

A survey of super-heavy elements from a theoretical perspective

P.-G. Reinhard¹, J. Erler², P. Klüpfel³, K.-H. Langanke⁵, H.-P. Löns⁵,
G. Martinez-Pinedo⁵, J.A. Maruhn⁴.

¹Institut für Theoretische Physik, Friedrich-Alexander-Universität, Erlangen/Germany

²Physics Division, Oak Ridge National Laboratory, Oak Ridge/USA

³Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

⁴Institut für Theoretische Physik, Johann-Wolfgang-Goethe Universität, Frankfurt/Germany

⁵Gesellschaft für Schwerionenforschung, Darmstadt/Germany

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Outline

- 1 The Skyrme energy functional and its performance
- 2 Shell gap and magic numbers
- 3 Fission of SHE
- 4 Competing decay channels

The Skyrme energy functional and its performance

The Skyrme energy functional

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

The Skyrme energy functional

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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.

The diagram illustrates the decomposition of the total Skyrme energy functional E_{tot} into several components. The total energy is given by the equation:

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

Arrows point from four boxes below the equation to specific terms in the equation:

- A pink arrow points from the box labeled "kinetic energy" to the first term E_{kin} .
- A pink arrow points from the box labeled "effective potential energy" to the second term $\int d^3r \mathcal{E}_{\text{Skyrme}}(\rho, \tilde{\rho}, \tau, \tilde{\tau}, \mathbf{J}, \tilde{\mathbf{J}}, \dots)$.
- A pink arrow points from the box labeled "pairing functional" to the third term $\int d^3r \mathcal{E}_{\text{pair}}(\chi_p, \chi_n, \rho)$.
- A pink arrow points from the box labeled "Coulomb en. (exchange = Slater appr.)" to the fourth term E_{Coul} .

The fifth term, $-E_{\text{corr}}$, is highlighted with a pink bracket and has a pink arrow pointing to it from the text "correlations from low energy modes: c.m., rotation, vibrat."

The Skyrme energy functional

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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.

functional of local densities and currents:

density	$\rho(r) = \sum_{\alpha} v_{\alpha}^2 \varphi_{\alpha} ^2$
kinetic density	$\tau(r) = \sum_{\alpha} v_{\alpha}^2 \nabla \varphi_{\alpha} ^2$
spin-orbit density	$\mathbf{J}(r) = -i \sum_{\alpha} v_{\alpha}^2 \varphi_{\alpha}^{\dagger} \nabla \times \boldsymbol{\sigma} \varphi_{\alpha}$
spin density	$\sigma(r) = \sum_{\alpha} v_{\alpha}^2 \varphi_{\alpha}^{\dagger} \hat{\boldsymbol{\sigma}} \varphi_{\alpha}$
current	$\mathbf{j}(r) = -i \sum_{\alpha} v_{\alpha}^2 \varphi_{\alpha}^{\dagger} \nabla \varphi_{\alpha} + \text{c.c.}$
spin-kinetic density	$\tau(r) = -i \sum_{\alpha} v_{\alpha}^2 \varphi_{\alpha}^{\dagger} \nabla \sigma \nabla \varphi_{\alpha}$
total & difference	$\underbrace{\rho}_{\text{isoscalar}} = \rho_n + \rho_p, \underbrace{\tilde{\rho}}_{\text{isovector}} = \rho_n - \rho_p$
pair density	$\chi(r) = \sum_{\alpha} u_{\alpha} v_{\alpha} \varphi_{\alpha} ^2$
pairing amplit.	u_{α}, v_{α}

The Skyrme energy functional

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

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mean-field equations:

variation s.p. wave functions φ_{α}^*
variation of occupation amplitudes u_{α}

... and its parameterization

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

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

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

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

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

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

... and its parameterization

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incompressibility	K	, symmetry energy	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

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

The parameters are adjusted to empirical data (\leftrightarrow least squares fits).

... and its parameterization

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Fit to ground state properties \implies fix parameters  \leftrightarrow parameterization 

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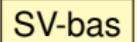
	isoscalar	isovector
bulk: bulk equilibrium	$E/A, \rho_{0,\text{equil}}$	
incompressibility	K	, symmetry energy
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proton and neutron pairing strengths: $V_{\text{pair},p}, V_{\text{pair},n}$

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Fit to ground state properties \implies fix parameters  \leftrightarrow parameterization  SV-min

Info from giant resonance & neutron radius \implies fix also parameters  \leftrightarrow  SV-bas

... and its parameterization

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Fit to ground state properties \Rightarrow fix parameters  \leftrightarrow parameterization  SV-min

Info from giant resonance & neutron radius \Rightarrow fix also parameters  \leftrightarrow  SV-bas

\Rightarrow : some aspects vaguely determined \Rightarrow some uncertainty in extrapolations

... and its parameterization

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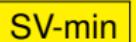
$\mathcal{E}_{\text{Skyrme}}$:

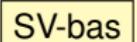
	isoscalar	isovector
bulk: bulk equilibrium	$E/A, \rho_{0,\text{equil}}$	
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Fit to ground state properties \Rightarrow fix parameters  \leftrightarrow parameterization  SV-min

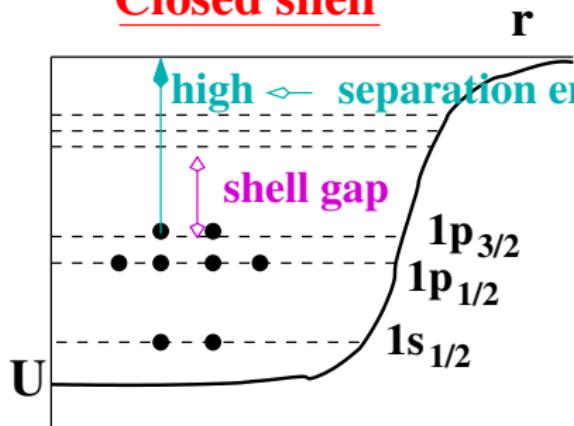
Info from giant resonance & neutron radius \Rightarrow fix also parameters  \leftrightarrow  SV-bas

\Rightarrow : some aspects vaguely determined \Rightarrow some *freedom* in extrapolations

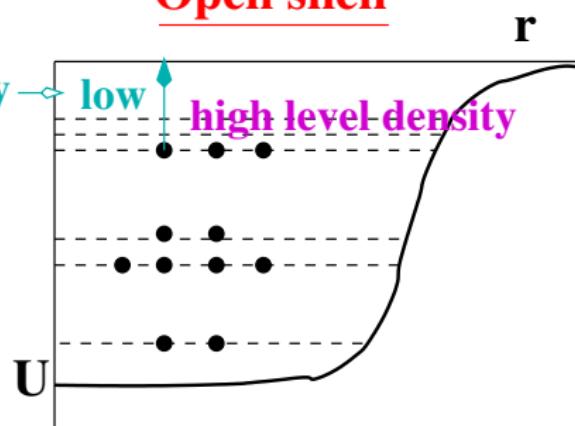
Shell gap and magic numbers

Separation energies, halting points and shell gaps

Closed shell



Open shell

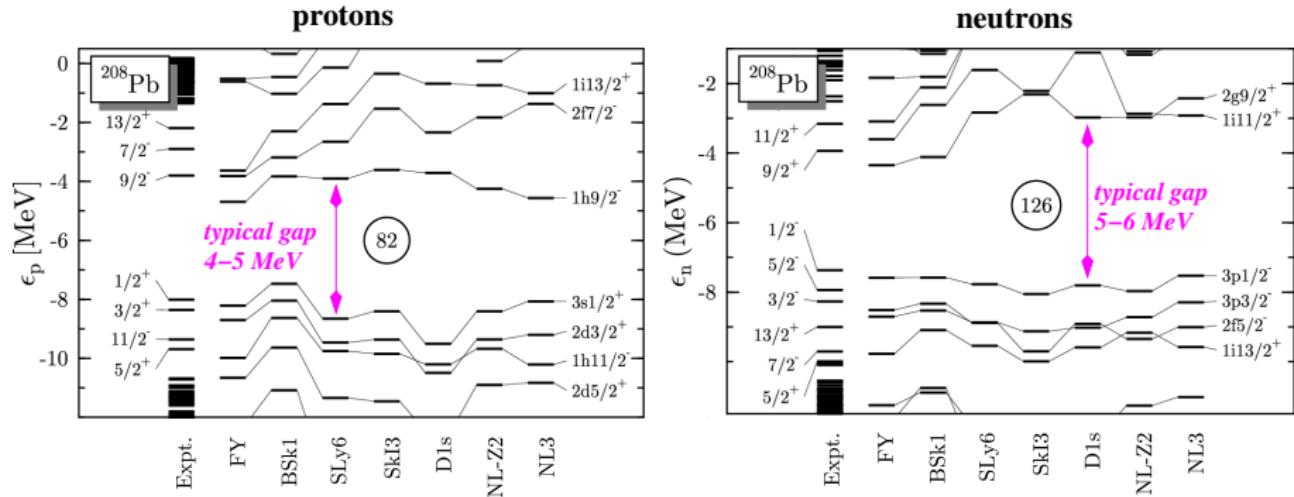


(example: nuclear potential, harmonic osc. labelling, l^*s)

- large separation energy (S_{2n}, S_{2p})
- enhanced binding ("shell correction")
 \Rightarrow high abundance
- enhanced fission stability
- low separation energy (S_{2n}, S_{2p})
- reduced prob. in evaporation chains
(e.g. r -process)
- less stable against fission

Well developed shell gaps – example ^{208}Pb

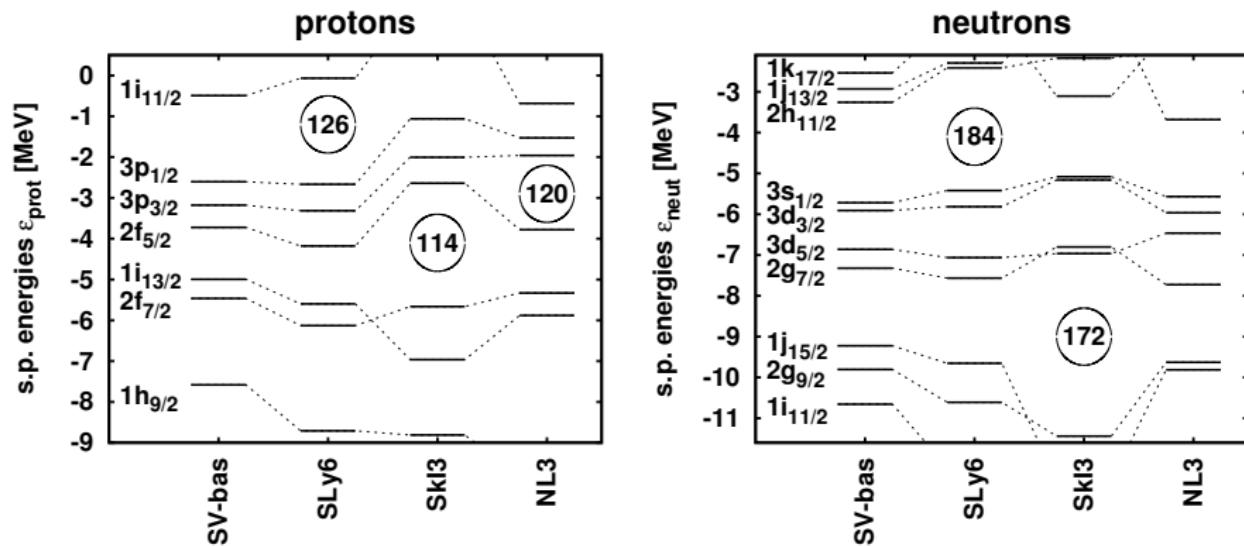
single nucleon spectra near the Fermi energy for ^{208}Pb for a variety of models



proton and neutron shell gaps are well developed for all models and forces
⇒ the “magic numbers” $Z = 82$ and $N = 126$ well visible

