Construction of continuous collective energy landscape

An opportunity for TDGCM approach to describe scission and include dissipation

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I. Nuclear fission dynamics within TDGCM approach

Physica Scripta. Vol. 10 A, 118–121, 1974

Quantum Theory of Dissipation for Nuclear[1] Collective Motion

Arthur K. Kerman and Steven E. Koonin[2]

Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology Cambridge, Massachusetts

Received November 30, 1974

Abstract

Quantum theory of dissipation for nuclear collective motion. A. K. Kerman and S. E. Koonin (Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA).
Physica Scripta (Sweden) 10 A, 118–121, 1974.

We present a theory of energy dissipation in heavy ion and fission processes. Beginning with the time-independent coupled channels generator coordinate equations, a statistical treatment leads to a quantal equation in the collective coordinates *and* excitation energy. Assumptions of adiabaticity lead to a momentum coupled Schroedinger-like equation for the statistical wave-function. This equation describes, in a statistical manner, quantum mechanical collective motion, including dissipation. Therefore, average inelastic cross sections or fragment excitation energies may be obtained. Of course, phenomenologically known functions such as the nuclear mass parameter or potential energy surface can be simply utilized. The new dissipation function (like all the others) is determined by averages of microscopically calculable quantities. Numerical results for a model calculation exhibiting the structure of the equation are presented.

Of course, there will still be some redundancy in the basis, which will appear, as usual, in the treatment of the overlap matrix.

By varying the f_n of eq. (1) so as to minimize the expectation value of the many body hamiltonian H, we obtain matrix integral equations of the form

$$\sum_{n'} \int d\alpha' \langle n\alpha | H - E | n'\alpha' \rangle f_{n'}(\alpha') = 0 \quad (2)$$

or, schematically

$$(H - EN) f = 0 \quad (3)$$

with the hamiltonian and overlap kennels given by

$$H_{nn'}(\alpha, \alpha') = \langle n\alpha | H | n'\alpha' \rangle \quad (4)$$

$$N_{nn'}(\alpha, \alpha') = \langle n\alpha | n'\alpha' \rangle \quad (5)$$

and the energy E arising as a lagrange multiplier for the normaliza-

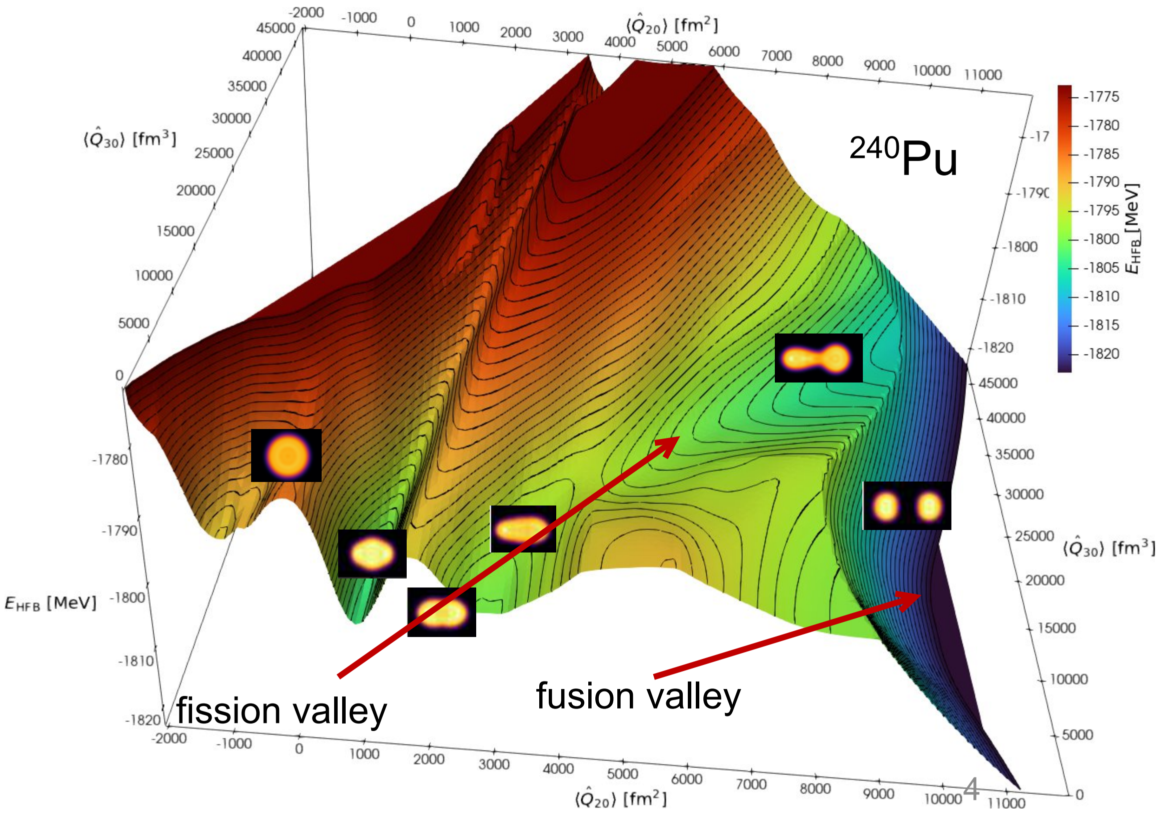
Emergence of two ways of solving
this Time-dependent Hill-Wheeler equation for **fission**:

- Statistical treatment of intrinsic excitations with T-dependent HFB (grand-canonical ensemble)
  D. Vretenar et al. (2022)

- Explicit treatment of discrete intrinsic excitations for low energy fission: **Schrödinger Collective-Intrinsic Model** (SCIM)
  R. Bernard et al. (2011)

- [high energy fission: K. Dietrich, JJ. Niez and JF Berger, Nucl. Phys. A 832 (2010), “Microscopic transport theory of nuclear process”
  =>Rigorous equation of motion+ Markov approx.]

I. Nuclear fission dynamics within TDGCM approach



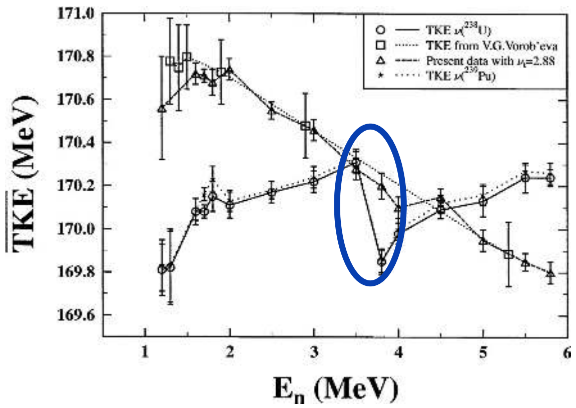
Adiabatic PES
(HFB states, 2 CT HO basis, D1S)

Main degrees of freedom in fission

- Collective deformations
- Superfluidity
- Shell effects

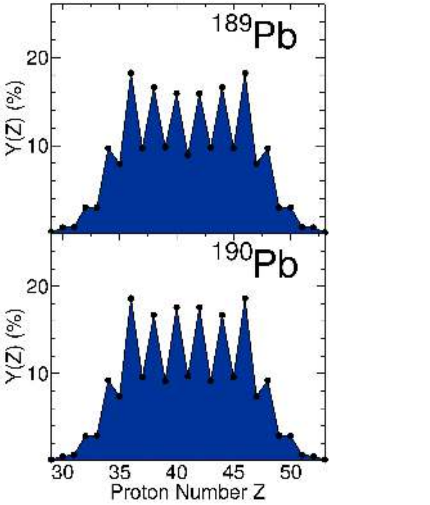
- Intrinsic excitations (pair breaking phenomenon):

Sudden drop of $\overline{\mathrm{TKE}}$
(F. Vives et al., Nucl.Phys. A662 (2000))



Pair breaking energy: 2.3MeV

Odd-even staggering
(SOFIA data, P. Morfouace et al.)



I. Nuclear fission dynamics within TDGCM approach

Schrödinger Collective-Intrinsic Model (SCIM)

Adiabatic states

Excited states

- **Trial wave function** :

$$|\Psi_{SCIM}\rangle = \int dq f(q)|\Phi(q)\rangle + \sum_{i=1,N} \int dq f_i(q)|\Phi^{(i)}(q)\rangle$$

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$$\delta(\frac{1}{2^n}\sum_j\sum_i\int d\bar{q}\int ds f_j^*(\bar{q}-s)\langle\Phi^{(j)}(\bar{q}-s)|\hat{H}-E|\Phi^{(i)}(\bar{q}+s)\rangle f_i(\bar{q}+s)) = 0$$

Taylor expansion →

$$\delta(\frac{1}{2^n}\sum_j\sum_i\int ds\int d\bar{q} f_j^*(\bar{q})e^{s\frac{\partial}{\partial q}}\langle\Phi^{(j)}(\bar{q}-s)|\hat{H}-E|\Phi^{(i)}(\bar{q}+s)\rangle e^{s\frac{\partial}{\partial q}} f_i(\bar{q})) = 0$$

Non local equation!

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- **Non-locality in "s" fully treated** with the Symmetric Ordered Products of Operators (SOPO) technics

$$\begin{cases} \mathcal{H}_{ji}(\bar{q},s) = \langle\Phi^{(j)}(\bar{q}-s)|\hat{H}\quad|\Phi^{(i)}(\bar{q}+s)\rangle \\ \mathcal{N}_{ji}(\bar{q},s) = \langle\Phi^{(j)}(\bar{q}-s)|\Phi^{(i)}(\bar{q}+s)\rangle \end{cases}$$

SOPO

$$[AB]^{(n)} = \sum_{k=0}^{n}\binom{n}{k} B^k A B^{n-k}$$

$$\begin{cases} e^{s\frac{\partial}{\partial q}}\mathcal{H}_{ji}(\bar{q},s)e^{s\frac{\partial}{\partial q}} = \sum_{k=0}^{+\infty}\frac{1}{k!}[\mathcal{H}_{ji}(\bar{q},s)(s\frac{\partial}{\partial q})]^{(k)} \\ e^{s\frac{\partial}{\partial q}}\mathcal{N}_{ji}(\bar{q},s)e^{s\frac{\partial}{\partial q}} = \sum_{k=0}^{+\infty}\frac{1}{k!}[\mathcal{N}_{ji}(\bar{q},s)(s\frac{\partial}{\partial q})]^{(k)} \end{cases}$$

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's' dependence in SOPO

Moments of operators

$$\begin{cases} \mathcal{H}_{ji}^{(p)}(\bar{q}) = \int ds \mathcal{H}_{ji}(\bar{q},s)s^p \\ \mathcal{N}_{ji}^{(p)}(\bar{q}) = \int ds \mathcal{N}_{ji}(\bar{q},s)s^p \end{cases}$$

I. Nuclear fission dynamics within TDGCM approach

Schrödinger Collective-Intrinsic Model (SCIM)

Adiabatic states ↘ Excited states ↘

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By integrating within the SOPO →

$$\begin{cases} \bar{\mathcal{H}}_{ji}(\bar{q}) = \sum_{k=0}^{+\infty}\frac{1}{k!}[\mathcal{H}_{ji}^{(p)}(\bar{q})\frac{\partial}{\partial q})]^{(k)} \\ \bar{\mathcal{N}}_{ji}(\bar{q}) = \sum_{k=0}^{+\infty}\frac{1}{k!}[\mathcal{N}_{ji}^{(p)}(\bar{q})\frac{\partial}{\partial q})]^{(k)} \end{cases}$$

special norm and Hamiltonian kernels

Moments of operators

I. Nuclear fission dynamics within TDGCM approach

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- **Hill-Wheeler equation including intrinsic excitations :**

$$\boxed{\mathcal{H}_{SCIM}\, g = E g} \quad \text{with} \quad \begin{cases} \mathcal{H}_{SCIM} = \bar{\mathcal{N}}^{-1/2}\bar{\mathcal{H}}\bar{\mathcal{N}}^{-1/2} \\ g = \bar{\mathcal{N}}^{1/2} f \end{cases}$$

Local equation!

