DE LA RECHERCHE À L'INDUSTRIE

PES topology and interplay with shell effects

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IRESNE / DER / SPRC / LEPh

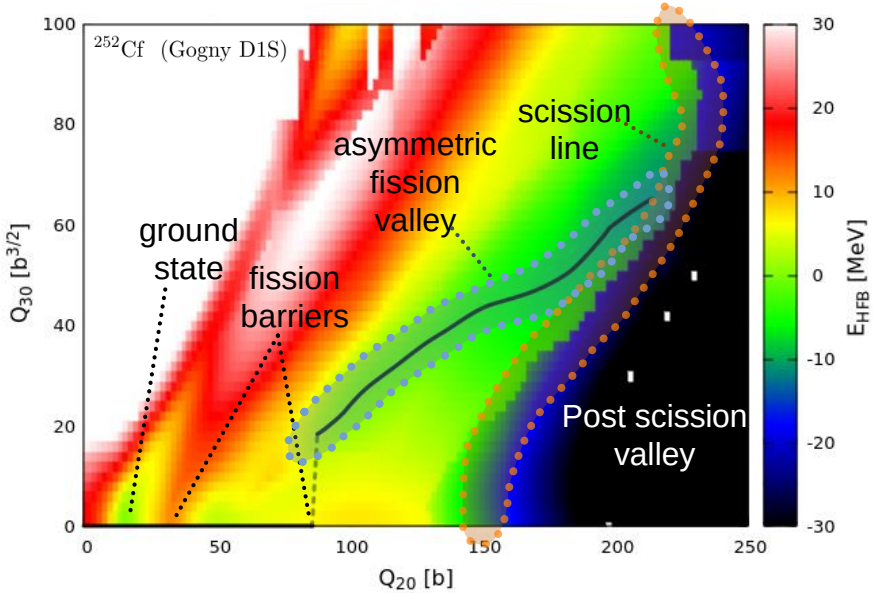
CONTENT

- Smoothing discontinuities from Potential Energy Surfaces
  - Motivations
  - The Dynamic Programming Method in 1 D
  - The Dynamic Programming Method in 2 D

- Shell effects in fission
  - Level densities at the Fermi surfaces
  - Connection to (pre)fragments
  - 180Hg case

MOTIVATION : POTENTIAL ENERGY SURFACE

Hartree-Fock-Bogoliubov (or any other mean field) under constraints calculations to generate the PES



<u>Adiabatic hypothesis</u> : the PES is built from mean field state minima for each deformation.

→ It implies discontinuities in unconstraint variables.

→ Missing the physics at the discontinuity

How to deal with discontinuities before the scission line ?

→ Adding a dimension in the calculations ?

→ Linear interpolation ?

→ Other ?

MOTIVATION : TDGCM

The Time-Dependent Generator Coordinate Method

$$\left|\Psi_{\mathrm{GCM}}(t)\right\rangle = \int d\mathbf{q}\; f(\mathbf{q},t)\left|\Phi(\mathbf{q})\right\rangle$$

⇩

Hill-Wheeler equation

$$\int d\mathbf{q}'\left(\underbrace{\mathcal{H}(\mathbf{q},\mathbf{q}')}_{\mathcal{H}(\mathbf{q},\mathbf{q}')=\langle\Phi(\mathbf{q})|\hat{H}|\Phi(\mathbf{q}')\rangle} - i\hbar\underbrace{\mathcal{N}(\mathbf{q},\mathbf{q}')}_{\mathcal{N}(\mathbf{q},\mathbf{q}')=\langle\Phi(\mathbf{q})|\Phi(\mathbf{q}')\rangle}\frac{d}{dt}\right) f(\mathbf{q}',t) = 0$$

