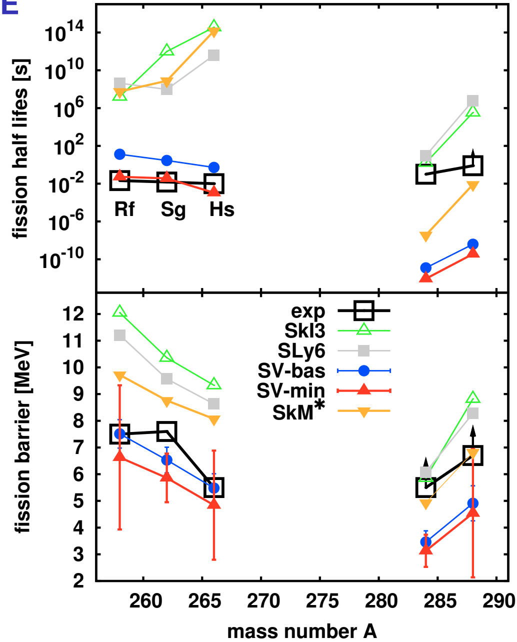
Systematics of barriers in SHE – several forces



pattern similar for all forces – but barrier heights vary dramatically

barrier height $\longleftrightarrow$ average d.o.s. $\longleftrightarrow$ effective mass m^*/m

Test fission lifetimes for SHE



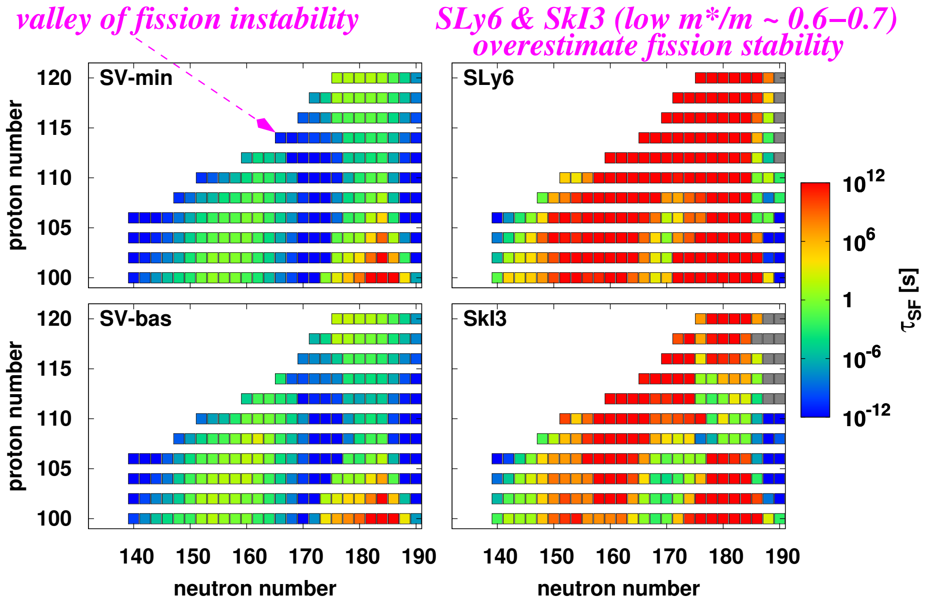
unresolved trend:

