Uncertainties in the evaluation of fission observables

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Observables

- Lifetimes (t_{sf})
- Fragments
  - Mass distribution
  - Kinetic energy
  - Excitation energy
- Fission isomer properties
- Barriers (?) ← Model dependent (?)

both for spontaneous and induced fission

Theory

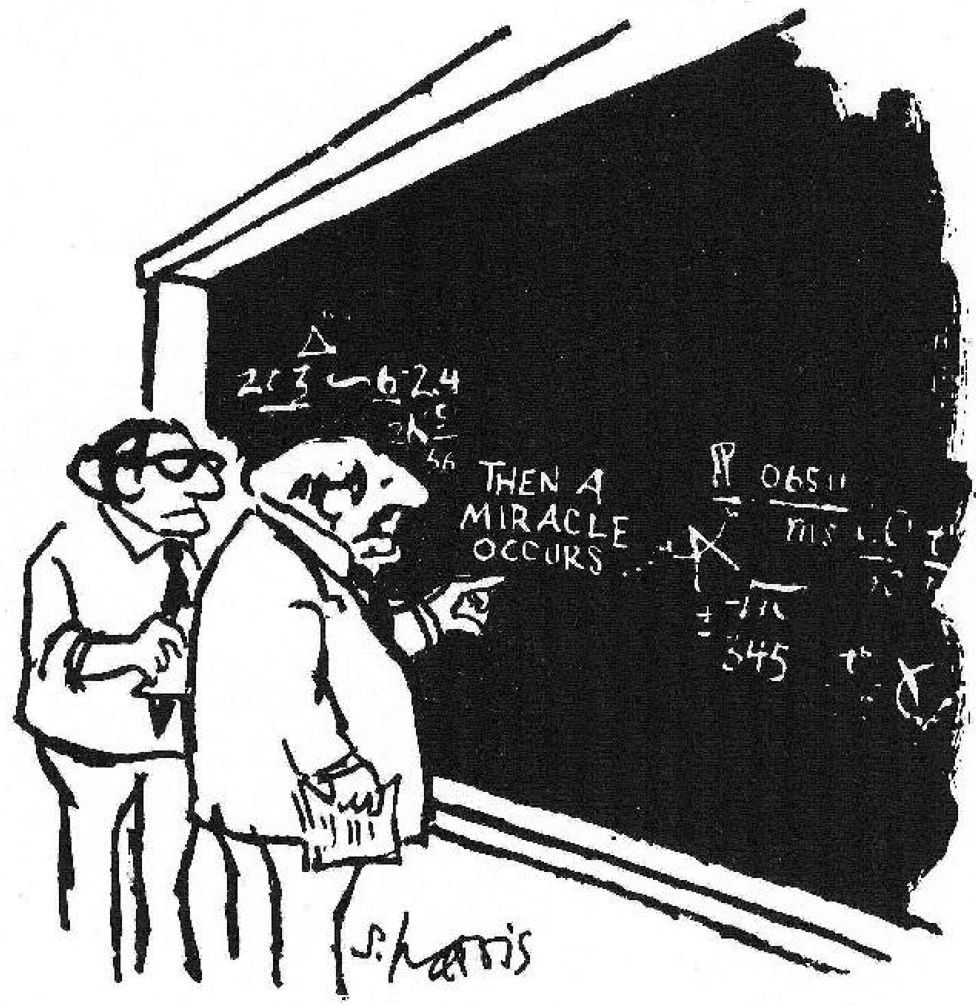
$$\mathcal{P}_{i\to f} = \left|\langle \Psi_f | \hat{U}(\infty, -\infty) | \Psi_i \rangle\right|^2$$

$|\Psi_i\rangle$ Nuclear ground state, Excited state, Nuclear state and an incident neutron, etc

$|\Psi_f\rangle$ the final state can be any of the exit channels

$$|f_1(\alpha_1)\rangle|f_2(\alpha_2)\rangle$$

All the wave functions are the **exact** ones but we do not know how to determine the exact wave functions and the evolution operator ….



"I think you should be more explicit here in step two."

we end up with a variety of different **mean field based** models used to compute the *observables*

we are interested in lifetimes: WKB model

$$t_{\rm sf} = t_0 \exp(2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)})$$

$$B(s) = \sum_{ij} B_{ij} \frac{dq_i}{ds} \frac{dq_j}{ds}$$

zero point energy

$$V(s) = \langle \phi(s) | H | \phi(s) \rangle - \epsilon_0(s)$$

$|\phi(s)\rangle$ is a constrained HFB mean field wave function

Uncertainties

Effective interaction

- ph channel (Skyrme, Gogny, relativistic)

  Influences PES. Under control if the interaction is properly adjusted (D1S, UNDEF1, …)

- pp channel (Global or locally adjusted)

  Influences B(q). Worth to explore

  Pairing strength gets multiplied by a factor eta

- "Exotic" terms (Coulomb exchange+antipairing)

  Relevant at extreme elongations (3rd minimum)

  Antipairing

Gogny

Finite range, density dependent interaction

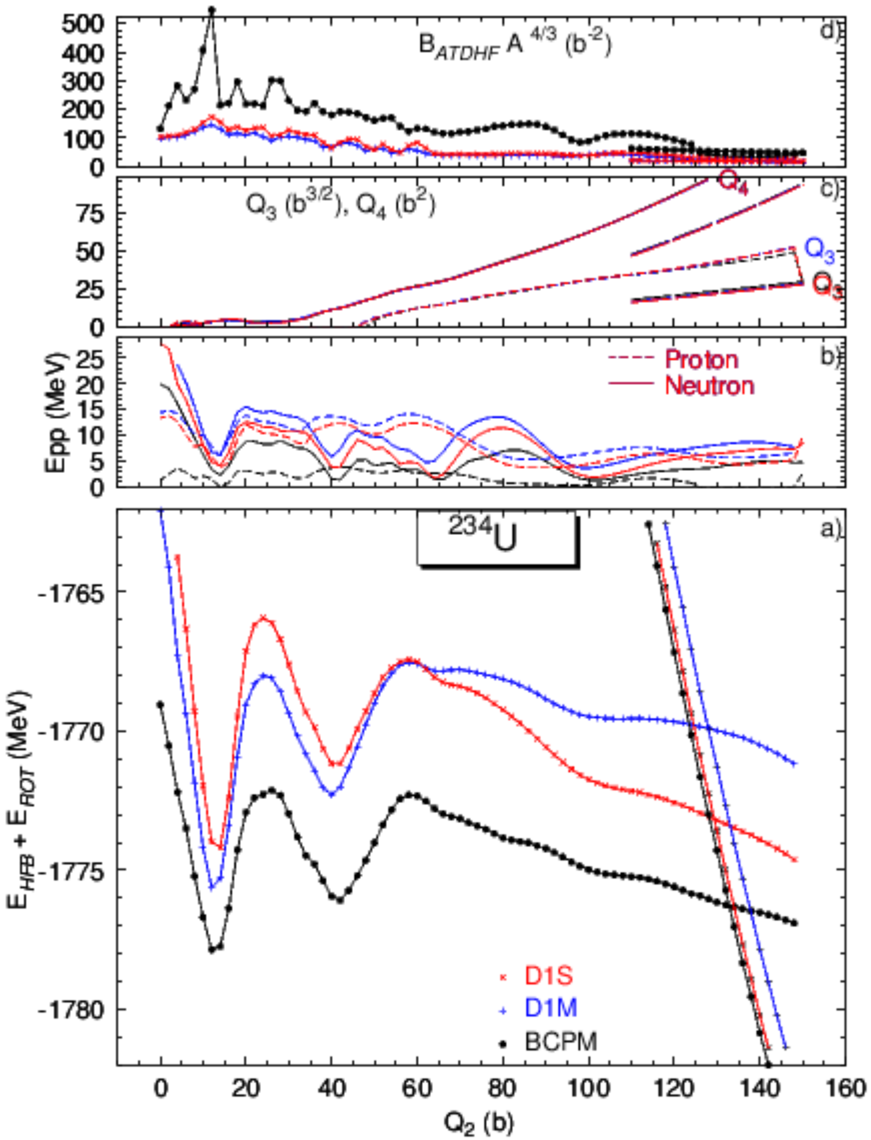
- D1S
    - Fit includes a few selected finite nuclei
    - Fission information in the fit.
    - Poor descriptions of masses
    - Good in describing collective phenomena