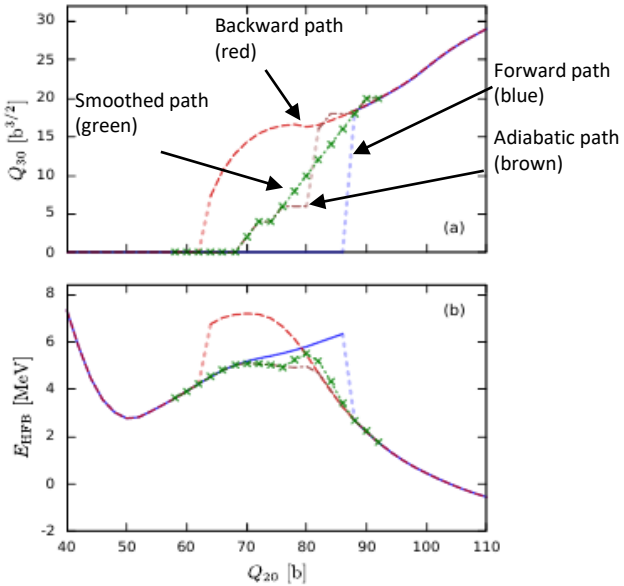
Hamiltonian kernel — overlap kernel

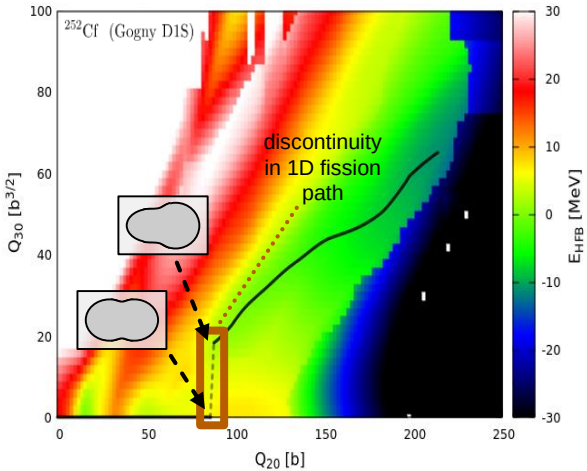
Overlap and Hamiltonian kernels

- Inversion of the square root of the overlap kernel usually done to solve the TDGCM equation
- Any inertia formula is based on wrong mean field states locally

→ issue for the TDGCM wave function evolution

PART IA : DISCONTINUITIES IN PES IN 1 DIMENSION





N.-W. T. Lau, et al, Phys. Rev. C 105, 034617 (2022)

Useful tools to detect discontinuities :

– Overlaps (Onishi Formula) between adjacent states $\mathcal{N}(\mathbf{q},\mathbf{q}') = \langle \Phi(\mathbf{q}) | \Phi(\mathbf{q}') \rangle$

– Density distance

Smoothing discontinuities : Requirements

N.-W. T. Lau, et al, Phys. Rev. C 105, 034617 (2022)

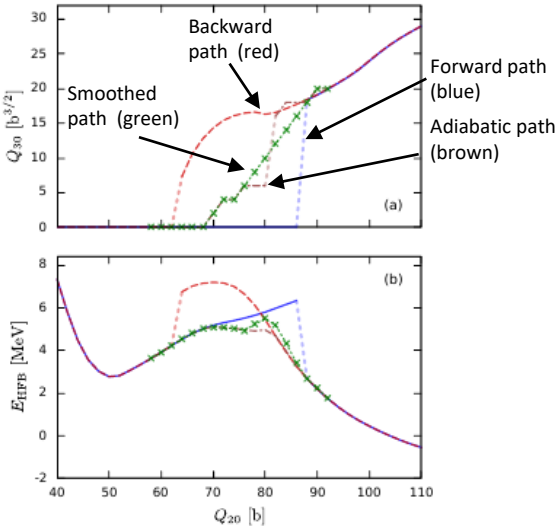
The method to clean the discontinuities is built from the following criteria :

- Minimizing the total energy

- Remaining smooth in energy

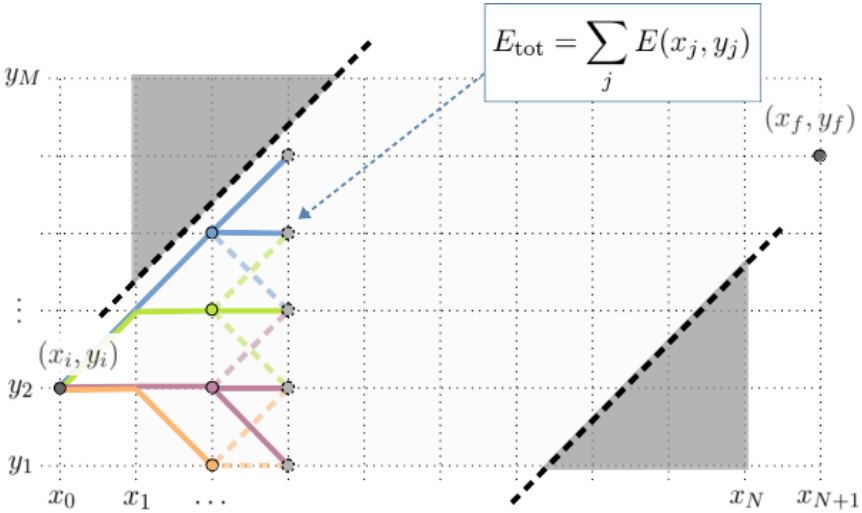
- The 1D/2D PES must be continuous in terms of overlap or density distance

- Method must be efficient to facilitate its application to many discontinuities and PESs at a reasonable cost



The solution is not unique, one may start from other requirements or add some extra criteria...