Single nucleon spectra and shell gaps in SHE

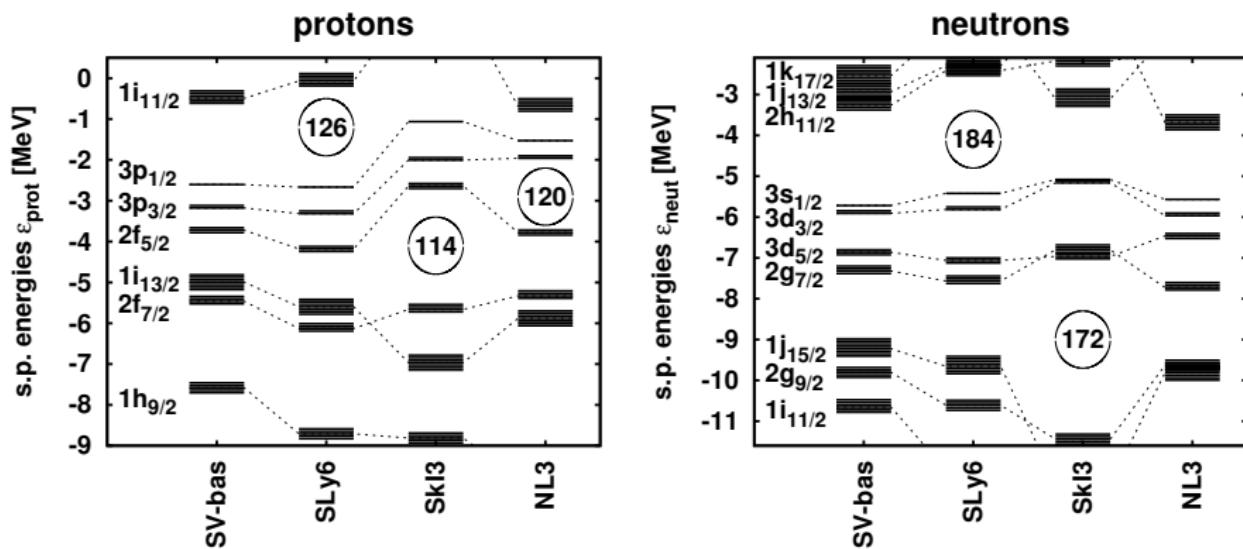
single nucleon spectra near the Fermi energy for SHE Z=114/N=184
computed for a variety of mean-field models



spectrum much more diffuse than in ^{208}Pb

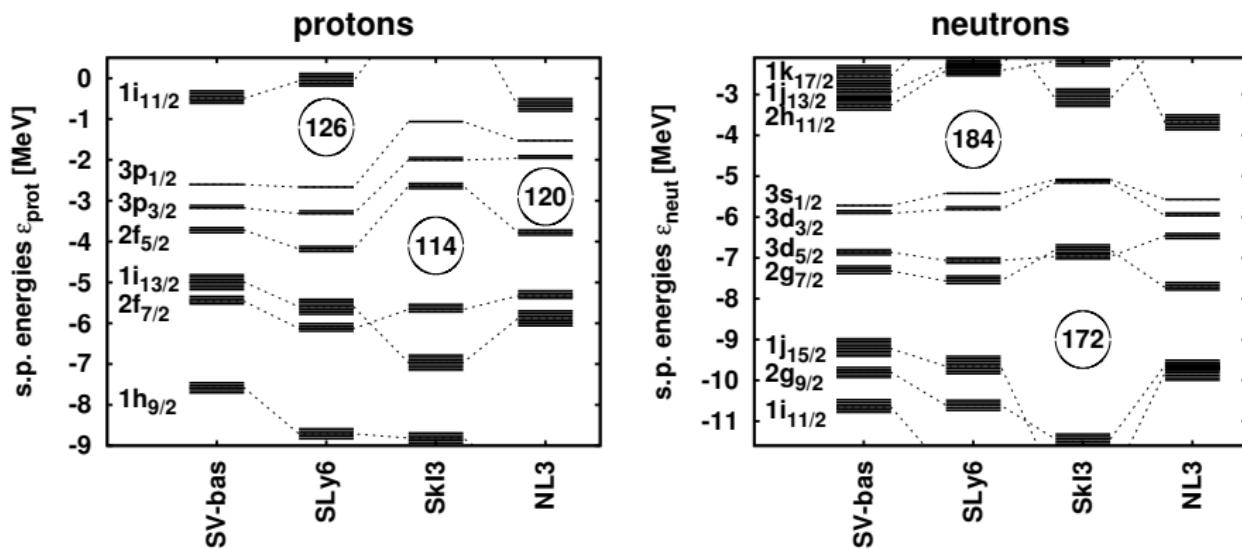
Single nucleon spectra and shell gaps in SHE

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)



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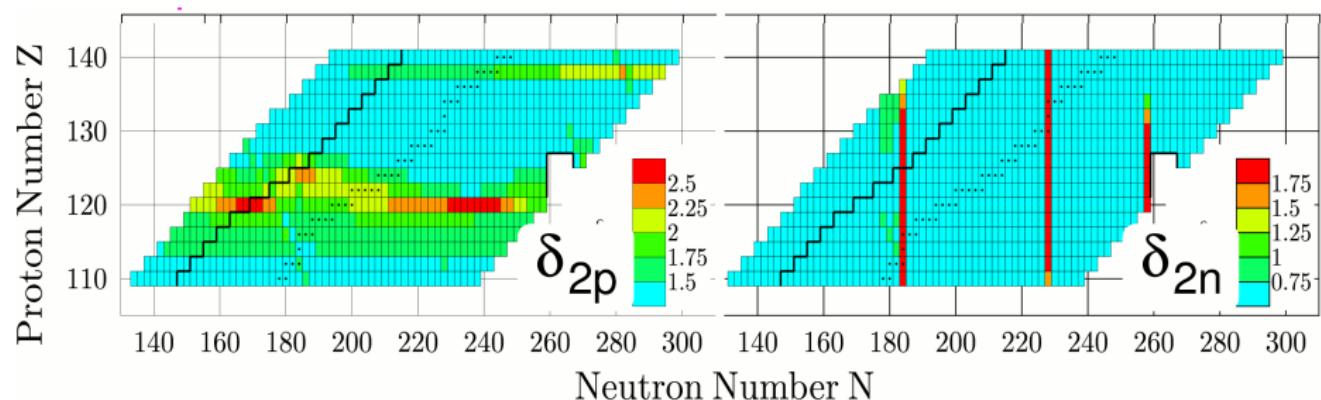
protons: high d.o.s. $Z \approx 114$ & $Z \approx 126$, loosely filled $114 < Z < 126$
 \implies floating & weak shell closures, broad region of shell stabilization

Two-nucleon shell gaps in SHE

Compute spectral shell gaps from two-nucleon energy differences:

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

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



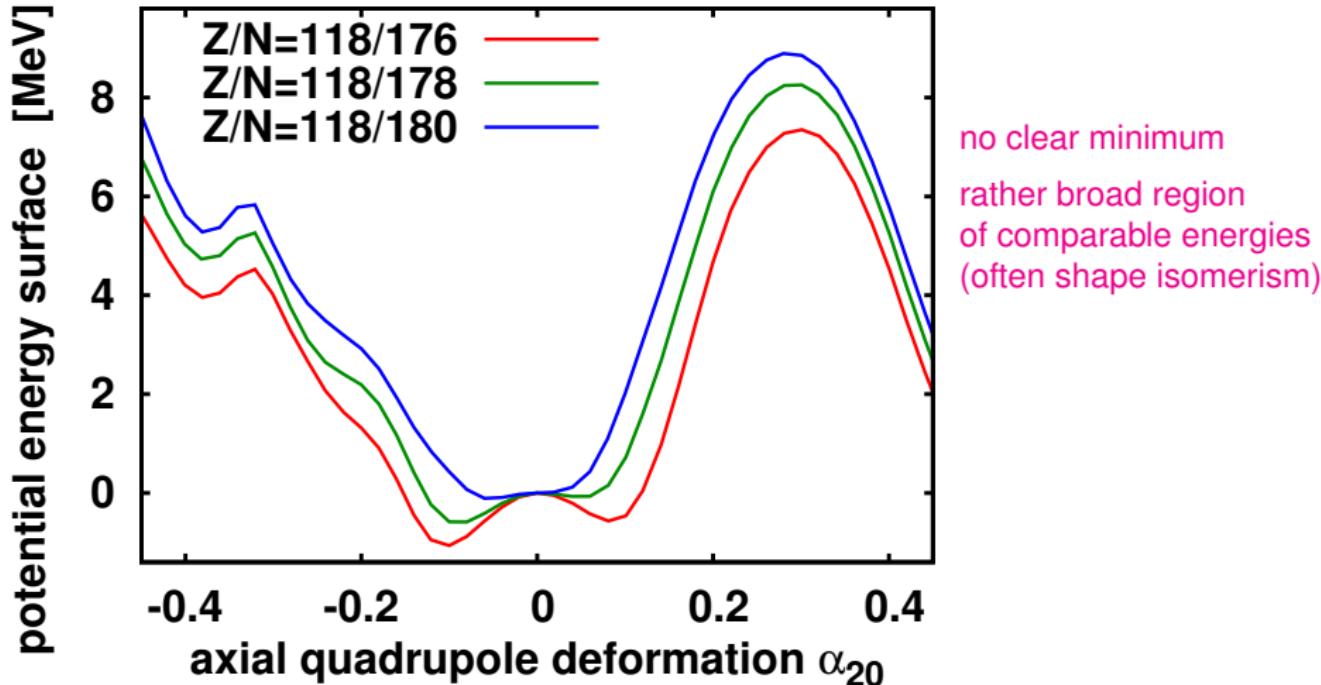
proton and neutron shell gaps are very weak $\longleftrightarrow \Delta_{2N} \approx 2$ MeV
particularly for protons: broad regions of enhanced gaps

The softness of SHE ($Z \gtrapprox 114$)

intruders in “energy gap” \longleftrightarrow soft potential-energy surface expected