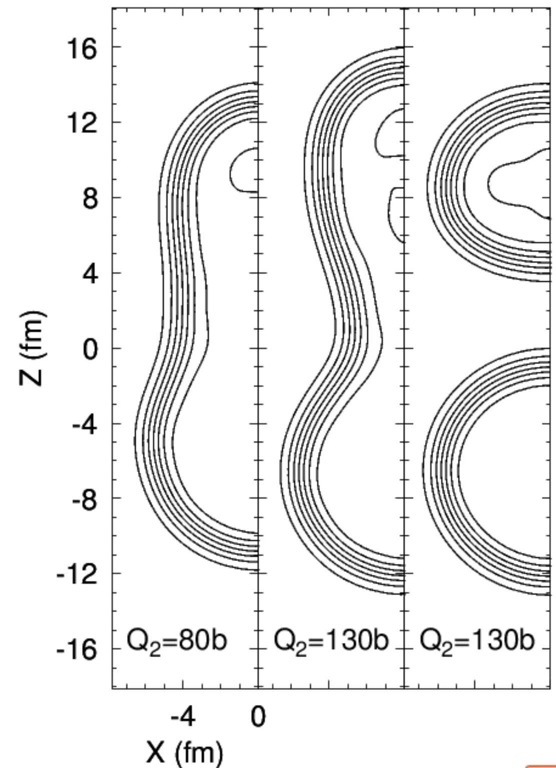
- D1M
    - Global mass fit
    - No fission information in the fit
    - Very good description of masses (rms 0.7 MeV)
    - Not as thoroughly tested as D1S

BCPM

Density functional inspired in microscopic EoS

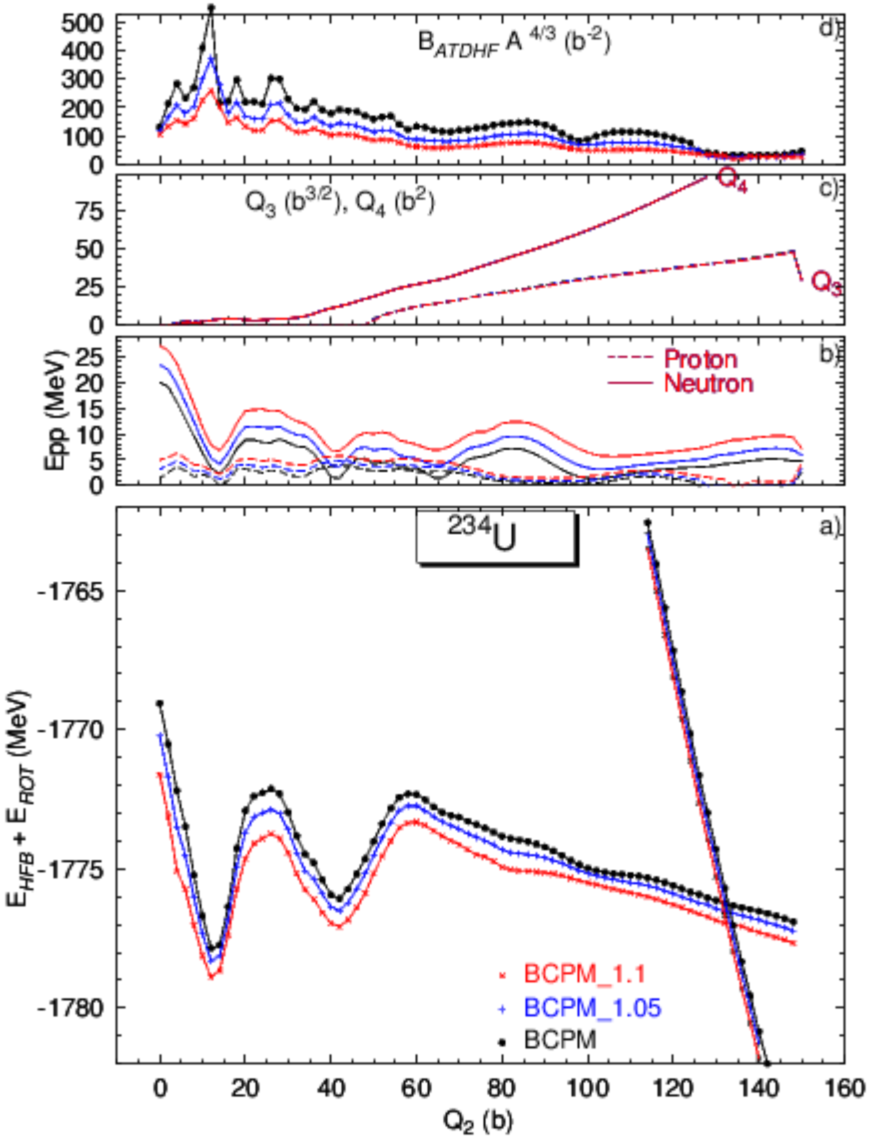
- Global (even-even) mass fit
- No fission information in the fit
- Not bad at masses (rms 1.6 MeV, even-even nuclei)





$t_{sf}^{(S)}$	D1S	D1M	BCPM
GCM	1.3E+23	4.7E+29	2.3E+38

Big differences due to pairing properties



Pairing strength is multiplied by a factor η =1.05 (5%) or 1.10 (10%)

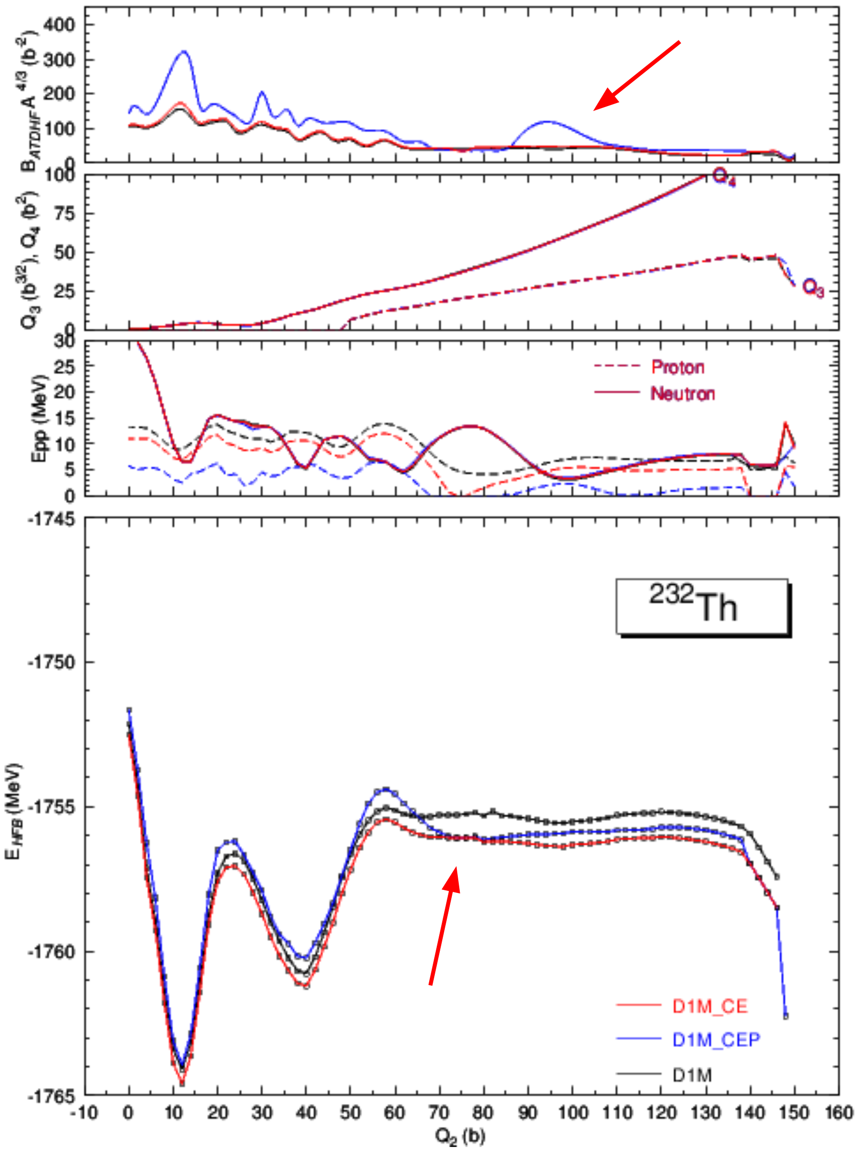
Huge impact on lifetimes

η	t_{sf} (s)
1.0	2.3 E+38
1.05	8.0E+27
1.10	6.7E+21

consequence of the reduction of the collective mass

Little impact on binding energies and other properties like deformation

Coulomb repulsion is a fundamental concept in fission that should be treated exactly: ⇨ Exact Coulomb exchange and Coulomb antipairing