The Dynamic Programming Method in 1D

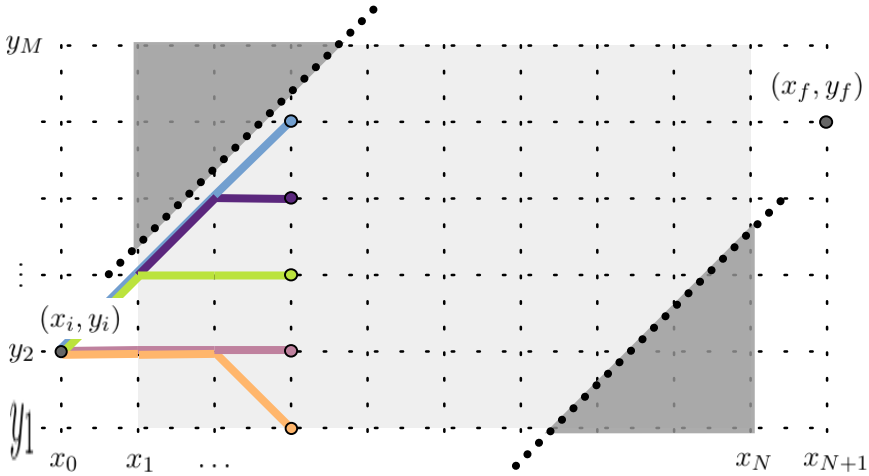


Conventional tree search:
M^N paths

Dynamic Programming Method (DPM):
MN trajectories by keeping the best path for each point

A. Baran et al. 1981 Nuclear Physics A361 83-101
J. Sadhukhan et al. 2013 Phys. Rev. C 88 064314

The Dynamic Programming Method in 1D



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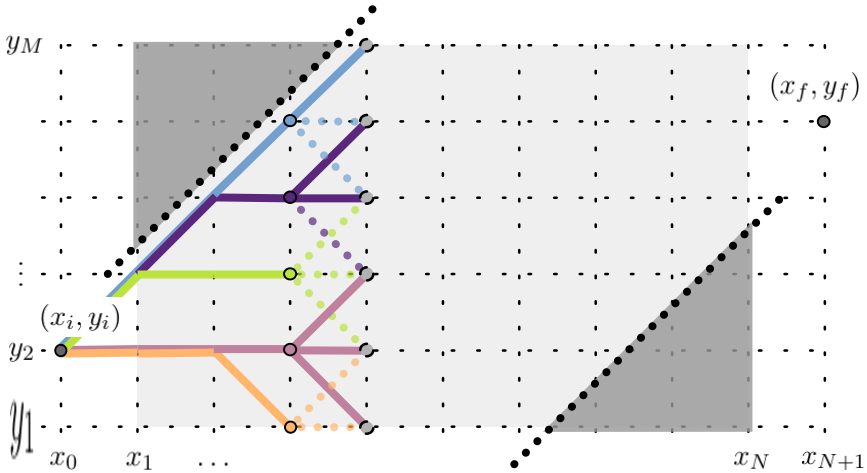

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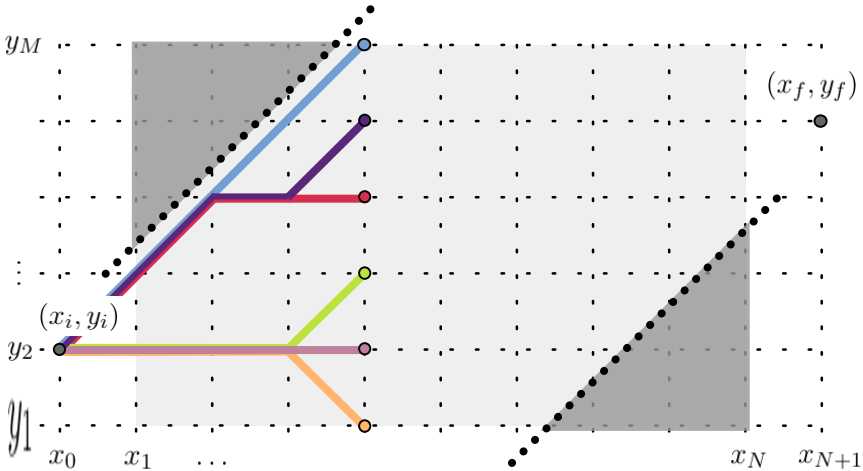

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M^N paths

Dynamic Programming Method (DPM):
MN trajectories by keeping the best path for each point

1D DPM : for M = 9 and N = 19; an extremely short run (of few seconds on the CDC-CYBER 7316 computer) allows us to choose the minimal trajectory from among a huge number, 919 x 1018, of all trial paths. (Baran NPA 81)

