Nuclear uncertainties in the evaluation of fission observables

L.M. Robledo
Universidad Autónoma de Madrid
Spain

Nucleo-synthesis of elements

A large chemical elements are produced in violent stellar environments

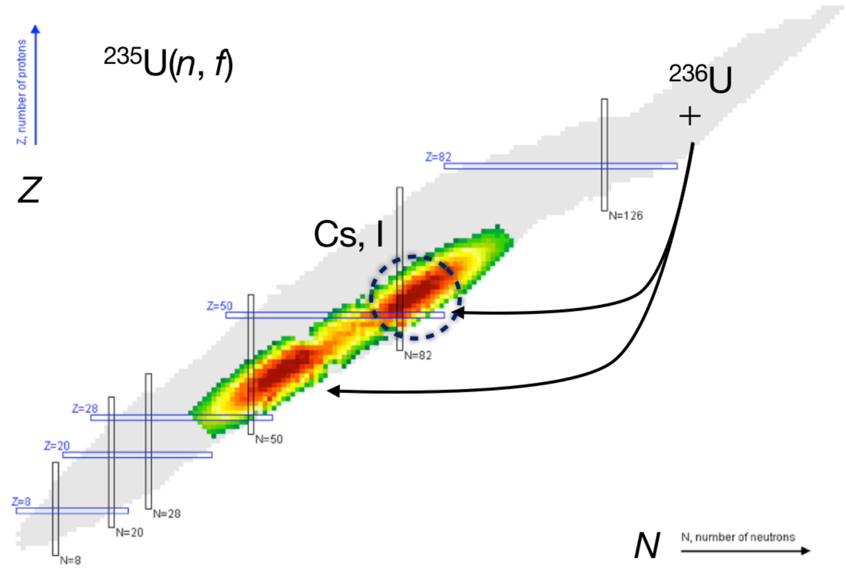
- Supernova explosions
- Ejecta of neutron star mergers

Neutron rich environments produce a large amount of Super Heavy (SE) elements

SHs can fission, feeding back the abundances of medium-mass nuclei

Understanding fission is also important in the quest to create super-heavy elements in the laboratory

Finally, technological applications cannot be overlooked



Fission observables in NS

Computing abundances in this scenario requires nuclear input (reactions) for many (a few thousand) neutron rich SH nuclei.

As there is no experimental data in the region, theoretical input is needed

- Lifetimes (t_{sf})
- Fission fragments
  - Mass distribution
  - Kinetic energy
  - Internal excitation energy
- Fission isomer properties
- Barriers (?) ⇐ Model dependent (?)

both for spontaneous and (any kind of) induced fission (mostly neutron induced)

Theory of fission

Not much since Bohr and Wheeler's theory of fission

SEPTEMBER 1, 1939 PHYSICAL REVIEW VOLUME 56

The Mechanism of Nuclear Fission

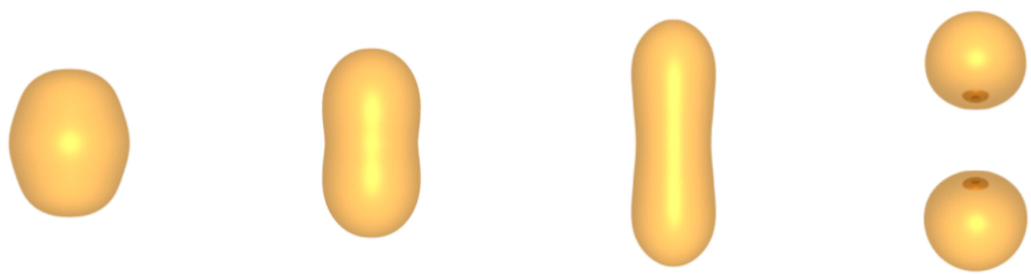
NIELS BOHR
University of Copenhagen, Copenhagen, Denmark, and The Institute for Advanced Study, Princeton, New Jersey

AND

JOHN ARCHIBALD WHEELER
Princeton University, Princeton, New Jersey

(Received June 28, 1939)

On the basis of the liquid drop model of atomic nuclei, an account is given of the mechanism of nuclear fission. In particular, conclusions are drawn regarding the variation from nucleus to nucleus of the critical energy required for fission, and regarding the dependence of fission cross section for a given nucleus on energy of the exciting agency. A detailed discussion of the observations is presented on the basis of the theoretical considerations. Theory and experiment fit together in a reasonable way to give a satisfactory picture of nuclear fission.

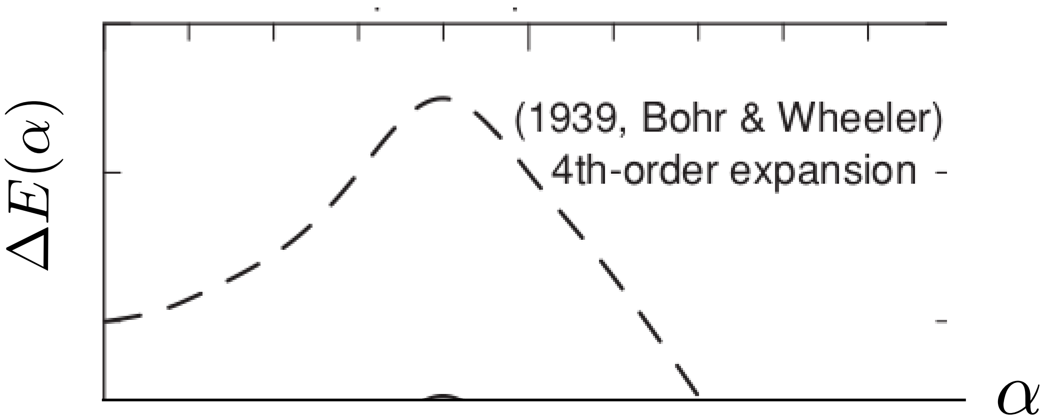


Fission is pictured as the gradual deformation of the parent nucleus as to split it in two pieces. Results from the balance between:

- Surface energy: short range of nuclear interaction, similar to surface tension of a water drop
- Coulomb repulsion among protons

$$\Delta E(\alpha) = E_s^{(0)}\left(\frac{2}{5}(1-x)\alpha^2 - \frac{4}{105}(1+2x)\alpha^3\right)$$

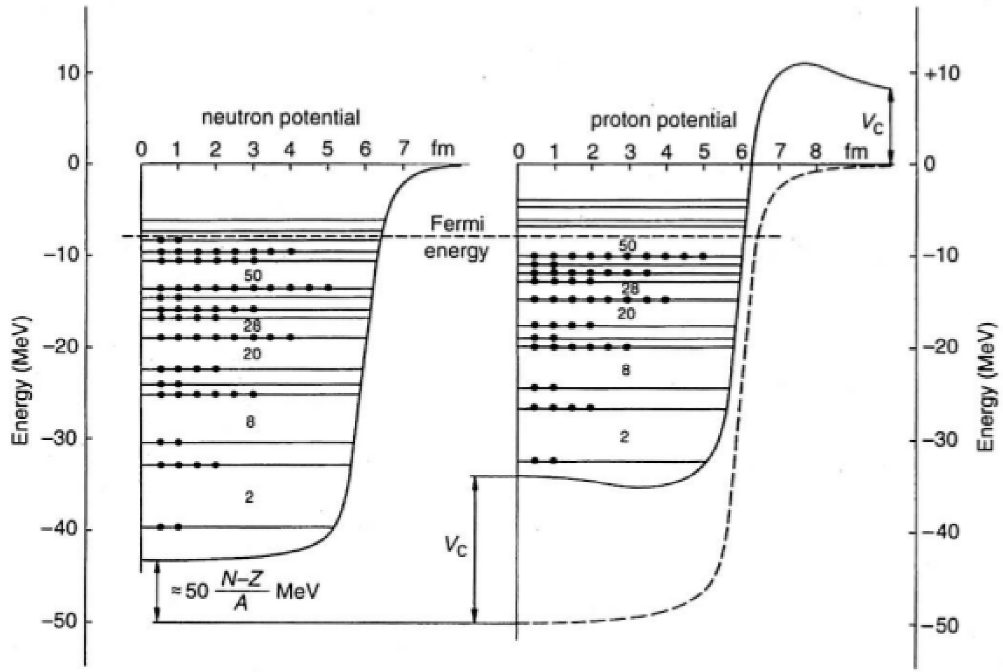
$$x = \frac{E_c}{2E_s^{(0)}}$$ Fissibility parameter $$\frac{Z^2}{A}$$



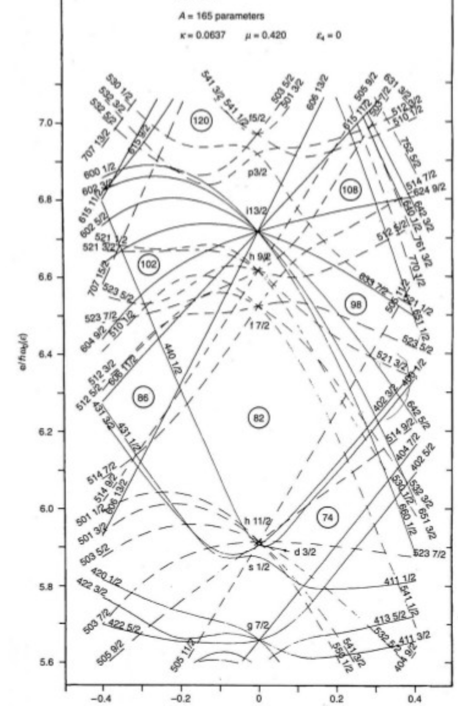
From the liquid drop model of the nucleus

α Def parameter

Nowadays we know that quantum mechanics is important in fission (shell effects)