Non-locality absorbed in special norm and Hamiltonian kernels

I. Nuclear fission dynamics within TDGCM approach

Schrödinger Collective-Intrinsic Model (SCIM)

- **Collective-Intrinsic Hamiltonian at second order in SOPO**

$$\mathcal{H}_{SCIM}(\bar{q}) = V(\bar{q}) + [D(\bar{q})\frac{\partial}{\partial q}]^{(1)} + [B(\bar{q})\frac{\partial}{\partial q}]^{(2)}$$

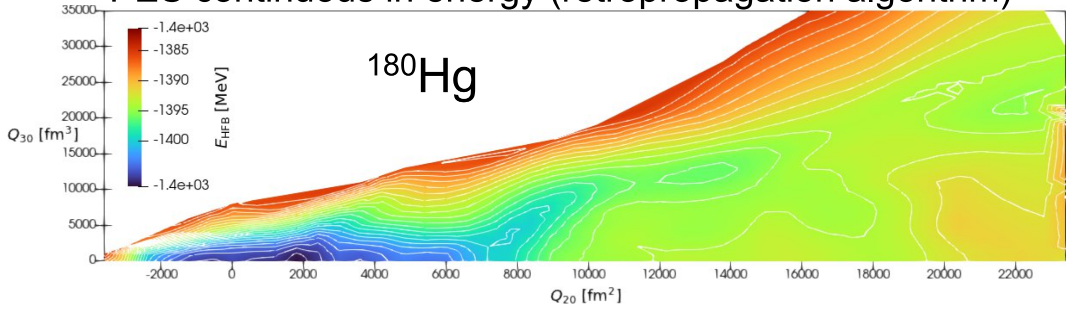
  - Zero order: potential $V(\bar{q})$
  - First order: “dissipation” tensor $D(\bar{q})$
  - Second order: inertia tensor $B(\bar{q})$

- **Time-dependent Schrödinger equation with intrinsic excitations**
  - Trial Wave function: $|\Psi_{SCIM}(t)\rangle = \int dq f(q,t)|\Phi(q)\rangle + \sum_{i=1,N} \int dq f_i(q,t)|\Phi^{(i)}(q)\rangle$
  - Schrödinger equation: $\mathcal{H}_{SCIM}\, g(t) = i\hbar\frac{\partial}{\partial t}g(t)$

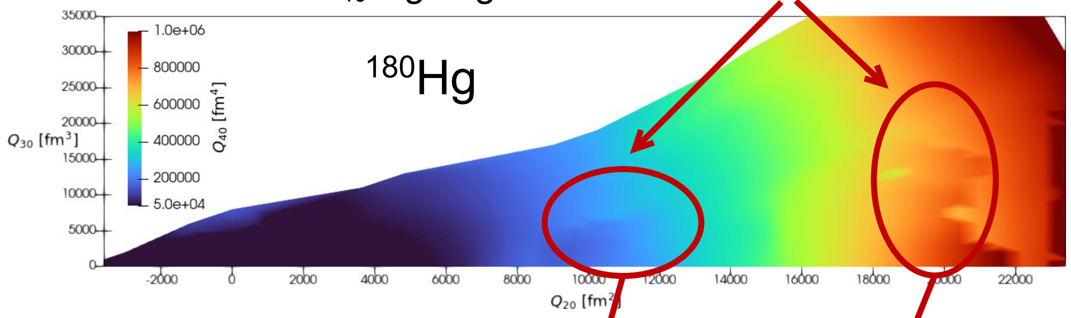
- **Continuous and regular overlaps required** for the Norm and Hamiltonian moment kernels to be continuous and regular (**strong hypothesis of the SCIM!**)

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

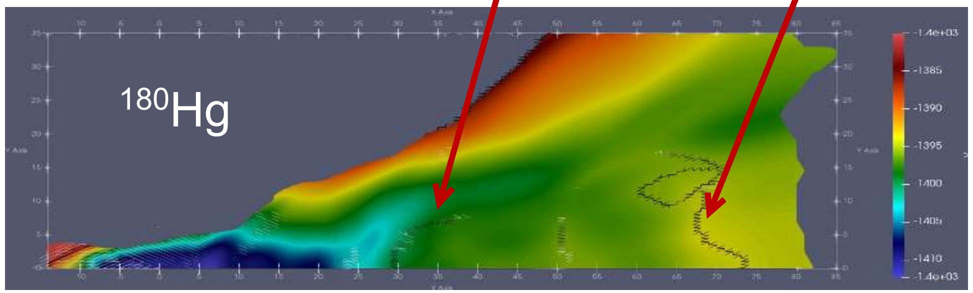
PES continuous in energy (retropropagation algorithm)



Evolution of Q_{40} signing state discontinuities



Small values of the overlaps signing states discontinuities

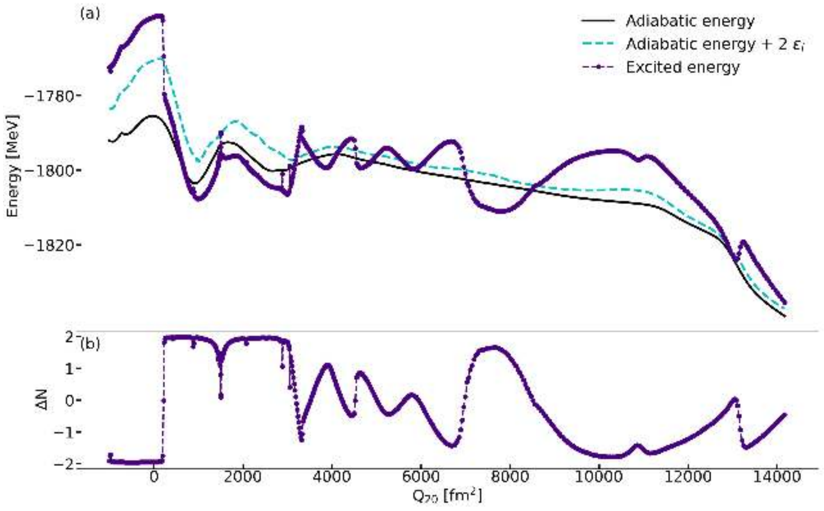


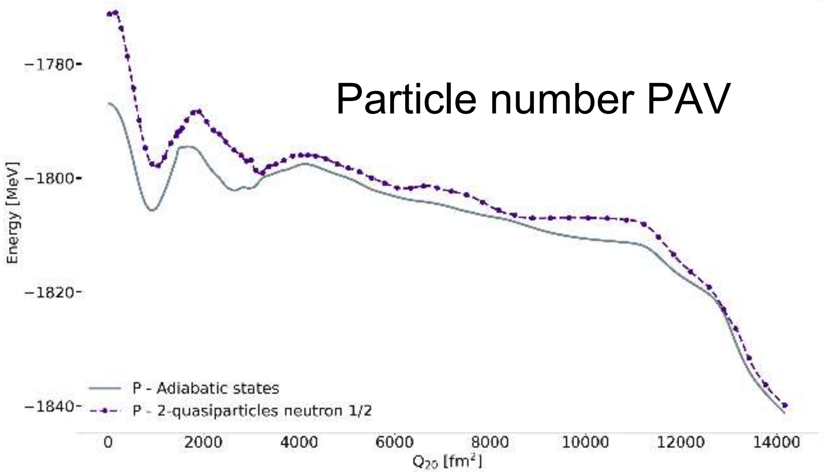
Discontinuity issues in the adiabatic states

- **Discontinuities in energy**
  - Origin: HFB solver a non-ideal minimizer that can fall in local minima
  - Solved numerically by a retro-propagation algorithm based on the overlap wave functions
- **Discontinuities in states**
  - Reduction of the collective space to few multipoles
  - Signed by the overlap of neighbor wave functions in the PES
  - More delicate to solve

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

Non self-consistent 2QP excitations





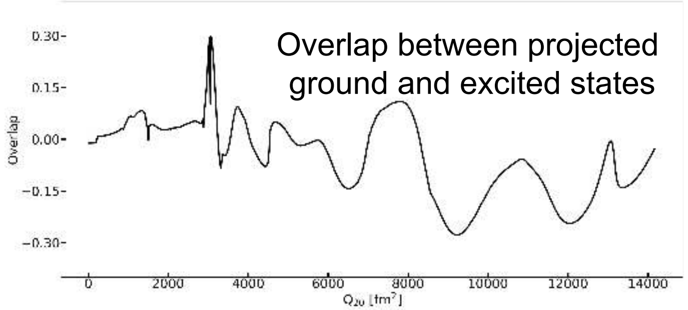
Particle number PAV

Discontinuity and irregularity issues in 2QP states

- **Non self-consistent 2QP excitations**
  - Original proposal of the SCIM
  - Time-even $|\Phi_{ij}\rangle = \alpha_{ij}(\xi_i^+\bar{\xi}_j^+ + \xi_j^+\bar{\xi}_i^+)|\Phi\rangle$
  - Followed by continuity

    $$|\langle\Phi_{ij}(q)|\Phi_{ij}(q+\delta q)\rangle| = \max_{i'j'}|\langle\Phi_{ij}(q)|\Phi_{i'j'}(q+\delta q)\rangle|$$
  - Minimizing average particle number breaking
  - **Not suitable**

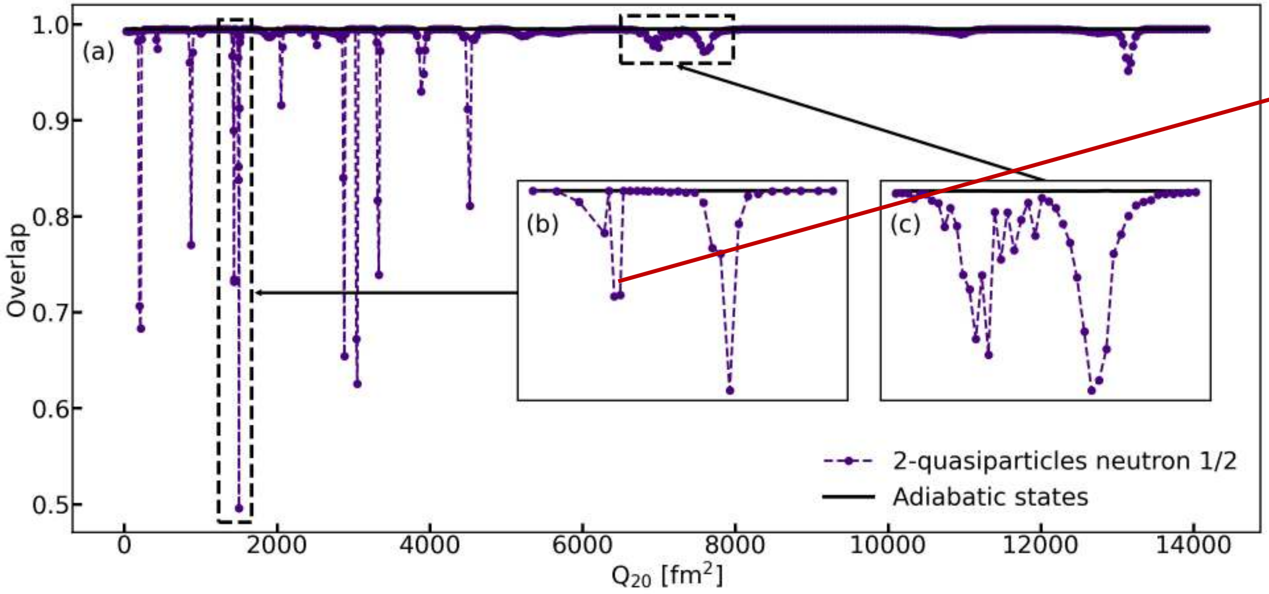
- **Particle number PAV for adiabatic and 2QP states**
  - Solve the energy problems
  - Creates ambiguous mixing