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1D Results for 222Th

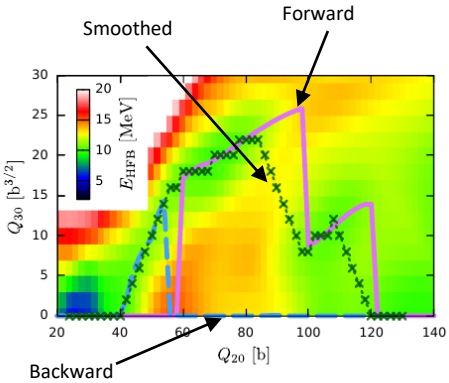
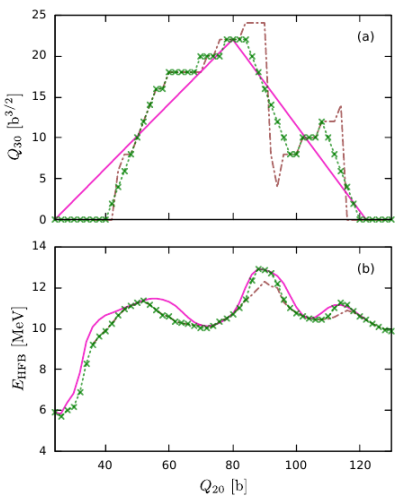
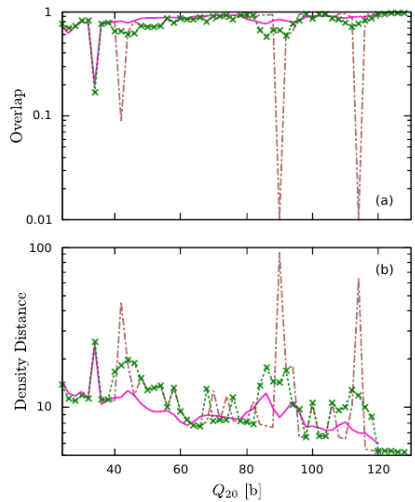


FIG. 8. A subsection of the 2D PES in Q_{20} and Q_{30} for ^{222}Th, generated with $N_\perp = 15$, $N_z = 22$ shells and fixed oscillator lengths $b_\perp = 2.0$, $b_z = 3.0$. Energies are shown relative to the ground state. The HFB paths propagated in the $+Q_{20}$ and $-Q_{20}$ directions are drawn with solid pink and dashed blue respectively, while the smoothed path generated using DPM is depicted in dotted green with crosses.

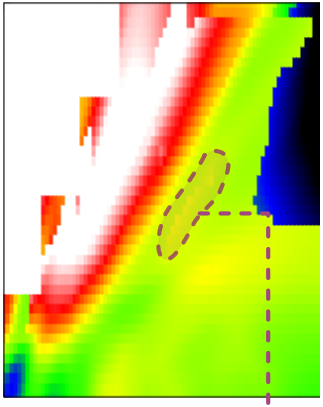




Pink : Linear interpolation
Brown : Adiabatic path
Green : Smoothed

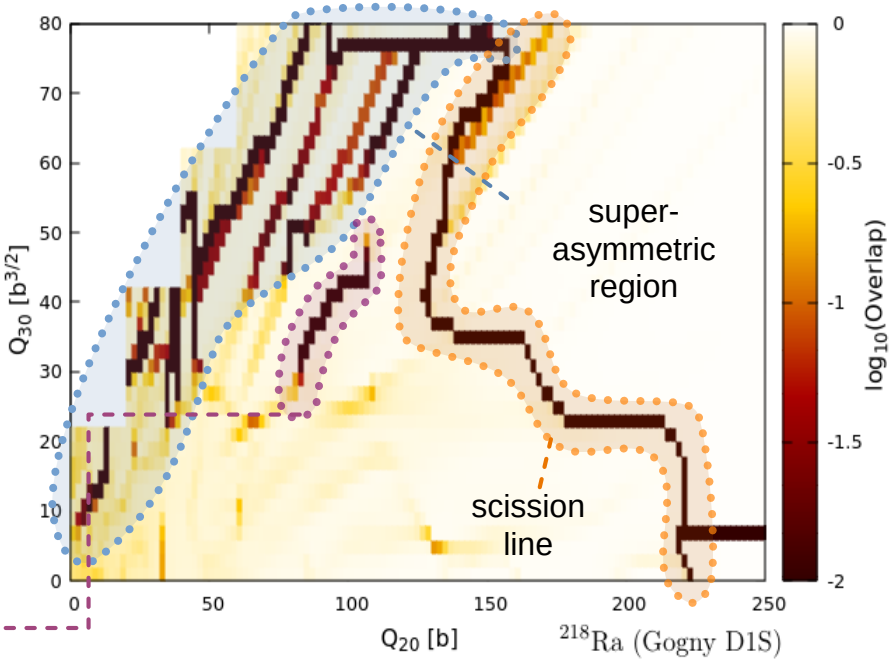
Identification : overlap or density distance