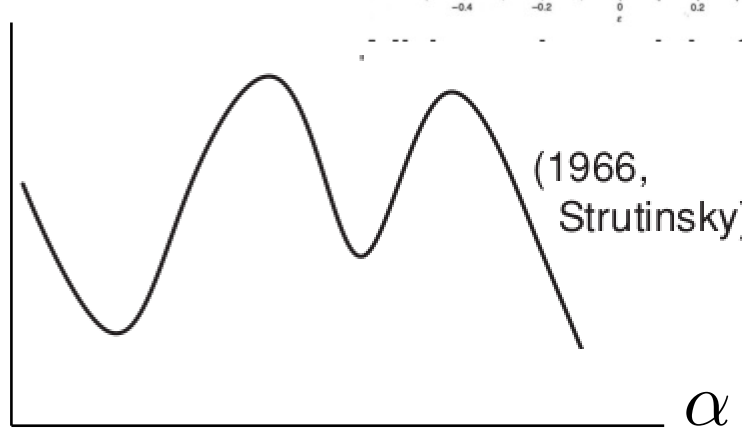
Jahn-Teller effect



Modify substantially the barrier shape, height and width

Double humped barriers, etc

Mic Mac models: Liquid drop+deformed potential



Theory

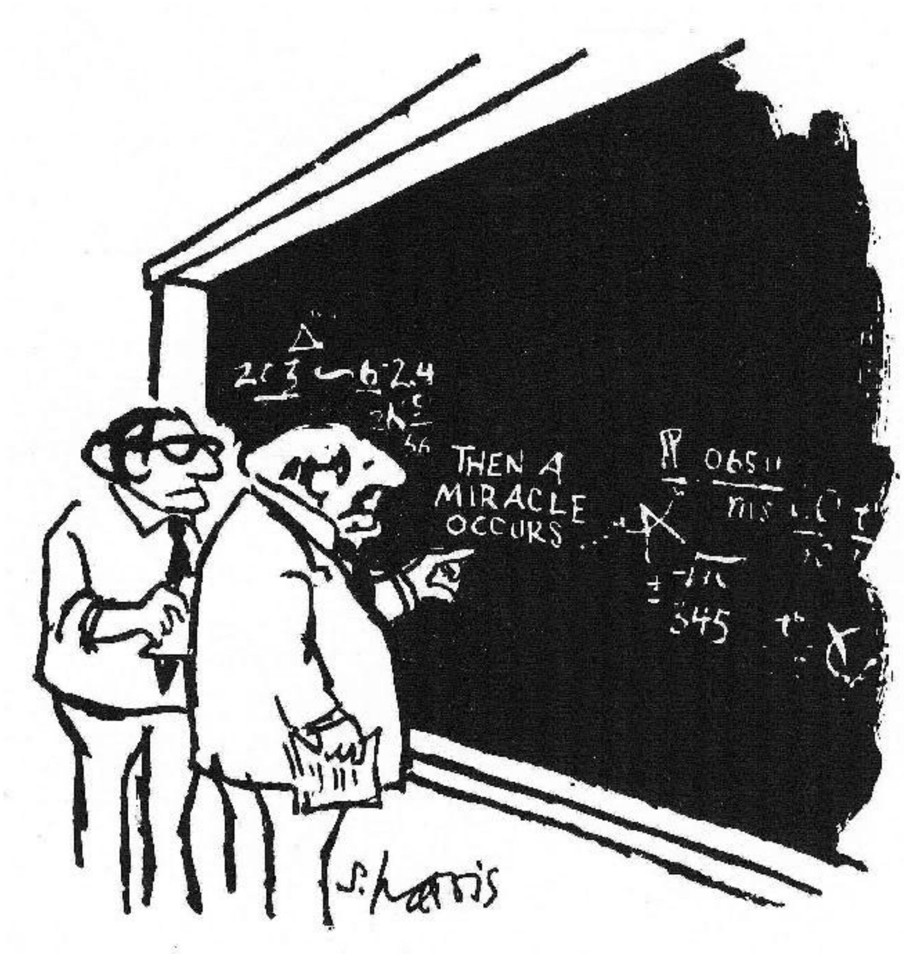
$$\mathcal{P}_{i\rightarrow f} = \left|\langle \Psi_f | \hat{U}(\infty, -\infty) | \Psi_i \rangle\right|^2$$

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

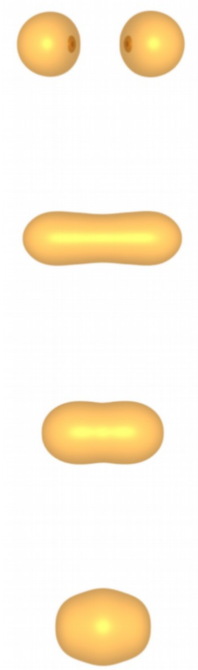
$|\Psi_f\rangle$ the final state can be any of the exit channels

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

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



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



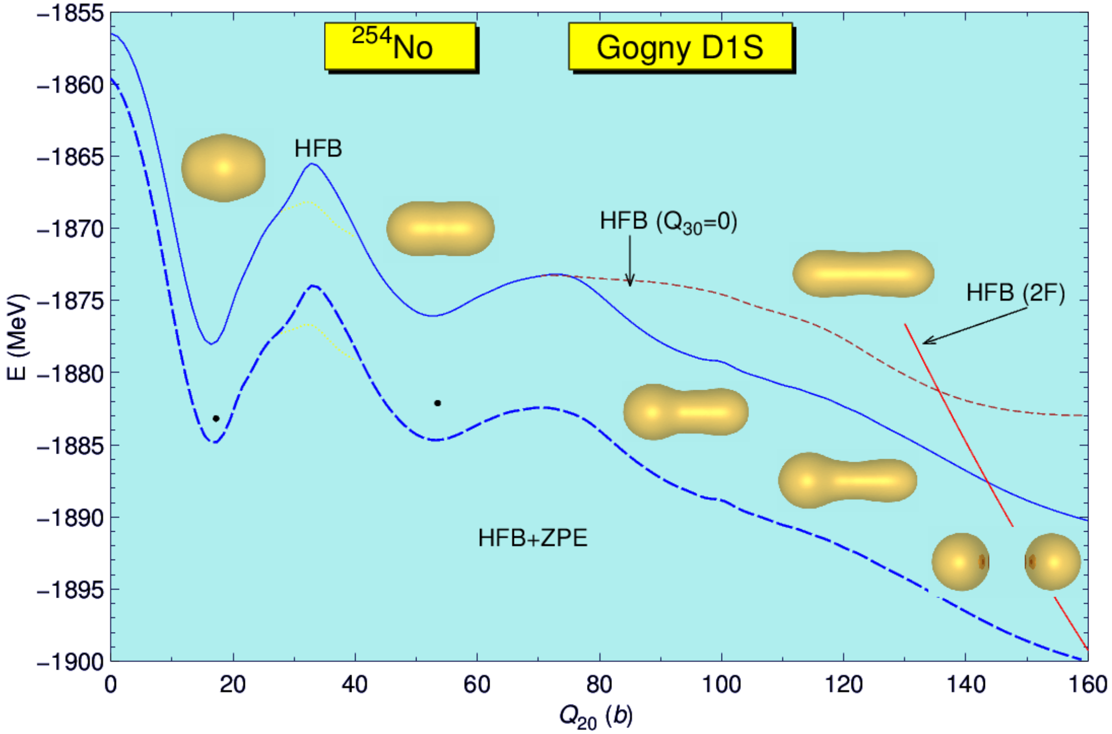
Inspired by BW ideas, let us try, as in any nuclear quantum many body problem, with a deformed mean field as the starting point of a microscopic description

Using Bohr-Wheeler's picture of a liquid drop, we assume the nucleus proceed from the initial state to scission by deforming its matter density.

Density computed from a mean field wave functions including pairing obtained from a realistic (effective) interaction

Deformation parameter: Many can be used but quadrupole moment is a popular choice

Compute the mean field with a constraint in the deformation parameter



Inner and outer barriers

Reflection symmetric and reflection asymmetric fission paths

Other degrees of freedom important (triaxiallity, hexadecapole, pairing)

Tunneling through the barriers

To compute half lives we use the WKB approximation

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

The action is given by

$$S = 2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)}$$

Where B(s) is the collective inertia along the path and V(s) the potential energy

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

Zero point energy correction

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

The inertia and zpe can be obtained from the mean field wf under certain assumptions

$|\phi(s)\rangle$ Is a mean field wave function of the Hartree-Fock-Bogoliubov type

Although not fully justified from a fundamental perspective (*), semi-classical arguments tells that fission should proceed through the least action path in the parameter space including all (or at least the most relevant) degrees of freedom. This is the so-called “dynamic path to fission”

$$S = 2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)}$$

- To minimize S we have to minimize the product of the inertia times the potential energy.
- If the inertia is roughly constant in the regions of relevance, then the configurations with the least energy would lead to the least action.
- Therefore, a good approximation to determine the path to fission is to minimize the energy, the “static path to fission”.
- The static approach is far simpler because the mean field wave functions are already determined as to minimize the energy (HFB equations).
- The dynamic approach implies exploring many mean field configuration increasing several orders of magnitude the complexity of the problem

(*) Some hints from path integral methods using instantons seem to justify it

The collective inertia can be visualized as the response of the nucleus to a given external field. Typically, the external field is one of the multipole moments describing fission dynamics (quadrupole moment)

The response can be computed in two different frameworks

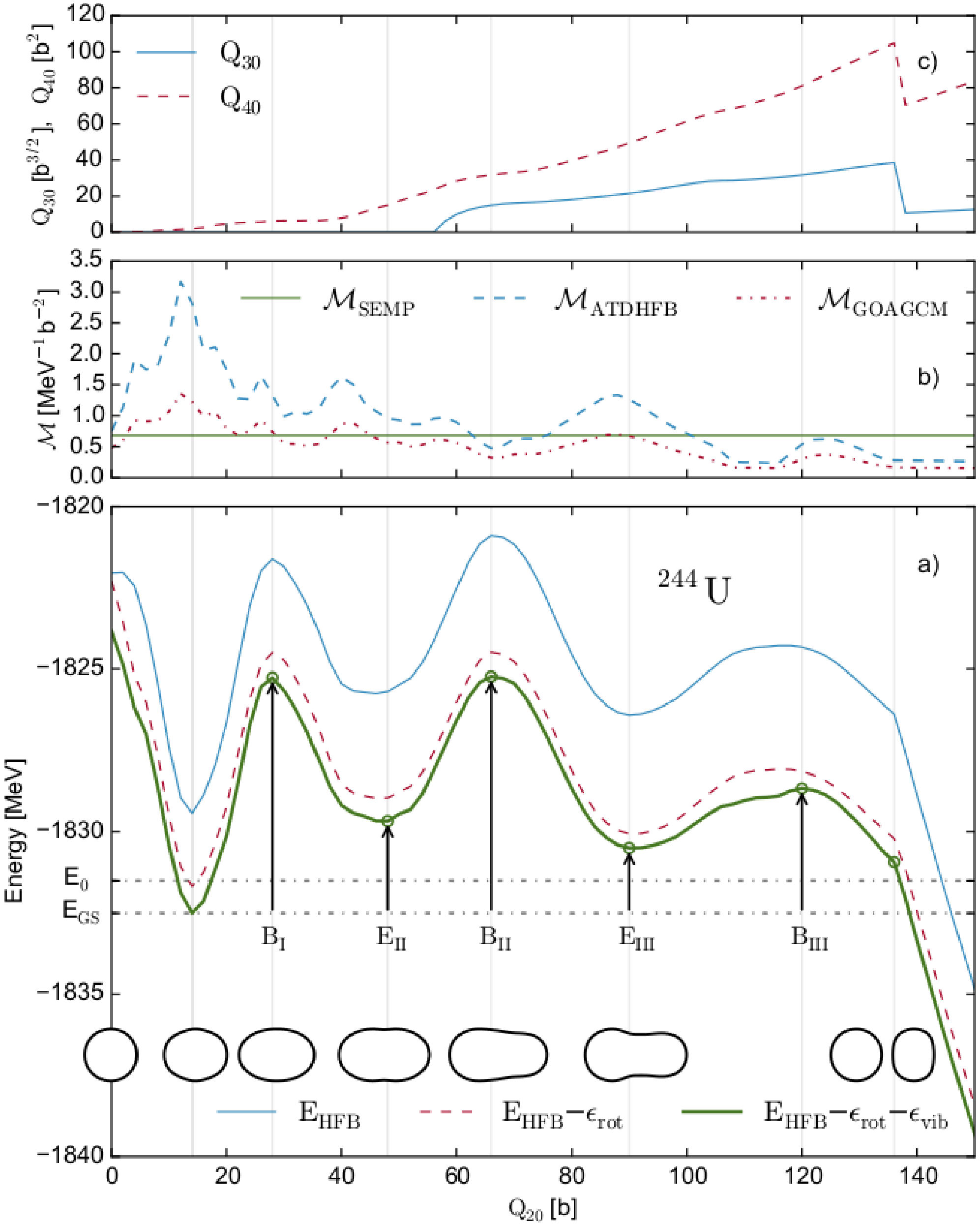
- ATDHFB: The time evolution of the HFB field, assuming adiabatic motion, is used. It takes into account time odd components of the nuclear interaction. If the external perturbation is a rotation the Thouless-Valatin moment of inertia is obtained, if a boost, the exact mass.