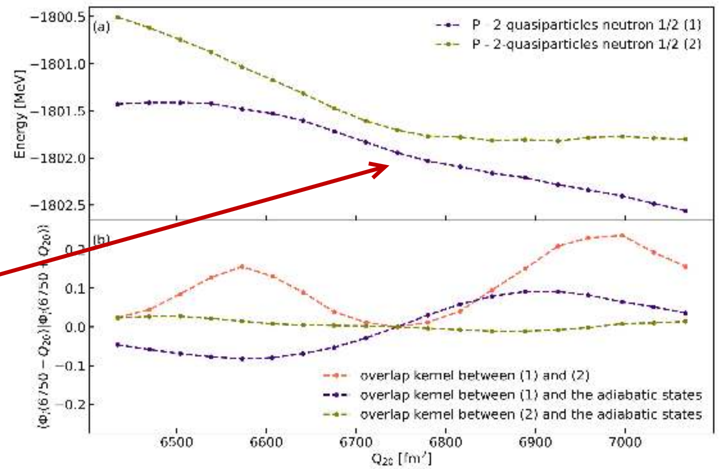


Overlap between projected ground and excited states

  - 2QP states produced by VAP also not suitable

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

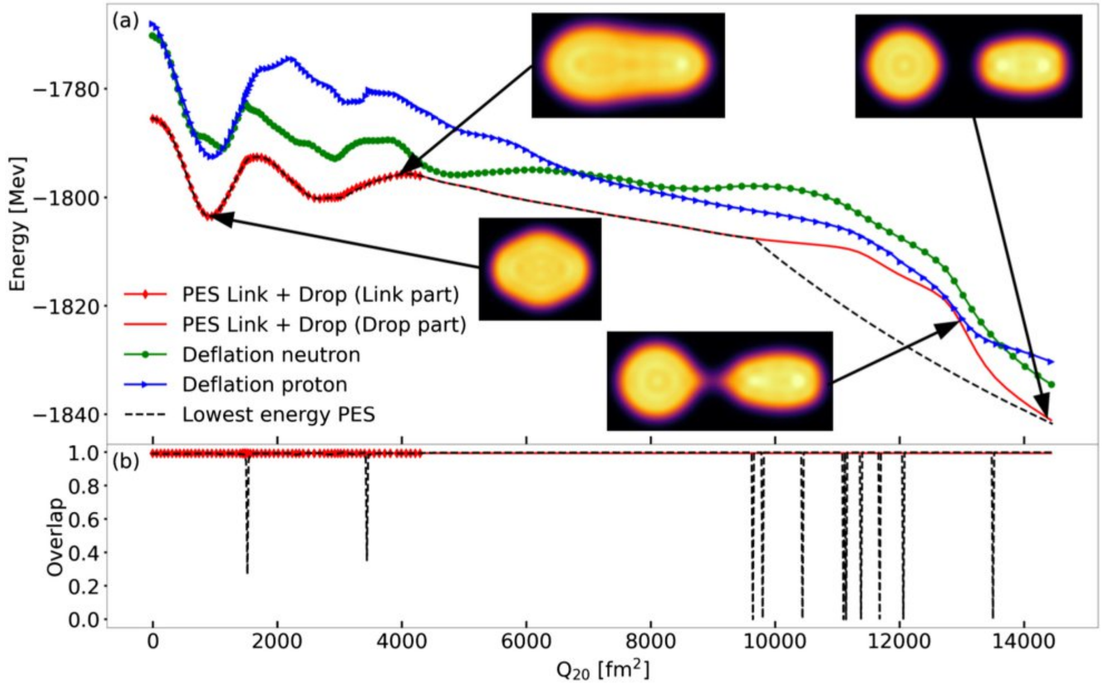




- **2QP excited states strongly irregular**
  - Even built from regular adiabatic states
  - Existence of numerous level repulsions along the path
  - Makes the SCIM unusable in practice
- **Need of another way of producing excited states!**

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

Adiabatic and excited asymmetric paths in ^{240}Pu



HFB approach under overlap constraints

$$\hat{H}_c = \hat{H} + \sum_{\alpha} \lambda_\alpha \hat{Q}_\alpha + \sum_{\beta} \gamma_\beta |\Phi_\beta\rangle\langle\Phi_\beta|$$

- **3 protocols**: Link, Drop and Continuous Deflation
  - continuous adiabatic path
  - continuous and orthogonal excited states
- Continuity: Link and Drop protocols

$$|\langle\Phi_i(q)|\Phi_i(q+\delta q)\rangle| \sim 1$$

- Orthogonality: Continuous Deflation protocol

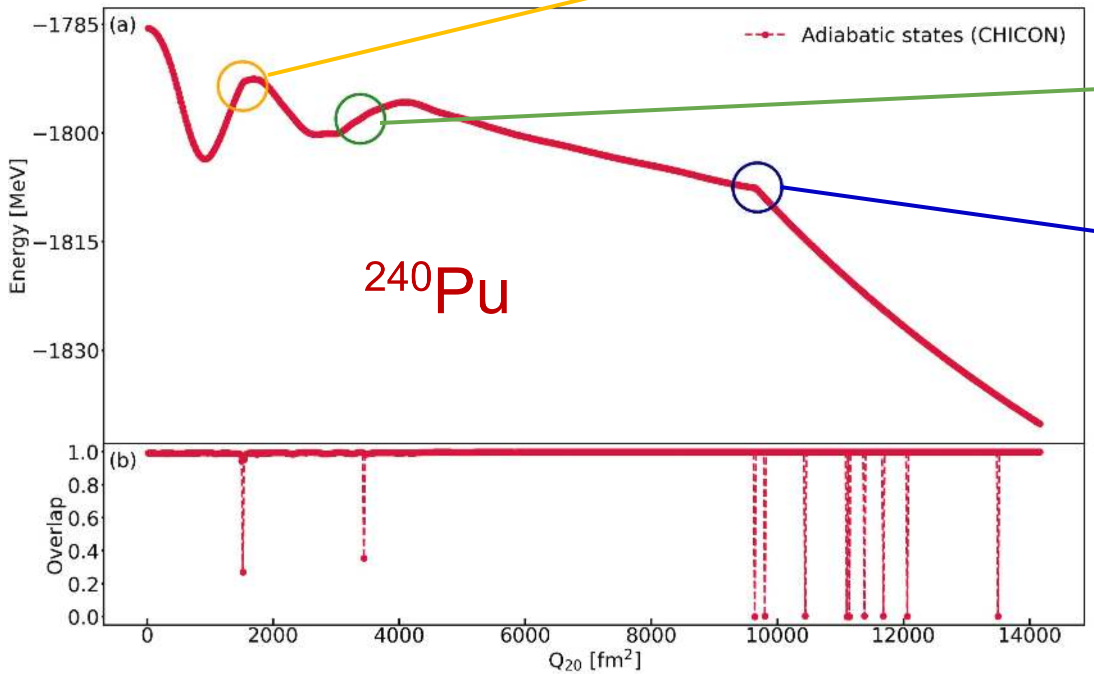
$$|\langle\Phi_i(q)|\Phi_i(q+\delta q)\rangle| \sim 0$$

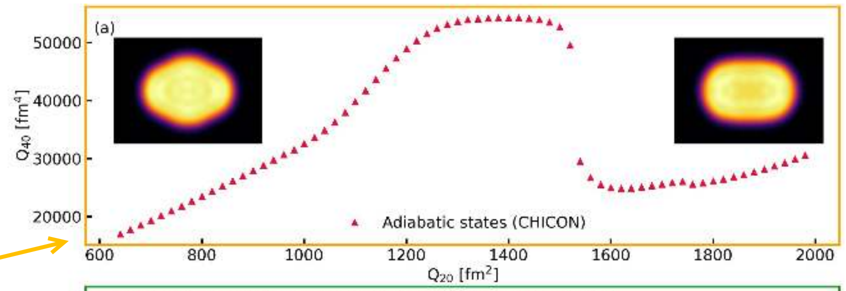
- Gradient method well-suited for these constraints

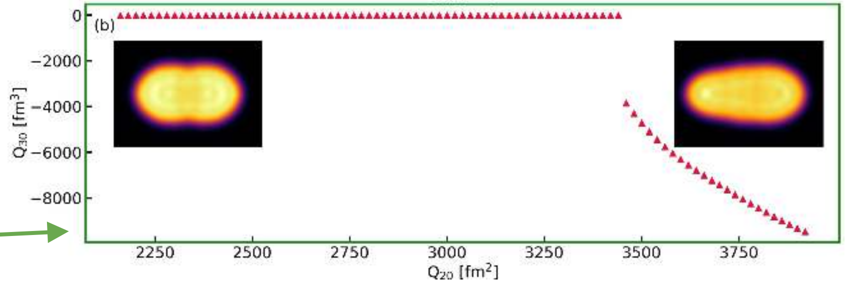
P. Carpentier, N. Pillet, D. Lacroix, N. Dubray and D. Regnier,
Phys. Rev. Lett.133, 152501 (2024)

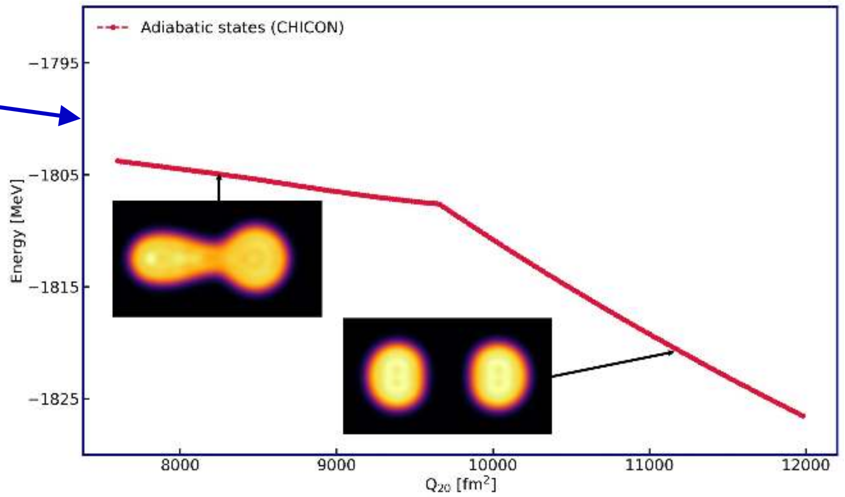
II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

- HFB adiabatic and asymmetric path of ^{240}Pu without overlap constraint
- **Spontaneous appearance of 3 discontinuities**
  - 2 simple state discontinuities (yellow and green)
  - Scission discontinuity (blue)