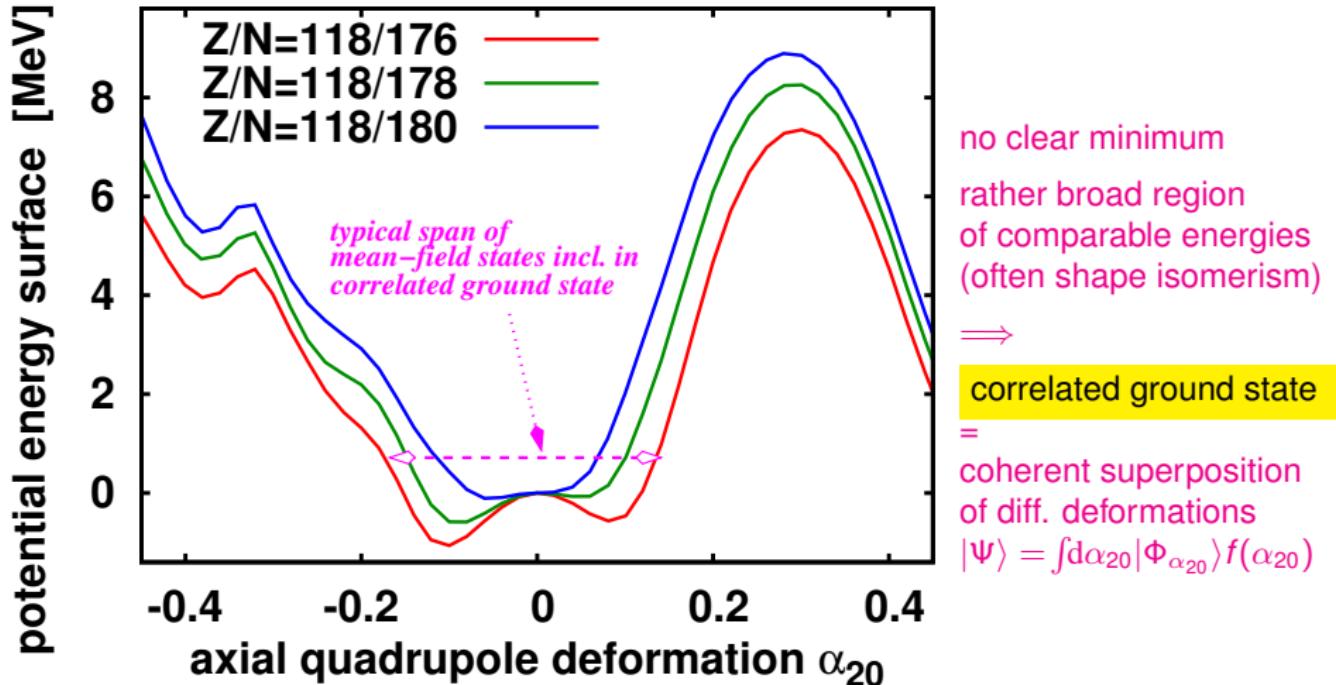
The softness of SHE ($Z \gtrsim 114$)

intruders in “energy gap” \longleftrightarrow soft potential-energy surface expected



The softness of SHE ($Z \gtrsim 114$)

intruders in “energy gap” \longleftrightarrow soft potential-energy surface expected



Fission of SHE

Coulomb instability and shell stabilization

potential energy surface along fission path

nuclear shapes along the fission path
(schematic)

actual microscopic path $\{|\Phi_{\alpha_{20}}\rangle\}$
computed self-consistently
by constrained H.F.

⇒

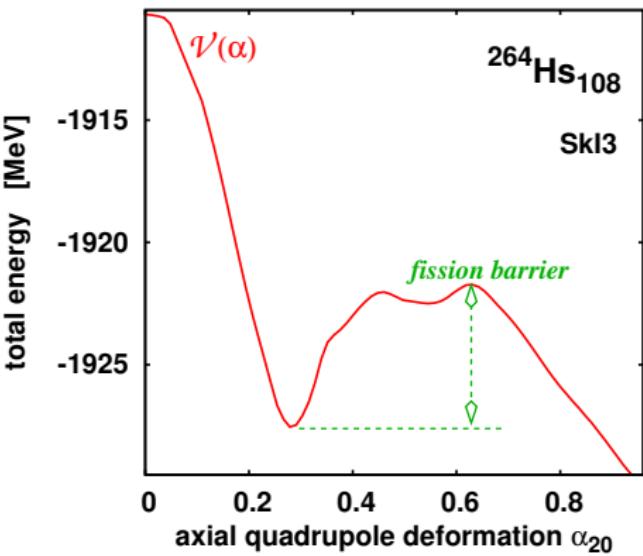
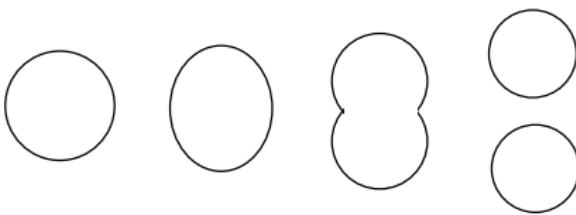
deformation energy surface $V(\alpha_{20})$,
basis for collective description
of the fission dynamics

shell structure adds energy correction

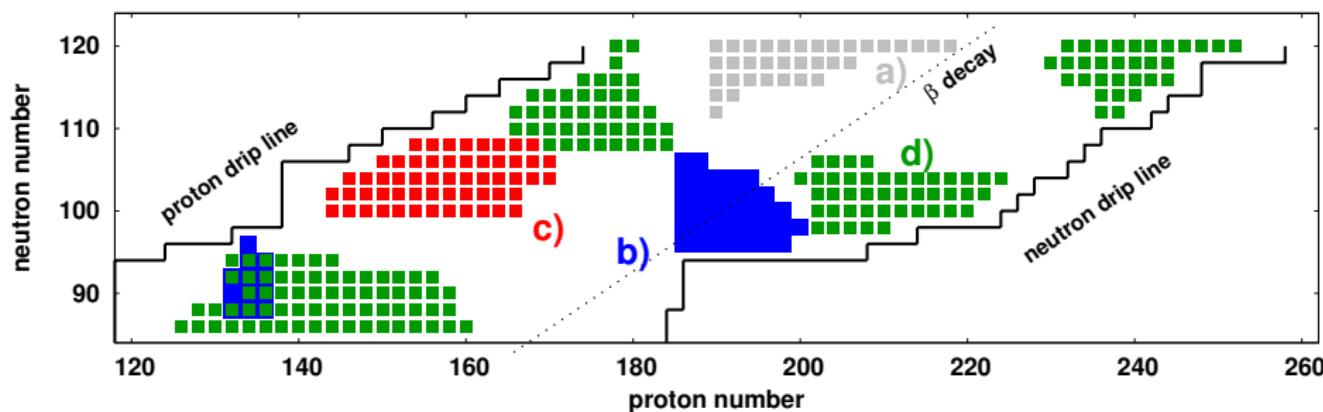
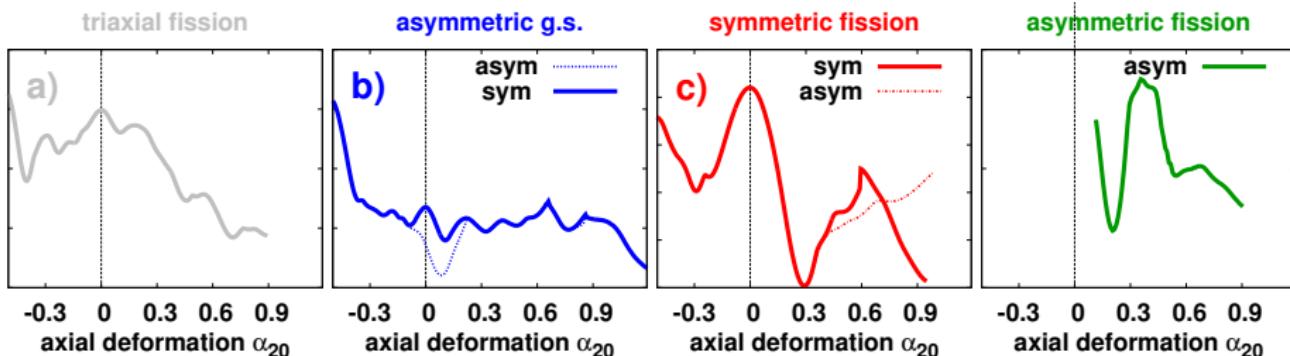
⇒ binding pocket ↔ low d.o.s.

⇒ fission barrier ↔ high d.o.s.

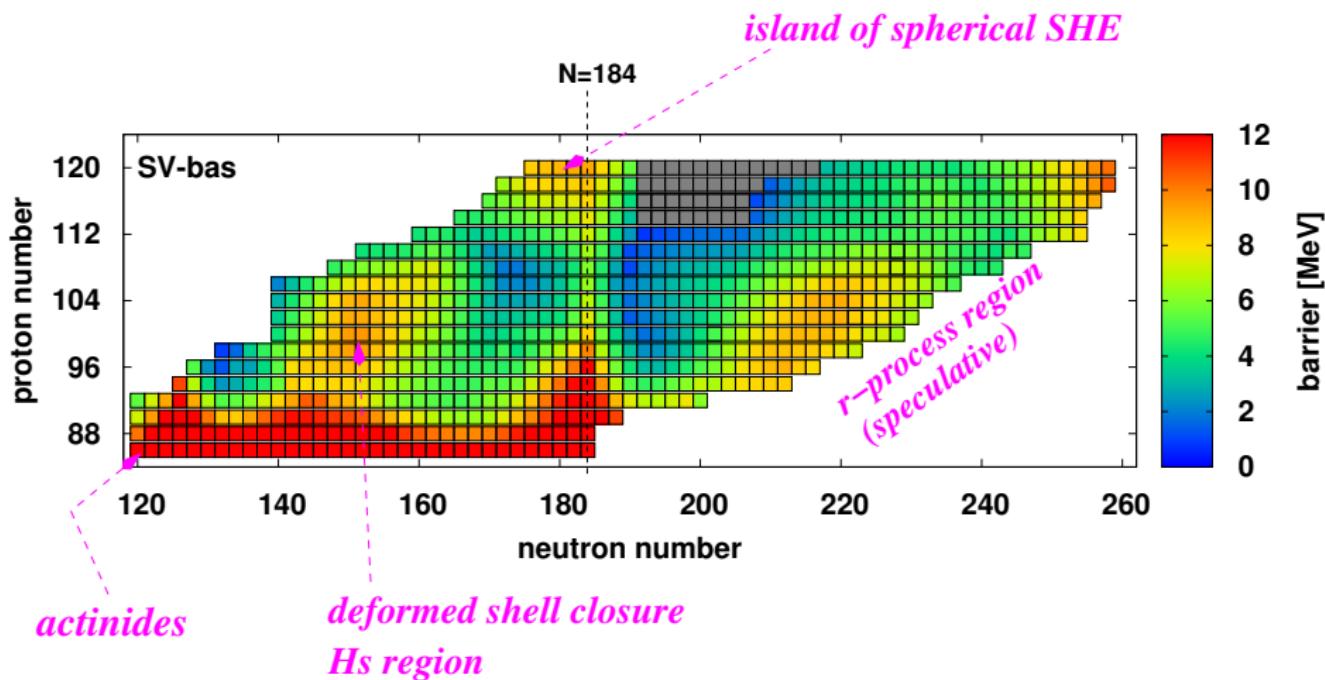
Note: "shell correction" automatically
in self-consistent calculations