214Ra Potential Energy Surface

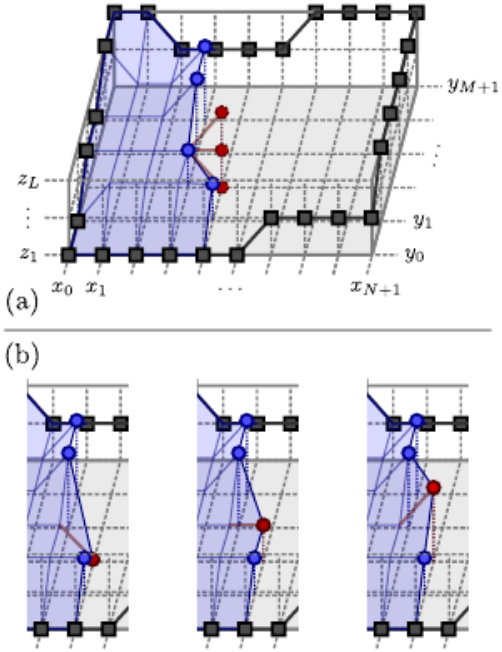


2D
discontinuity

Overlap N(q,q+dq) = <q|q+dq>



2D DPM procedure



Number of possible surfaces = L^(M.N)

(1) The initial set of partial surfaces contains only one surface consisting of the boundary points.

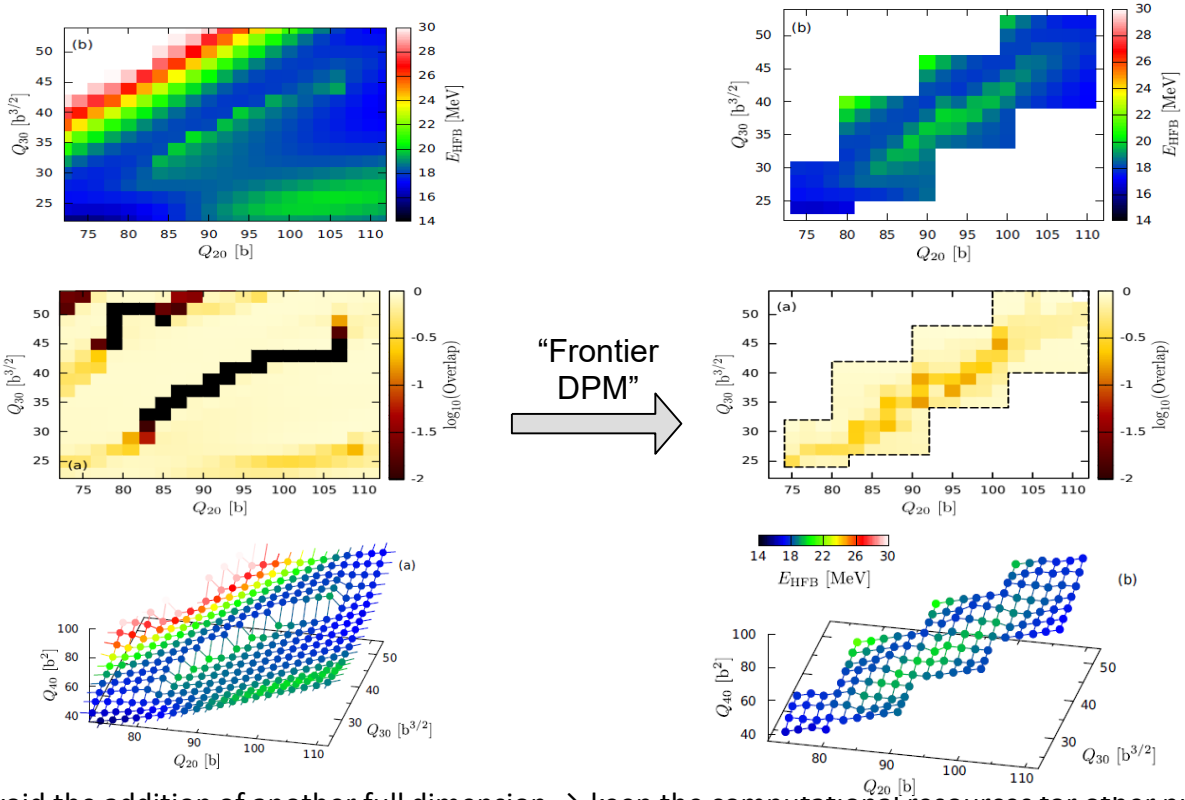
(2) Choose the next point in the (x, y) plane to add to the surface

(3) For each possible z-value at this point, generate a successor surface from each existing surface by the point. Keep the surface that lower the total energy

(4) Repeat from step 2 until the entire surface within the boundaries is filled.

Number of calculated surfaces in the 2D DPM = M.N. L^(M+1)

Application in 2D : 218Ra



Avoid the addition of another full dimension → keep the computational resources for other purposes

No need to get the adiabatic PES first

Part 2 : Shell effects in the PES

→ Shell effects have been studied by Strutinsky corrections to explain asymmetric fission on the way to fission

→ Recent studies based on microscopic theories are focused on the 1D path scission point

→ What are the compound nucleus shell effects along the asymmetric fission path?

→ What are the role of fragment spherical and deformed shell effect in fission ?