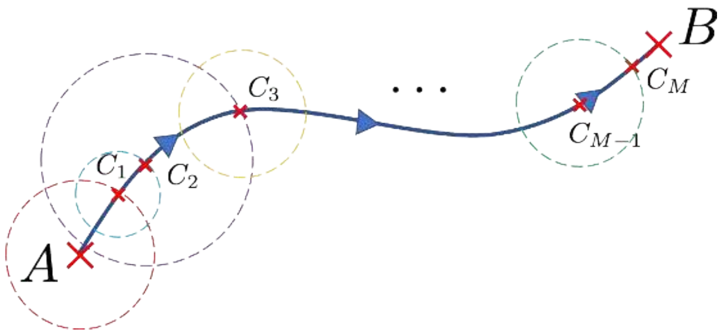


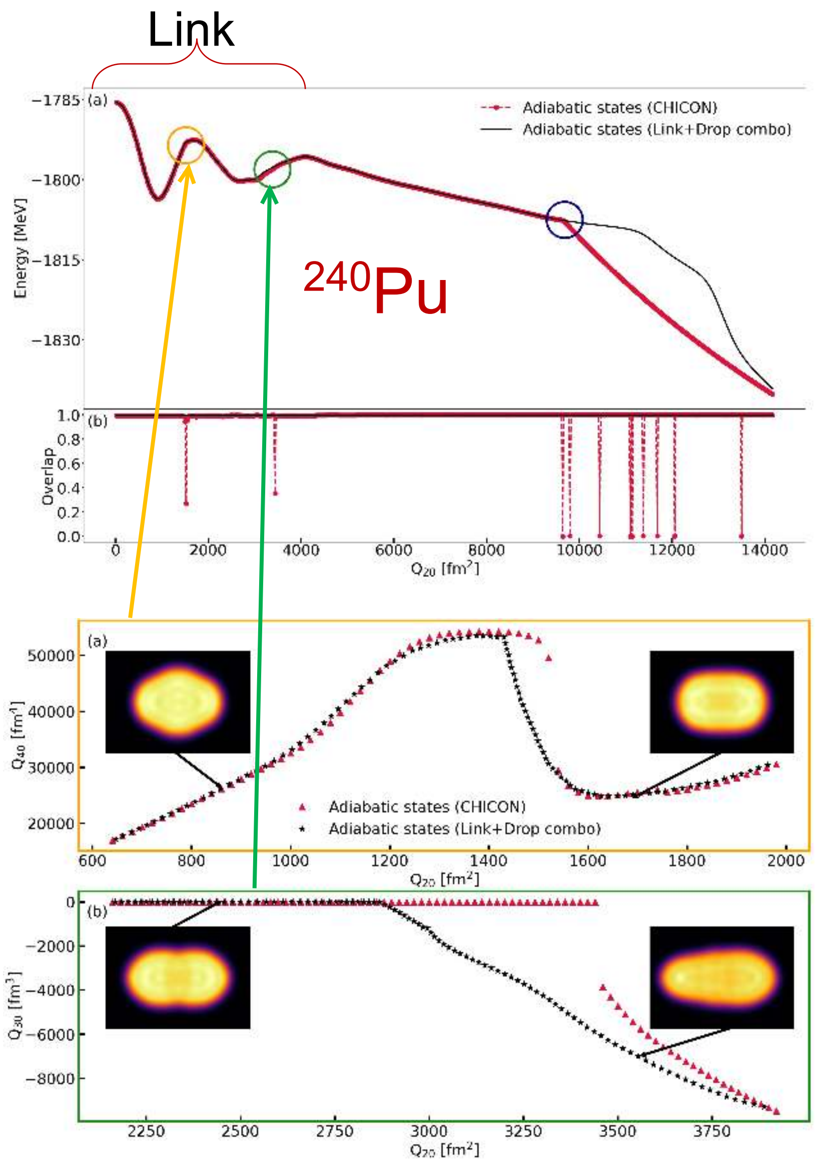




II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

Link protocol:



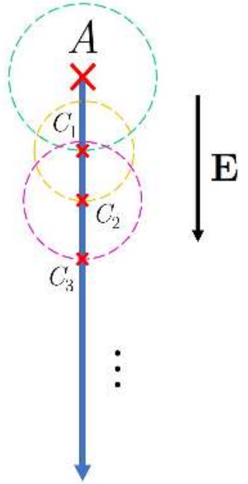


- **Objective:** To connect continuously 2 HFB vacua, A and B
- **Principle:** To create a set of HFB vacua $\{C_i\}$ such that the overlap squared between two adjacent states is equal to a fixed value $x_0 \approx 1$
- Shortest path ensured by a maximization of the overlap between $\{C_i\}$ and B

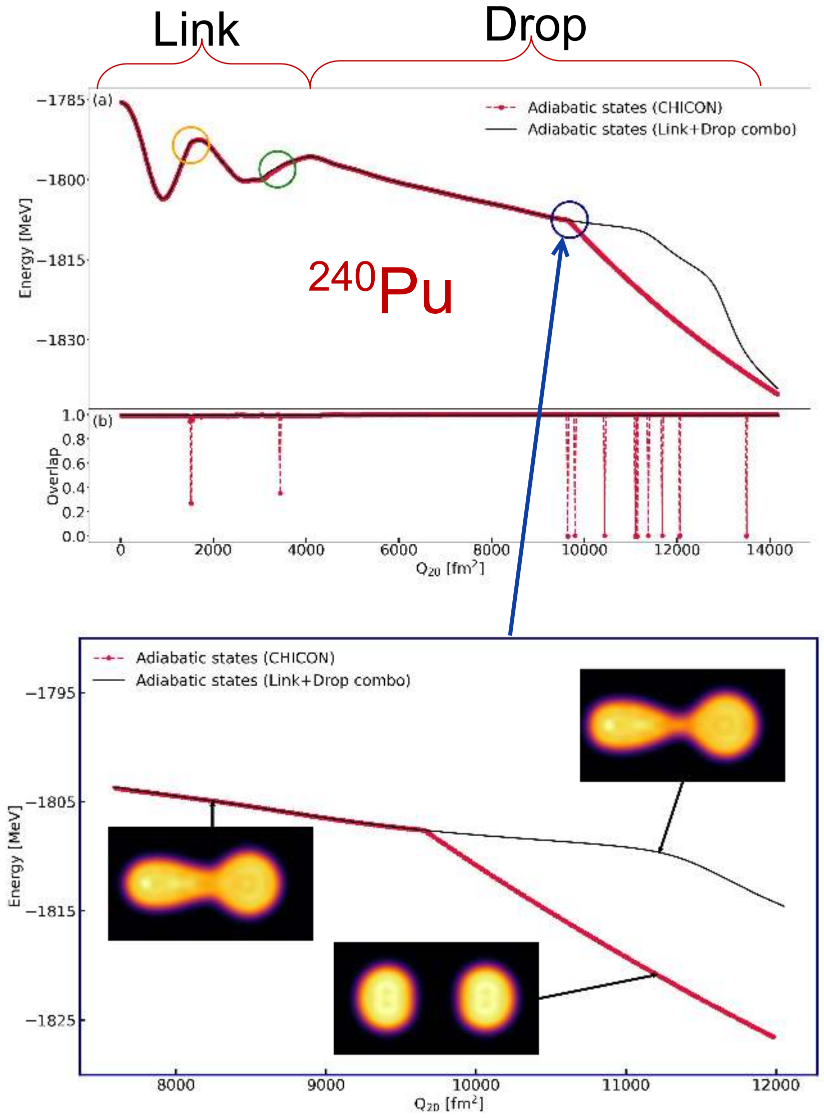
P. Carpentier, N. Pillet, D. Lacroix, N. Dubray and D. Regnier, Phys. Rev. Lett.133, 152501 (2024)

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

Drop protocol:



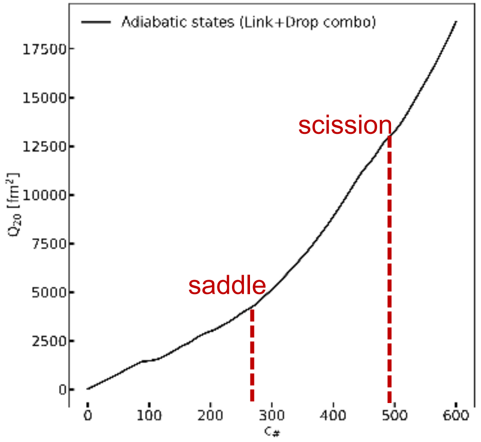
- **Objective:** To create a continuous and regular path of HFB vacua along an energy descent
- **Principle:** Starting from an HFB vacua "A", creation of HFB states {C_i} following an energy descent whose overlap squared between two adjacent states is equal to $x_0 \approx 1$

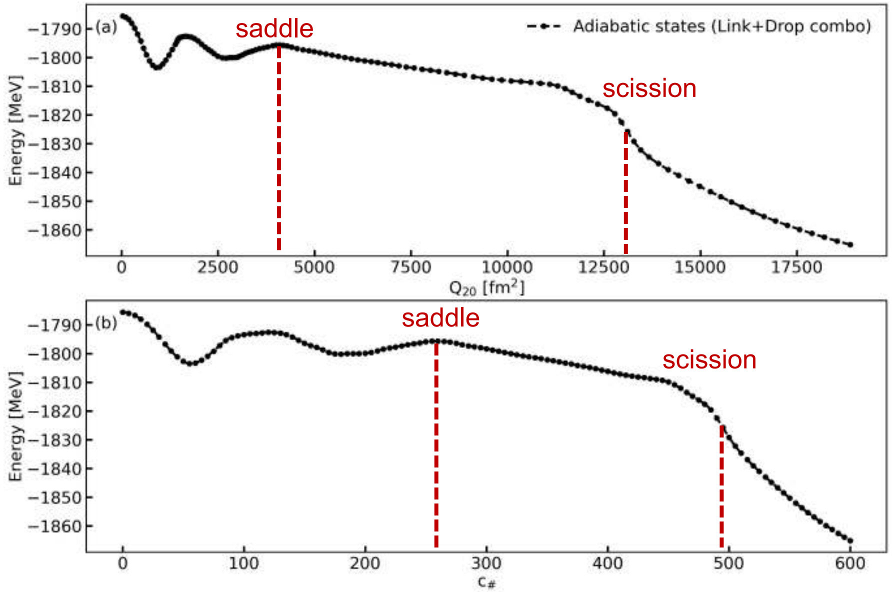


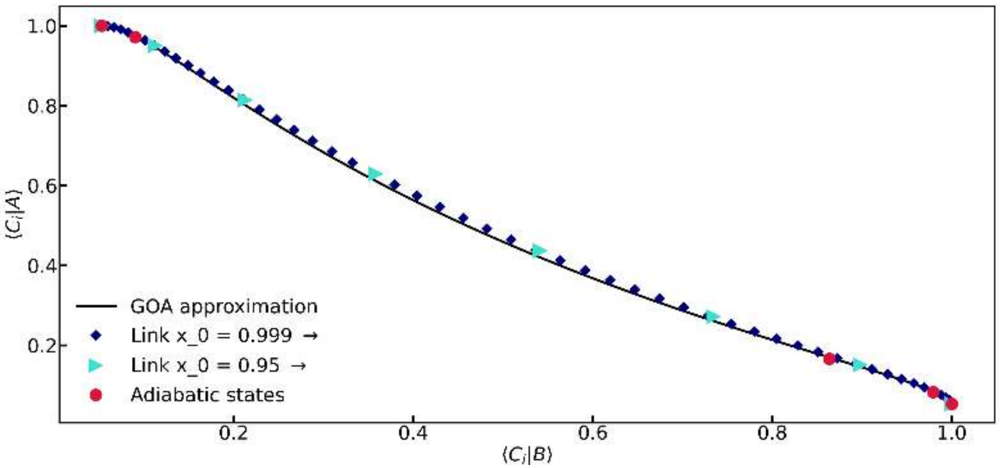
From the ground state of ^{240}Pu towards scission and beyond:

- a new continuous and regular path
- description of two fragments well-separated
- relaxation of fragments
- Connection to the Coulomb valley

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle







New collective variable $c_\#$

- Index of the states generated by the Link and Drop protocols naturally provides a new collective coordinate $c_\#$, canceling out the irregularities of the kernels:

$$\forall c_\#, c'_\#,\ \langle \Phi(c_\#)|\Phi(c_\# \pm 1)\rangle = \langle \Phi(c'_\#)|\Phi(c'_\# \pm 1)\rangle$$

- neighbors states are distant from a constant overlap x_0

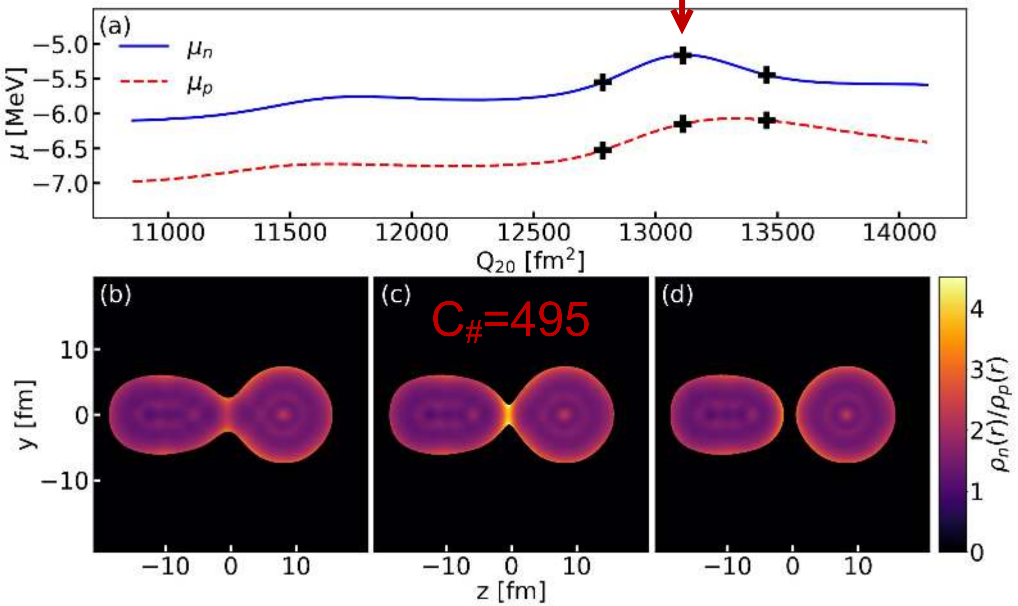
- $c_\#$ not a trivial coordinate as $Q_{20}(c_\#)$ is a non-linear function: different slope before and after saddle

