Building Continuous Potential Energy Surfaces for Nuclear Fission Dynamics

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Table of contents

1. Introduction

Table of contents

Recall of static SCIM Formalism

Wave-function Ansatz

$$\left|\Psi_{\text{SCIM}}\right\rangle = \sum_i \int dq\, f_i(q)\, \left|\phi^i(q)\right\rangle \tag{1}$$

- Energy minimization leads to a Hill–Wheeler–type equation

Collective Schrödinger Equation (static)

$$\hat{H}_{\text{SCIM}}\, g(q) = E\, g(q) \xrightarrow{\text{dynamics}} \hat{H}_{\text{SCIM}}\, g(t) = i\hbar \frac{\partial}{\partial t} g(t)$$

Key Ingredients

Continuity and regularity .

- Overlap kernels:

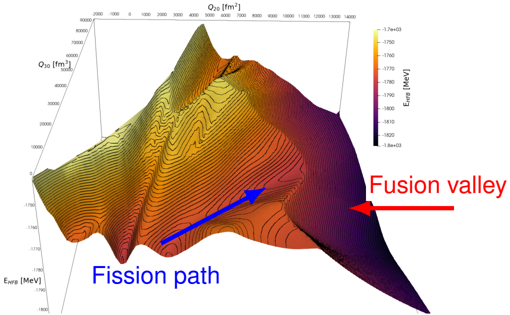
$$\mathcal{N}_{ij}(\bar{q}, s) = \left\langle \phi^i(\bar{q} - s) \middle| \phi^j(\bar{q} + s) \right\rangle \tag{2}$$

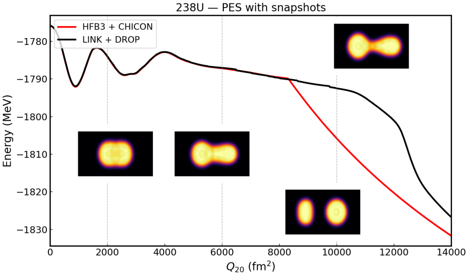
- Hamiltonian kernels:

$$\mathcal{H}_{ij}(\bar{q}, s) = \left\langle \phi^i(\bar{q} - s) \middle| \hat{H} \middle| \phi^j(\bar{q} + s) \right\rangle \tag{3}$$

Motivation

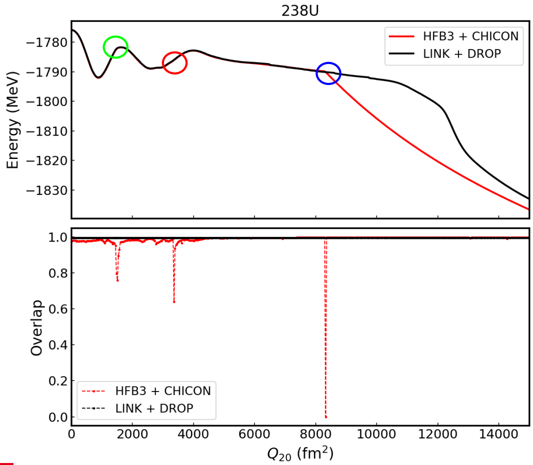
^{238}U





- HFB3 solver, 2 ct. HO basis, D1S Gogny interaction [1]
- Limited number of collective coordinates → state discontinuities

Origin of the Problem



- Potential energy surfaces (PES) are continuous in energy.
- However, discontinuities appear in the **overlap**.

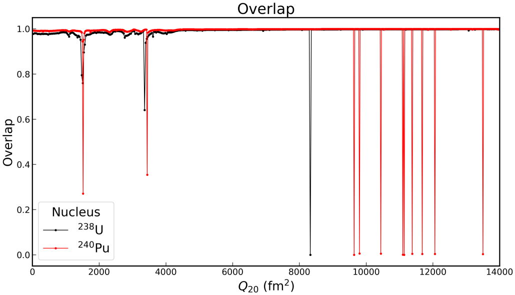
$$\mathcal{N}_{ij}(\bar{q}, s) = \left\langle \phi^i(\bar{q} - s) \middle| \phi^j(\bar{q} + s) \right\rangle \qquad (4)$$

Physical Origin of Discontinuities

- Truncation number of collective coordinates allows relaxation in unconstrained directions.
- Some discontinuities are associated with symmetry breaking.
- Example: parity breaking linked to the Q_3 operator.

At large deformations:

- The system may fall into the *fusion valley*.