- Exact Coulomb exchange is important for elongated configurations
- Coulomb pairing also important (enhances barriers, even the third one)
- Coulomb antipairing increases collective inertia
- Coulomb antipairing produces bumps in the inertia the favor the localization of wave function in the third minimum

t_{sf} with *ATDHFB* inertias

D1S	7.5 E+42	
D1S(CE)	3.9 E+43	!!!!
D1S(CE+CP)	2.9 E+51	
D1M	3.6 E+54	
D1M(CE)	4.8 E+56	!!!!
D1M(CE+CP)	5.1 E+69	

Inertias

$$t_{\rm sf} = t_0 \exp(2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)})$$

Two types of inertias

- ATDHFB: Contains time odd components
- GCM: No time odd components

Both are traditionally computed using the “cranking approximation”

ATDHFB

$$B(Q_{20}) = \frac{1}{2} \frac{M_{-3}}{(M_{-1})^2}.$$

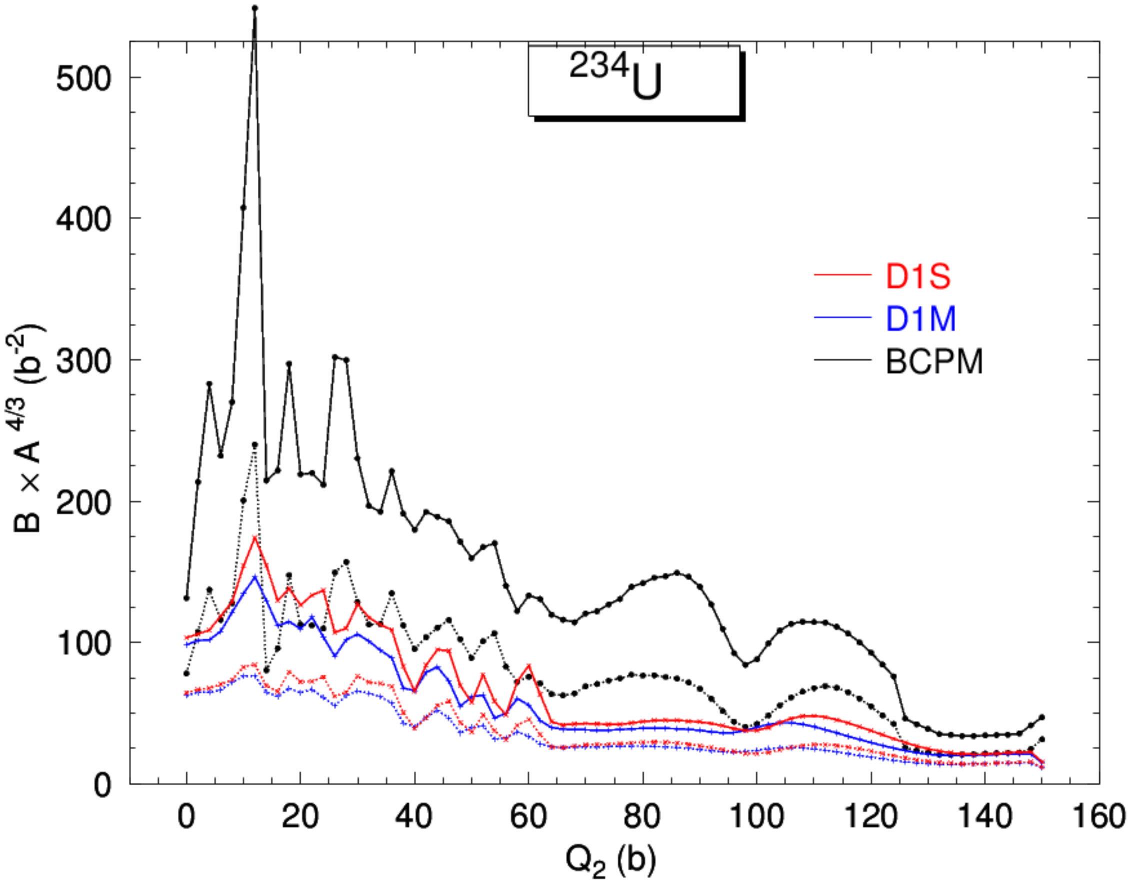
GCM

$$B(Q_{20}) = \frac{1}{2} \frac{M_{-2}^2}{(M_{-1})^3}.$$

$$M_{(-n)} = \sum_{\alpha > \beta} \langle 0 | Q_{20} | \alpha\beta \rangle \frac{1}{(E_\alpha + E_\beta)^n} \langle \alpha\beta | Q_{20} | 0 \rangle$$

Both can be computed exactly but the numerical cost involved is rather high (prohibitive up to now).

Exact inertias can be a factor 1.5 larger than the approximate ones.



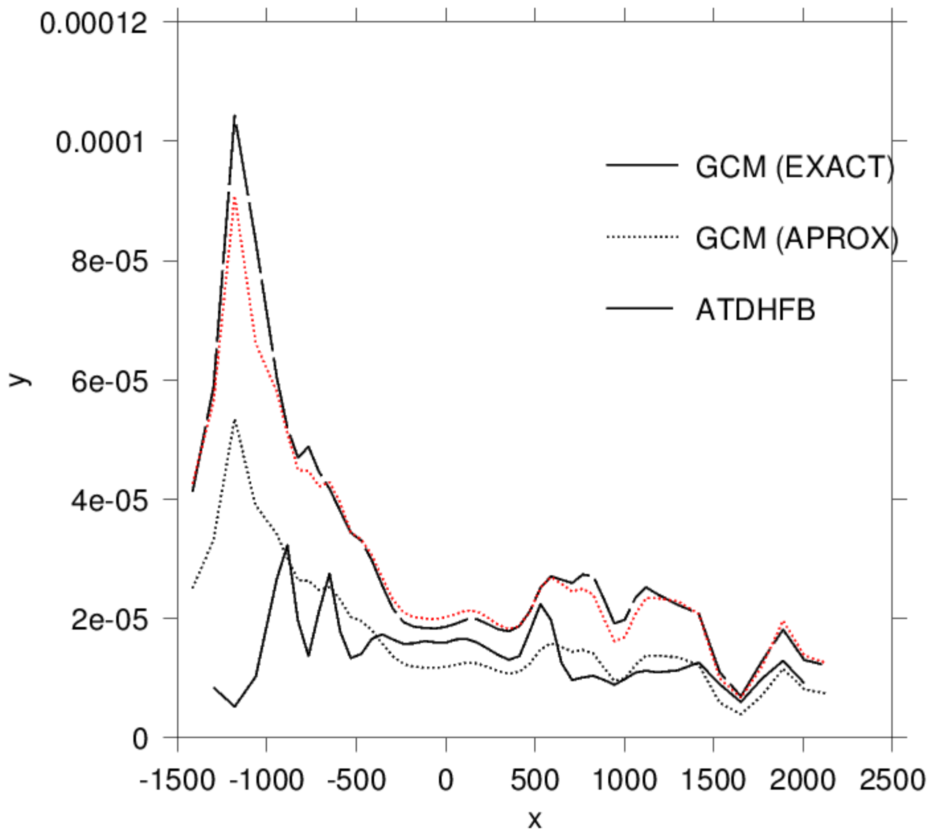
t_{sf}	ATDHFB	GCM
D1S	4.3 E+32	5.7 E+23
D1M	6.0 E+46	6.6 E+34
BCPM	3.0 E+54	1.6 E+40