- Distance between the states generated by the Link and Drop methods in line with the GOA predictions

- Collective space dimension left unchanged

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

C$_{\#}$=495



$$r_\rho(\vec{r}) = \begin{cases} \frac{\rho^{\tau_n}(\vec{r})}{\rho^{\tau_p}(\vec{r})} & \text{if } \rho(\vec{r}) > 5 \times 10^{-3} \\ 0 & \text{if } \rho(\vec{r}) \leq 5 \times 10^{-3} \end{cases}$$

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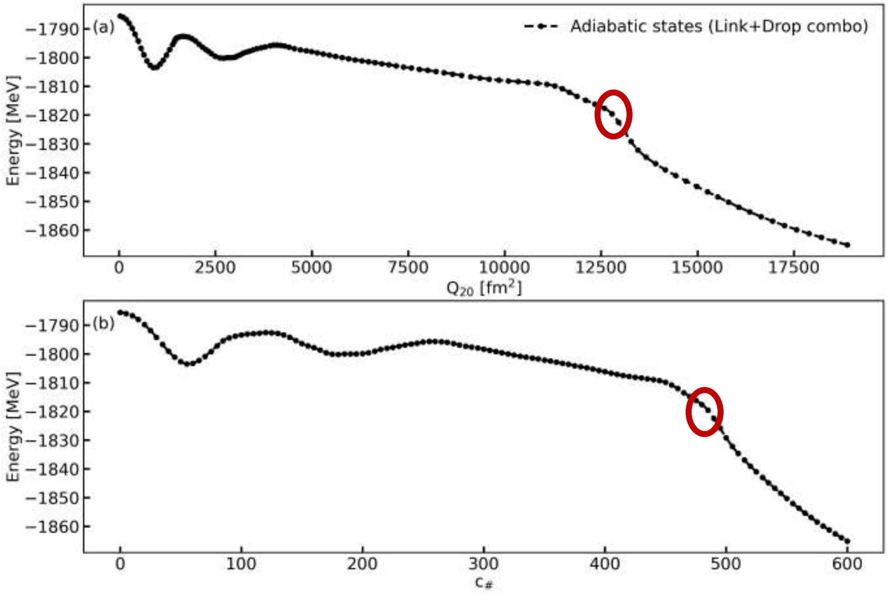
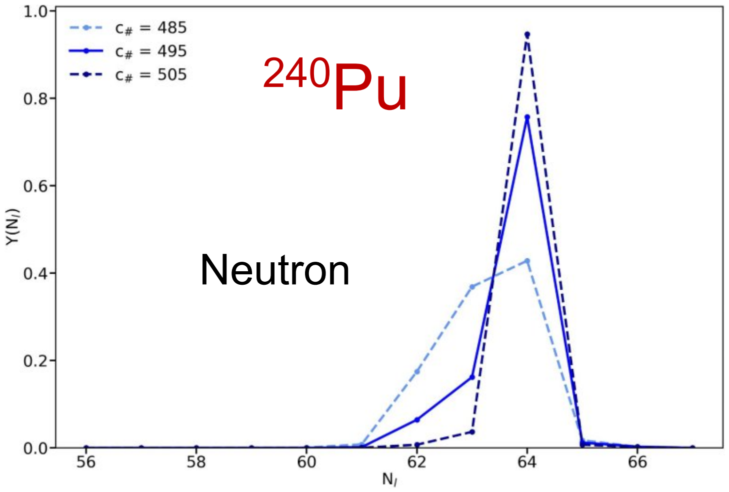
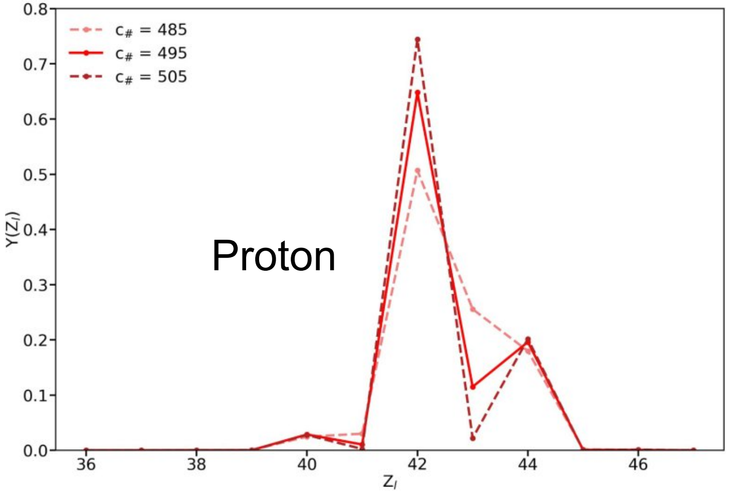
Where is scission?

- Chemical potentials peak at **$c_{\#}$ = 495** (Q_{20} ~ 13000 fm^2)
- Maximum of neutron necking at **$c_{\#}$ = 495**



II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

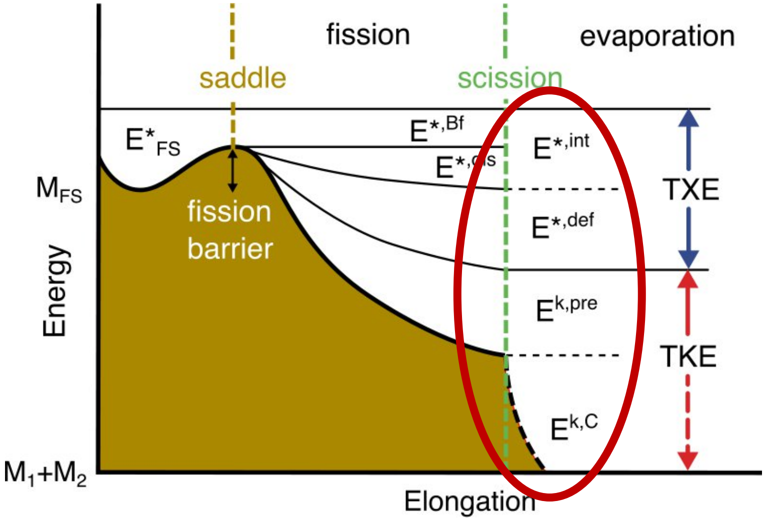




Particle distribution of the light fragment

- C. Simenel, PRL 105, 192701 (2010)
- Particle number projection
- **Neutrons**
  - Peak at N_l=64 (exp. 60)
  - Sharper distribution close to scission
- **Protons**
  - Peak at Z_l=42 (exp. 40)
  - Odd-even staggering close to scission

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle



Intrinsic excitations	**?**
Deformation energy	**26.7 MeV**
TXE	**?**

Pre-scission	**?**
Post-scission (Interaction energy)	**152.5 (178.7) MeV**
TKE	**?**

Static energy balance at scission

- W. Younes and D. Gogny, PRL 107, 132501 (2011)

$$E = E^{(l)} + E^{(r)} + E_{int}$$

- **Deformation energy**

$$E_{def} = E^{(r)}(495) - E^{(r)}(+\infty) + E^{(l)}(495) - E^{(l)}(+\infty)$$

- **Post-scission kinetic energy**

$$E_{int} = E_{int}(Nucl) + E_{int}(Coul)$$

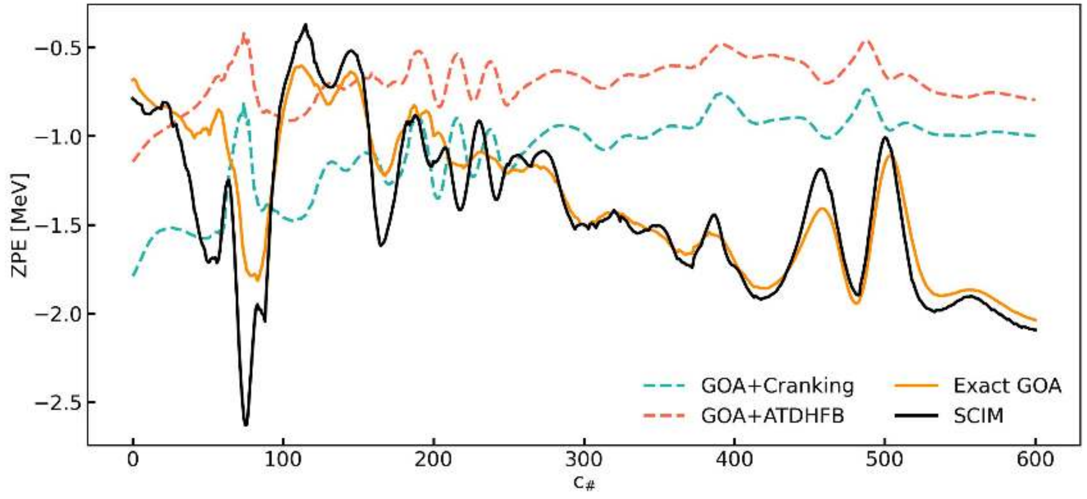
II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

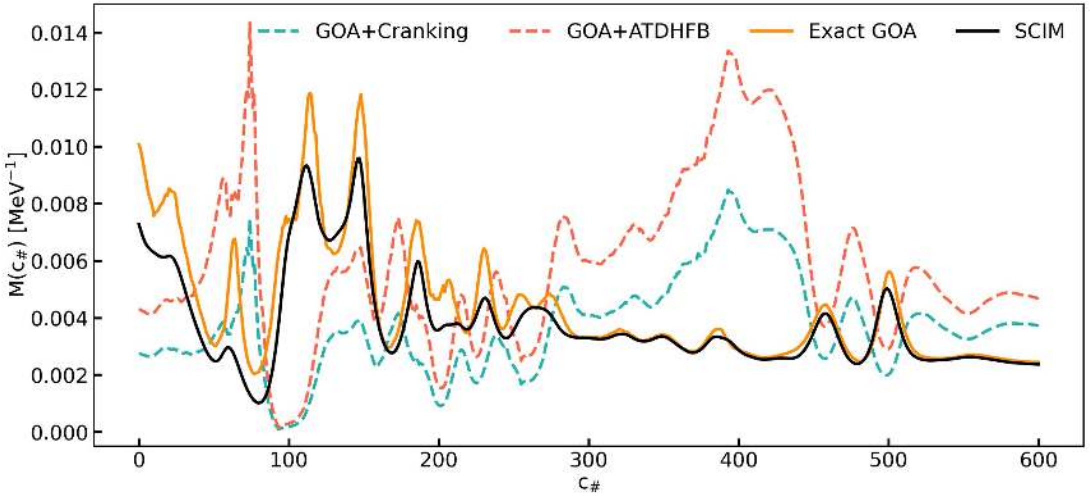
Adiabatic ZPE and collective mass of SCIM: Good agreement with exact GOA

$$\mathcal{H}_{SCIM} = V + [D\frac{\partial}{\partial q}]^{(1)} + [B\frac{\partial}{\partial q}]^{(2)}$$