Overlap Constraints for Continuous PES

Goal: Develop a method to obtain **continuous potential energy surfaces (PES)**. Make the procedure **independent of the PES topology** to enable **systematic studies of nuclei**.
Key idea:

- Constrain the **overlap with a reference state**, ensuring PES continuity [2].
- Inspired by quantum chemistry techniques used to obtain excited states via orthogonality constraints [3].

$$H_c = H + \underbrace{\sum_\tau \lambda_\tau \sum_i c_i^{\tau\dagger} c_i^\tau}_{\text{Particle number}} + \underbrace{\sum_\alpha \lambda_\alpha \sum_{ij} Q_{ij}^{(\alpha,0)} c_i^\dagger c_j}_{\text{Multipole moment}} + \underbrace{\sum_\beta \gamma_\beta \left|\phi_\beta\right\rangle \left\langle\phi_\beta\right|}_{\textit{Overlap}}$$

Methods based on this concept:

- Link method – adiabatic
- Drop method – adiabatic
- Deflation and Continuous deflation – excited states

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Thouless Theorem and Gradient Method

- **Goal:** Minimize the Hamiltonian with constraints under Bogoliubov transformations.
- **Thouless theorem:** Any Bogoliubov-transformed vacuum can be written as

$$|\phi(Z)\rangle = e^{\hat{Z}}|\phi_0\rangle$$

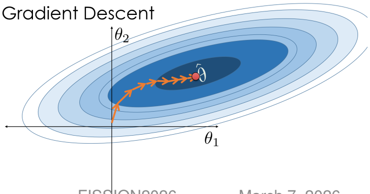
where

$$\hat{Z} = \sum_{k<k'} Z_{kk'}\, \xi_k^\dagger \xi_{k'}^\dagger$$

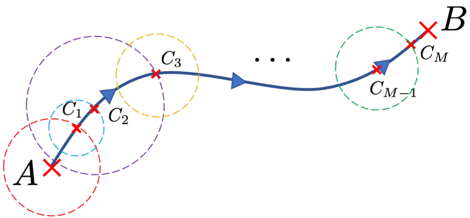
Gradient descent: Choose Z along the energy gradient to minimize the constrained Hamiltonian:

$$Z_{kk'} = -\eta \frac{\partial}{\partial Z_{kk'}} \frac{\langle \phi(Z)|H_c|\phi(Z)\rangle}{\langle \phi(Z)|\phi(Z)\rangle}\Bigg|_{Z=0}$$

$$= -\eta \left(H^{20}_{kk'} + \sum_\alpha \lambda_\alpha C^{20}_\alpha \right)$$



Link Method



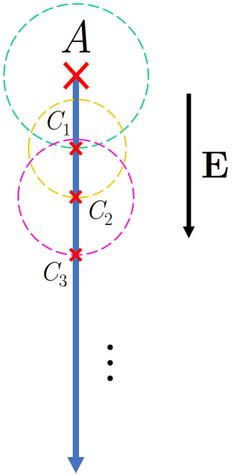
- Connects two different HFB states $|A\rangle$ and $|B\rangle$ through a set of intermediate HFB states $|C_i\rangle$ with contiguous overlaps fixed to x_0.

Practical steps:

1. Start from the original PES points.
2. Select anchor points using an overlap threshold.
3. Apply Link between $|A\rangle$ and $|B\rangle$: find $|C_i\rangle$ solutions with maximum overlap with B and fixed overlap x_0 with $|C_{i-1}\rangle$.
4. Keep the last Link solution as the new starting point $|A\rangle$.

$$\frac{\partial}{\partial Z_{kk'}} \gamma_\beta \left\| \langle \phi(Z) | \phi_\beta \rangle \right\|^2 \Big|_{Z=0} = 2 \sum_\beta \langle \phi_\beta | \xi^\dagger \bar{\xi}^\dagger | \phi \rangle \langle \phi_\beta | \phi \rangle$$

Drop Method



- Start from the last iteration of the Link method.
- Drop the state along the energy gradient while imposing continuity with the previous solution.
- We implemented both Link and Drop method in an automatic way to make a systematic study for different nuclei.

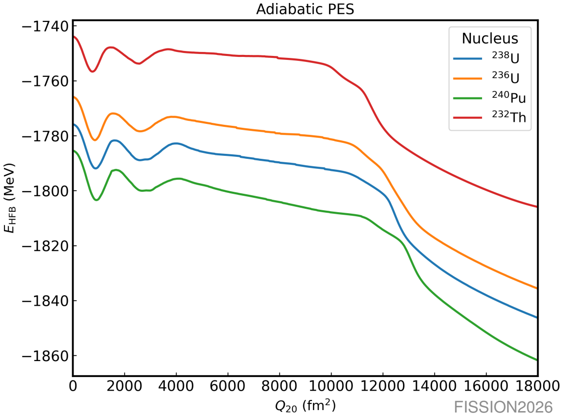
$$Z_{kk'} = -\eta \left(H^{20}_{kk'} + \sum_{\alpha} \lambda_\alpha C^{20}_\alpha \right)$$