Up to 14 orders of magnitude difference

Full line: ATDHFB (Cranking) mass
Dashed: GCM (Cranking) mass

ATDHFB is a factor of 1.8 larger than GCM

Exact versus approximate GCM masses



Quadrupole inertia

If inertia gets multiplied by a factor f the actions is multiplied by sqrt(f) as the expected change in the exponent of t_{sf}

- Exact GCM is computed with second derivatives of energy overlap
- Approximate GCM using the “cranking” formulas. Red curve: approximate x 1.6
- ATDHFB computed using “cranking” formulas

Zero point energies

- Symmetry restoration
  (Rotational, PNP, parity, Center of mass)
- Fluctuations on quadrupole, octupole, etc

Typically, symmetry restoration energies are considered in the spirit of Projection After Variation

$$\frac{\langle \Delta \vec{J}^2 \rangle}{2\mathcal{J}_{Yocc}}$$

Rotational energy correction well approximated by rotational formula if exact Yoccoz is used.

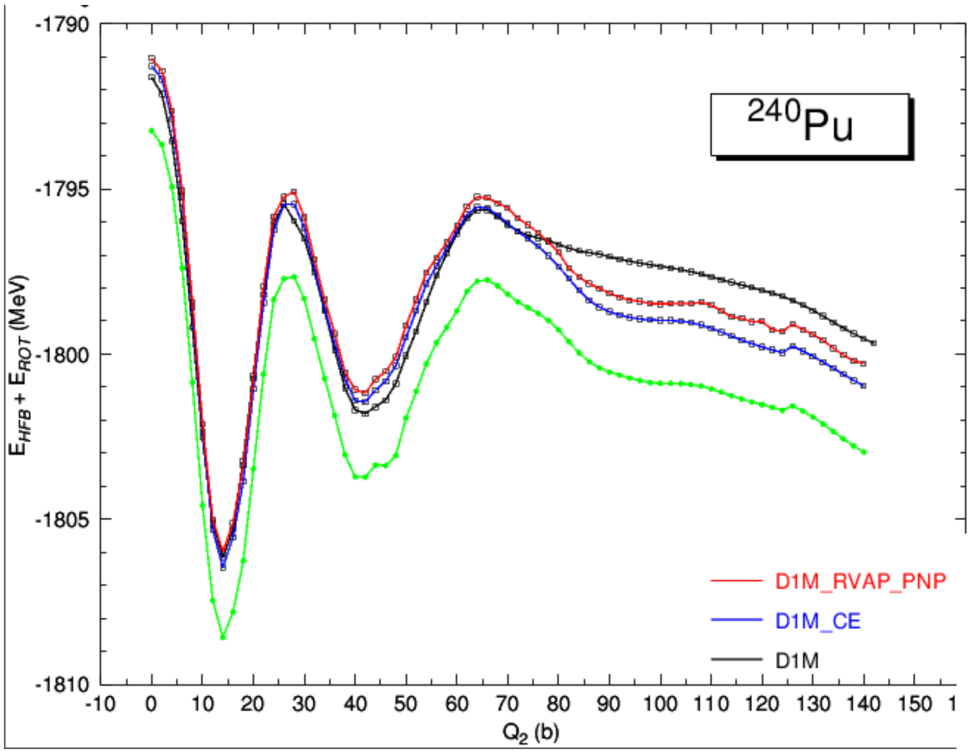
A good approximation to Yoccoz is to use “cranking” formula and multiply by a phenomenological facto

Rotational correction substantially modifies energy landscape (3 - 7 MeV)

Parity projection and PNP-PAV have little impact on energy landscapes

PNP-VAP increases pairing correlations: the inertia decreases !

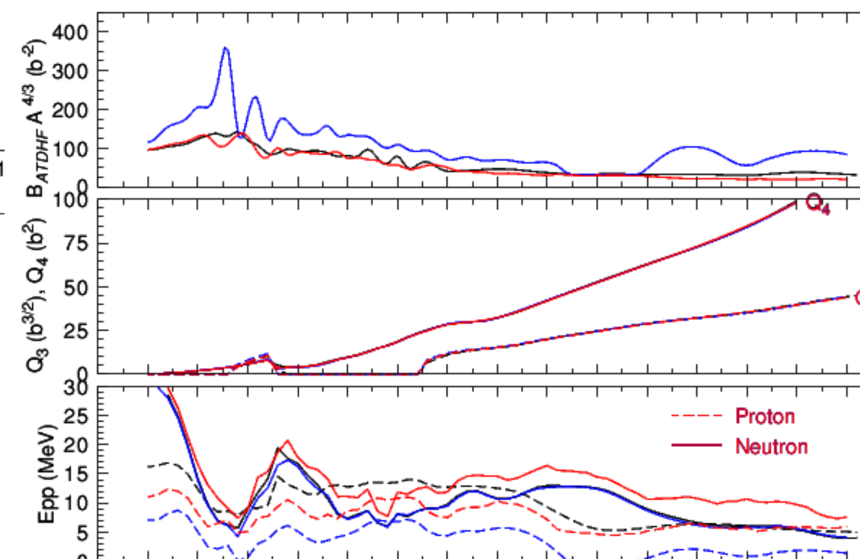
PNP-RVAP: Minimize projected energy on a restricted subspace (fluctuations in proton and neutron number)



Coulomb exchange and antipairing has to be considered to avoid pathologies in the evaluation of overlaps