$$ZPE = V - E_{HFB}$$

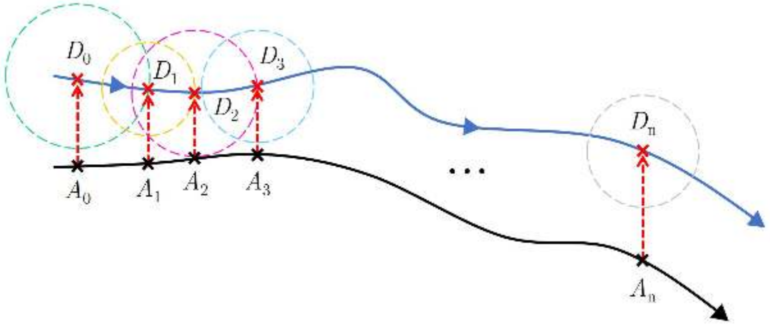
$$M = -\frac{1}{2B}$$





II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

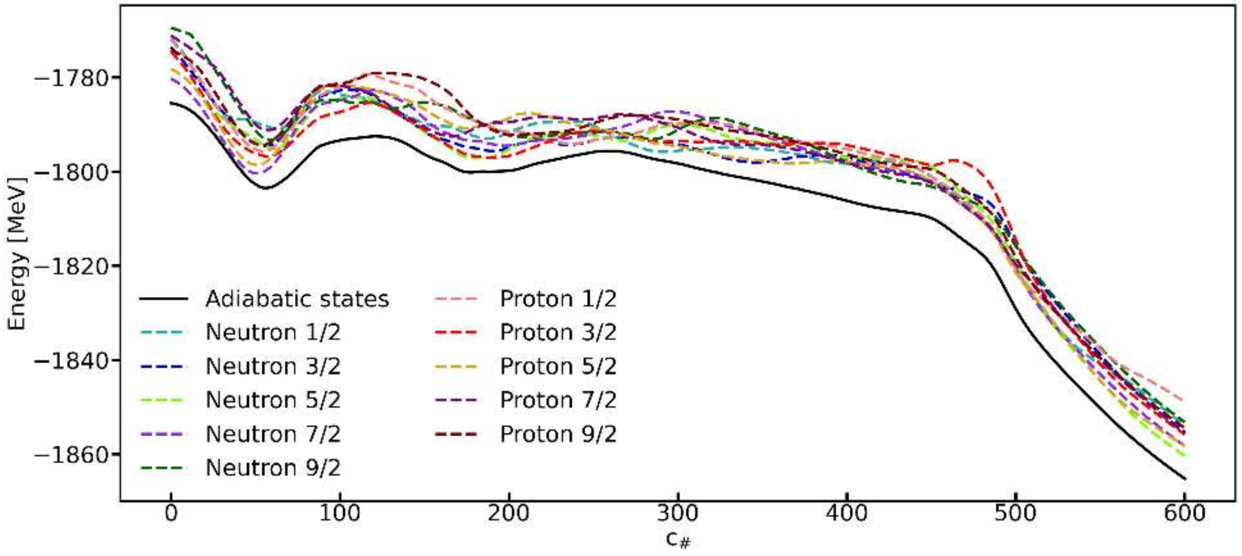
Continuous Deflation protocol:



- **Objective:** To create variational excited HFB vacua above the continuous adiabatic path

- **Principle:** For each state A_i, an excited state D_i is built imposing
  - an overlap $x_1 \approx 0$ with A_i to obtain orthogonality
  - an overlap $x_0 \approx 1$ with D_{i-1} to obtain continuity

Adiabatic and excited asymmetric paths in ^{240}Pu



P. Carpentier, N. Pillet, D. Lacroix, N. Dubray and D. Regnier,
Phys. Rev. Lett.133, 152501 (2024)

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

Content of excited HFB vacua: mixing of 2n-QP

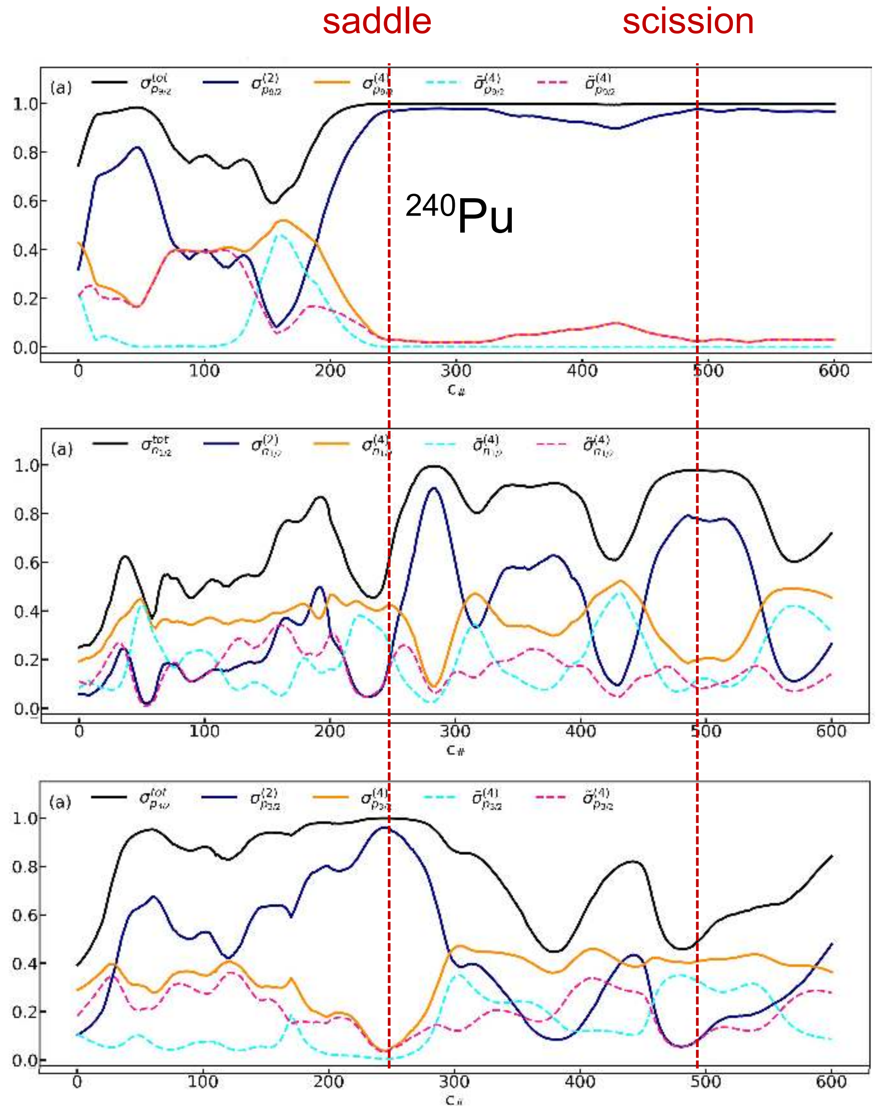
- 2-QP component :

$$\sigma^{(2)} = \sum_{ij} \left|\langle \Phi^* | \xi_i^+ \bar{\xi}_j^+ | \Phi \rangle\right|^2$$

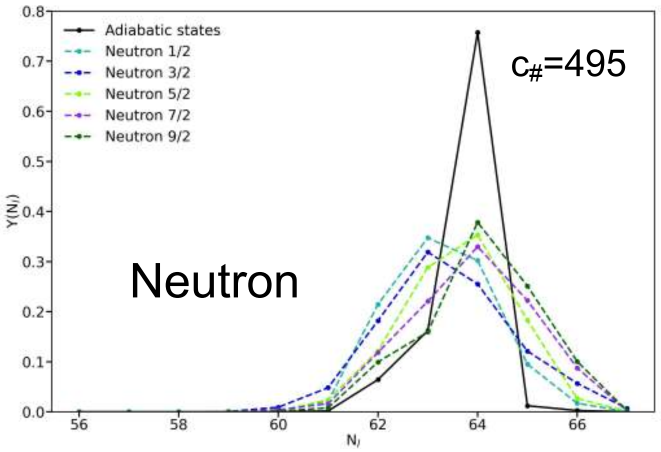
- 4-QP component:

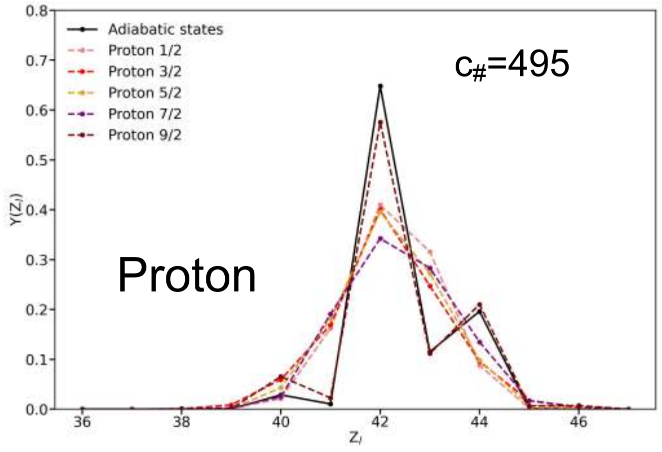
$$\sigma^{(4)} = \frac{1}{2}\sum_{\alpha\beta} \sum_{ij,\, (\Omega_{\alpha\beta},\tau_{\alpha\beta})\neq(\Omega_{ij},\tau_{ij})} \left|\langle \Phi^* | \xi_\alpha^+ \bar{\xi}_\beta^+ \xi_i^+ \bar{\xi}_j^+ | \Phi \rangle\right|^2 + \frac{1}{4}\sum_{\alpha\beta} \sum_{ij,\, (\Omega_{\alpha\beta},\tau_{\alpha\beta})=(\Omega_{ij},\tau_{ij})} \left|\langle \Phi^* | \xi_\alpha^+ \bar{\xi}_\beta^+ \xi_i^+ \bar{\xi}_j^+ | \Phi \rangle\right|^2$$

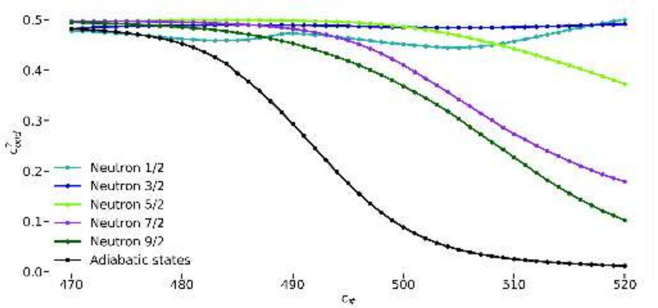
- Intrinsic excitations:
  - ❖ Configuration mixing changing with $c_{\#}$
  - ❖ Dominant 2-QP and 4-QP components but not only
  - ❖ Pair breaking mechanism included

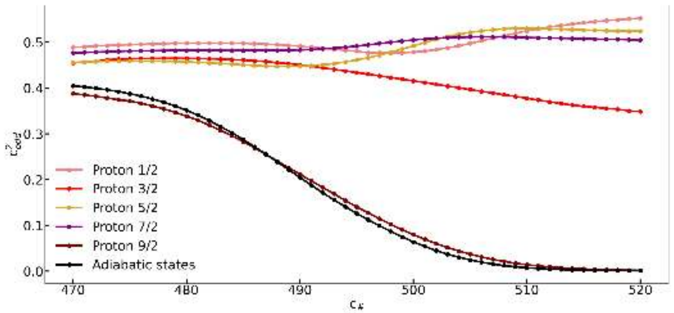


II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle









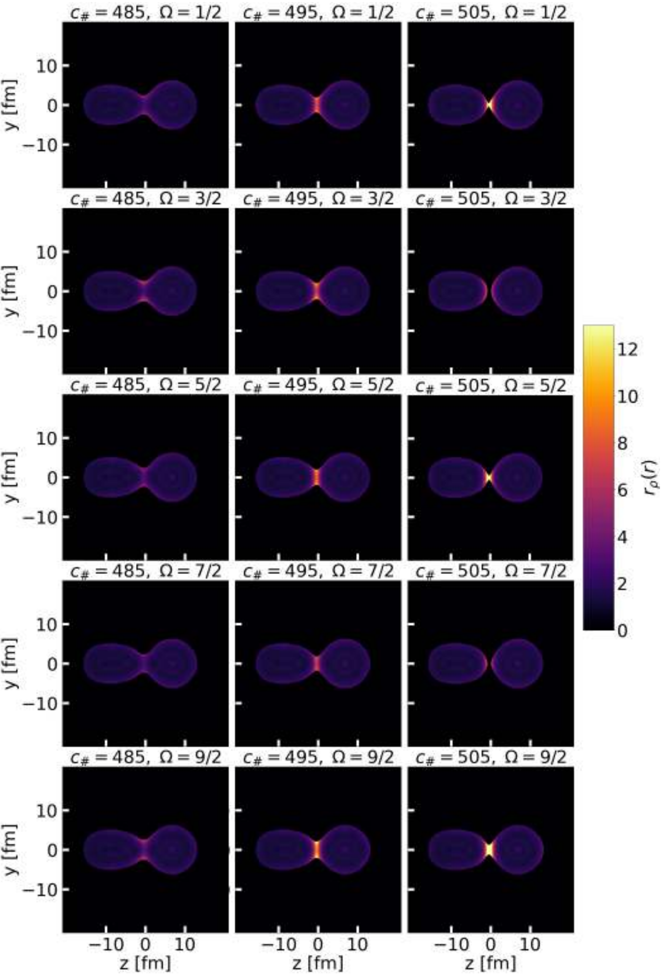
Particle distribution of the light fragment