2. Application to Pu, U and Th isotopes

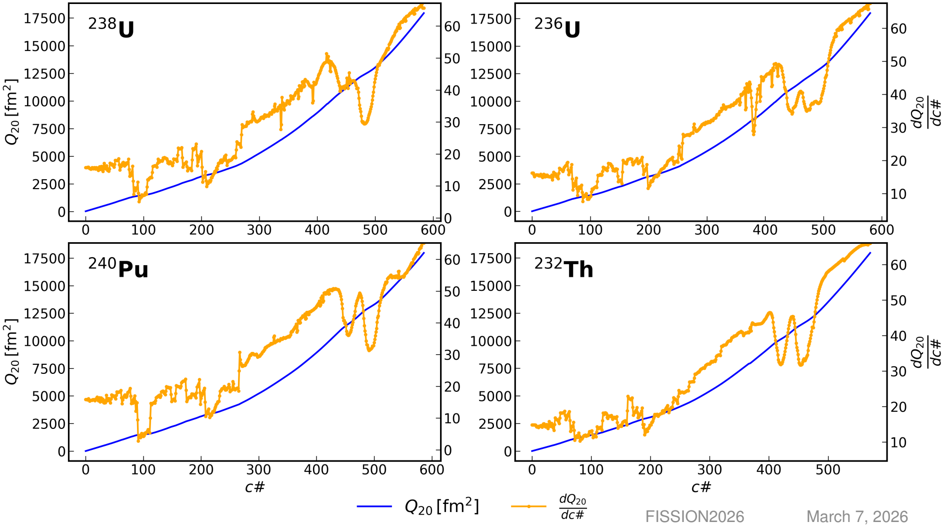
Table of contents

Continuous 1D PES Generation: Link and Drop Methods

- Applied **Link** and **Drop** methods to different nuclei.
- Obtained continuous PES for each nucleus, extending beyond scission.



New Collective Coordinate: Q_{20} vs c#



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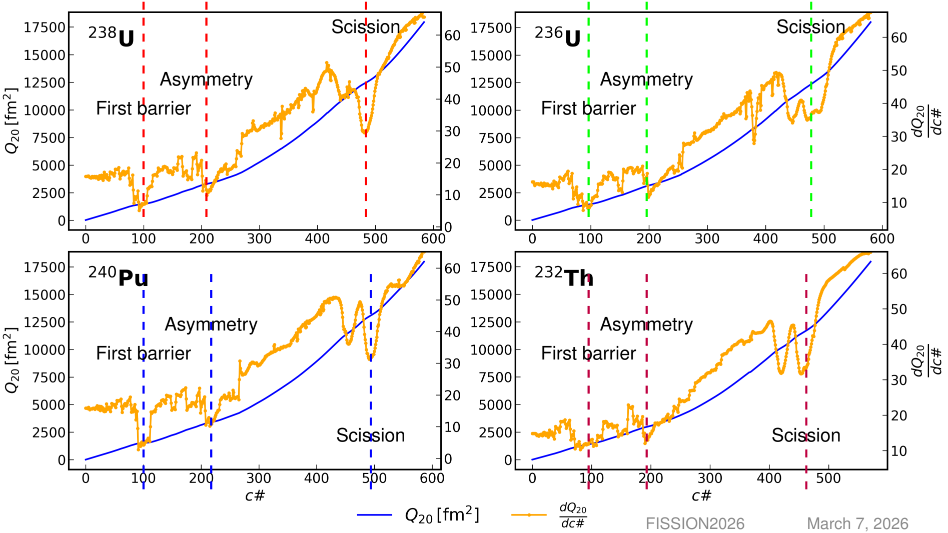
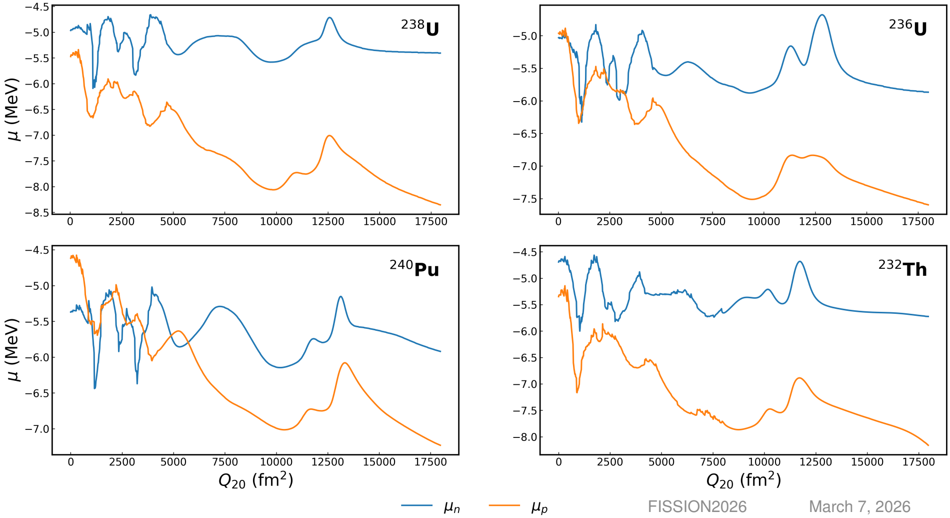


Where does scission take place?