$$i\hbar\frac{\partial\mathcal{R}}{\partial t} = [\mathcal{H},\mathcal{R}]$$

- GCM: The generator coordinate method with the external field as generating coordinate is used to derive, under certain assumptions, a “collective energy” and a “collective moment” that allow to define an inertia. The corresponding moment of inertia is that of Yoccoz and in the case of a boost it does not yield the exact nuclear mass.

$$|\Psi_\sigma\rangle = \int dq f_\sigma(q)|\phi(q)\rangle$$

Both inertias require for their evaluation the inversion of a huge matrix (the linear response matrix), a feat that has started to be possible only recently.



c)
Q_{30}
Q_{40}
Q_{30} [$b^{3/2}$], Q_{40} [b^2]
b)
$\mathcal{M}_{SEMP}$
$\mathcal{M}_{ATDHFB}$
$\mathcal{M}_{GOAGCM}$
$\mathcal{M}$ [$MeV^{-1} b^{-2}$]
a)
^{244}U
Energy [MeV]
E_0
E_{GS}
B_I
E_{II}
B_{II}
E_{III}
B_{III}
E_{HFB}
$E_{HFB} - \epsilon_{rot}$
$E_{HFB} - \epsilon_{rot} - \epsilon_{vib}$
Q_{20} [b]

Uncertainties

- Static vs Dynamic calculations: which degrees of freedom are relevant ?
- Nuclear Energy Density Functional (NEDF): Variance with the choice of NEDF, should unusual terms (Coulomb exchange, for instance) be included ?
- Collective inertias: Which of the two schemes ATDHFB or GCM is appropriate ?
- Collective inertias: Impact of the various approximations used to compute them
- Zero point energy corrections: Same as in collective inertias
- Choices for the ground state energy E_0

In addition a fully consistent theory of fission from excited states is missing (only averages, using finite temperature formalism)

Minimizing the action

Long ago (Funny hills paper) the minimization of the action was proposed to determine the fission path

$$S = 2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)}$$

$$s(q_1, q_2, \ldots)$$

Requires fixing which degrees of freedom q1, q2, … are to be explored

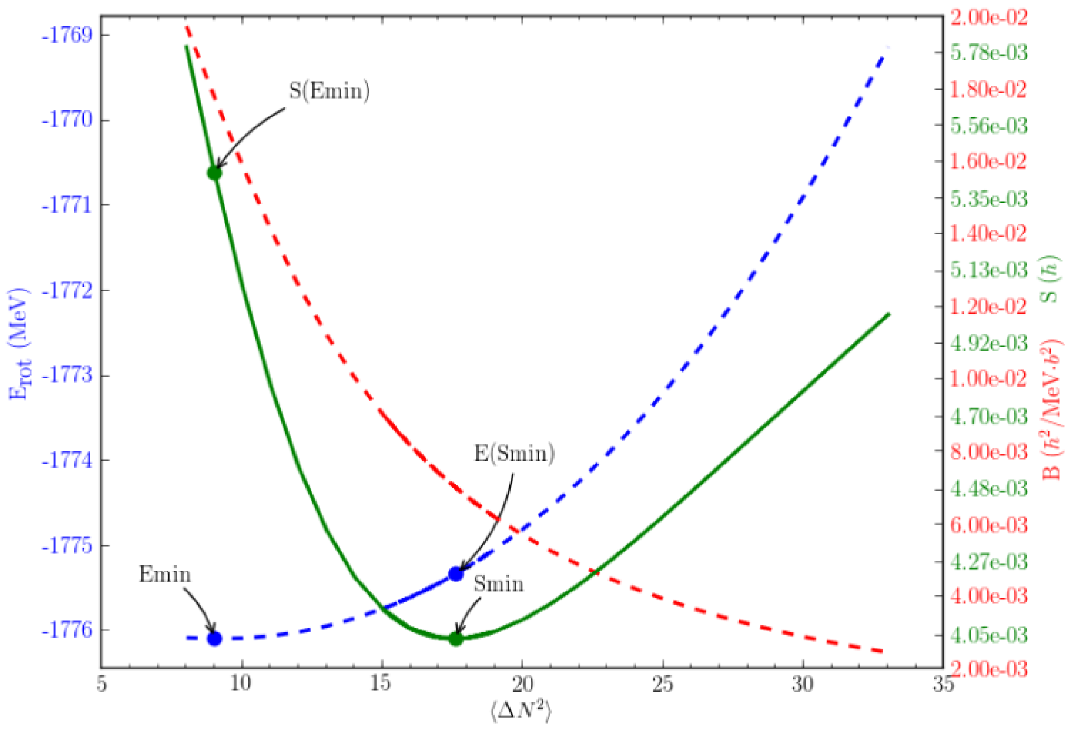
If only multipole moments of the matter density are explored, several calculations have shown that the “dynamic path” is very similar to the “static path”

This is the reason why, so far, most of the fission calculations are “static”

However, Moretto proposed long ago to include pairing correlations as additional degrees of freedom to explore in dynamic calculations.

The reason is the expected dependence on the “pairing gap” Δ

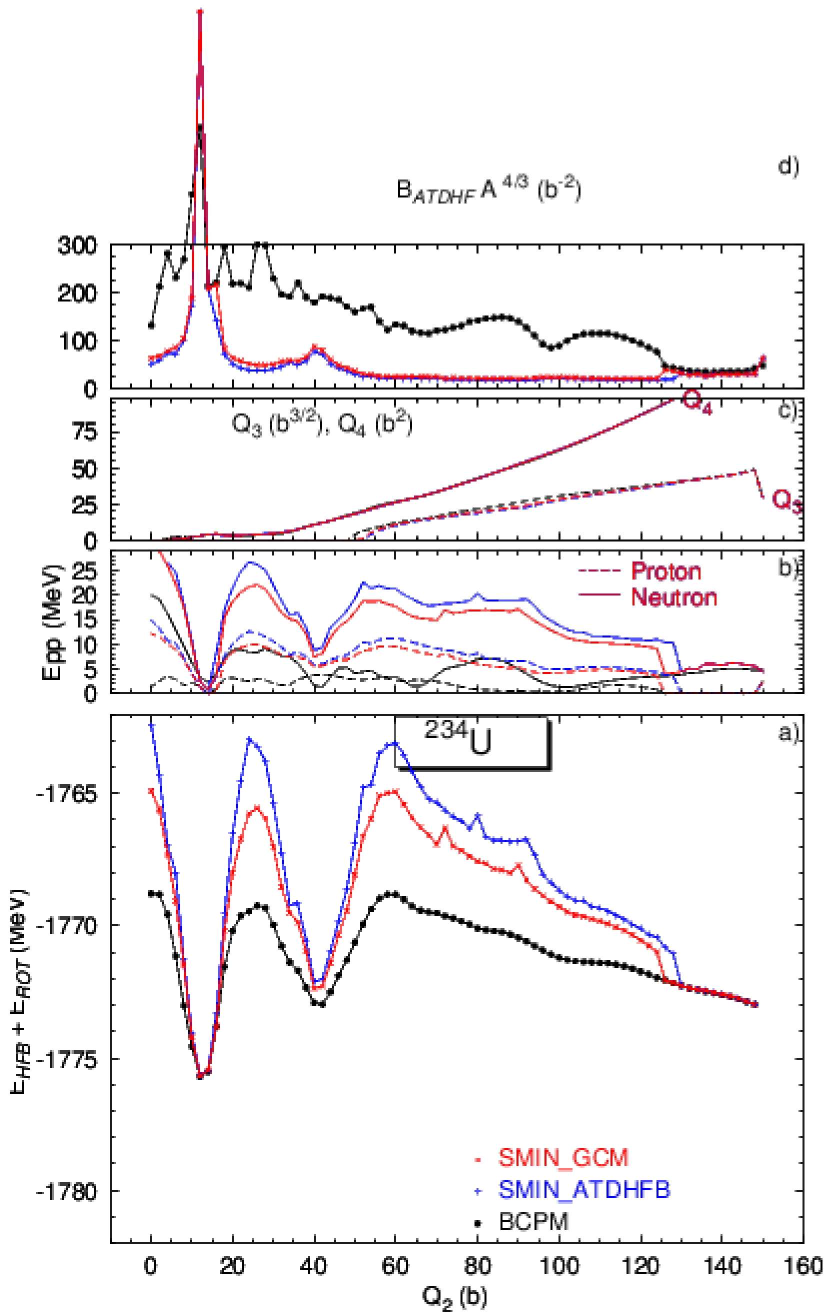
$$B \approx \frac{1}{\Delta^2} \qquad V(\Delta) = V(\Delta_0) + g(\Delta - \Delta_0)^2$$



For this degree of freedom, the least action configuration has a much lower collective inertia with a modest increase on the energy

The equilibrium action is much lower than in the “static” case leading to strong reductions in t_{sf}

The dependence of B on Δ is a general property of the inertia (Bertch and Flocard)



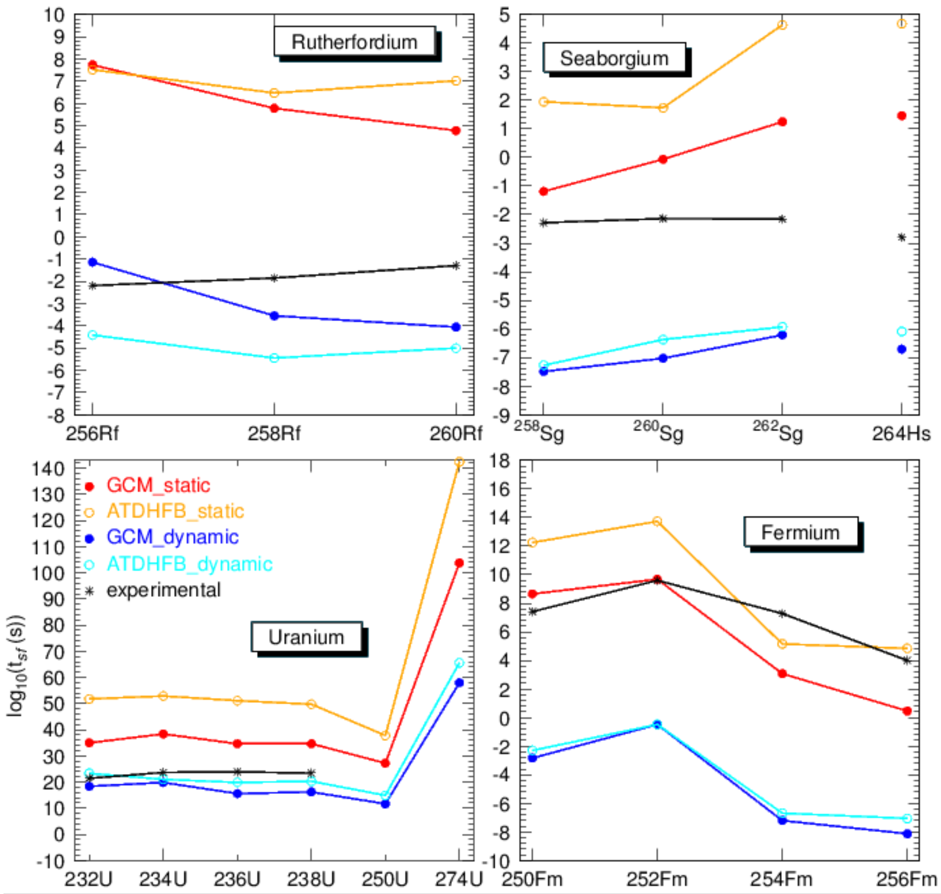
We have explored the idea using $\langle \Delta N^2 \rangle$ instead of the gap to search for a minimum of the action for each quadrupole moment

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}

Huge impact on t_{sf}



A reduction of many orders of magnitude in t_{sf} is observed

The ATDHFB and GCM results seem to "converge"

This is still a very preliminary calculation where protons and neutrons were not treated separately and some simplifying assumptions were made.