Different types of fission paths and their regimes

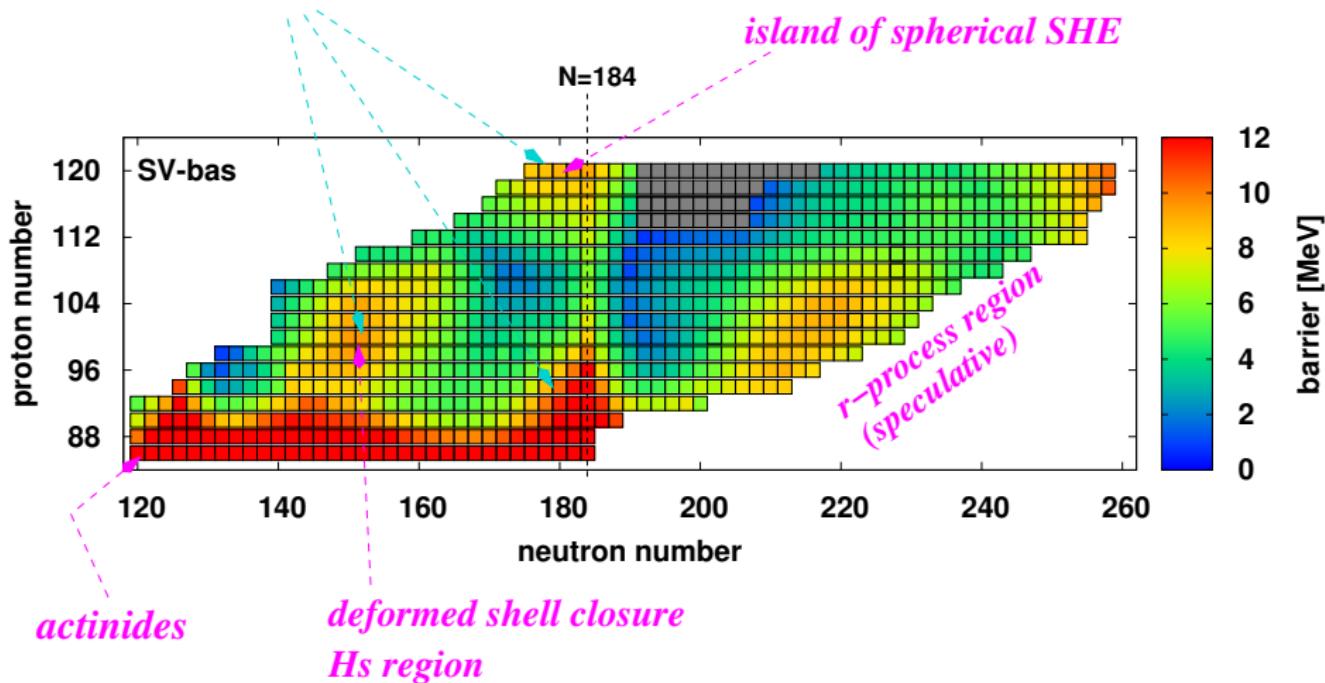


Systematics of barriers in SHE – for the parameterization SV-bas



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

*broad regions of fission stability
(as anticipated by shell structure)*

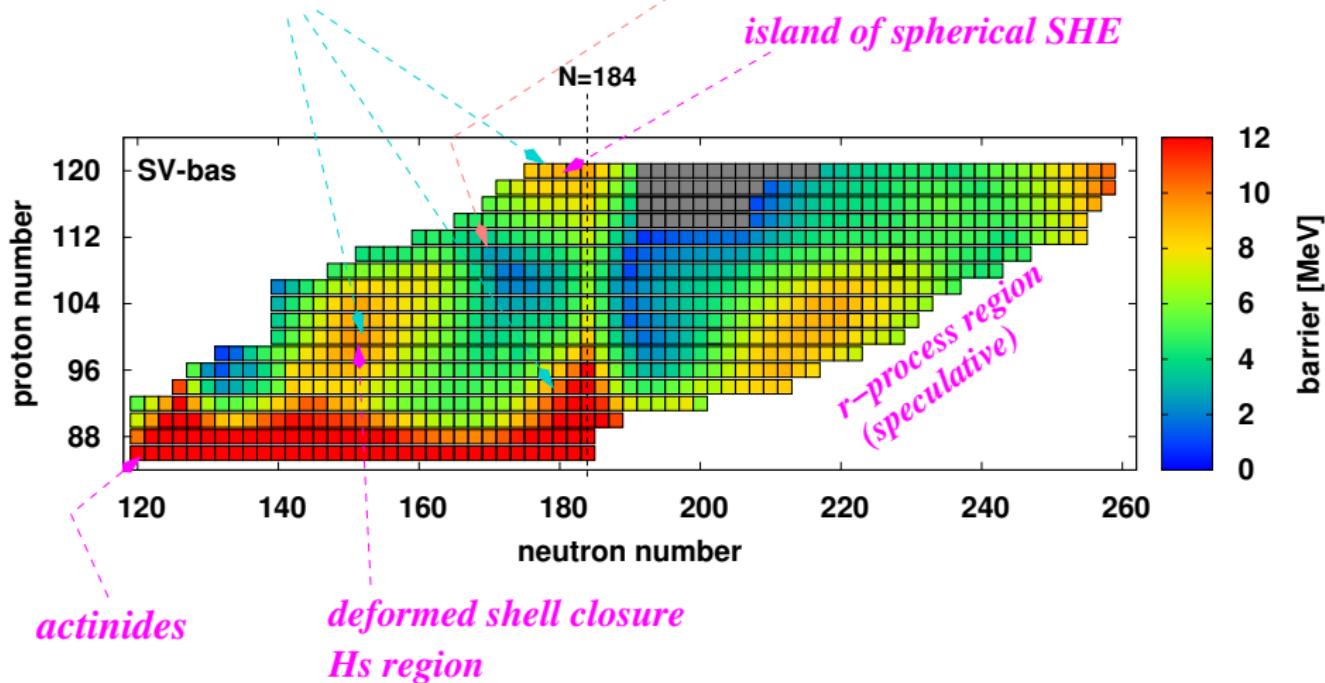


Systematics of barriers in SHE – for the parameterization SV-bas

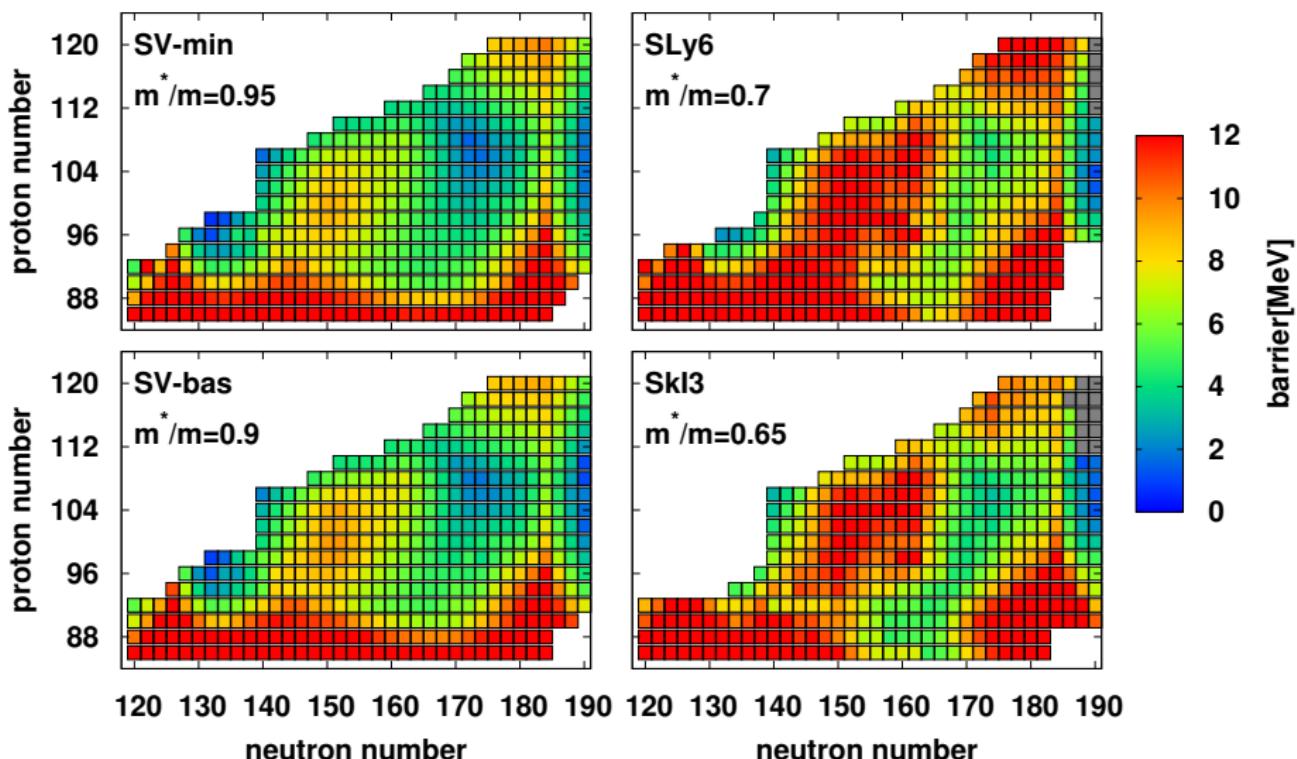
*broad regions of fission stability
(as anticipated by shell structure)*

*valley of fission instability
between Z~120 and Z~104*

island of spherical SHE



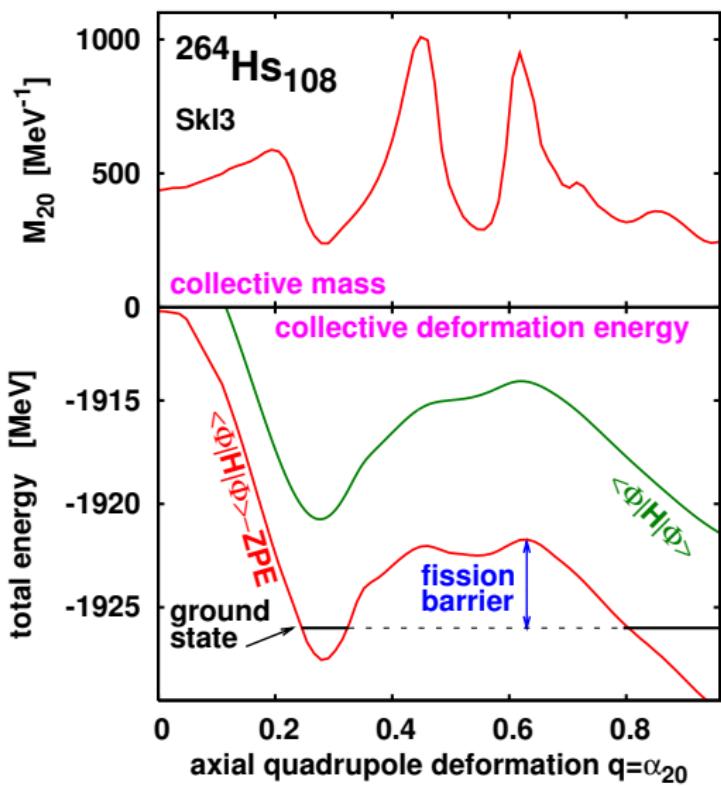
Systematics of barriers in SHE – several forces



pattern similar for all forces – but barrier heights vary dramatically
barrier height \longleftrightarrow average d.o.s. \longleftrightarrow effective mass m^*/m

Computation of fission 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} :

$$\mathcal{V}(q) = \langle\Phi_q| \hat{H} |\Phi_q\rangle$$
 - 3) Collective mass \mathcal{M} (lin.resp.):