- **Neutrons**
  - Peak at N=64 for adiabatic state (exp. N=60)
  - No odd-even staggering
  - Increase of odd components with the excited states: pair breaking
  - Enlargement of distribution with excitations

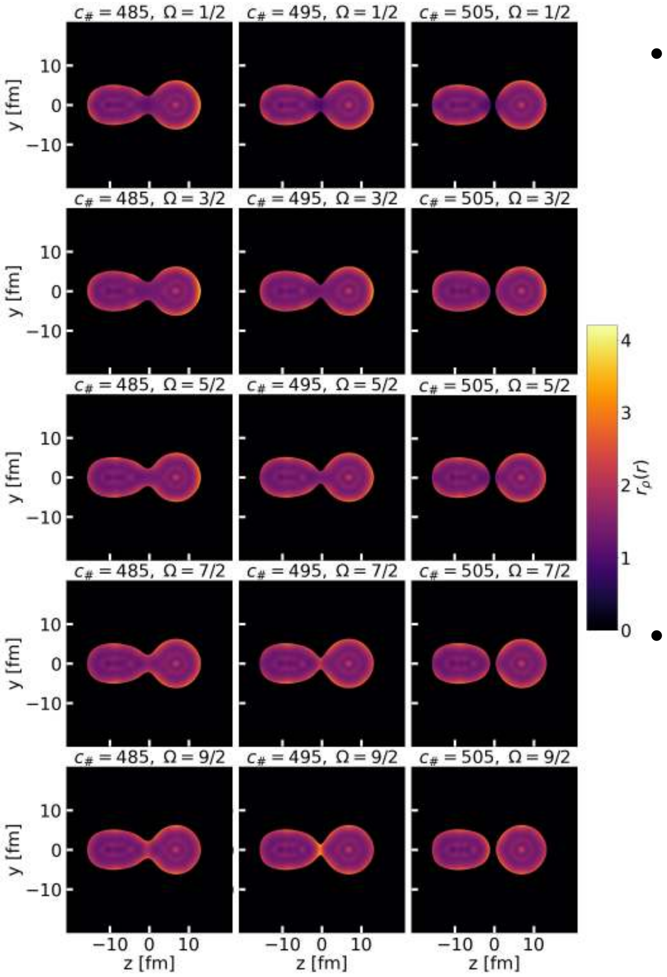
- **Protons**
  - Peak at Z=42 for adiabatic state (exp. Z=40)
  - Odd-even staggering in both adiabatic and few excited states
  - Increase of the odd components with the excited states (excepted the 9/2 state)

II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle

Neutron intrinsic excitations



Proton intrinsic excitations

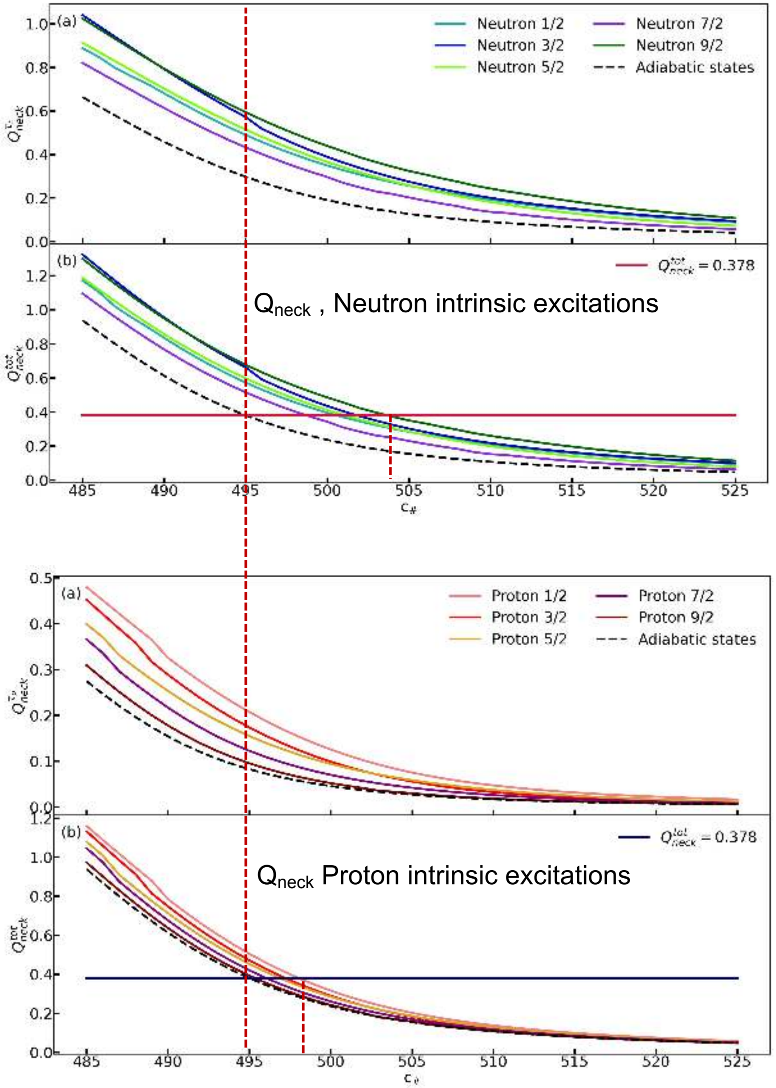


- **Neutron intrinsic excitations:**
  - Local ratio rρ higher than in the adiabatic state
  - Differences from one excited state to another
  - Differences in the separation: the greater the maximum of rρ the later the separation

	$n_{1/2}$	$n_{3/2}$	$n_{5/2}$	$n_{7/2}$	$n_{9/2}$
$c_\# = 485$	5.56	8.62	5.65	4.66	7.65
$c_\# = 495$	10.40	12.38	11.30	8.73	14.22
$c_\# = 505$	20.21	9.23	20.48	9.41	29.13

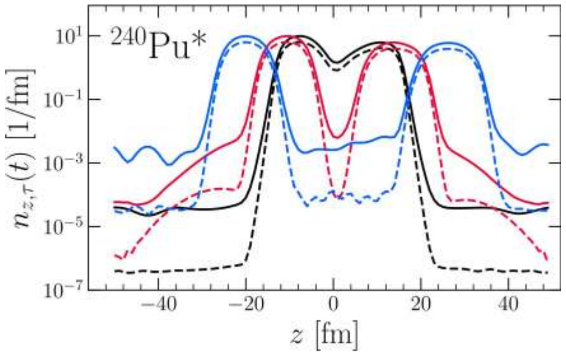
- **Proton intrinsic excitations:**
  - local ratio rρ quite similar to the adiabatic state and smaller between pre-fragment than in the adiabatic state
  - Neutron necking clearly visible only in the 9/2 state
  - More proton in the neck than in the adiabatic case

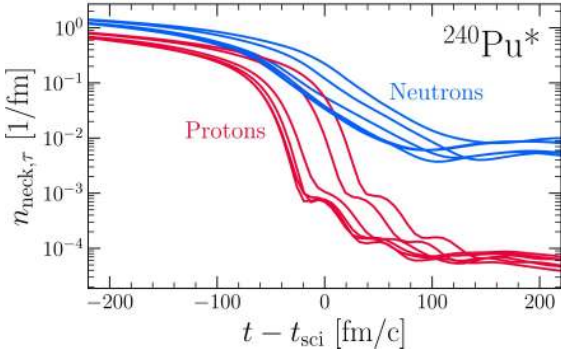
II. Building continuous adiabatic and excited HFB vacua with overlap constraints in the variational principle



- Q_{neck} (neutron)> Q_{neck} (proton)
- Neutron intrinsic excitation with a total Q_{neck} larger than the one of the proton intrinsic excitations
- Neutron intrinsic excitations hold pre-fragments together in the scission area
- Neutron as the ultimate glue
- Results in agreement with the recent study of I. Abdurrahman et al. using TDDFT approach

I.Abdurrahman et al.,
PRL 132, 242501 (2024)





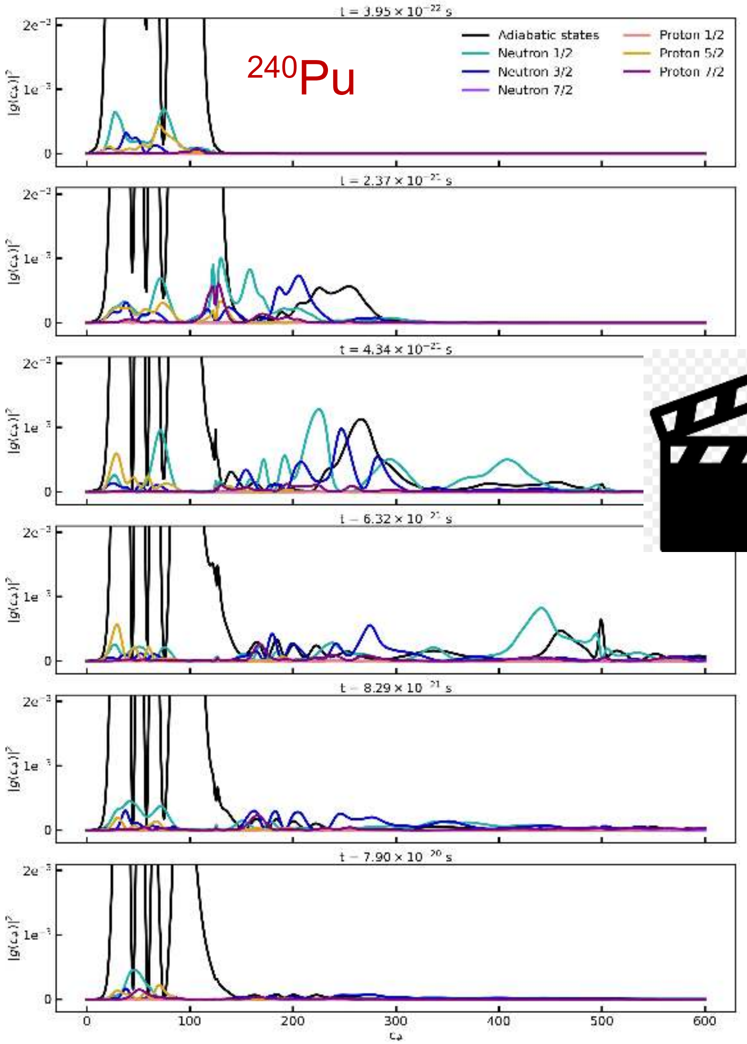
III. Application to ^{240}Pu fission along the asymmetric path including intrinsic excitations

Schrödinger equation handled numerically

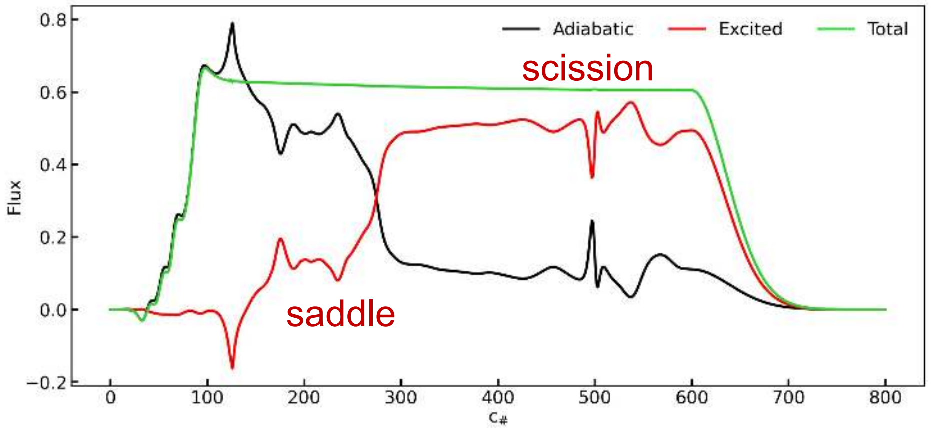
$$\mathcal{H}_{SCIM}\, g(t) = i\hbar \frac{\partial}{\partial t} g(t)$$