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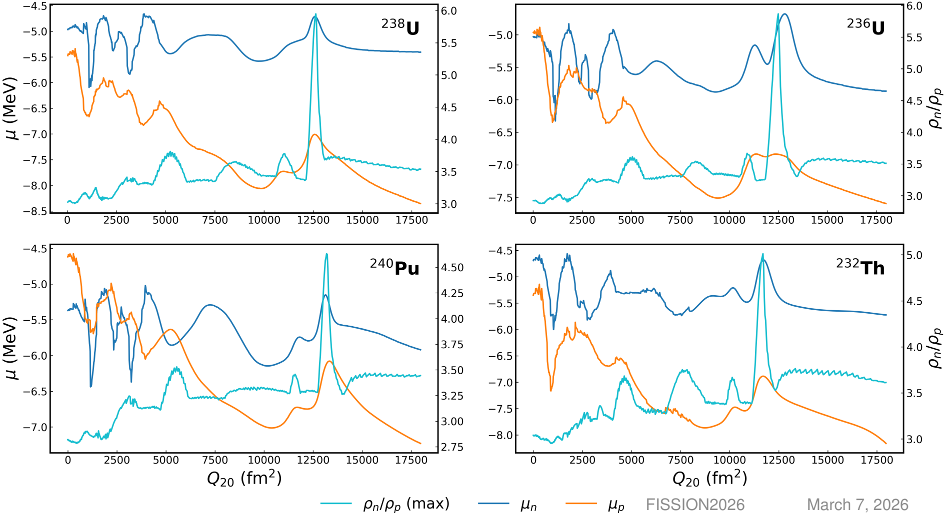
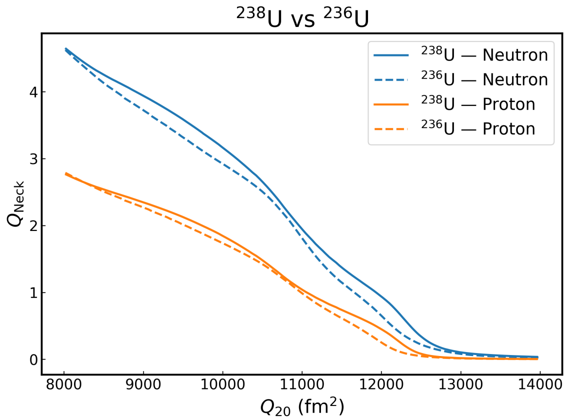
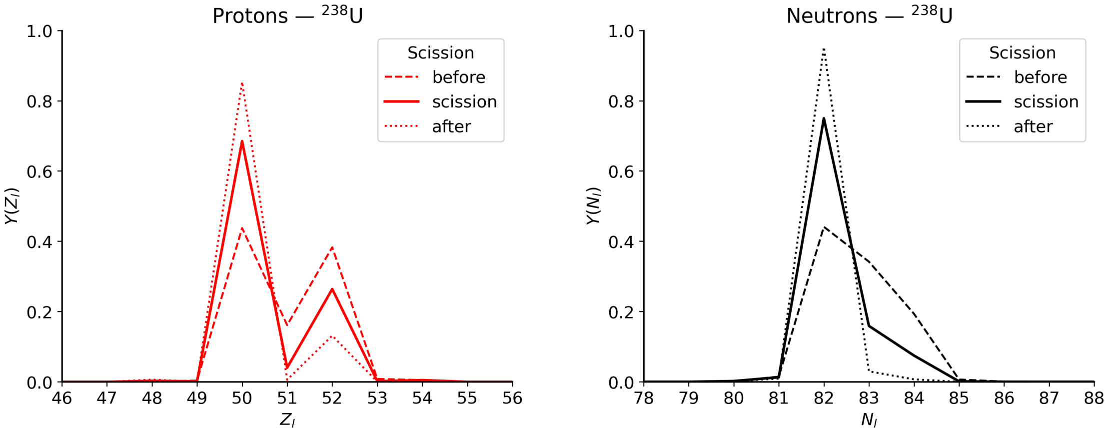