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

$$\mathcal{M}^{-1} = \langle\Phi_q| [\hat{R}, [\hat{H}, \hat{R}]] |\Phi_q\rangle$$
 - 4) Momentum of inertia $\Theta \leftrightarrow \mathcal{M}$
 - 5) Quantum corrected energy V :

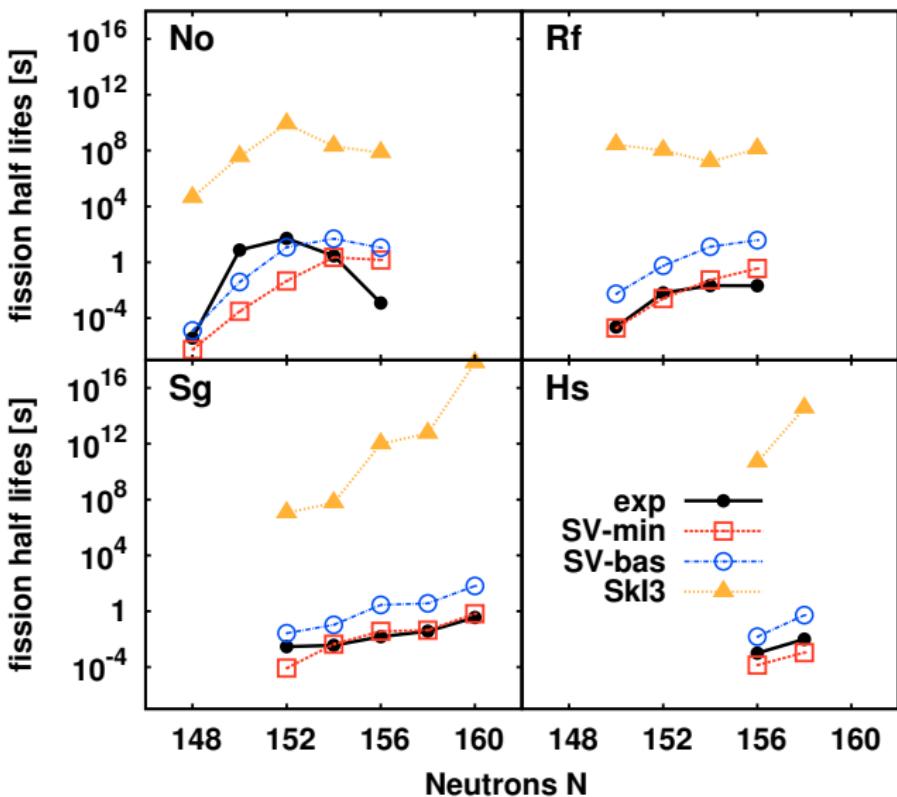
$$V = \mathcal{V} - \mathcal{Z}_{\text{vib}} - \mathcal{Z}_{\text{rot}}$$

 $(\mathcal{Z} \equiv \text{zero-point energy})$
 - 6) Ground state energy E_{gs} :
 solve Schr.eq. with V and \mathcal{M}
 - 7) Tunneling probability $P \leftrightarrow \text{WKB}$
 - 8) Repetition time $T_{\text{rep}} \leftrightarrow \text{WKB}$
- ⇒ fission lifetime $\tau_{\text{fis}} = T_{\text{rep}}/P$

"ab initio" – no free parameters

Test fission lifetimes for transactinides

predictions vary sizeably
 τ_{fiss} depends on m^*/m
 $m^*/m = 0.9 - 1$
⇒ reasonable results



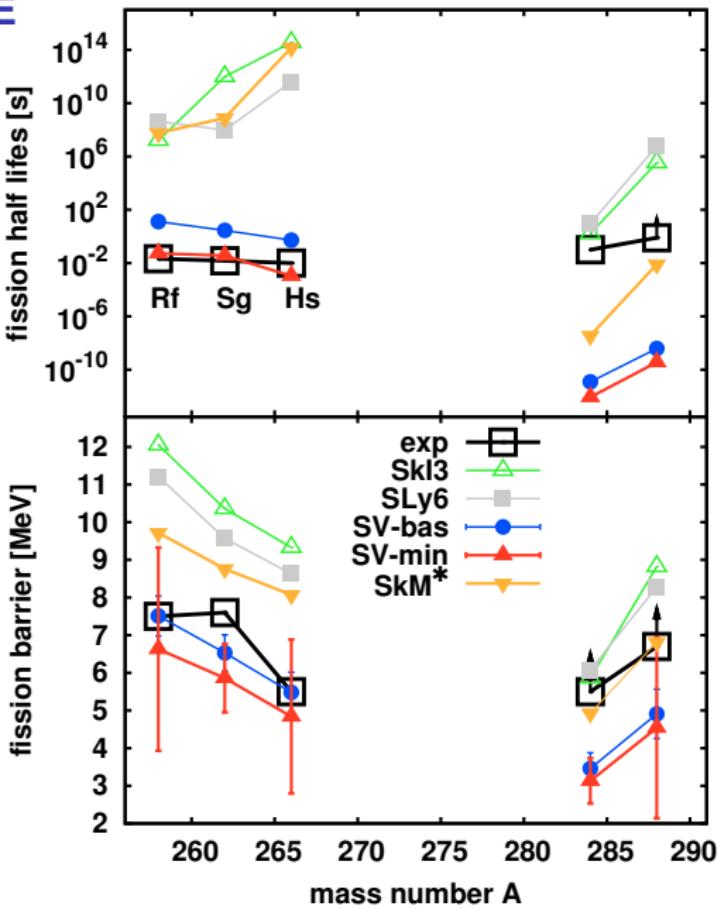
Test fission lifetimes for SHE

unresolved trend:

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

underestimate τ_{fiss} for $Z \approx 114$

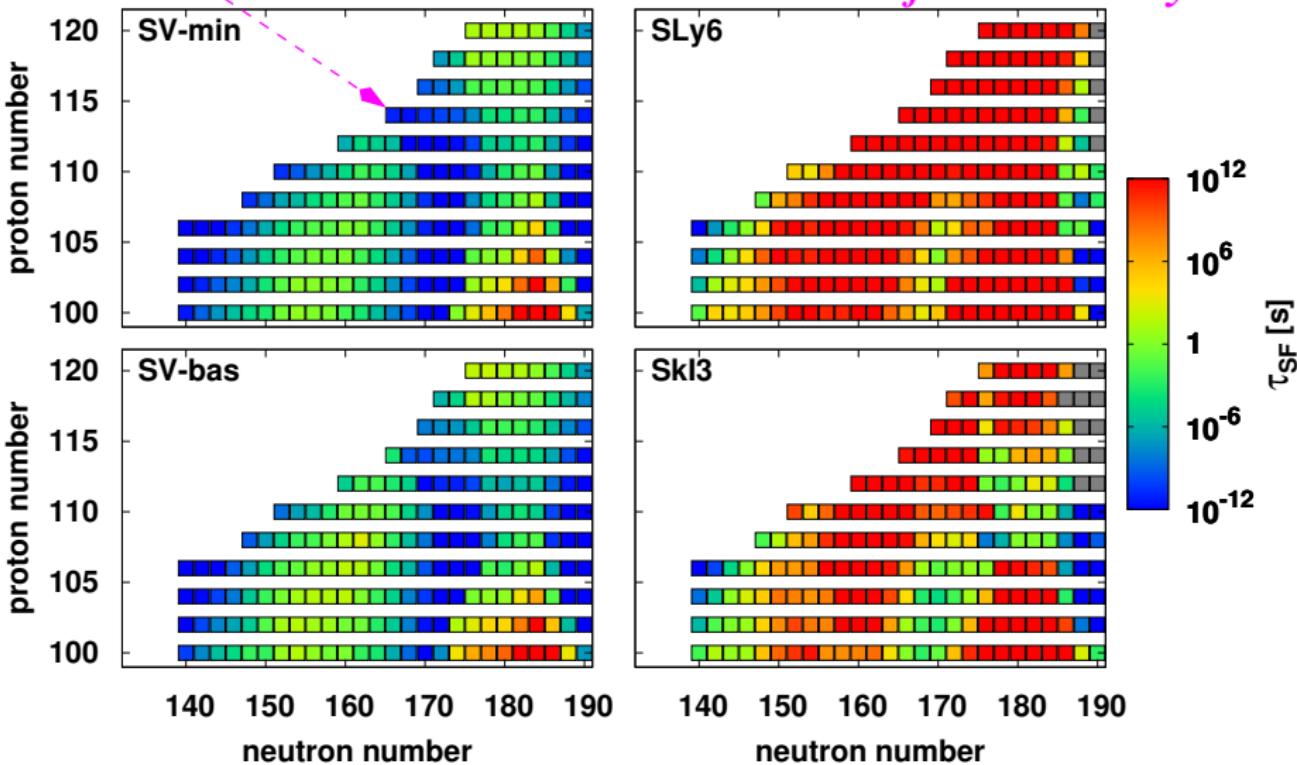
and vice versa



Systematics of lifetimes for a variety of forces

valley of fission instability

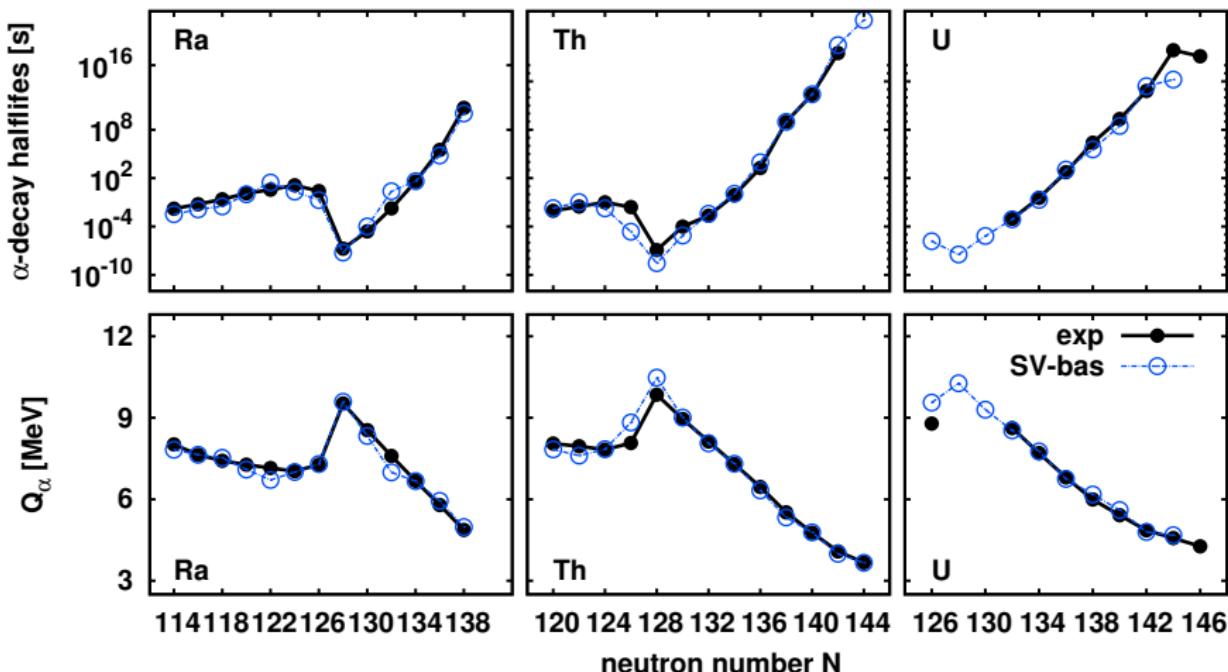
SLy6 & SkI3 (low $m^/m \sim 0.6-0.7$)
overestimate fission stability*