Quantum shells stabilizing fission fragments with various shapes have been invoked as a factor determining the distribution of nucleons between the fragments at scission.
Spherical : Z = 50, N = 82
Deformed : Z = 52,54,56 N = 88

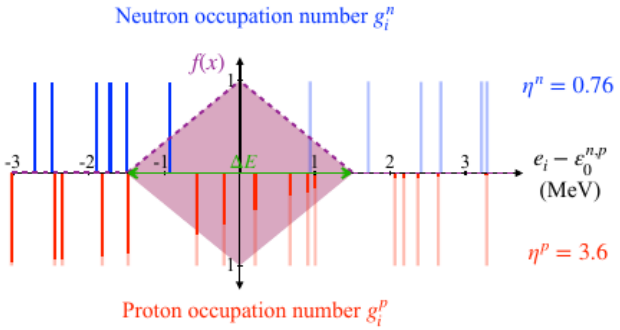
Other shells are also expected in the fissioning nucleus.

Shell effect at the Fermi surface

Idea : looking at the shell effects only at the Fermi level within all the PES

- counting the number of single particle energy states in an energy window around the Fermi level

- applying a smoothing function f

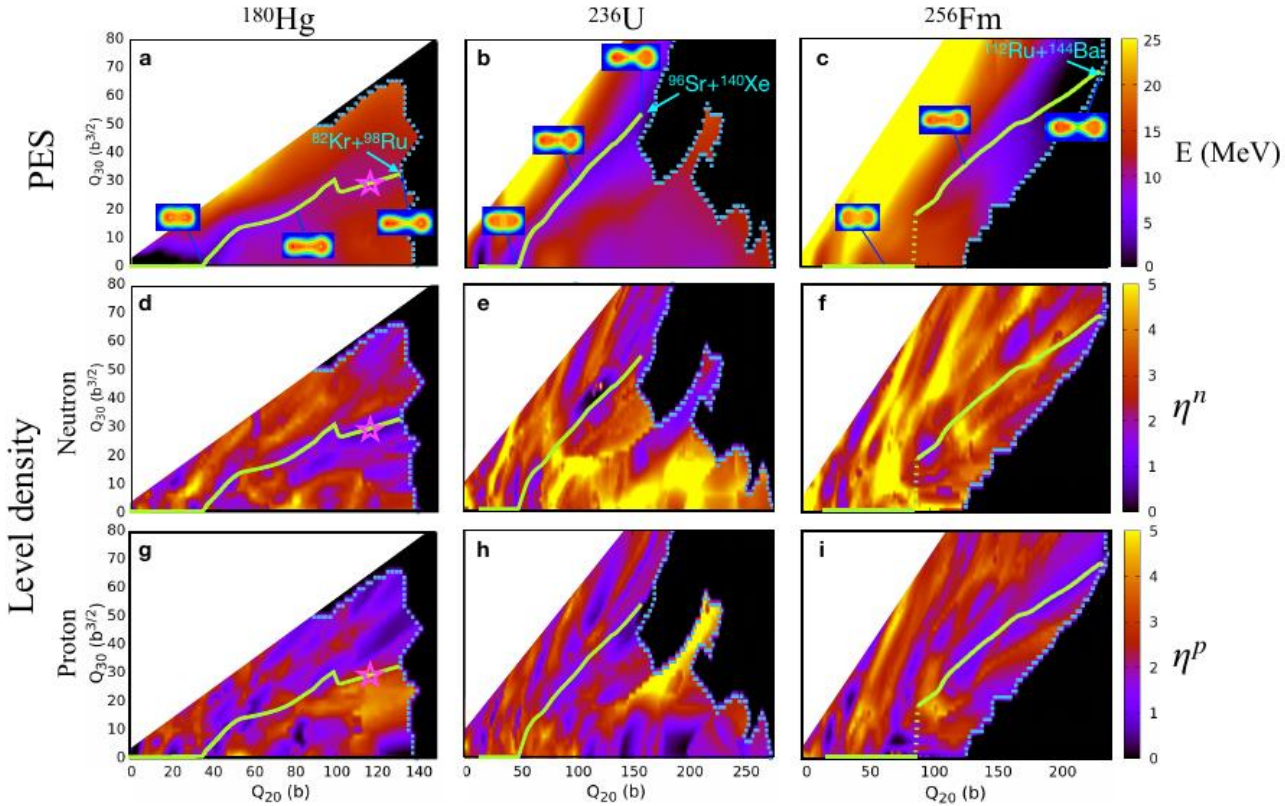


- Diagonalisation of the h part of the Bogoliubov matrix to get Single Particle Energy