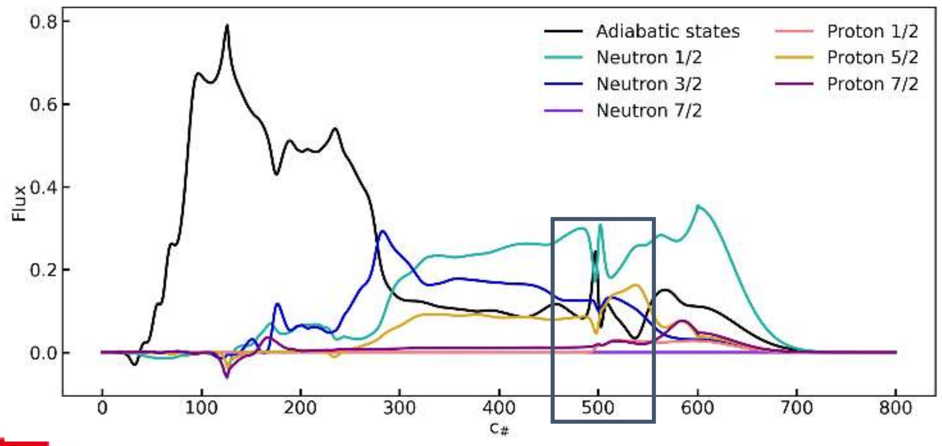
- **Crank-Nicolson** method
- Initial state built in the ground state well
- Initial average energy **E_0= first barrier top**
- Initial energy standard deviation = **0.5 MeV**
- Absorption is added after scission

$$\mathcal{H}_{SCIM}(\bar{q}) = V(\bar{q}) + [D(\bar{q})\frac{\partial}{\partial q}]^{(1)} + [B(\bar{q})\frac{\partial}{\partial q}]^{(2)}$$



III. Application to ^{240}Pu fission along the asymmetric path including intrinsic excitations





Probability fluxes extracted from a continuity equation

$$\phi(c_s, t_f) = \int_0^{t_f} \mathrm{d}t \frac{\mathrm{dP}(c_\# > c_s)}{\mathrm{d}t}(t)$$

- t_f = 7.90 10^{-20} s
- Averaged over **[445,545]**
- Neutron > Proton

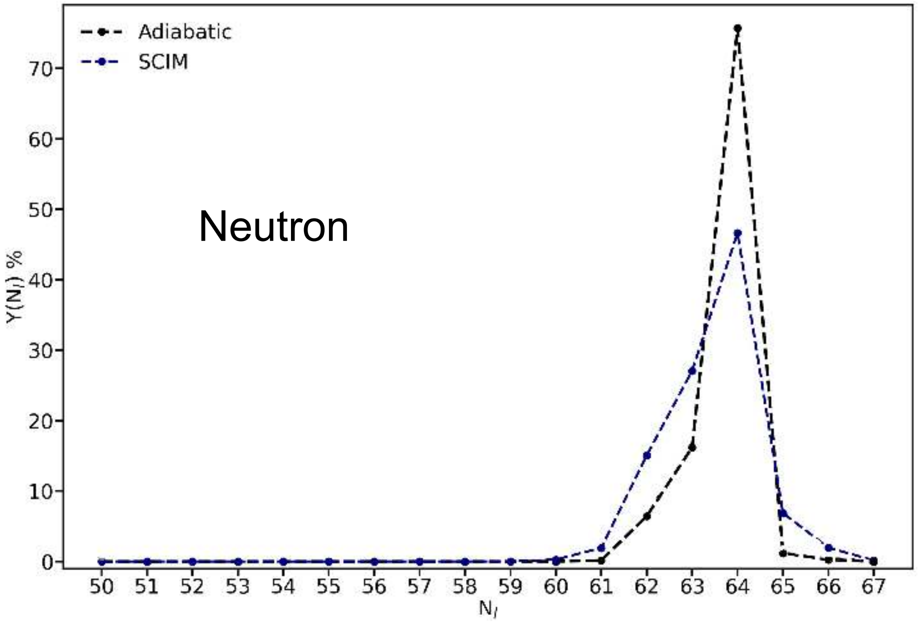
	1/2	3/2	5/2	7/2
Neutron	**41.5 %**	**20.3 %**	**-**	**0.0 %**
Proton	**2.1 %**	**-**	**17.5 %**	**2.8 %**

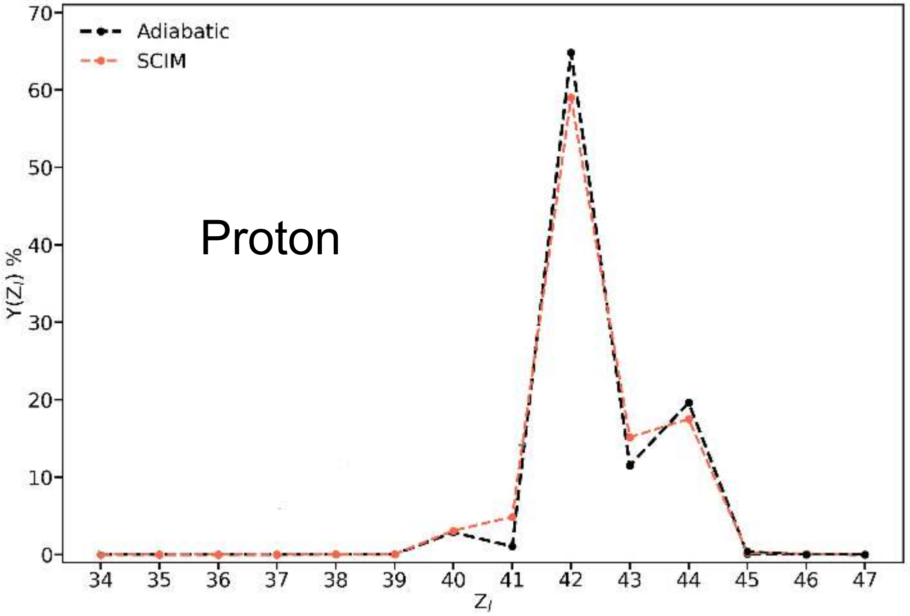
Adiabatic
15.8 %

III. Application to ^{240}Pu fission along the asymmetric path including intrinsic excitations

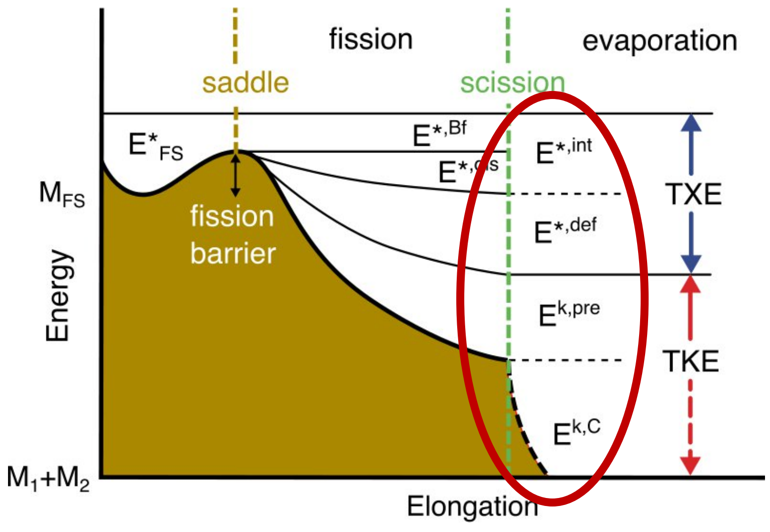
With the intrinsic excitations

- Enlargement of the distribution on the neutron side
- Smoothing of the odd-even staggering on the proton side





III. Application to ^{240}Pu fission along the asymmetric path including intrinsic excitations

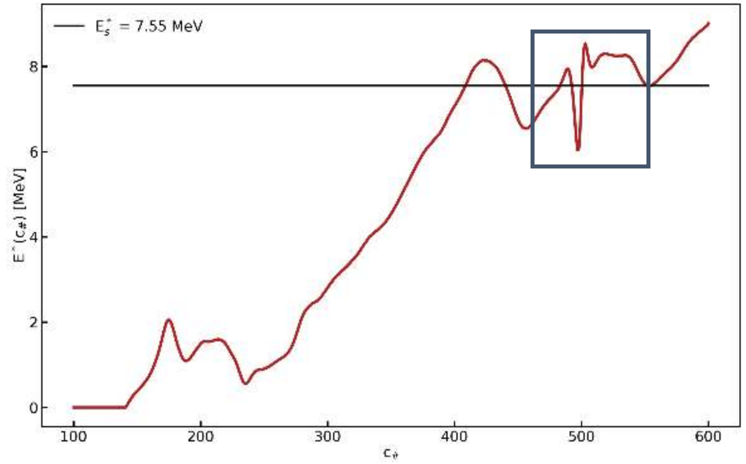


Intrinsic excitations	7.6 MeV
Deformation energy	26.7 MeV
TXE: Exp.= ~ 30 MeV	34.3 MeV

Pre-scission	25.8 MeV
Post-scission (Interaction energy)	152.5 (178.7) MeV
TKE: Exp.= ~ 181.2 MeV	178.3 (204.5) MeV

Energy balance at scission

- **Intrinsic excitation energy** $$E^* = \frac{1}{101}\sum_i \sum_{c_\#=455}^{545} \phi_i(c_\#, t_f)\Delta E_i(c_\#)$$



- **Post-scission kinetic energy**

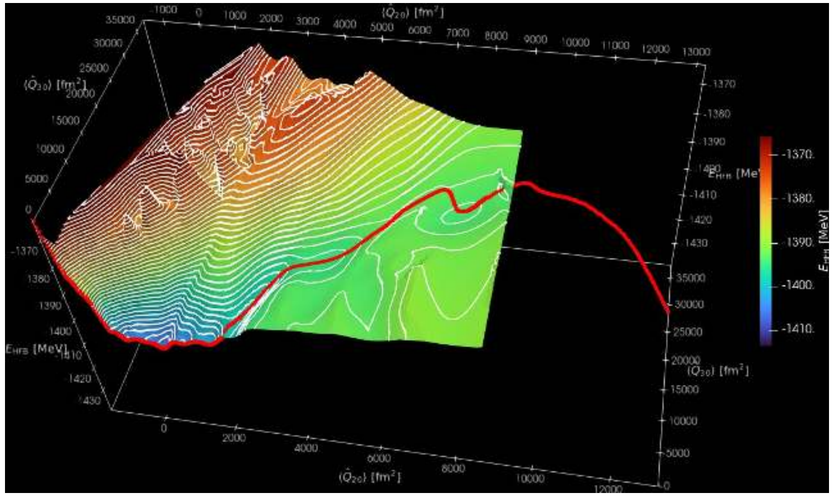
$$E_{PS} = E_0 - (E_{HFB}(495) + E^*)$$

IV. Conclusions and Perspectives

Conclusions:

- First application of SCIM on the asymmetric path of ^{240}Pu
- Need of continuity et regularity
- Creation of new protocols based on overlap constraints (Link, Drop, Continuous deflation) pour définir des états compatible with the SCIM and dynamics in general
- Importance to include intrinsic excitations within the description of fission
- ...

^{180}Hg with Link+Drop



Perpspectives:

- Improvement of energy balance by improving the fragment separation
- Improvement of energy balance by considering intrinsic excitations

- Application of 1D SCIM to other systems (in progress)
- Better understanding of the Deflation method
- Study of half-lives

- Generalization of SCIM to 2D for an exhaustive comparison to experiment (in progress)
- ...