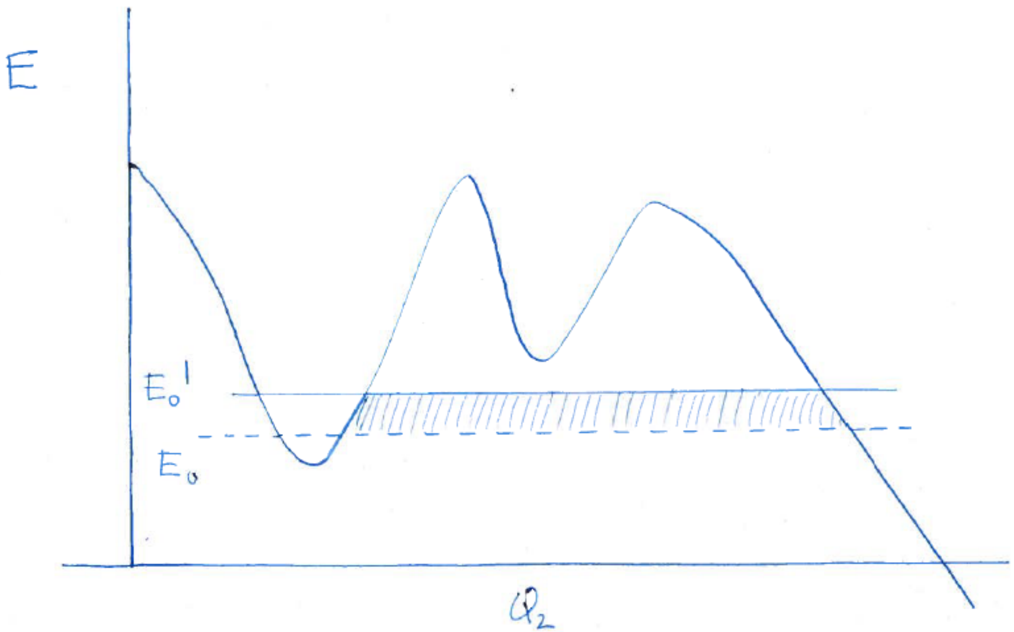
PES affected by PNP-RVAP

Collective mass similar to HFB one !
Effect of Coulomb antipairing cancells out



The E_0 parameter

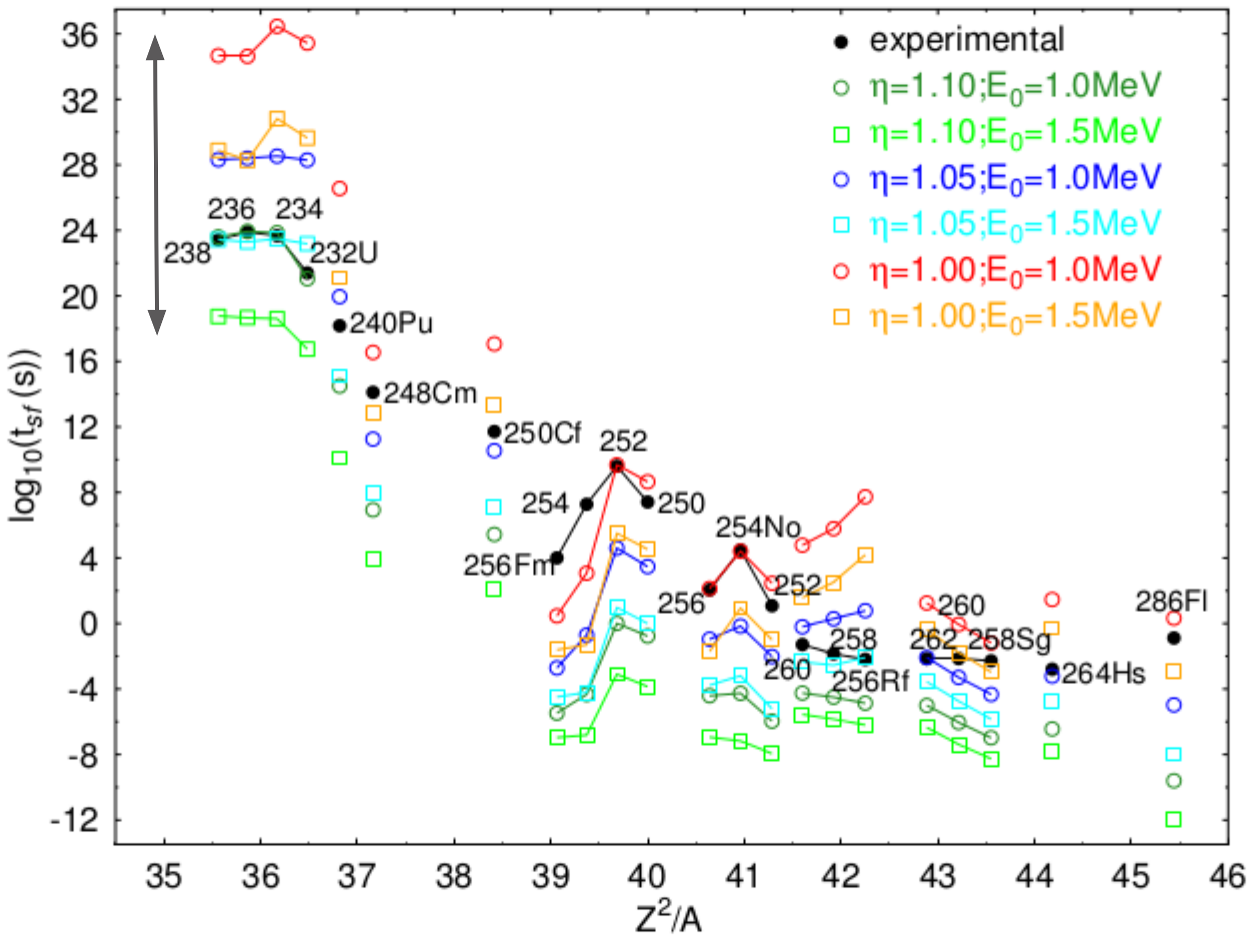
$$t_{\rm sf} = t_0 \exp(2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)})$$



E_0 is taken as the HFB ground state energy plus the zero point energy of the quadrupole motion: typically some value in between 0.5 and 1.5 MeV

Increasing E_0 makes the integration interval in the action sorter and the action smaller. Reduces lifetimes (up to 5 orders of magnitude)