- Fermi level as the middle of the gap

- Energy window : a few MeV around the Fermi level

Smoothed level densities around the Fermi level

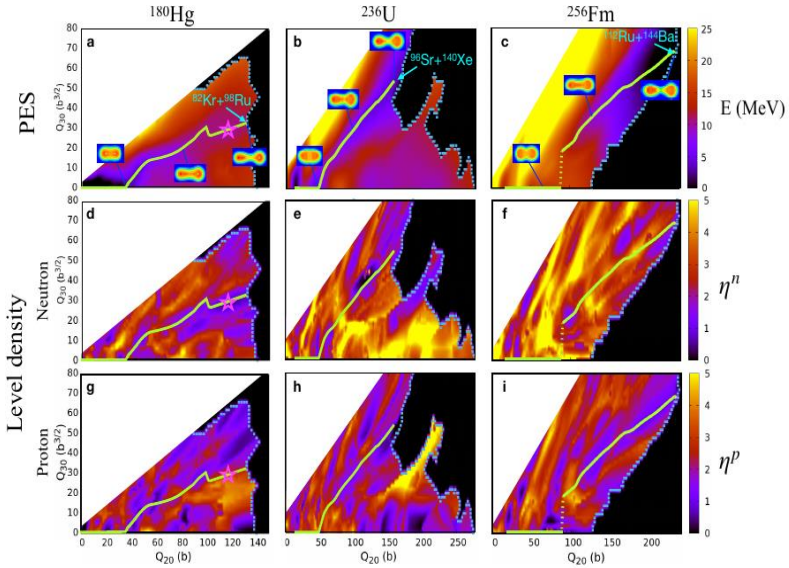


Smoothed level densities

- Asymmetric paths follow Fermi shell effects

- 2 to 3 proton/neutron shell effects are on the path of asymmetric fission

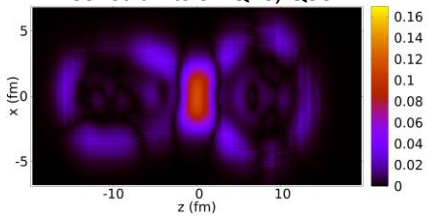
- some 1D path discontinuities may be understood looking at the competition of shell effects



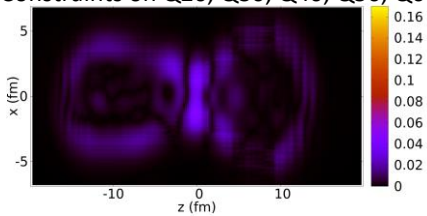
Compound nucleus – (pre)fragments shell effects connection

Total density difference $\left|\rho_{comp}(\vec{r}) - \rho_{frag}(\vec{r})\right|$

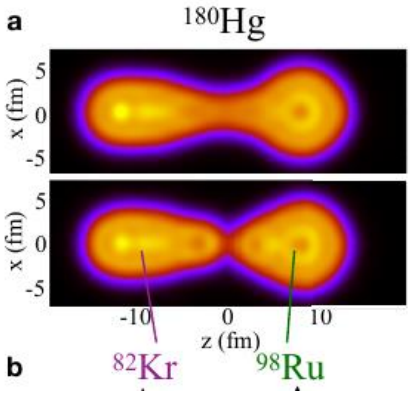
Constraints on Q20, Q30



Constraints on Q20, Q30, Q40, Q50, Q60



Total density



- Localizing the density minimum in the neck

- Integrating the space densities to get the fragment properties

- HFB calculation for (pre)fragments with 5 constraints on multipole moments from Q20 to Q60 to lower $\int d\vec{r}\left|\rho_{comp}(\vec{r}) - \rho_{frag}(\vec{r})\right|$ from 3,76 (2 constraints) to 1,90 (5 constraints)

180Hg Prefragments sld

Prefragments remains the 82Kr and 98Ru within the last 180 neutron shell effect

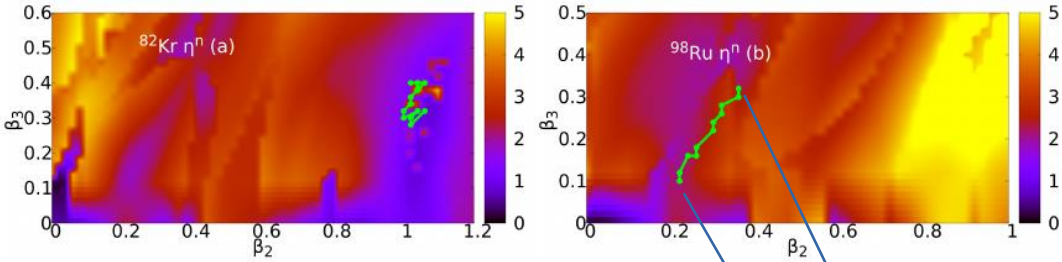
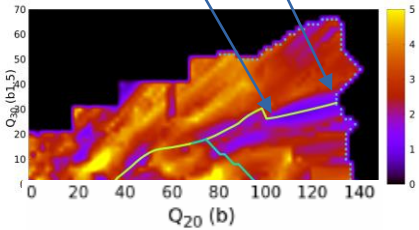


FIG. 2: Neutron sld of ^{82}Kr in panel (a) and ^{98}Ru in panel (b). The green dotted lines give the prefragment deformation during the final stages of the asymmetric ^{180}Hg fission. The energy window around the Fermi level is fixed to 5 MeV for medium mass nuclei. Constraints are done on Q_{20} and Q_{30} and higher multipole moments are let free.