Q-Neck Evolution - ^{236}U and ^{238}U

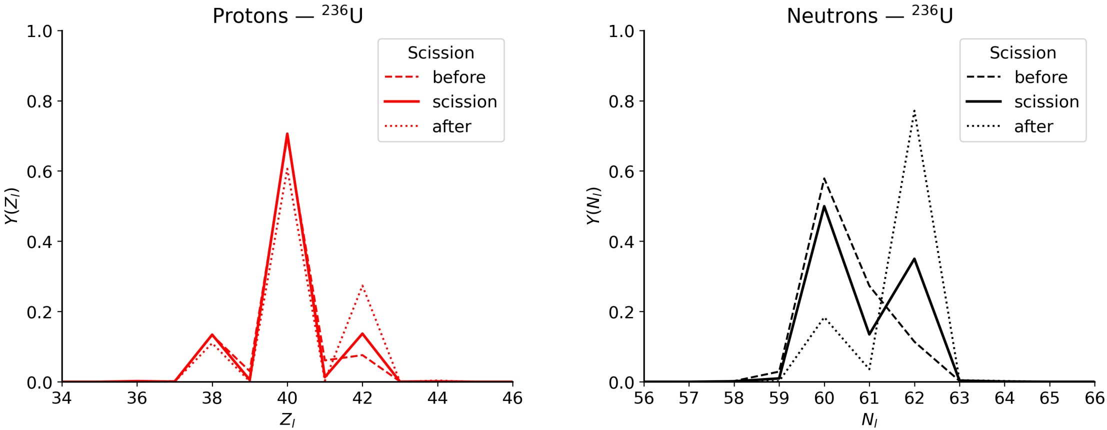


- **Protons leave the neck more rapidly**, whereas neutrons stay longer
- The **chemical potential** reflects localization of quasiparticles.
- For ^{236}U and ^{238}U, **localization** behaves differenly due to the interplay between Coulomb and nuclear forces.

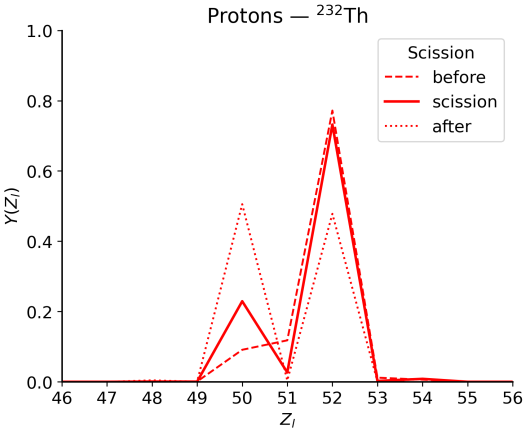
Fragmentation at Scission

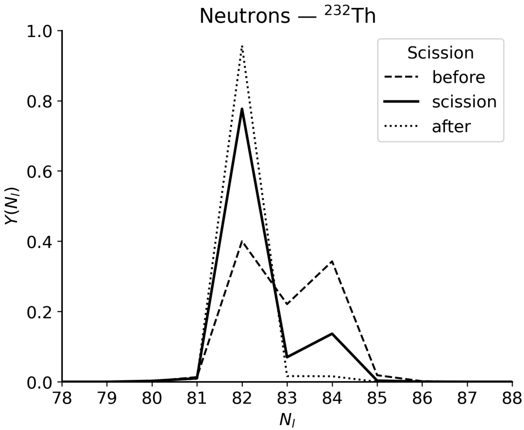


Fragmentation at Scission



Fragmentation at Scission



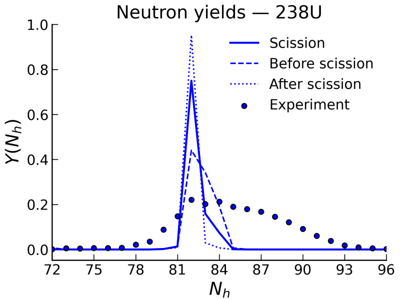


3. Conclusions and Perspectives

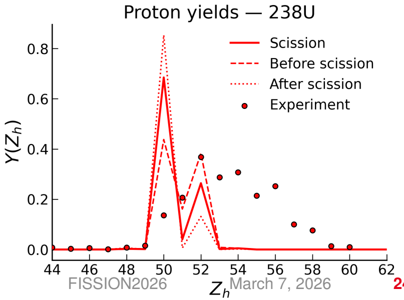
Table of contents

Conclusions

- **Built** continuous 1D PES for several nuclei (^{240}Pu, ^{236}U, ^{238}U, ^{232}Th).
- **Analyzed** the origin and behavior of discontinuities and improved the methodology for a systematic study.
- **Studied** the evolution of chemical potentials and neck properties, showing proton and neutron localization and flow along the fission path.
- **Determined** scission configurations and extracted static fragment properties.
- Compared proton and neutron yield distributions with experimental data [4].