The computational cost of a "dynamic" calculation with the quadrupole moment and the pairing gaps of protons and neutrons as dynamical variables is three orders of magnitude larger than a "static" calculation.

Too expensive when 3000 nuclei are to be considered !

Nuclear energy density functionals

- Long range term (ph channel)
  (Skyrme, Gogny, relativistic)
  Influences PES.
  (Some interactions fitted to fission data: D1S, UNDEF1, …)
- Short range term (pp channel)
  (Different strategies depending on the ph channel)
  Strong impact on inertias
- "Exotic" terms which are often ignored
  (Coulomb exchange+antipairing)
  Relevant at extreme elongations (3rd minimum)
  Antipairing impacts inertias

Gogny

Finite range, density dependent interaction

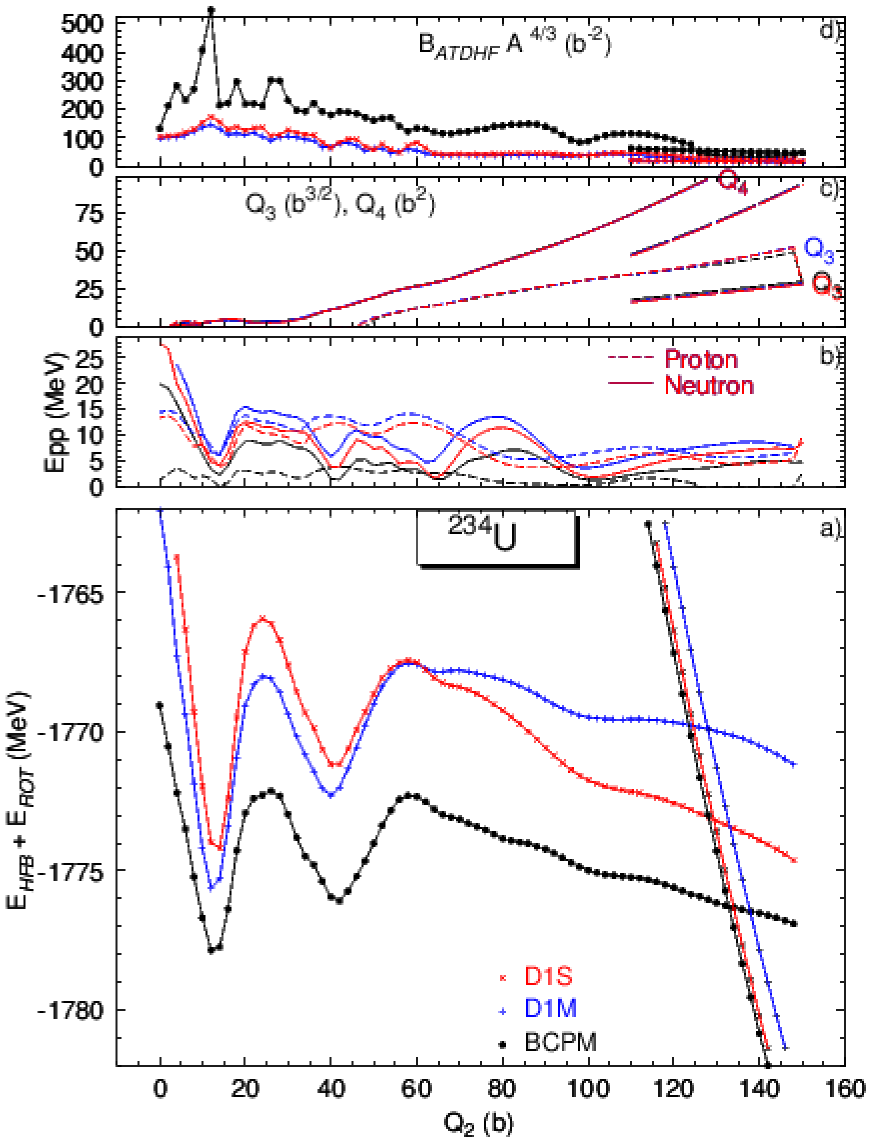
- D1S
  - Fit includes a few selected finite nuclei
  - Fission information in the fit.
  - Poor descriptions of masses
  - Good in describing collective phenomena

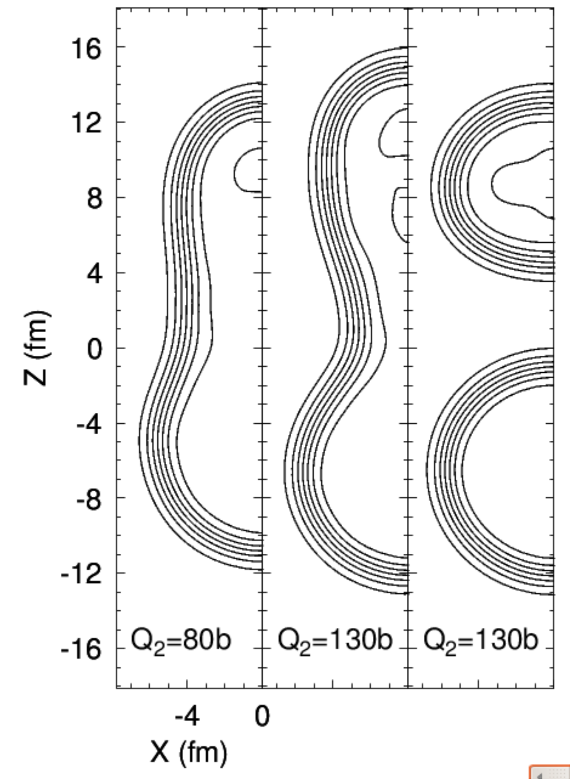
- D1M
  - Global mass fit
  - No fission information in the fit
  - Very good description of masses (rms 0.7 MeV)
  - Not as thoroughly tested as D1S

BCPM

Density functional inspired in microscopic EoS

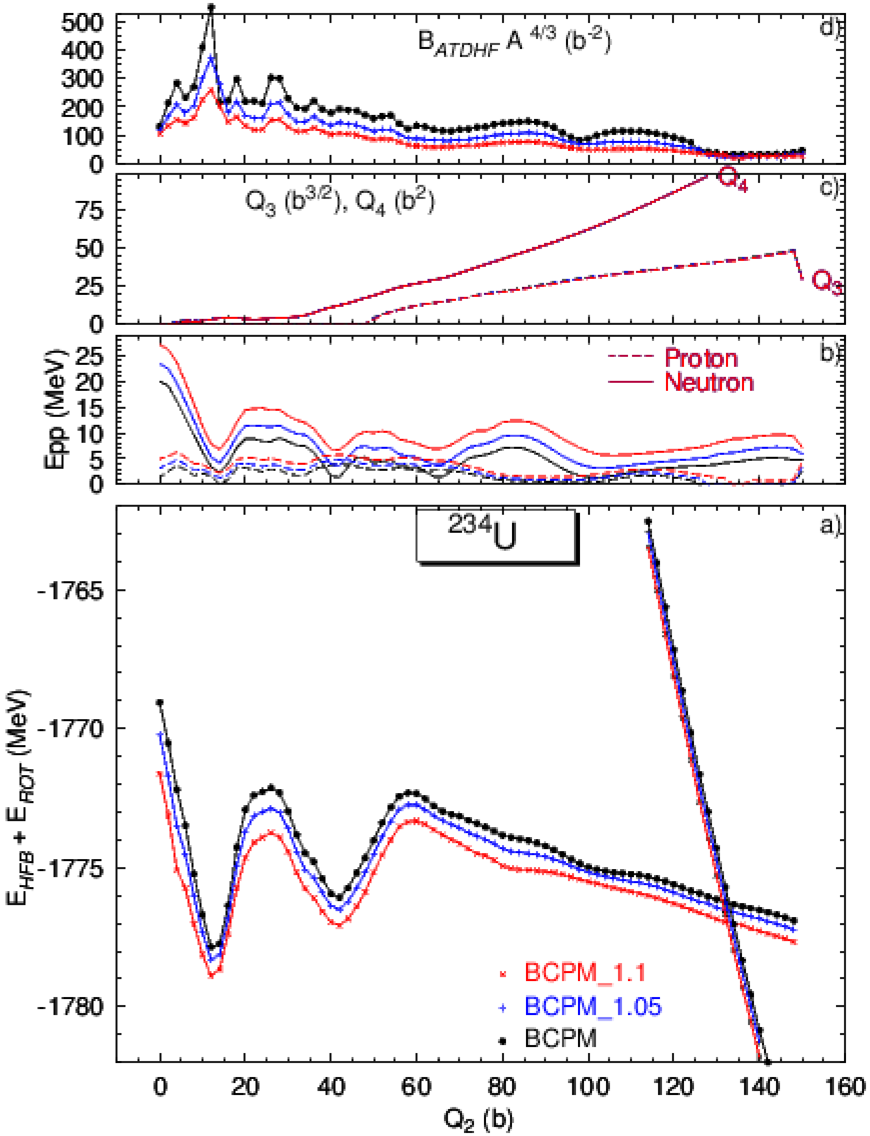
- Global (even-even) mass fit
- No fission information in the fit
- Not bad at masses (rms 1.6 MeV, even-even nuclei)





$t_{sf}^{(S)}$	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%)