Some physics with BCPM



Nuclei with known experimental data on t_{sf}

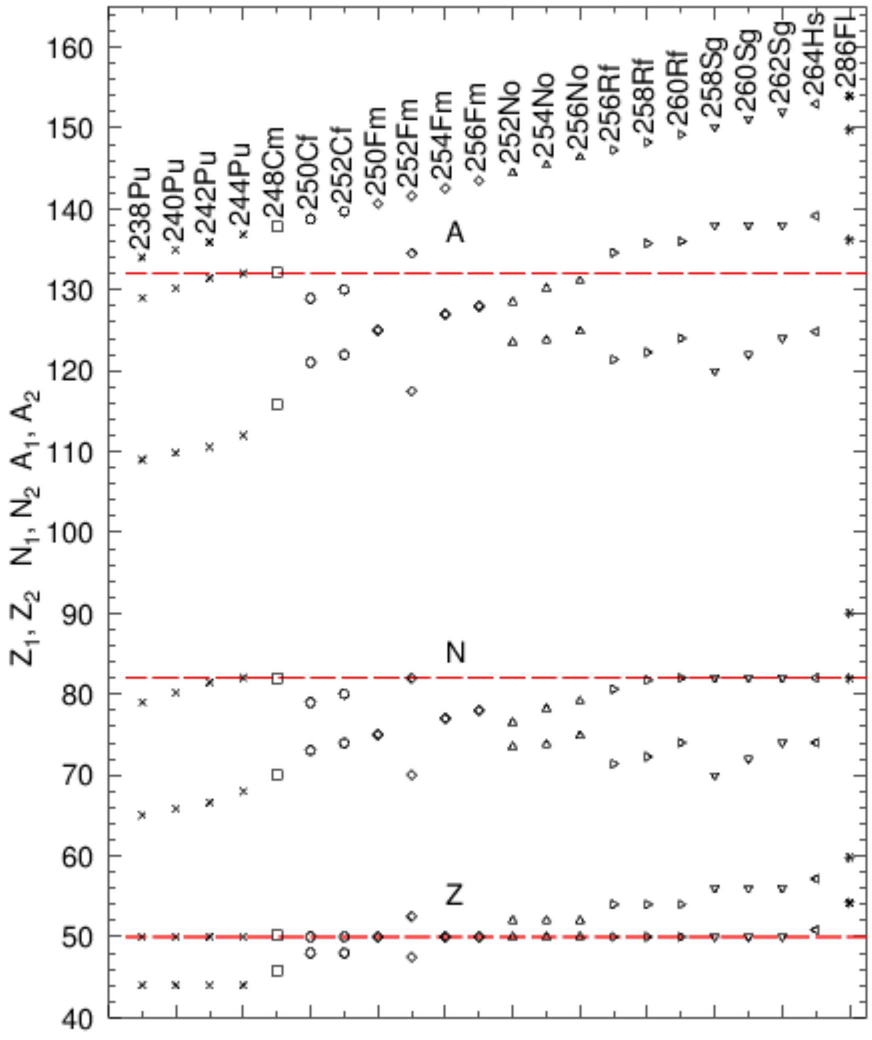
GCM inertias

Large variability with eta and E_0

Isotopic trend reproduced

Trend with mass number reproduced

Z, N of each fragment



Consider a large Q20 value

Constrain the neck to a small value

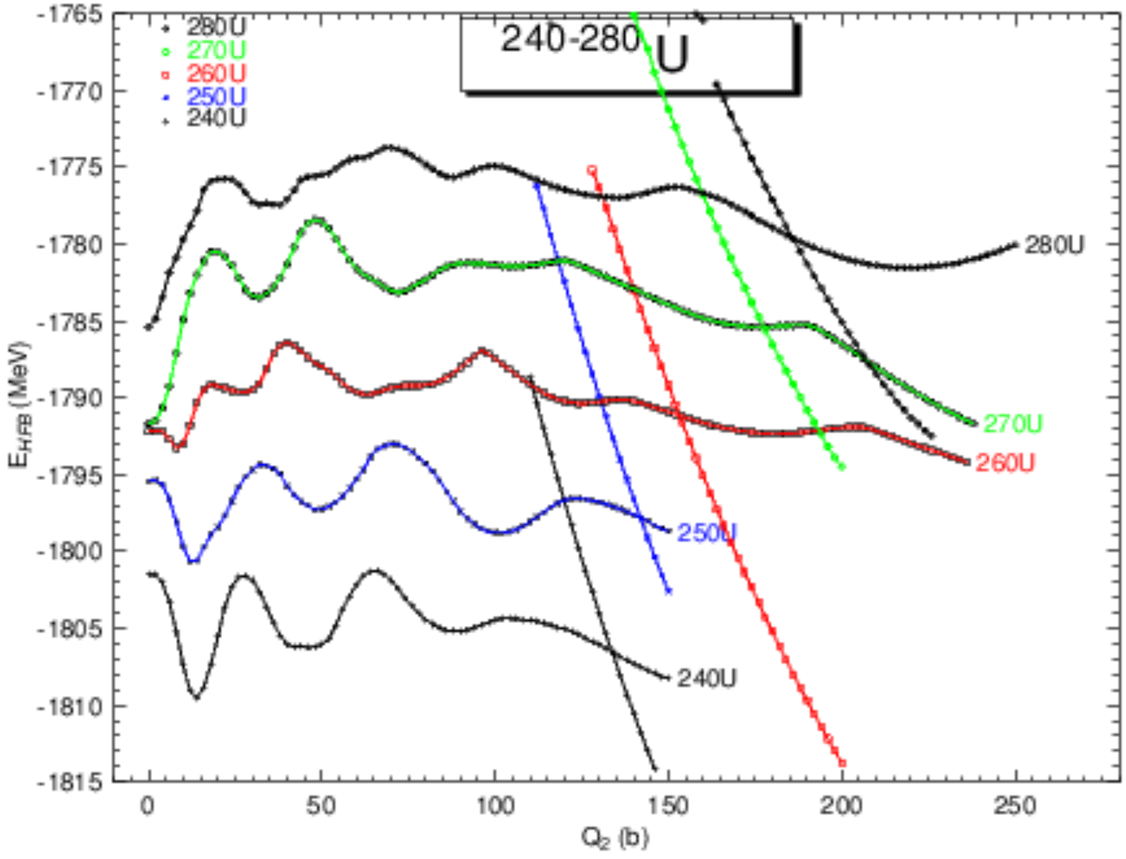
Release the constraint to obtain a solution with two fragments

Use that solution to seed a calculation for larger values de Q20 (i.e. increase the separation between fragments)

Continue the calculation until the Z and N values of the fragments do not change significantly as Q20 is increased

Neutron rich uranium (predictions!)