2D



Perspectives

Short-term goals

- Systematic study including more nuclei *(neutron deficient actinides, different isospin asymmetries and isotopic chains)*.
- Inclusion of excitations and dynamics via SCIM: *evolution from ground state through scission*.

Long-term goals

- **Extension to 2D collective coordinates**
  - Necessary for meaningful comparison with experimental fragment distributions
  - Currently under development
- Integration with experimental observables (e.g., charge and mass yields, fragment energy and angular momentum) *for validation*.
- Explore systematic trends in scission and necking behavior across isotopic chains.

References

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Thank you!

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A. Appendix

Table of contents

Appendix 1

Bla

Additional Constraints and Limitations

Historically, additional constraints such as Q_{Neck} have been introduced to avoid fusion configurations.

Advantages:

- Helps avoiding fusion configuration of the system for larger deformations

Difficulties:

- Non-trivial evolution with respect to other multipole operators.
- Numerical instabilities near scission
- Difficult recovery of full fragment separation

Consequences

These discontinuities:

- Prevent construction of a physically reasonable fission path
- Difficult description of the nucleus from ground state to scission

In this work:

- We propose a method to overcome these issues based on overlap constraints
- Make this methods independent of the PES and study nuclei in a systematic way
- Present some preliminary results.

Gradient Method with Constraints

- **Goal:** Minimize Hamiltonian with constraints under Bogoliubov transformations.
- **Variables:** U and V matrices defining the HFB state.
- **Densities:**

$$\rho = VV^\dagger, \quad \kappa = VU^T$$

- **One-body Hermitian operator:**

$$F = \sum_{ll'} F_{ll'} c_l^\dagger c_{l'} + \frac{1}{2} \sum_{ll'} \left(g_{ll'} c_l^\dagger c_{l'}^\dagger + \text{h.c.} \right)$$

- **Quasiparticle representation:**

$$F = F^{00} + \xi^\dagger F^{11} \xi + \frac{1}{2} \left(\xi^\dagger F^{20} \xi^\dagger + \text{h.c.} \right)$$

- **Gradient:**

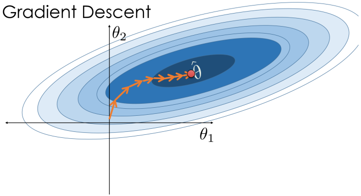
$$F^{20} = U^\dagger F V^* - V^\dagger F^T U^* + U^\dagger G U^* - V^\dagger G^* V^*$$

Bogoliubov Transformation

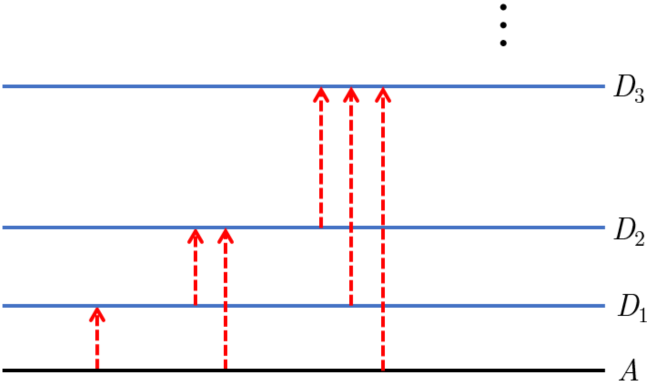
- **Transformed Bogoliubov matrices:**

$$U' = (U + VZ^*)(1 - ZZ^*)^{-1/2},$$
$$V' = (V + UZ^*)(1 - ZZ^*)^{-1/2}$$

- **Unitary condition:** The factor $(1 - ZZ^*)^{-1/2}$ ensures that U', V' are a canonical transformation.
- **Constraints:** Lagrange multipliers are corrected by solving a linear system to enforce the constraints.



Deflation and Continuous Deflation (soon)