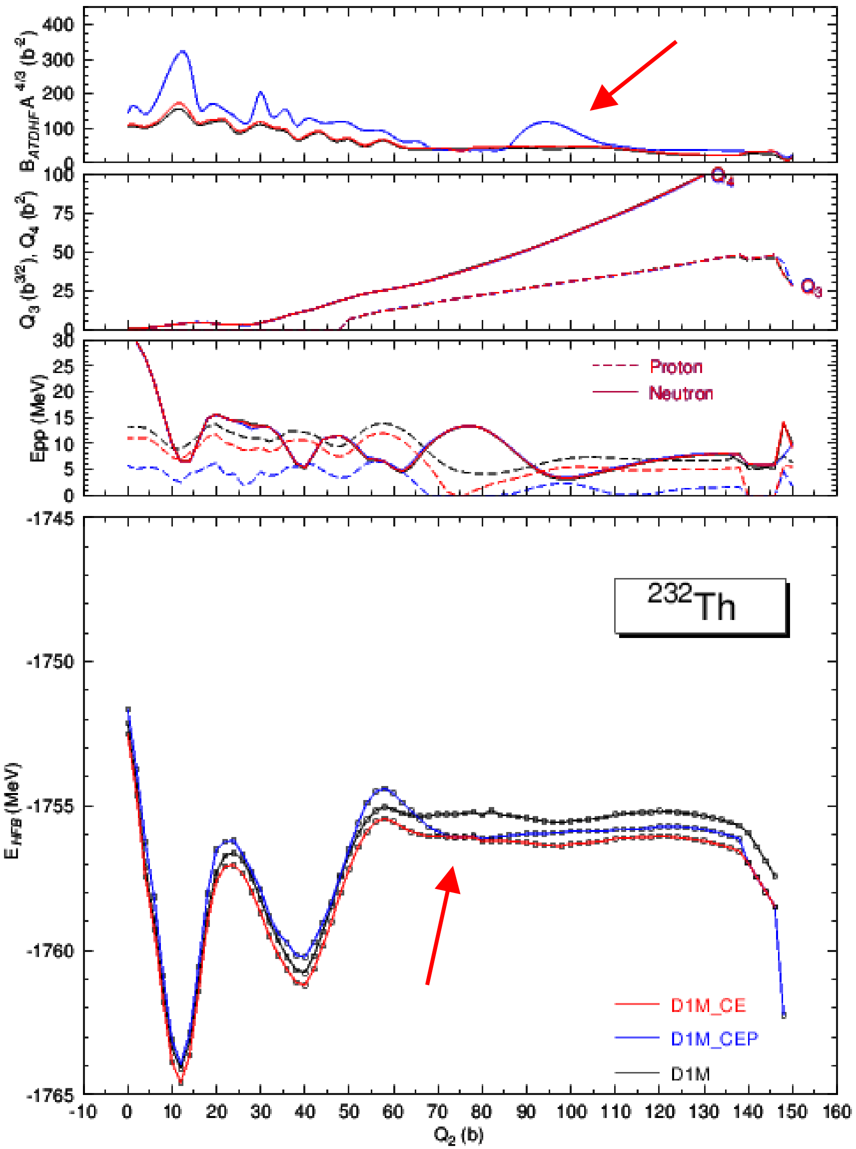
Huge impact on lifetimes

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 that 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

Two types of inertias

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

Both are traditionally computed using the “cranking approximation”

ATDHFB

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

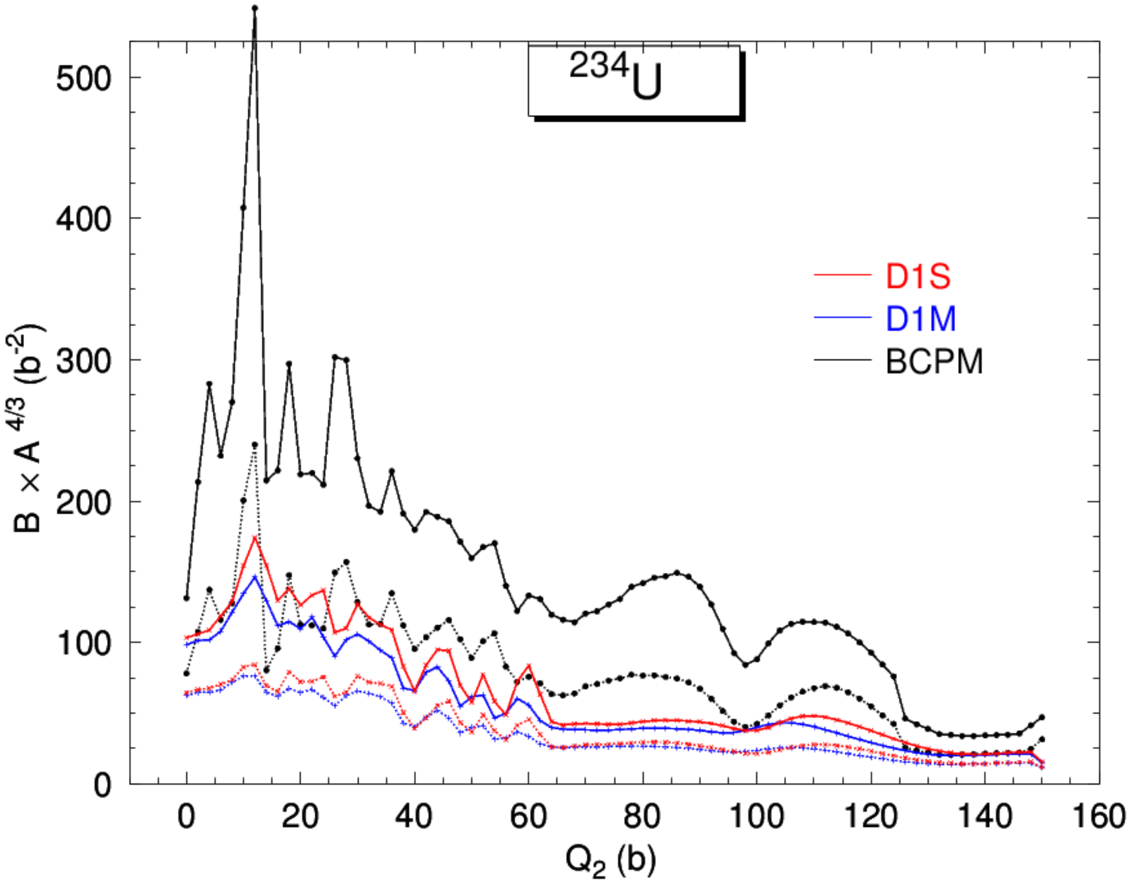
GCM

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

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

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.



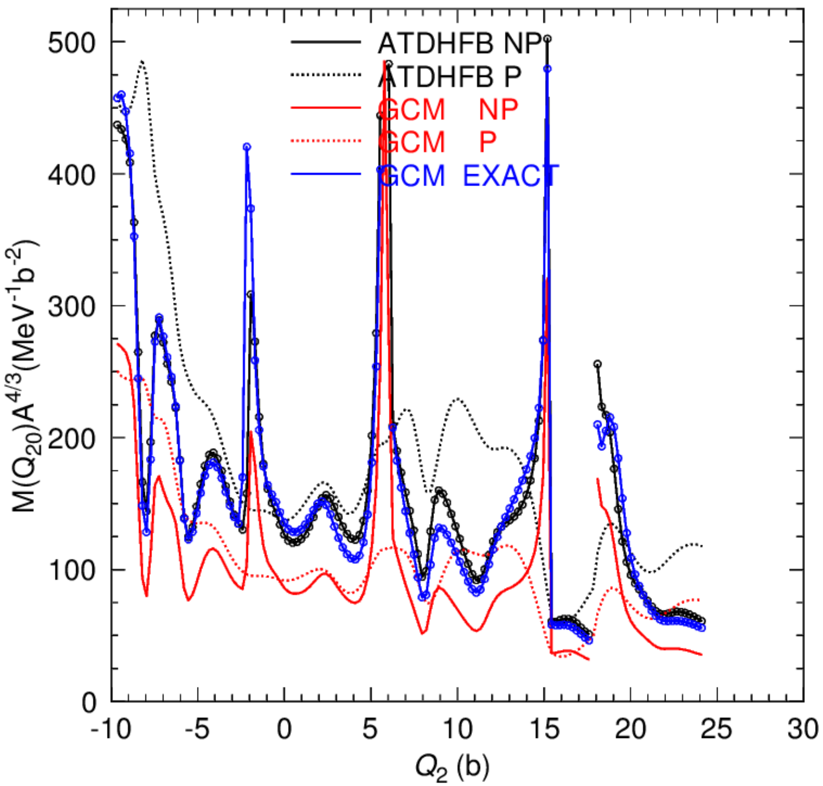
t_{sf}	ATDHFB	GCM
D1S	4.3 E+32	5.7 E+23
D1M	6.0 E+46	6.6 E+34
BCPM	3.0 E+54	1.6 E+40

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

The NP approximate GCM inertia follows the trend of the exact GCM mass.

There is a factor around 1.5 between NP and exact

The trend is also similar for the ATDHFB inertia.

Work in progress to compute exact ATDHFB

- Exact GCM is computed with second derivatives of energy overlap
- “P” means Perturbative (Traditional cranking formulas)
- “NP” means “Non Perturbative”: momentum operator from numeric derivatives of densities

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

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

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

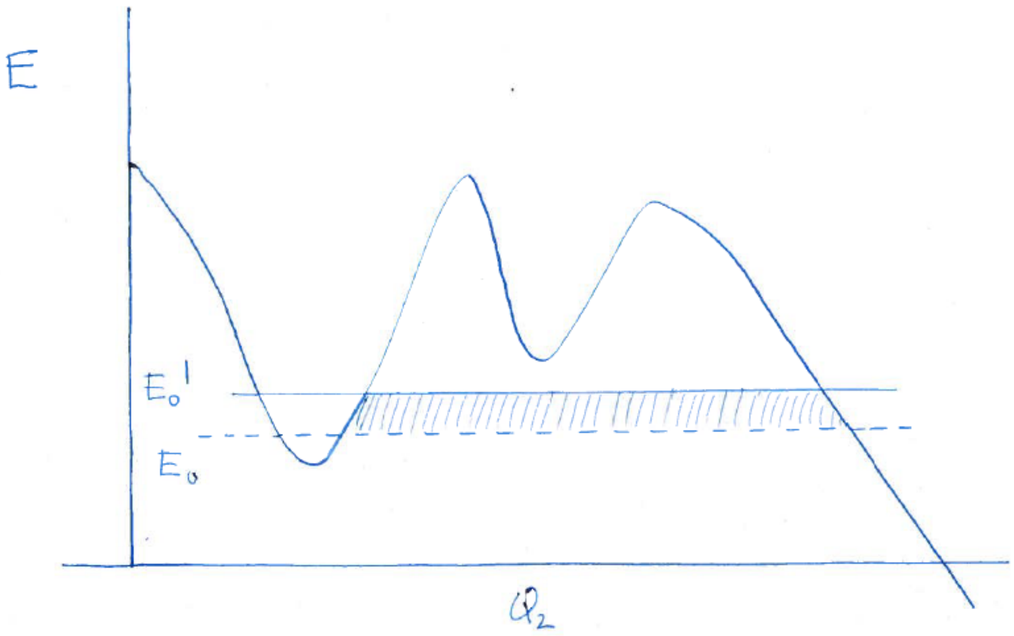
Rotational correction substantially modifies energy landscape (3 - 7 MeV)

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

PNP-VAP increases pairing correlations: the inertia decreases !