From ^{230} U up to ^{282} U

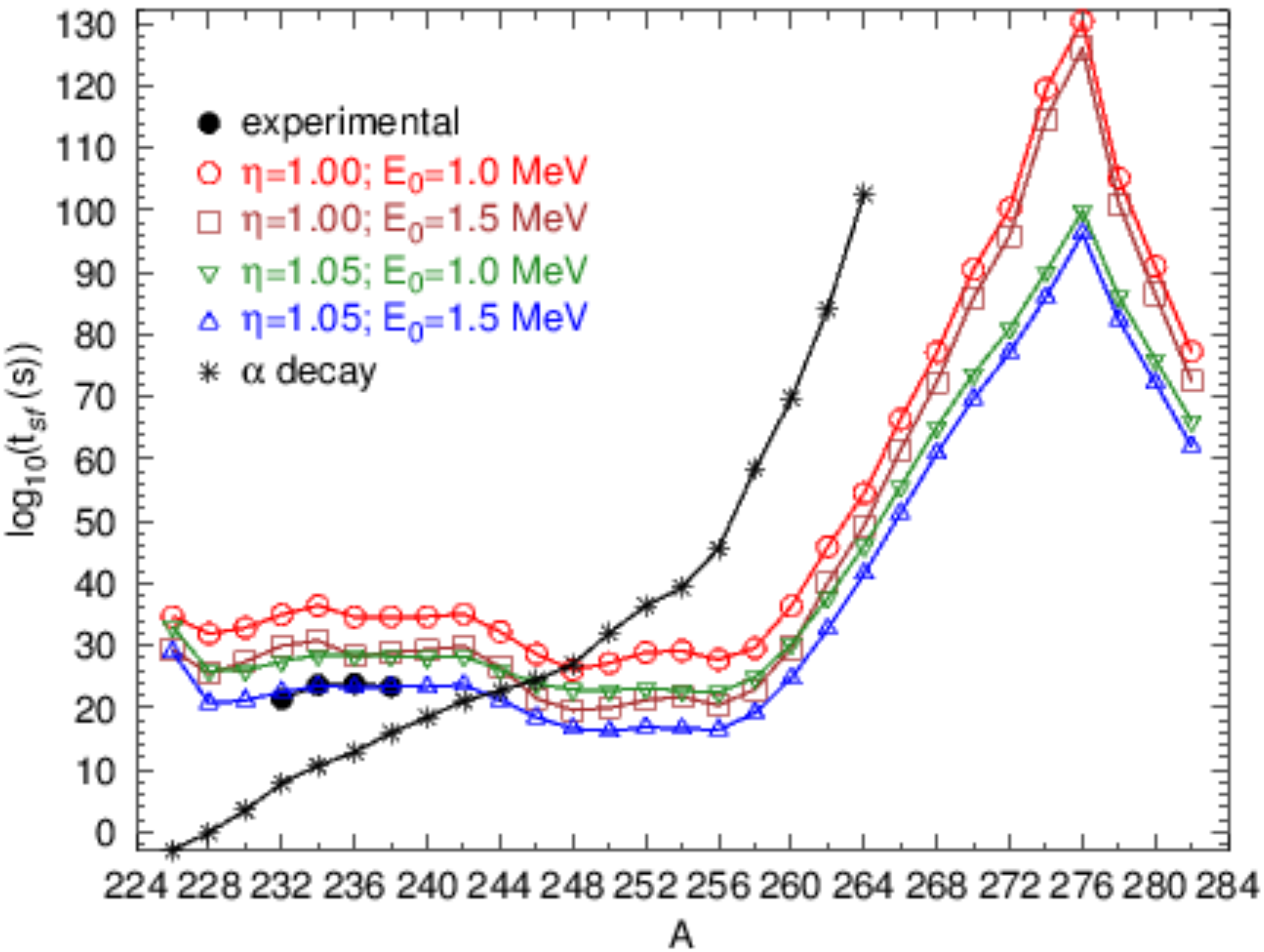


Emergence and evolution of the third minimum

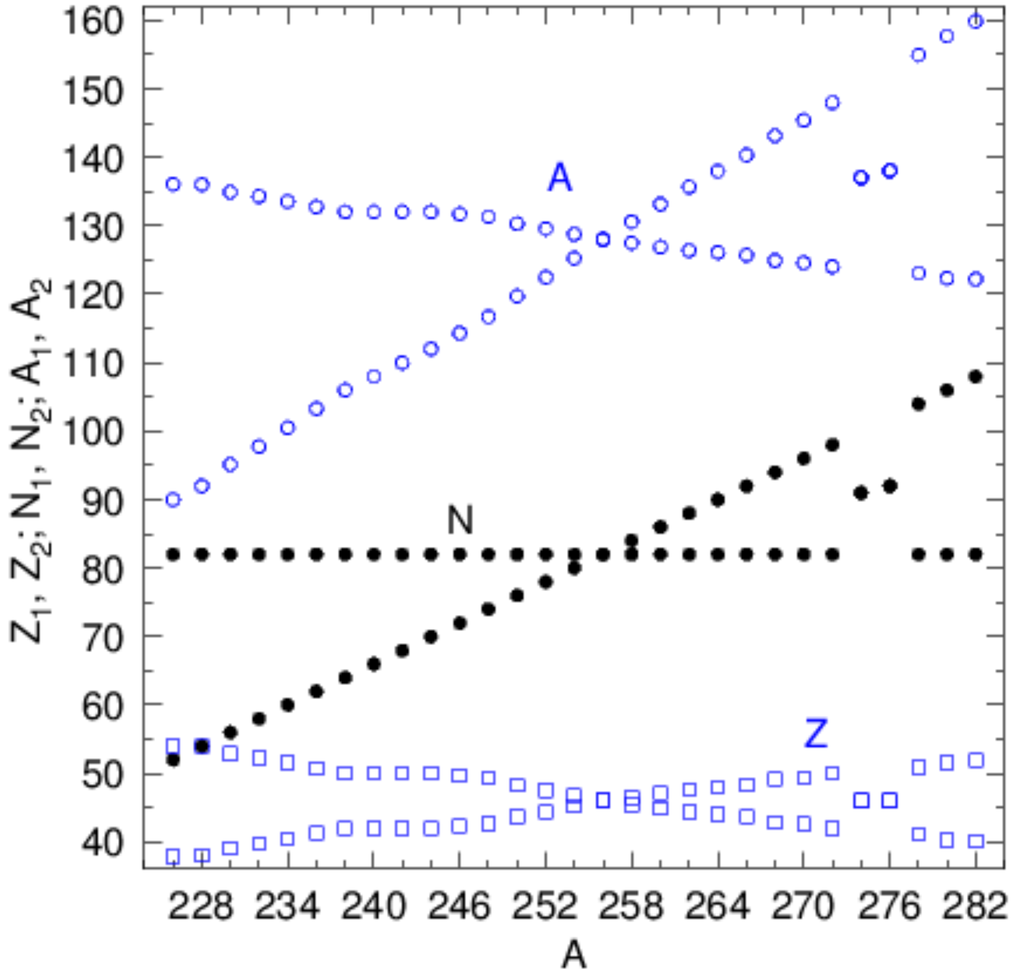
Barriers increase and become wider

alpha decay from Viola's formula (BCPM is good with masses)

Peak at ^{276}U

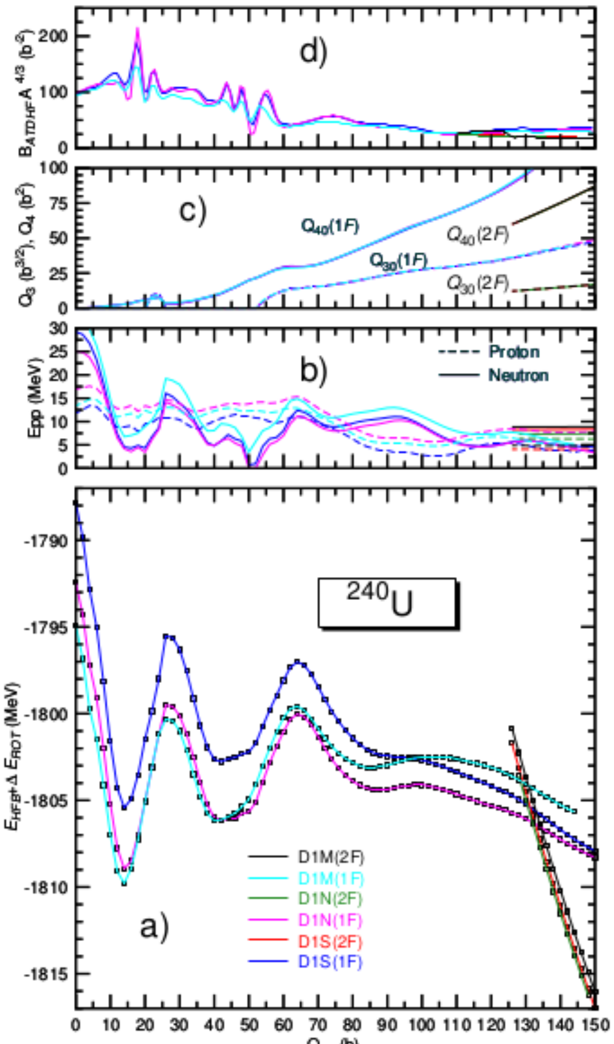


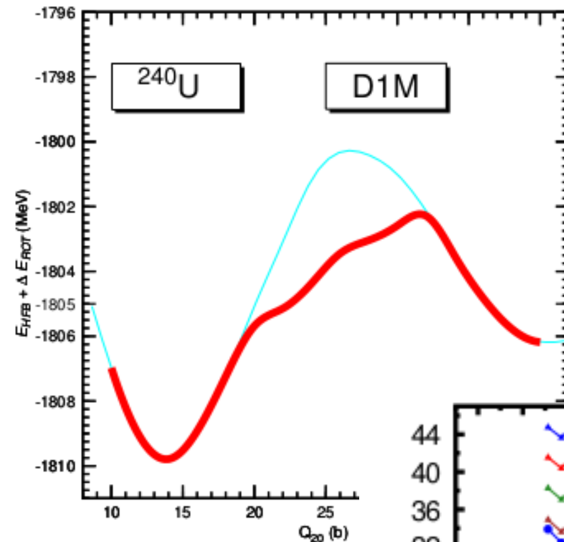
Fragments

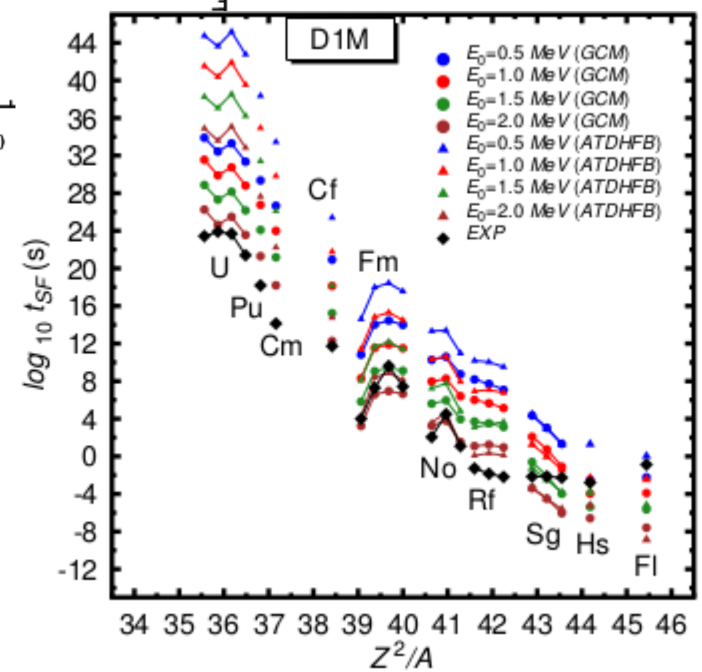


160
150
140
130
120
110
100
90
80
70
60
50
40
$Z_1, Z_2; N_1, N_2; A_1, A_2$
A
N
Z
228
234
240
246
252
258
264
270
276
282
A