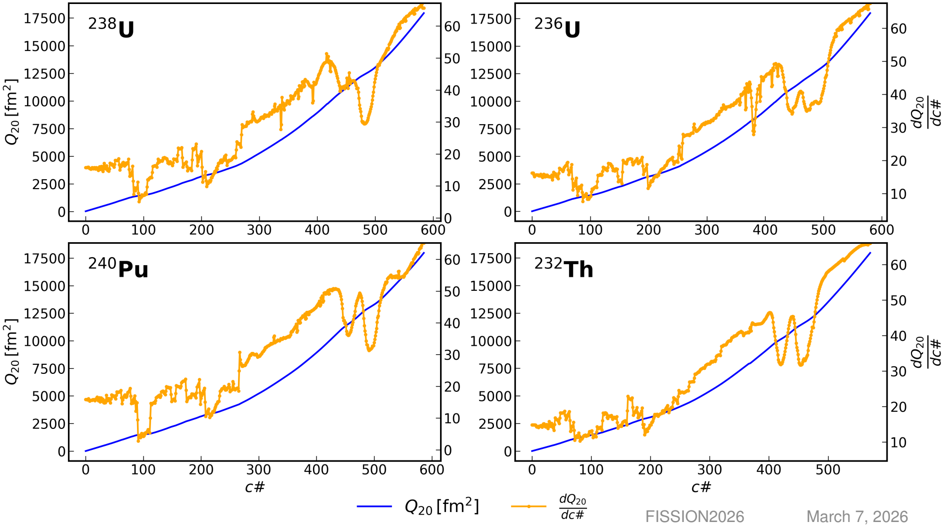


- Designed to obtain **excited states** by enforcing orthogonality with previously obtained states.
- Continuous deflation allows following a specific excited-state PES.