The E_0 parameter

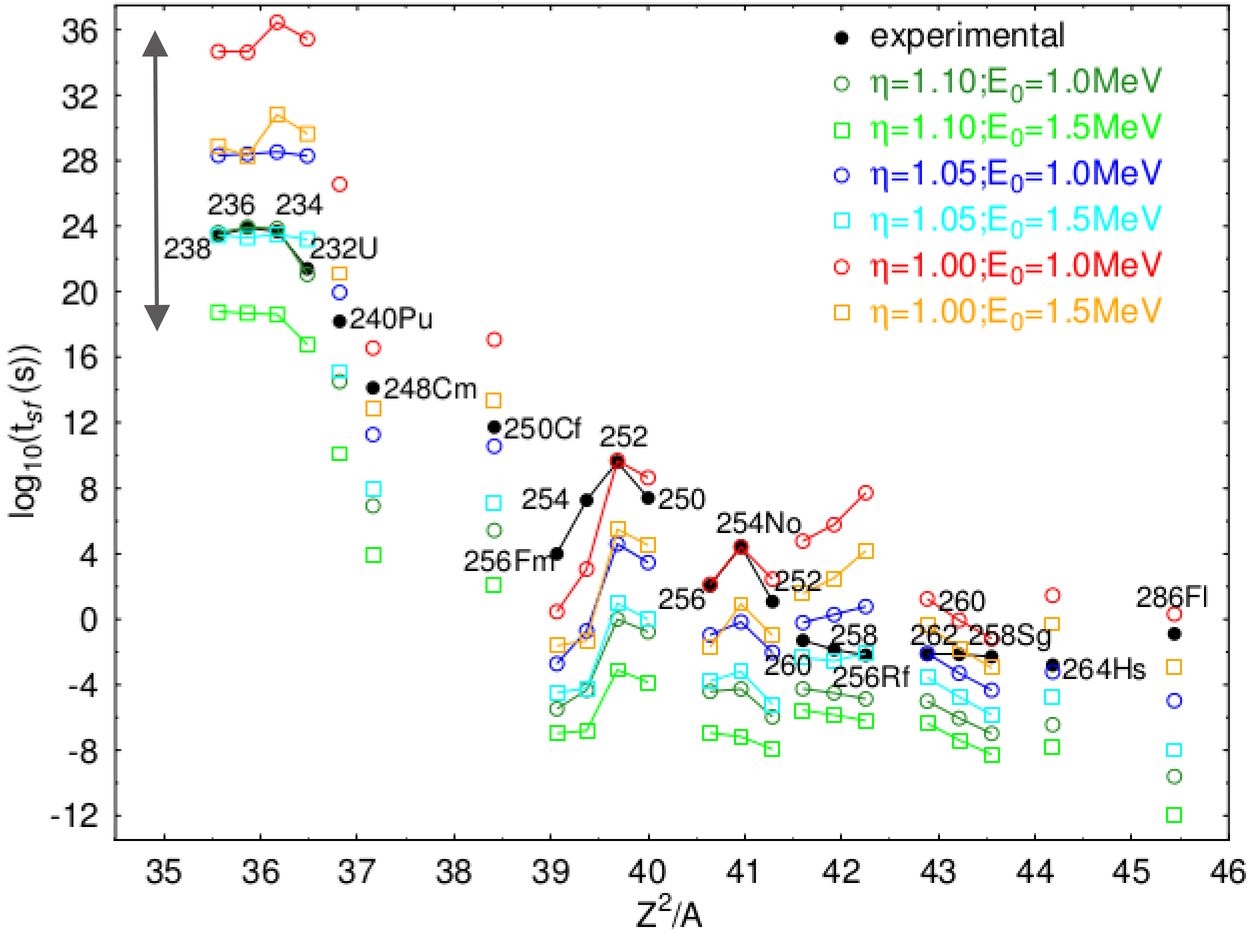
$$t_{\rm sf} = t_0 \exp(2/\hbar \int_a^b ds \sqrt{2B(s)(V(s) - E_0)})$$



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 results with BCPM



Nuclei with known experimental data on t_{sf}

GCM inertias

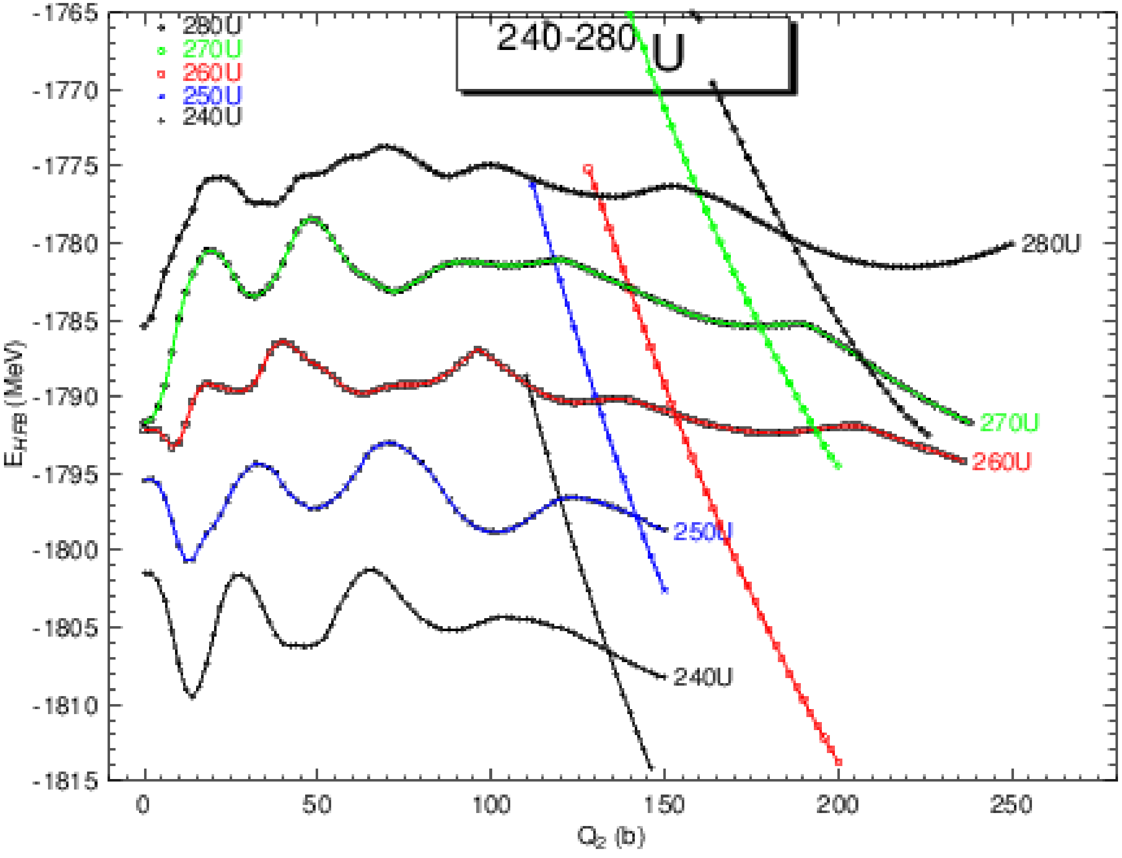
Large variability with eta and E_0

Isotopic trend reproduced

Trend with mass number reproduced

Neutron rich uranium (predictions!)