forces which perform very well for $Z \approx 100$

underestimate $\tau_{\rm fiss}$ for $Z \approx 114$

and vice versa

Systematics of lifetimes for a variety of forces

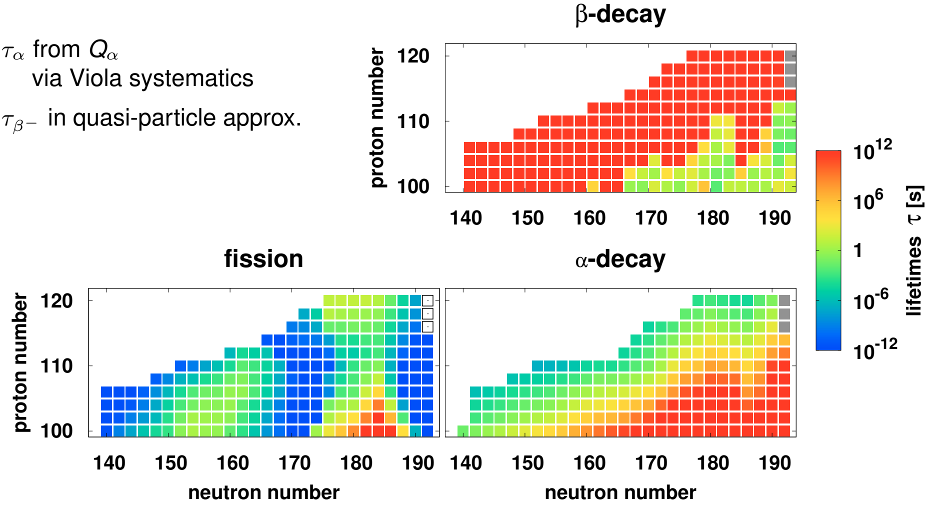


Competing channels: α- and β-decay

Compare lifetimes: fission – α decay – β^- decay

τ_α from Q_α
via Viola systematics

$\tau_{\beta-}$ in quasi-particle approx.

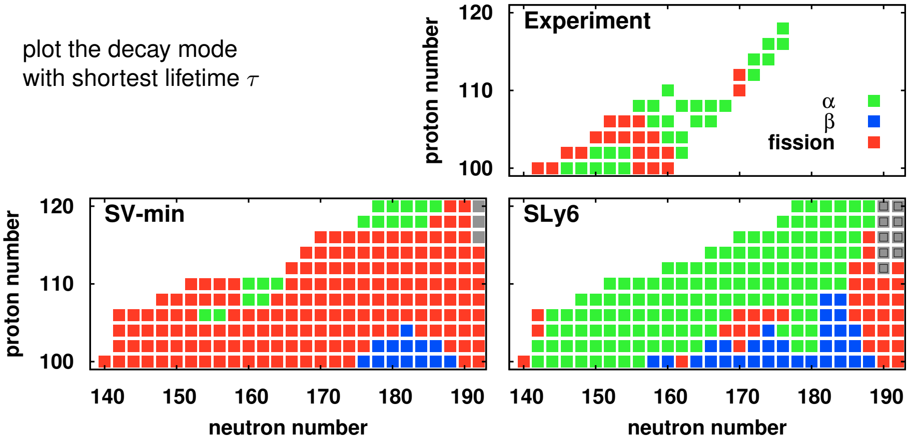


fission fluctuates strongly
pattern robust (shell structure)
magnitude depends on force

α- & β^--decay lifetimes vary smoothly
and are rather independent of force

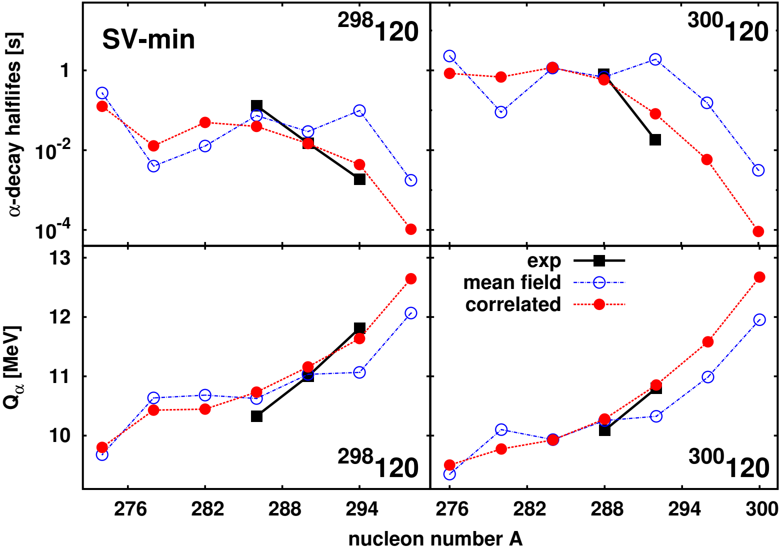
Dominant decay channel: fission – α decay – β^- decay