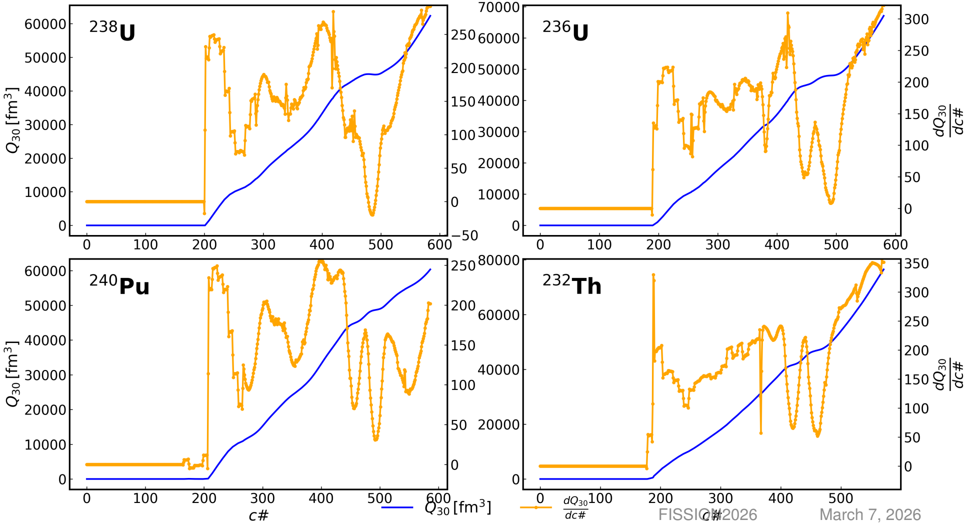
Appendix 2

Bli

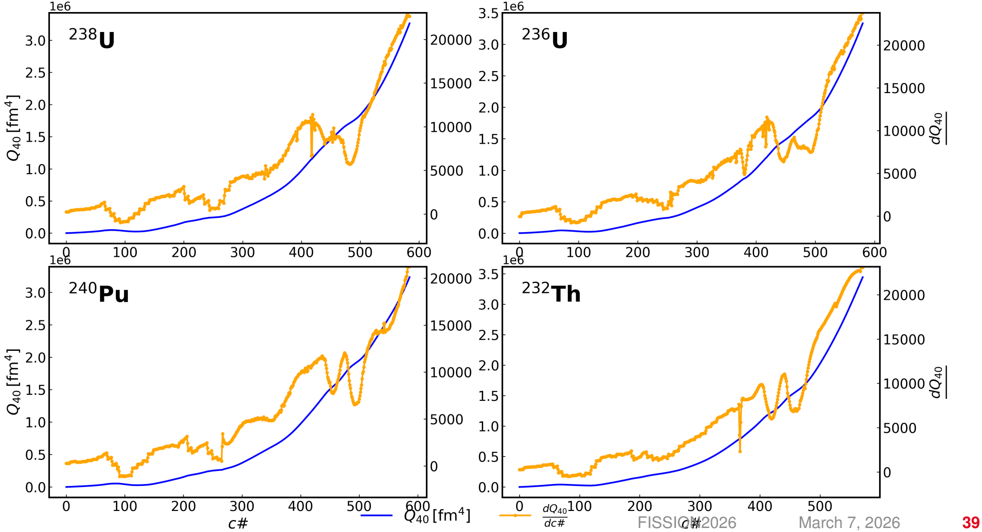
New Collective Coordinate: q_2 vs c#



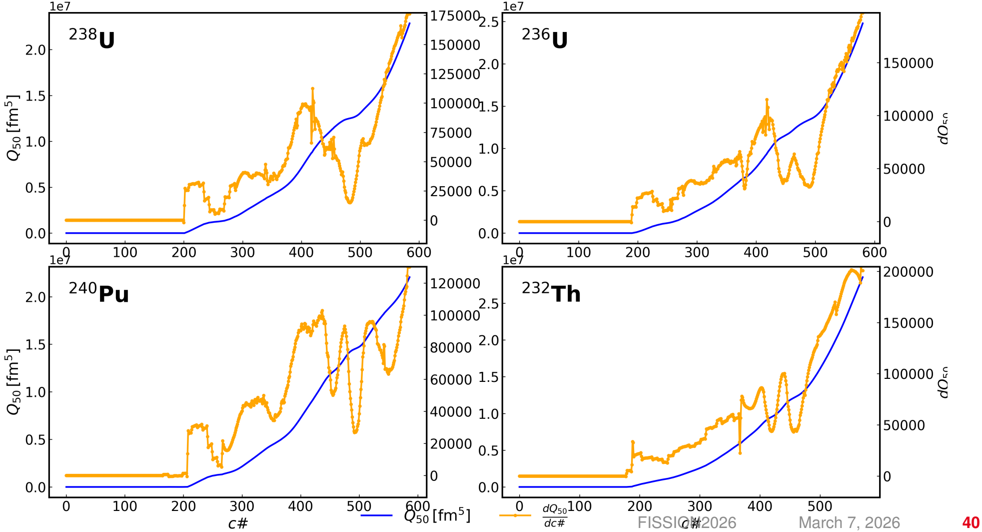
New Collective Coordinate: q_3 vs c#



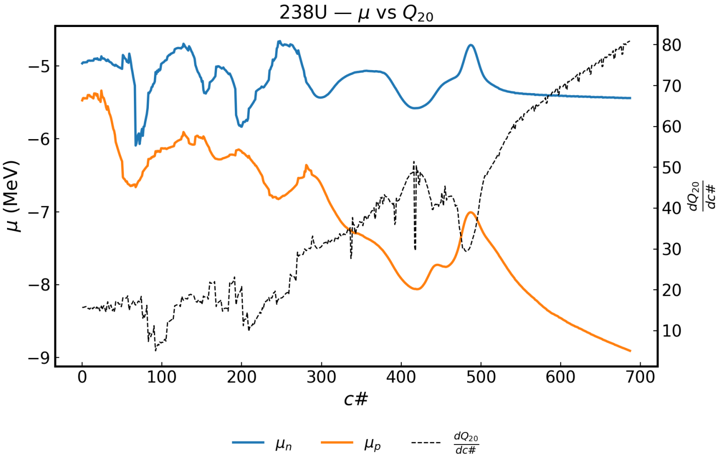
New Collective Coordinate: q_4 vs c#



New Collective Coordinate: q_5 vs c#



Chemical Potential + c# evolution



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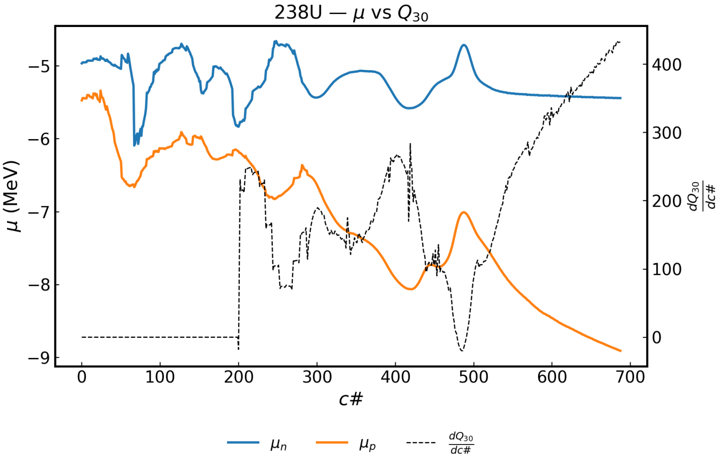

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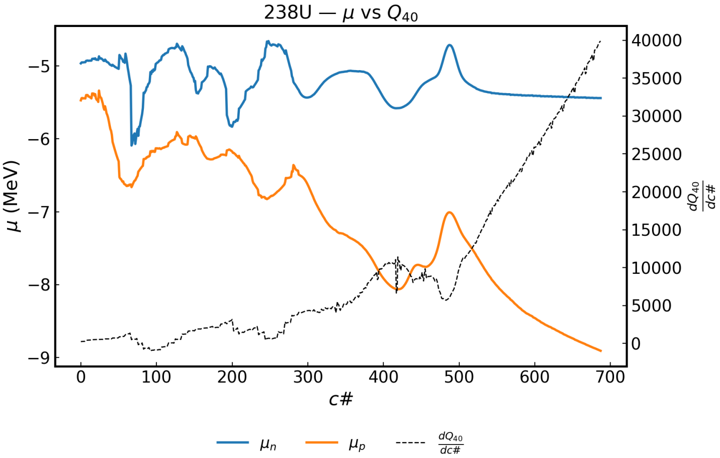

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