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

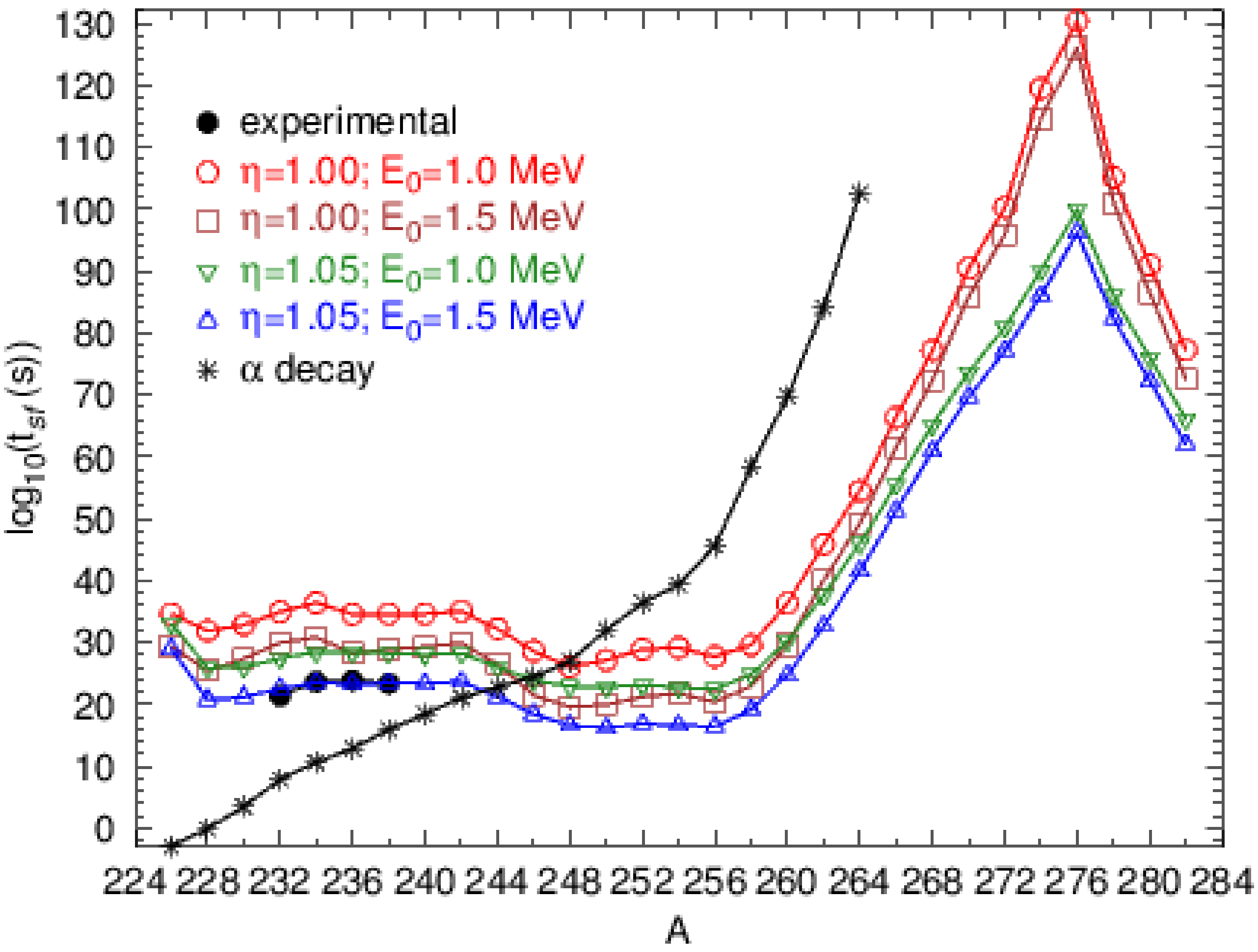


Emergence and evolution of the third minimum

Barriers increase and become wider

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

Peak at ^{276} U



Conclusions

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

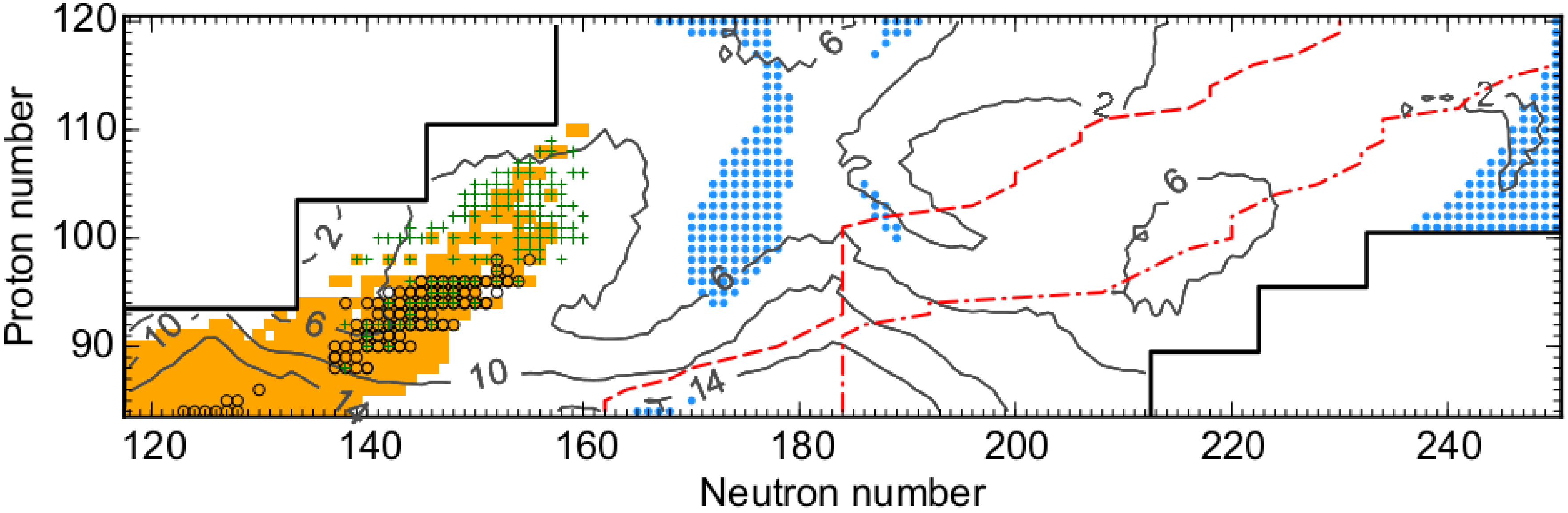
- To reach the "quantitative" level the dynamical aspects of fission have to be addressed

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

Most of the effects are related to the inertias and can be "mocked up" by playing with those quantities

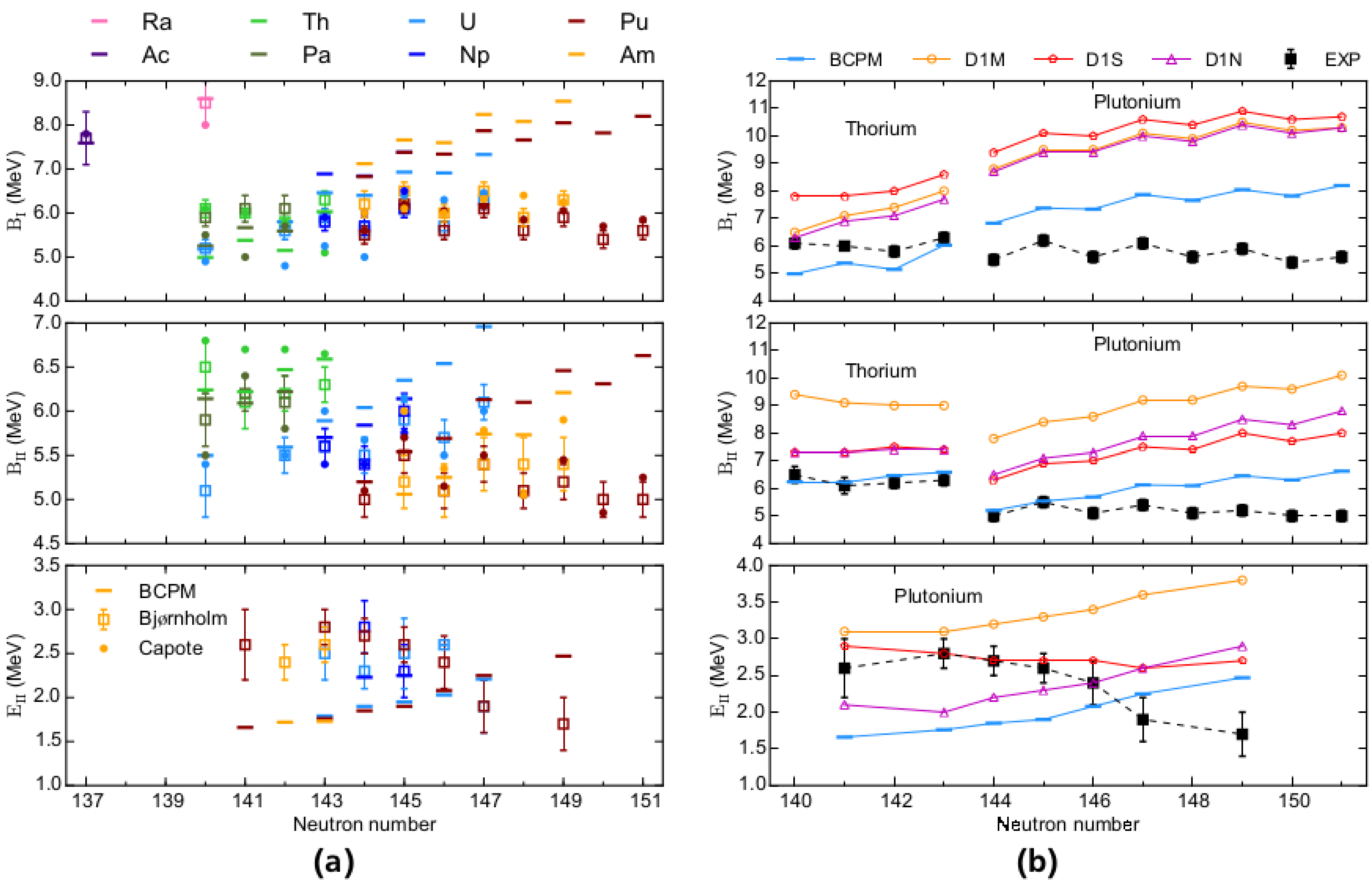
Some applications in astro

To run r-process simulations a table with fission properties of neutron rich SH elements has been produced using the BCPM NEDF



3640 SH neutron rich nuclei considered

Benchmarking with experimental data for B_I, B_{II} and E_{II}



Benchmarking with experimental data t_{sf}

	$\bar{R}_\tau$			σ_τ		
	ATDHFB	GCM	SEM	ATDHFB	GCM	SEM
BCPM	11.583	4.691	2.036	6.447	4.236	6.126
D1M	10.030	4.728	22.779	4.405	3.177	11.448
D1S	3.622	-0.748	8.423	3.585	4.050	6.325
D1N	5.460	0.771	12.480	3.388	3.249	6.993
BCPM-r	-0.007	-0.006	0.004	3.403	3.339	5.231

$$R_\tau = \log\left(t_{\mathrm{SF}}^{cal}/t_{\mathrm{SF}}^{exp}\right)$$

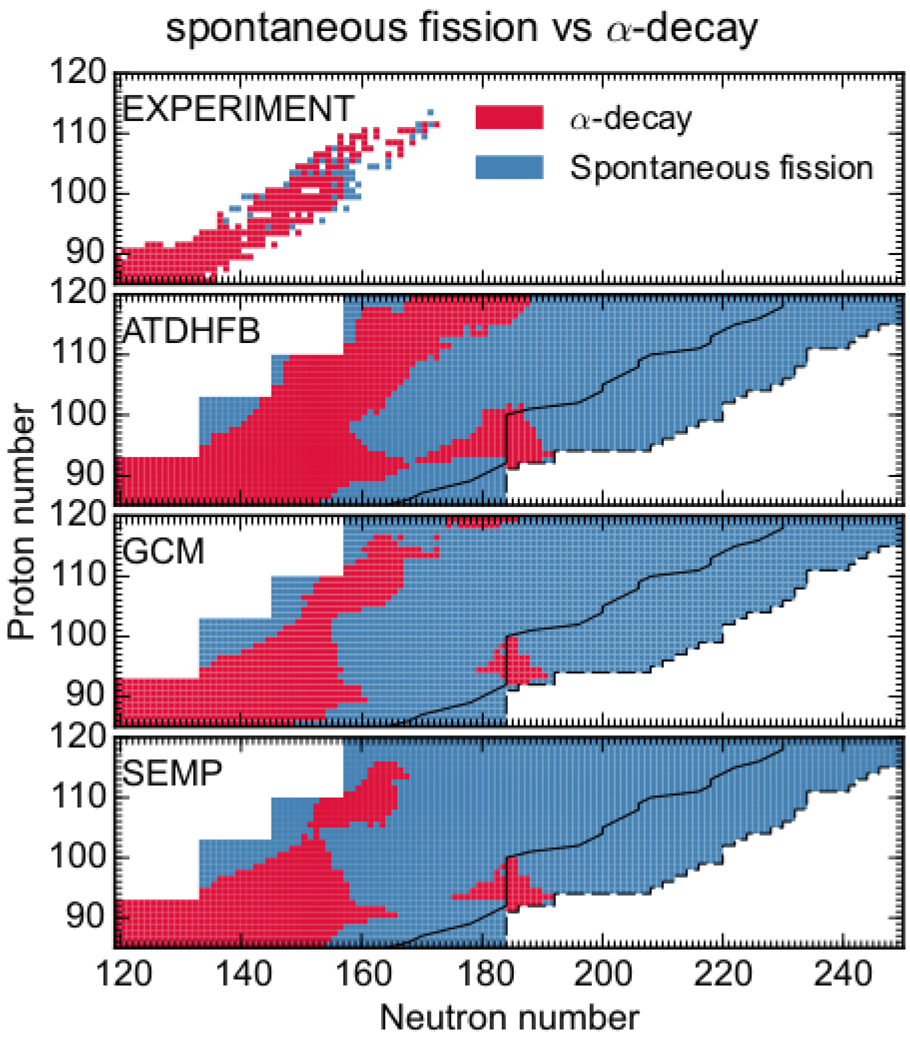
$$\bar{R}_\tau = \frac{1}{N}\sum_i^N R_{\tau,i}$$

$$\sigma_\tau = \frac{1}{N}\left(\sum_i^N (R_{\tau,i} - \bar{R}_\tau)^2\right)^{1/2}$$