Competing channels: α - and β -decay

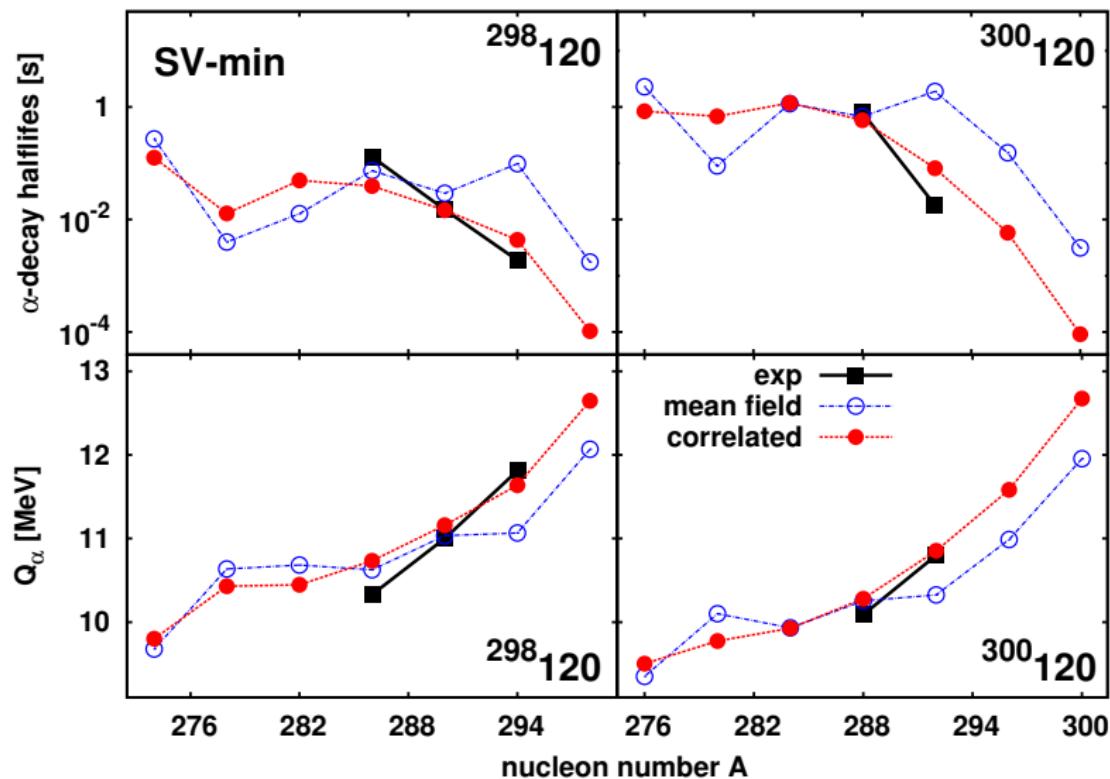
Test of α decay lifetimes

compute α -decay lifetimes τ_α from Q_α using Viola systematics



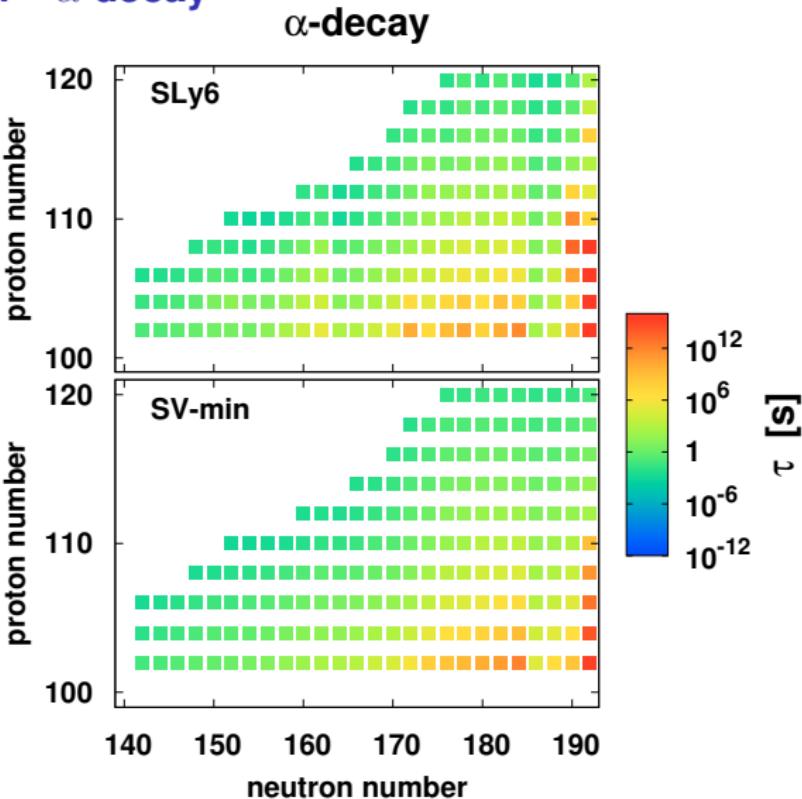
➡ recent Skyrme parameterizations describe α -decay in actinides very well

Test of α decay for SHE – correlation effects



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

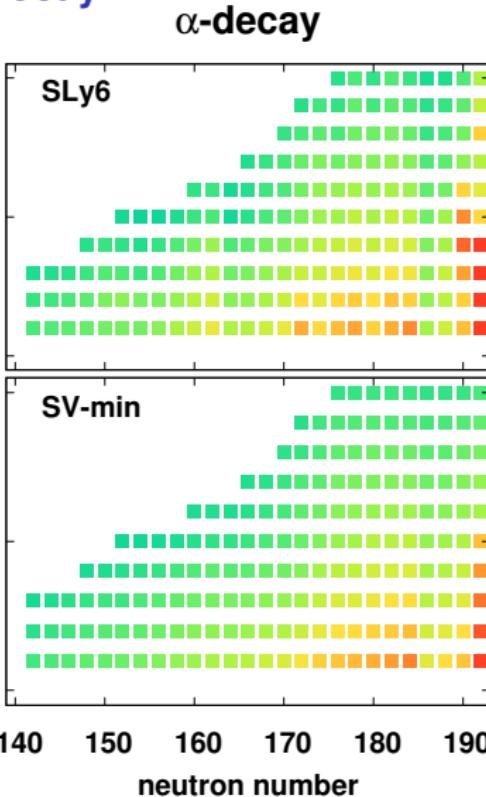
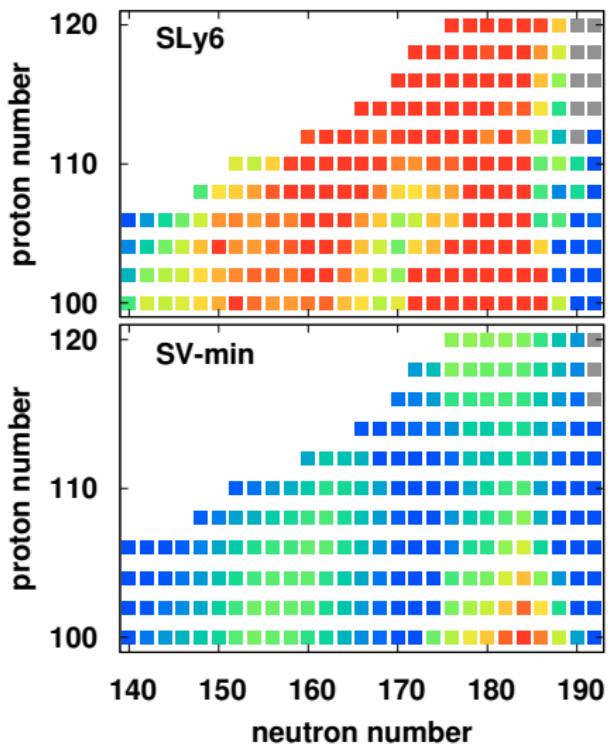
Compare lifetimes: fission – α decay



smoothly varying, independent of force

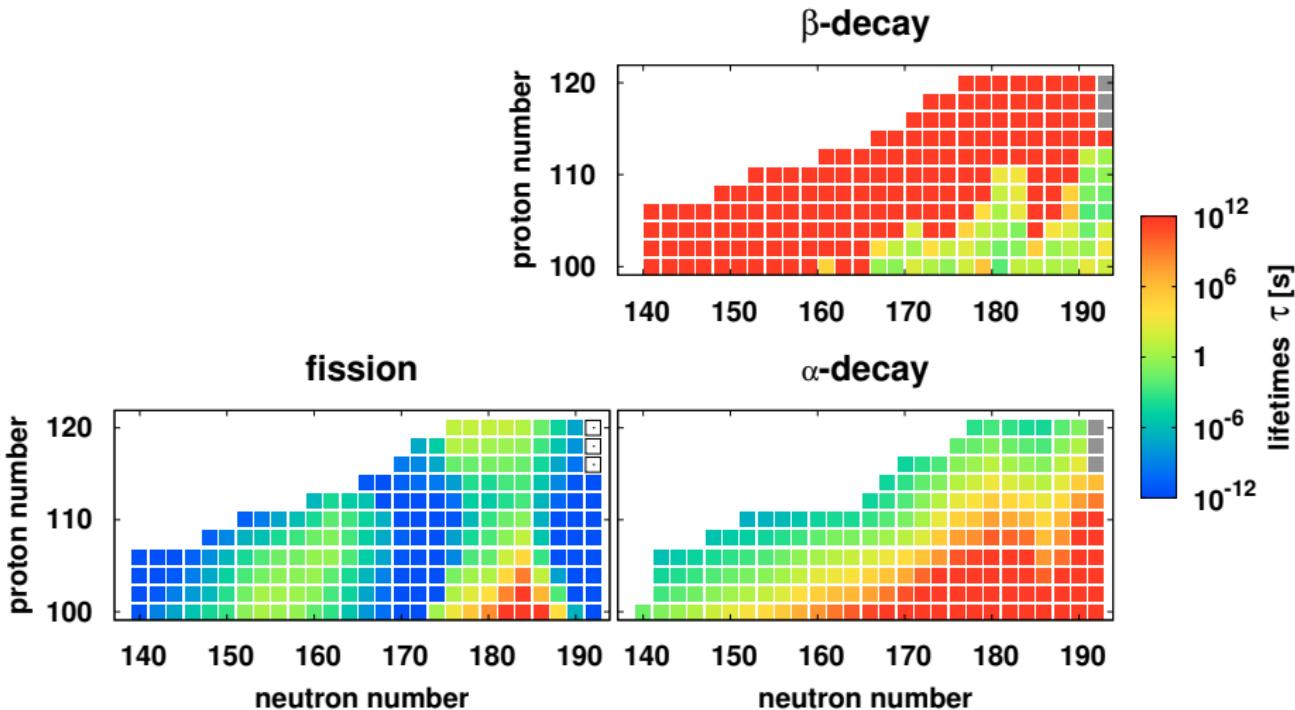
Compare lifetimes: fission – α decay

spontaneous fission



strong fluctuations, force dependent \longleftrightarrow smoothly varying, independent of force