- No low sld in the proton side

- *Andreyev PRL 2010* : « This is a new type of asymmetric fission, not caused by large shell effects related to fragment magic proton and neutron numbers, as observed in the actinide region. »

- Conclusions : N=46 driver at the last stages



Prefragments shell effects

Are the 1D path Z_frag and N_frag due :

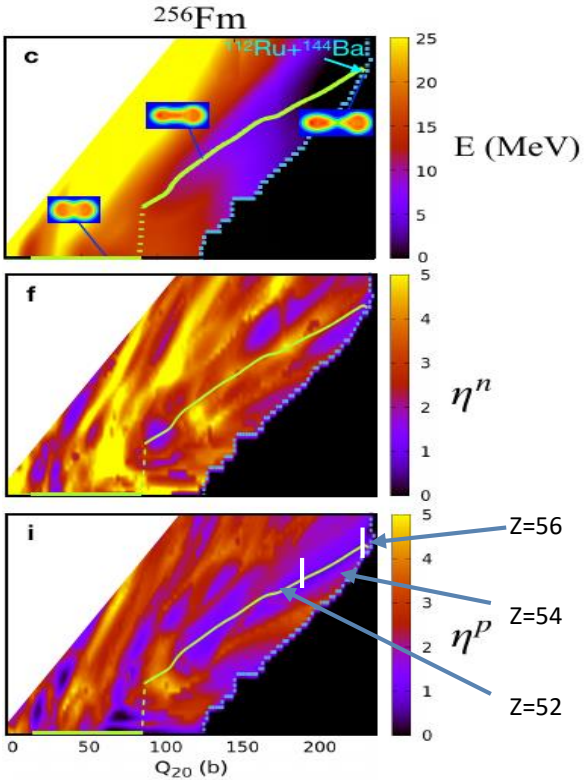
- Always to fragment shell effects ? (configuration at scission)
- To other Prefragment shell effects ? (configurations before scission)

→ stable prefragments before scission (82Kr and 98Ru)

→ successive shell effects from several prefragments during the last shell effect before scission

256Fm – Spherical Z=52
– Deformed Z= 54, 56

236U – Spherical Z=52, N=82
– Deformed Z=38, 40, 54, N=58,62



+ Local PES topolgy may be convex at the asymmetric valley around fission (ie 236U, ...)

Conclusions

Discontinuities :

- The cleaning of the Potential Energy Surfaces from discontinuities is required for the TDGCM wave function evolution

- Detection of discontinuities done with simples tools : mean field states overlap or density distance operator

- an adapted Dynamic Progamming Method used to clean discontinuities in 1 or 2 D involving a local N+1 dimension calculation

Shell effects :

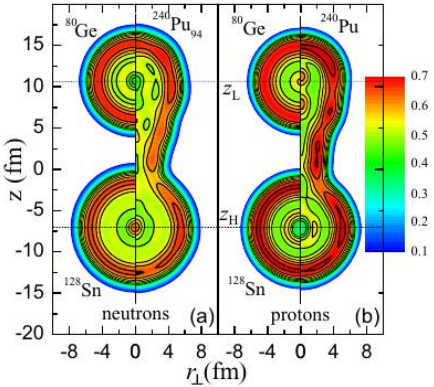
- The 1 D paths in PES favored by low sld at the Fermi surfaces

- Several proton and neutron shell effects guiding the asymmetric path

- Final shell effects correlated to (pre)fragment ones : several deformed and/or spherical fragment shell effects to lead the 1D path

Fragment separation methods

Localization function



Quantum loca. of the fragments

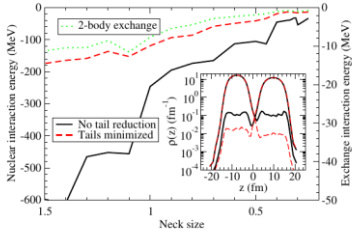
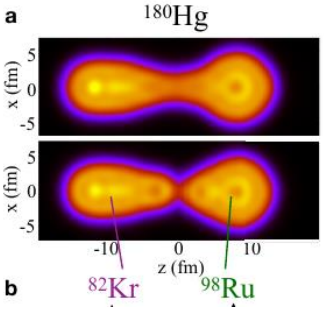


FIG. 1 (color online). Interaction energies plotted as a function of neck size (Q_N). The solid black and red dashed curves are the nuclear interaction energies before and after localization, respectively, (energy scale on the left y axis), and the dotted green curve is the exchange part of the 2-body component of the interaction energy (energy scale on the right y axis). The inset shows the effect of the localization on the densities of the fragments at scission.



Sadhukhan et al, PRC 2017

Younes et al, PRL 2011