BCM-r

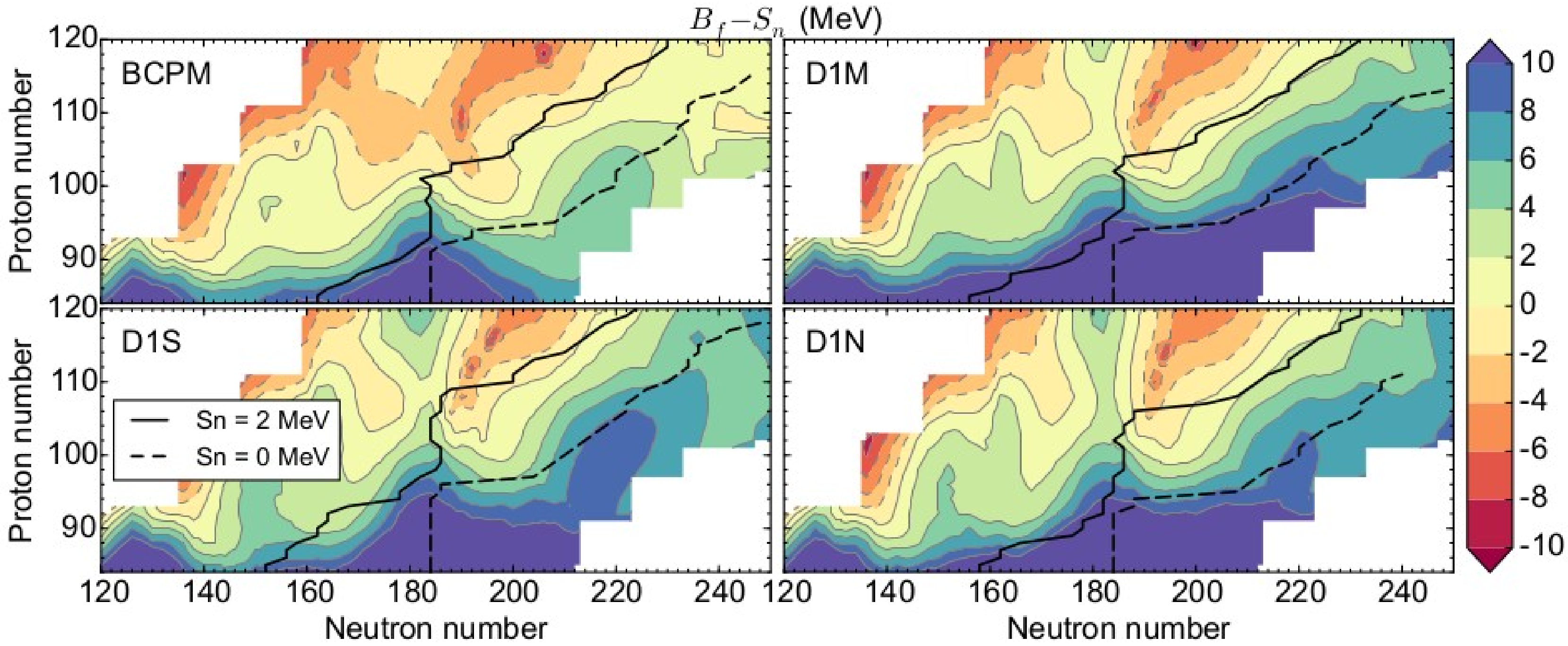
Inertias are renormalized by a constant factor
ATDHFB: 0.5
GCM: 0.73
SEM: 0.87

Fission vs α

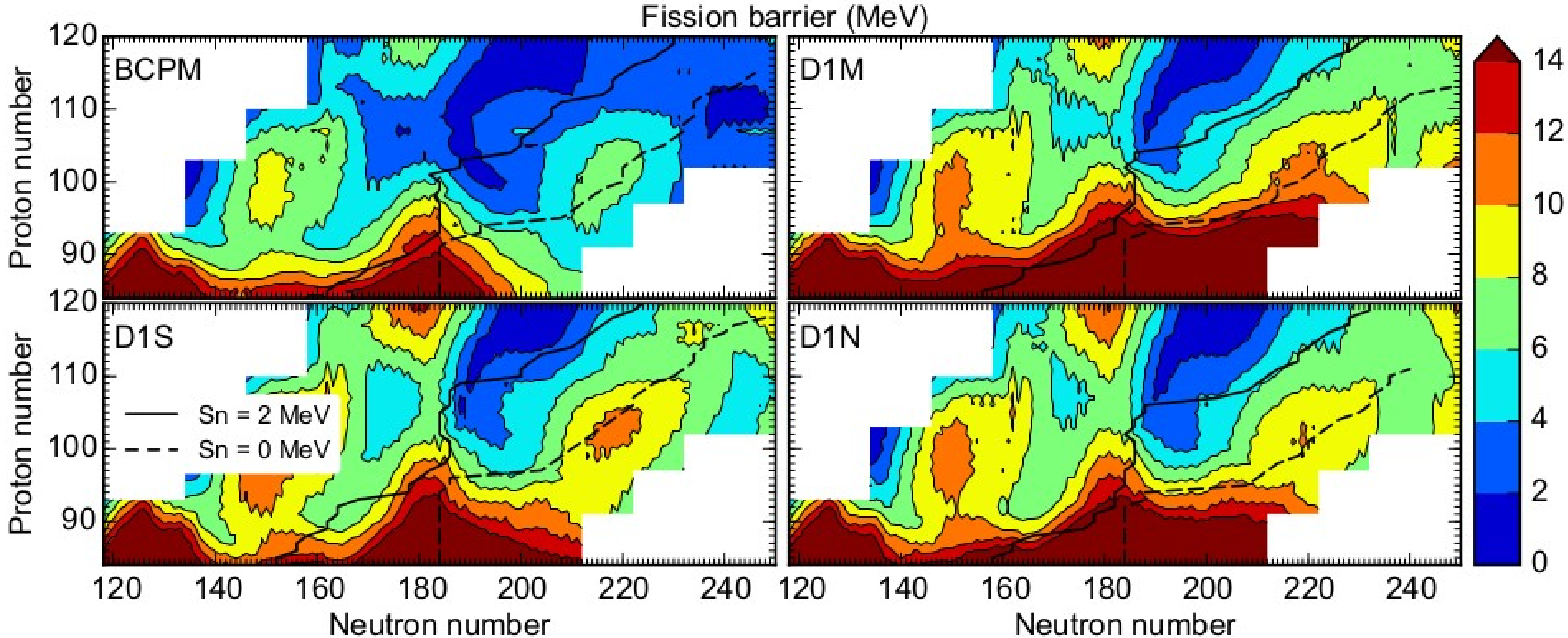


spontaneous fission vs α-decay
EXPERIMENT
α-decay
Spontaneous fission
ATDHFB
GCM
SEMP
Proton number
Neutron number
120
110
100
90
120
140
160
180
200
220
240

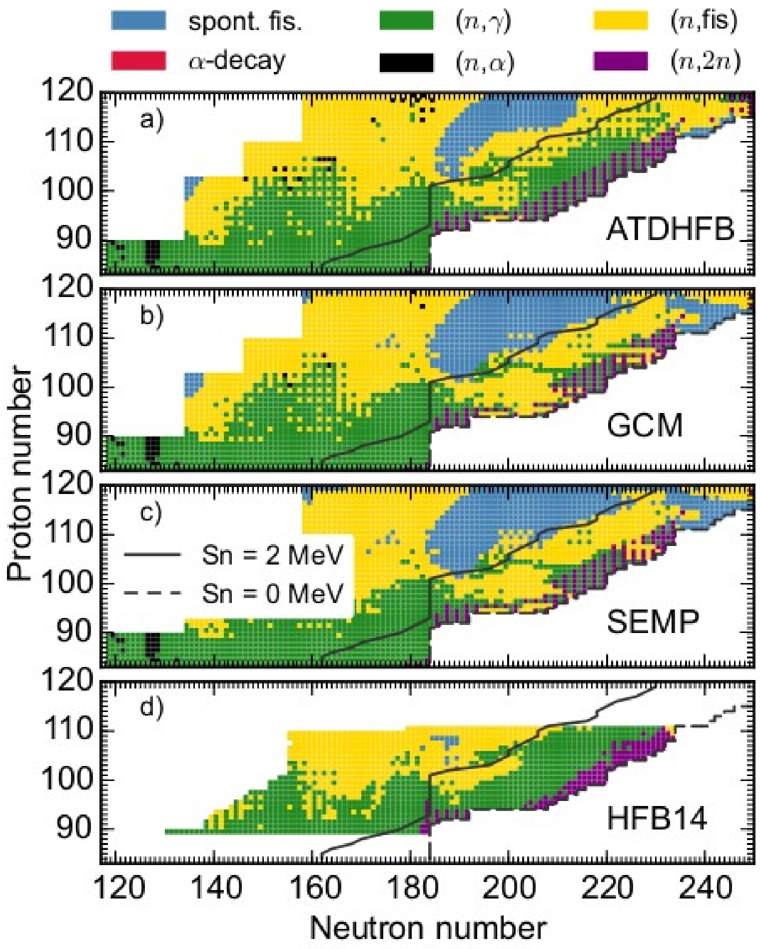
Neutron induced fission window



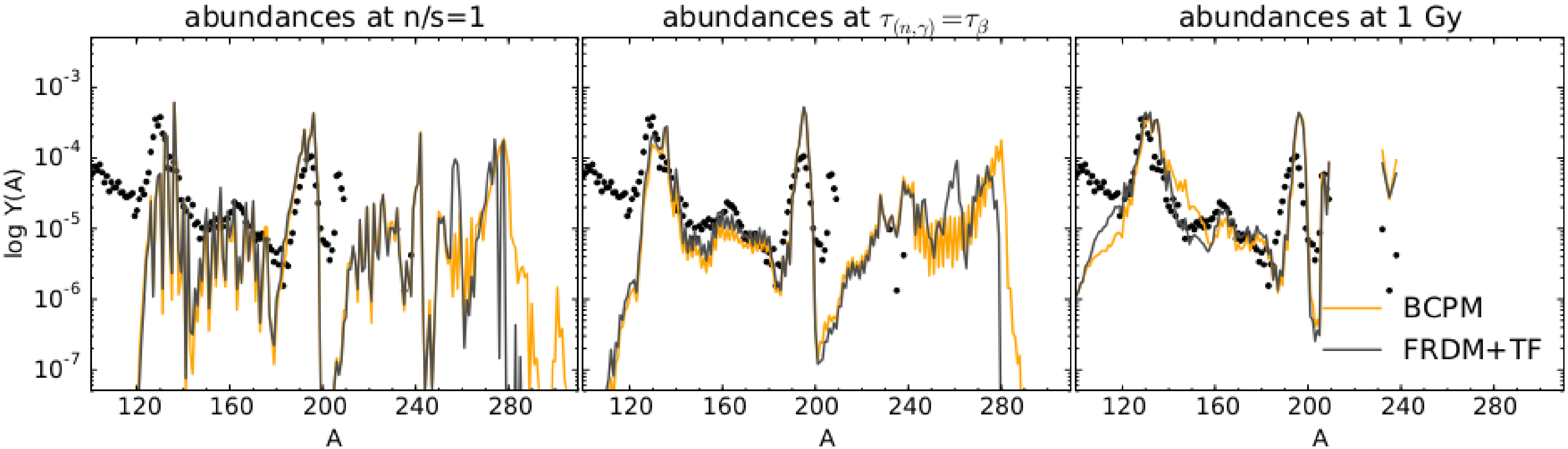
Fission barriers



Decay channels



Abundances



For more details contact Samuel Giuliani or Gabriel MP !

Thanks to ...

Samuel Giuliani and Gabriel MP