Compare lifetimes: fission – α decay – β decay

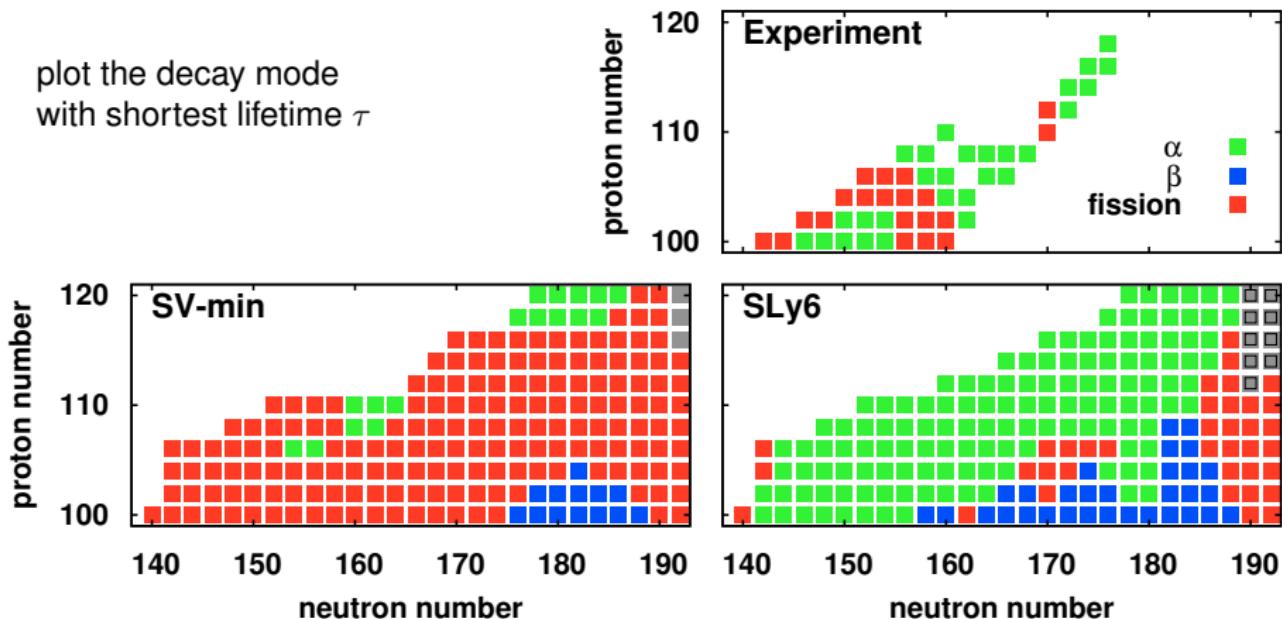


fission fluctuates strongly
pattern robust (shell structure)
magnitude depends on force

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 – SLy6 yields too much fission stability

Conclusions

Fading away of magic numbers

broad band of low density of states \leftrightarrow broad islands of shell stabilization

SHE $Z \gtrapprox 114$ are soft vibrators, may show pronounced shape isomerism

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broad islands stabilization ($Z/N \approx 104/150$ deformed, $Z/N \approx 116/172$ spherical)
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high m^*/m and/or high pairing \leftrightarrow low barriers & τ_{fiss} \leftrightarrow more realistic

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works fine for most recent Skyrme models with $m^*/m \approx 0.9$ (SV-min, SV-bas)

improvements in detail still needed (need slightly larger τ_{fiss} for $Z \geq 112$)

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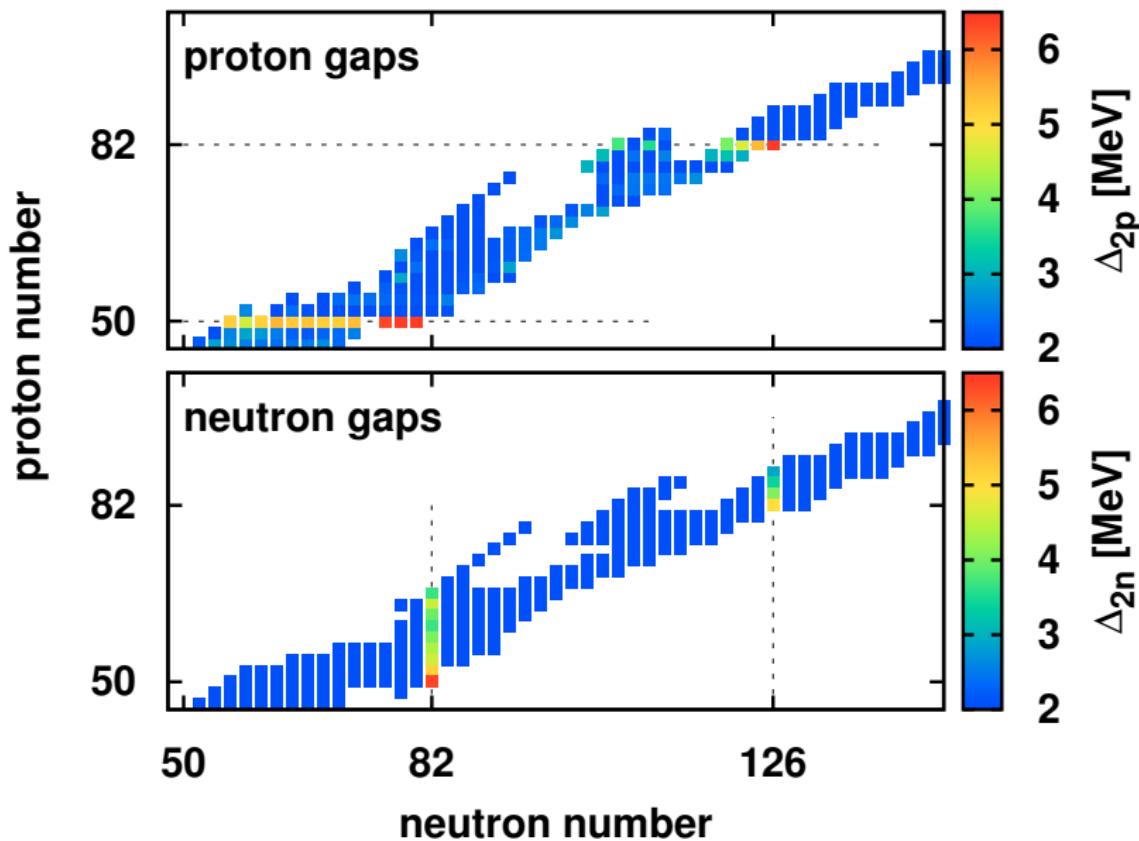
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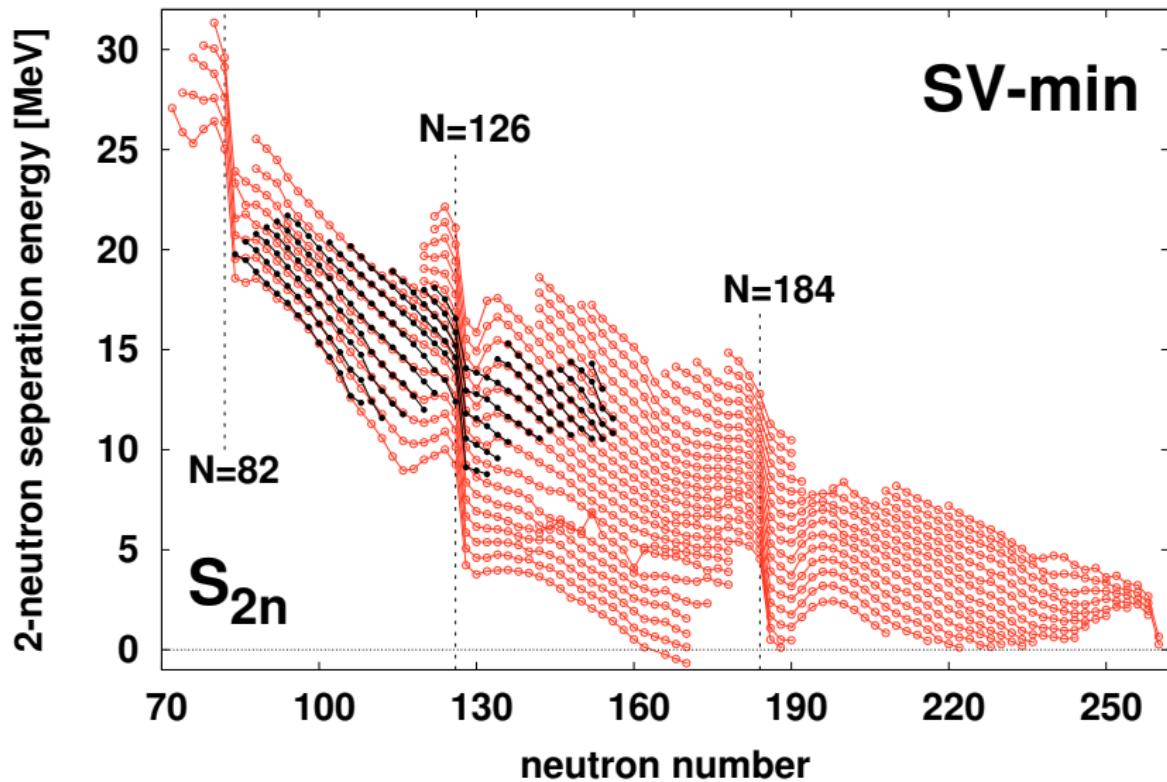
Open problems

wrong trend of τ_{fiss} from island $Z=104$ to island $Z=116$ (still for all Skyrme forces)

Experimental shell gaps



Test of performance for S_{2n}



Coulomb instability and shell stabilization

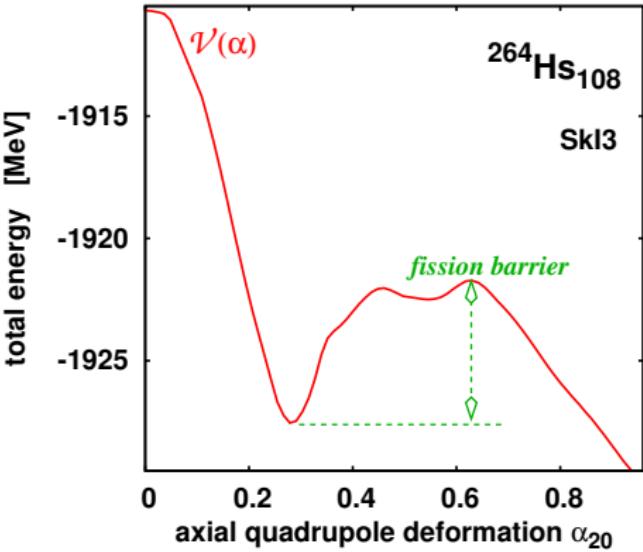
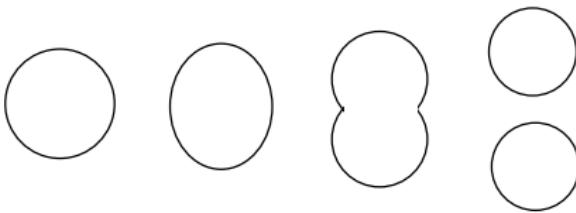
potential energy surface along fission path

nuclear shapes along the fission path
(schematic)

actual microscopic path $\{|\Phi_{\alpha_{20}}\rangle\}$
computed self-consistently
by constrained H.F.