plot the decay mode
with shortest lifetime τ



experimental trend roughly reproduced by SV-min

Test of α decay for SHE – correlation effects



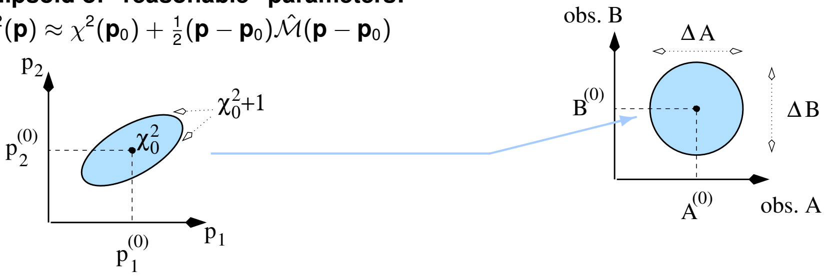
$\Longrightarrow$ 1) recent Skyrme parameterizations describe α-decay in SHE very well
2) ground-state correlations become important in SHE for a detailed description

Least-squares optimization and covariance (correlation) analysis

Error propagation – covariance analysis

ellipsoid of "reasonable" parameters:

$\chi^2(\mathbf{p}) \approx \chi^2(\mathbf{p}_0) + \frac{1}{2}(\mathbf{p}-\mathbf{p}_0)\hat{\mathcal{M}}(\mathbf{p}-\mathbf{p}_0)$



given by: $\Delta\mathbf{p}\cdot(\nabla\otimes\nabla\chi^2)\cdot\Delta\mathbf{p} = 1$

observables: $A = A(\mathbf{p})$, $B = B(\mathbf{p})$

$\Longrightarrow \quad \boxed{\overline{\Delta A\,\Delta B} = \nabla A \cdot \hat{\mathcal{M}}^{-1} \cdot \nabla B}$

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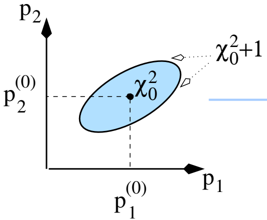

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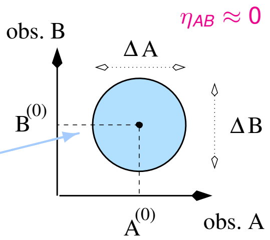
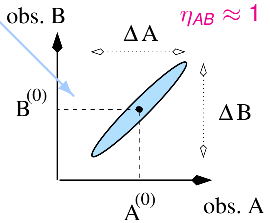
uncertainty: $\Delta A = \sqrt{\overline{\Delta A\,\Delta A}}$

correlation: $\eta_{AB} = \dfrac{\overline{\Delta A\,\Delta B}}{\sqrt{\overline{\Delta^2 A}\;\overline{\Delta^2 B}}}$

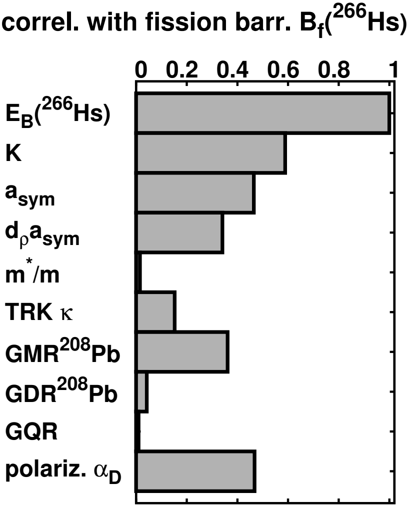
uncorrelated observables:



highly correlated observables:



Correlations with fission barriers in ^{266}Hs



fission barriers not correlated with one single LDM property

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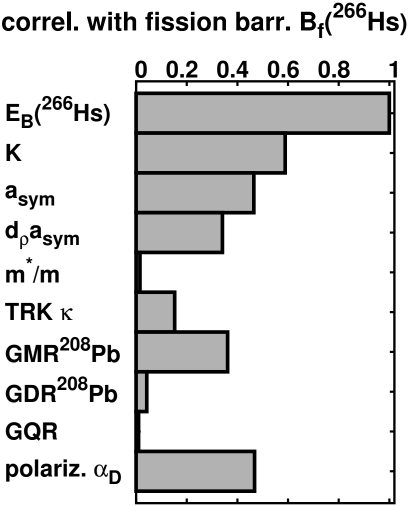
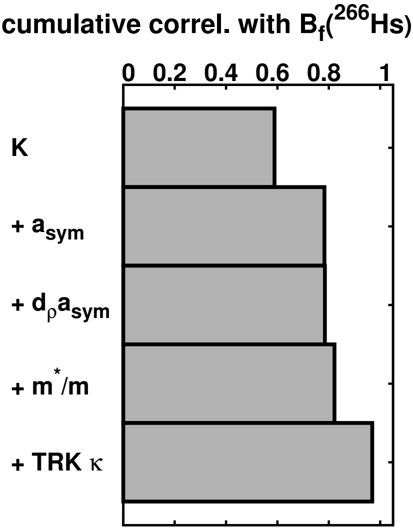
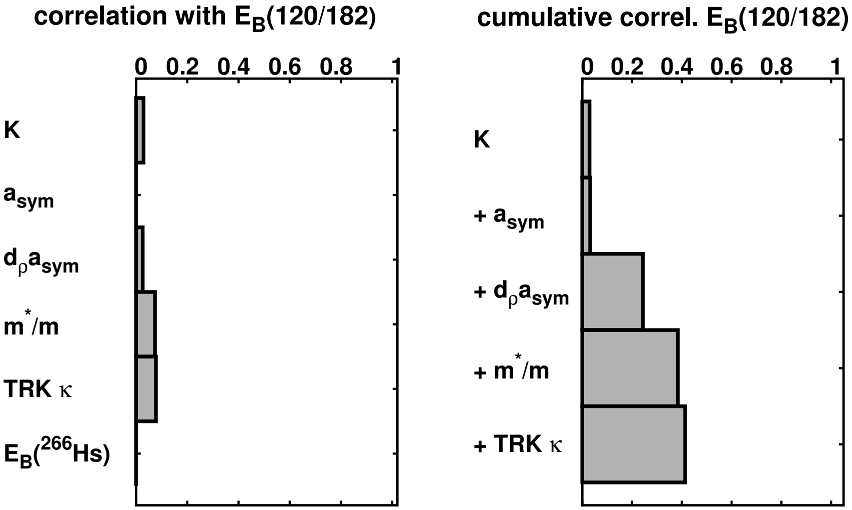




fission barriers not correlated with one single LDM property
but correlated with the full set of LDM properties

Correlations with fission barriers in Z=120/N=182 (for SV-min)



fission barriers in 120/182 show much less correlation – even for SV-min $\longrightarrow$??

Conclusions

Fully self-consistent description of fission (and α-, β-decay)
Skyrme-Hartree-Fock: effective energy-density functional, fitted to g.s. data
reliable extrapolations, estimate of uncertainty
fission: collective dynamics along 1D path fom Q_{20}-constraint

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Robust shell structure while magic numbers fade away
"gap" perturbed by intruders → broad band of low density of states
broad islands stabilization (Z/N≈104/150 deformed, Z/N≈116/172 spherical)

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"gap" perturbed by intruders $\rightarrow$ broad band of low density of states
broad islands stabilization (Z/N≈104/150 deformed, Z/N≈116/172 spherical)

Fair predictions for barrier heights and fission lifetimes
fine for actinides & lower SHE, $\Delta B_f \approx 1 - 2$ MeV, wrong trend higher SHE
low m^*/m and/or low pairing $\leftrightarrow$ high barriers & $\tau_{\rm fiss}$
competition with α- & β-decay qualitatively correct

Conclusions

Fully self-consistent description of fission (and α-, β-decay)
Skyrme-Hartree-Fock: effective energy-density functional, fitted to g.s. data
reliable extrapolations, estimate of uncertainty
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Open problems
wrong trend of $\tau_{\rm fiss}$ from island Z=104 to island Z=116 (still for all Skyrme forces)
$\leftrightarrow$ 1D fission path?, Q_{20} constraint?, triaxial sidewalk?, pairing model?