Gogny D1S, D1M and D1N







Minimizing the action

Long ago (Funny hills paper) the minimization of the action was proposed

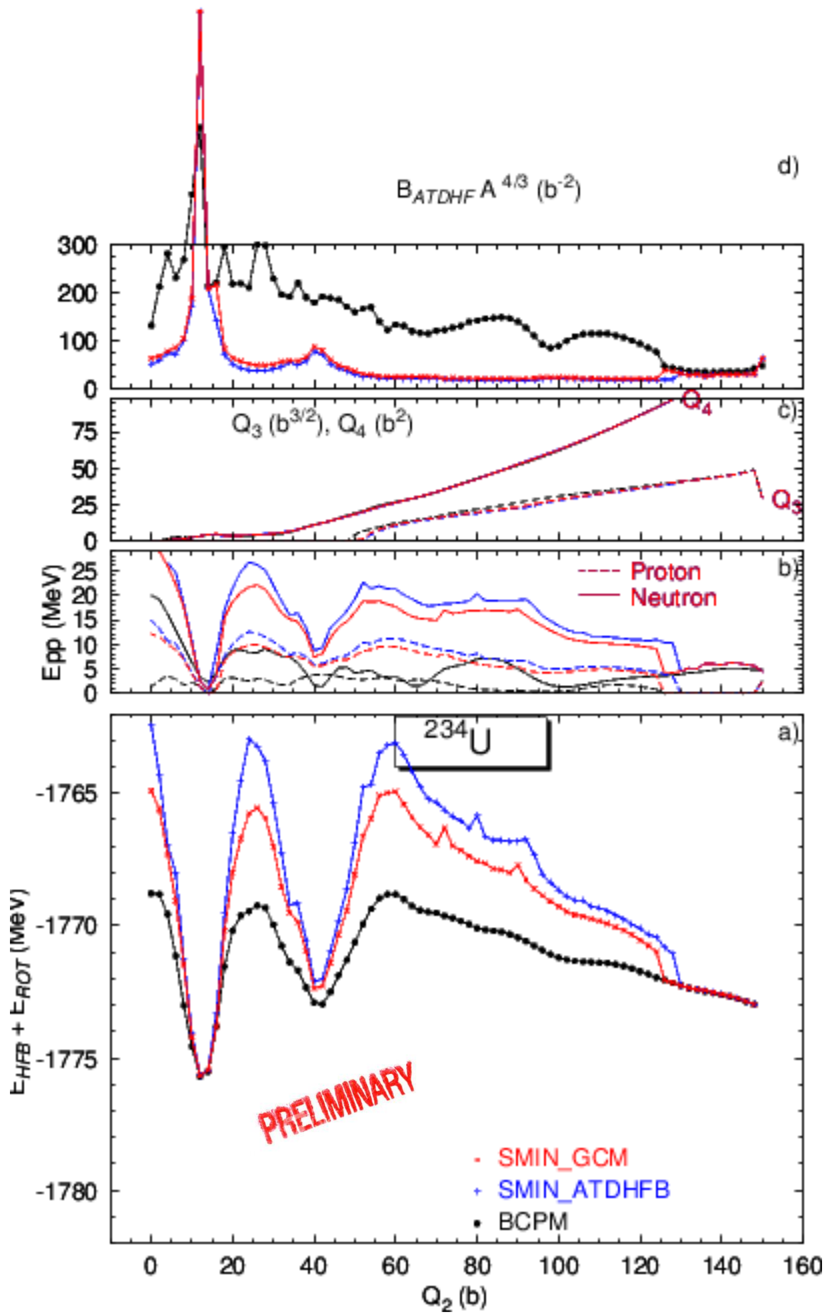
$$t_{\mathrm{sf}} = t_0 \exp(2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)})$$

Later, Moretto proposed a simple model of fission where the pairing gap is a relevant degree of freedom

$$B \sim \frac{1}{\Delta^2} \qquad V(s) = V_0(s) + 2g(\Delta - \Delta_0)^2$$

Minimization of the action using the pairing gap as degree of freedom decreases t_{sf} by several orders of magnitude

Pursued by Pomorski and others in the 80's

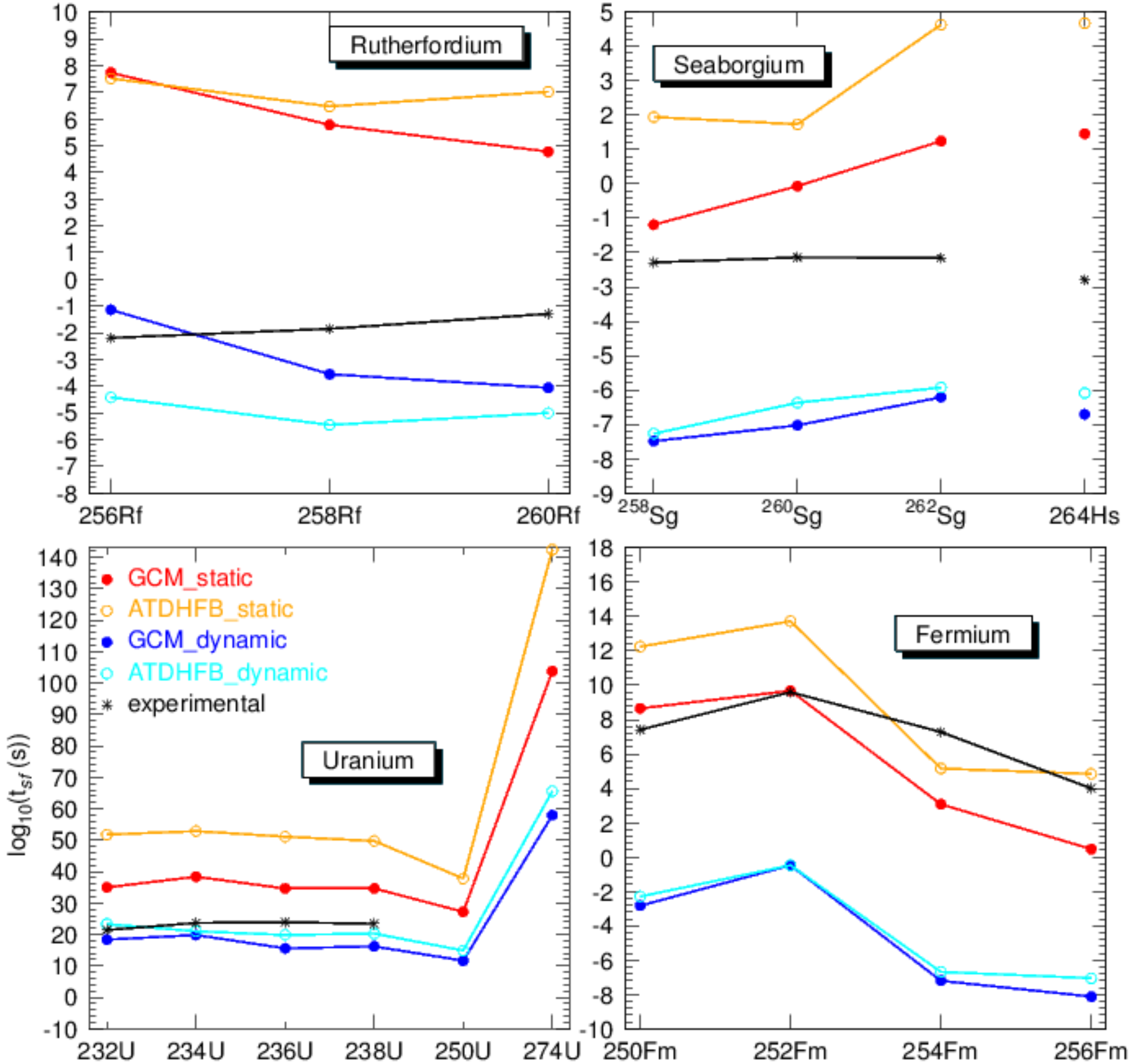


We have explored the idea using $\langle \Delta N^2 \rangle$ instead of the gap to search for a minimum of the action for each quadrupole moment

Strong quenching of the collective mass at the minimum of S.

Moderate increase of the potential energy (meaning of barrier heights here ?).

The action gets reduced by 20 % - 30 % implying a similar reduction of the exponent in t_{sf}



A reduction of many orders of magnitude is observed
The ATDHFB and GCM results seem to “converge”

also

- Numerical convergence with basis size, box size, step size, etc should be assessed
- An easy to implement extrapolation scheme to “infinite” basis will be beneficial
- Numerical accuracy of matrix elements, algorithms, etc should be tested (specially Coulomb)

Conclusions

- For a qualitative description of fission the present mean field methods are still valid

- To reach the “quantitative” level the dynamical aspects of fission have to be addressed

  - Pairing as a new degree of freedom
  - Least action versus Minimum energy
  - Exact evaluation of inertias
  - Particle number restoration
  - Full treatment of Coulomb

Thanks to ...

Previous studies

Michal Warda, K. Pomorski, S. Pérez, V. Martín and F de la Iglesia

Cluster radioactivity

Michal Warda

Present (in progress) studies

Samuel Giuliani (BCPM) and R.R. Rodriguez-Guzman (Gogny)