⇒

deformation energy surface $V(\alpha_{20})$,
basis for collective description
of the fission dynamics



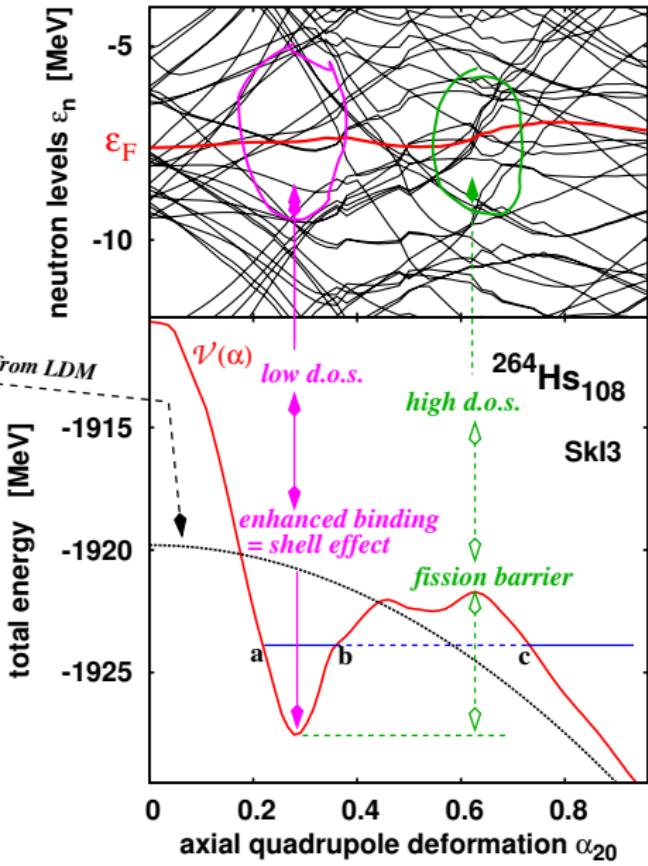
Coulomb instability and shell stabilization

density of state (d.o.s.)
at Fermi surface varies along path

^{264}Hs immediately fission unstable
in liquid drop model (LDM)

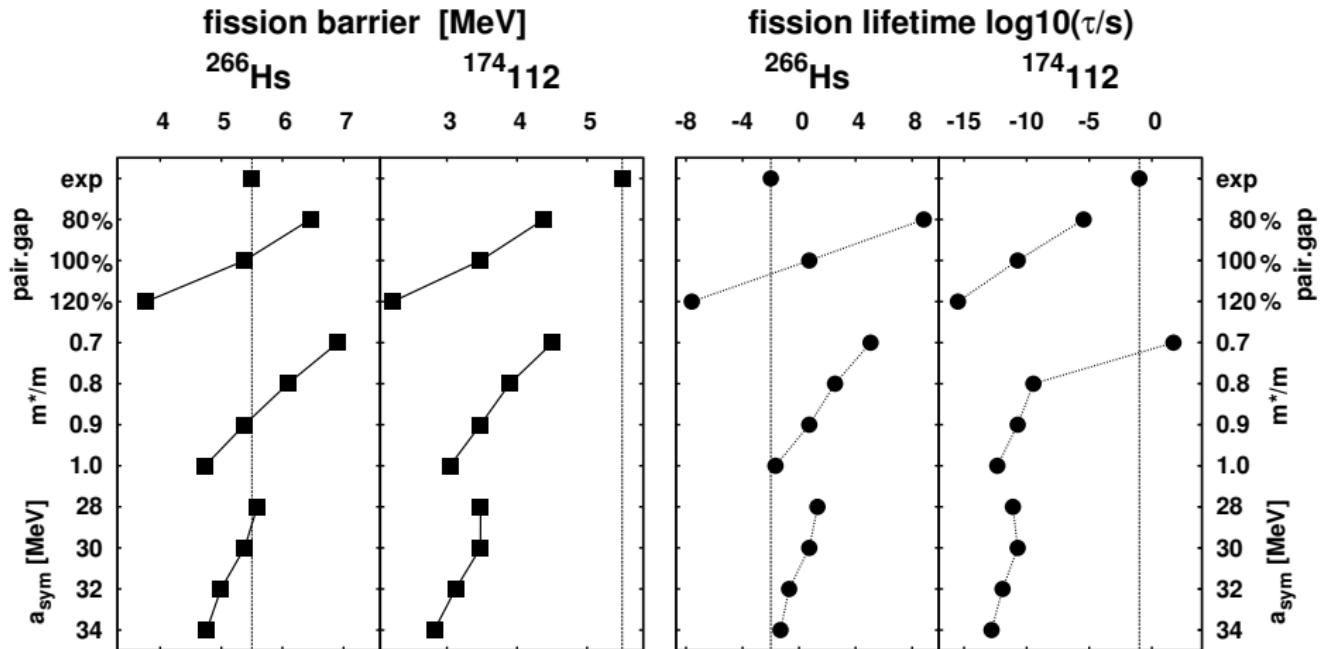
shell structure adds energy correction
⇒ binding pocket ↔ low d.o.s.
⇒ fission barrier ↔ high d.o.s.

Note: "shell correction" automatically
in self-consistent calculations



Fission properties for systematically varied Skyrme forces

exploit uncertainties in Skyrme parameterization to explore allowed variations



pairing has strongest effect on fission, next important is m^*/m (\leftrightarrow shell struct.) and a_{sym}
variations in ^{266}Hs and 112/174 go in parallel — no help for too short τ_{SF} in 112/174

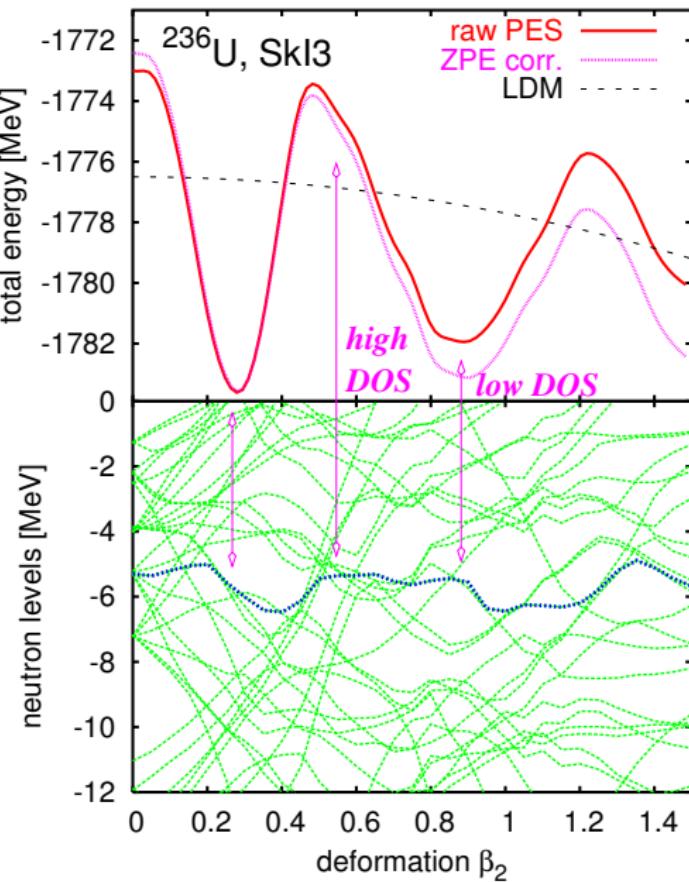
Fission path –example ^{236}U

pure LDM \Rightarrow unstable
stabilized by shell effects
 \Rightarrow subtle balance between
LDM and shell structure

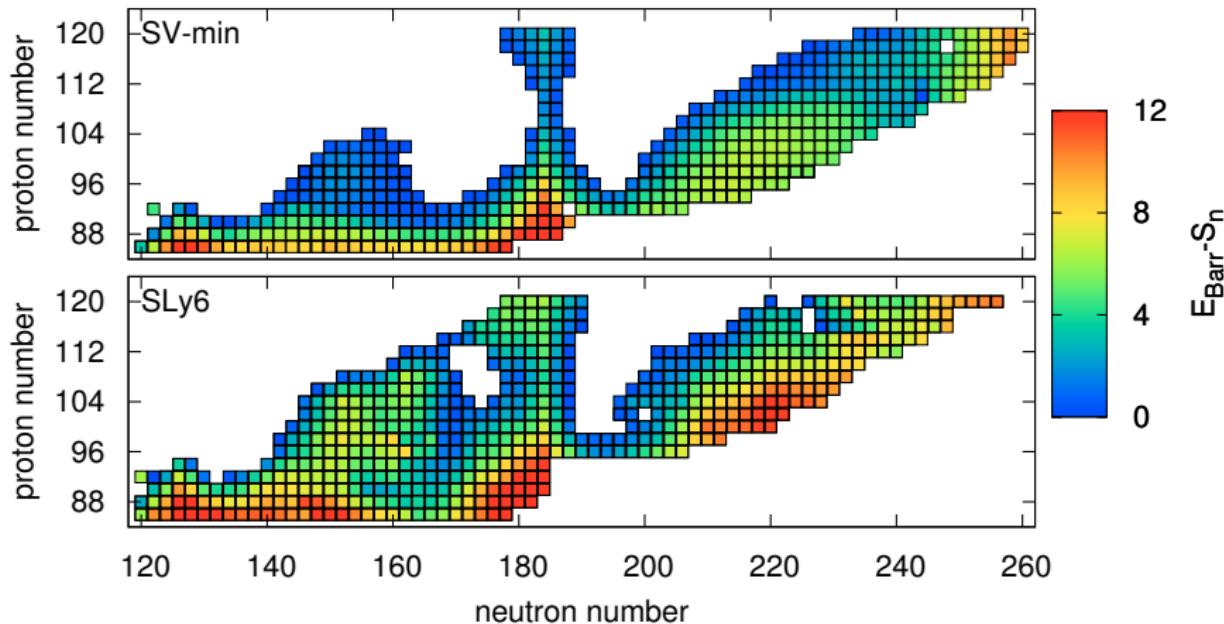
↓
 m^*/m effective mass
 κ sum rule enhanc.
(=isovector m^*/m)
 l^*s models

 K incompressibility
 a_{sym} symmetry energy

ZPE: lowering 0–0.5 MeV (1.barr.)
triaxiality: lowering 1. barr 0–2 MeV



Lifetimes for neutron induced fission



Computation of α -decay lifetimes nuclear fission

Estimate via the Viola-Seaborg relationship:

$$\log \left(\frac{\tau_\alpha}{\text{s}} \right) = (a * Z + b)(Q_\alpha / \text{MeV})^{-1/2} + (c * Z + d) + h_{\log}$$

$$a = 1.66175, b = -0.5166, c = -0.20228, d = -33.9069$$

Key ingredient is the Q_α value:

$$Q_\alpha = E(N-2, Z-2) - E(N, Z) + E(2, 2)$$

$$E(2, 2) = E_{\text{exp}}(^4\text{He}) = 28.3 \text{ MeV}$$

$E(N, Z)$ \longleftrightarrow deformed mean-field calculation

Test of β -decay halflives

