Spontaneous Fission from Self-Consistent Calculations

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“Nuclei in the laboratory and in stars”

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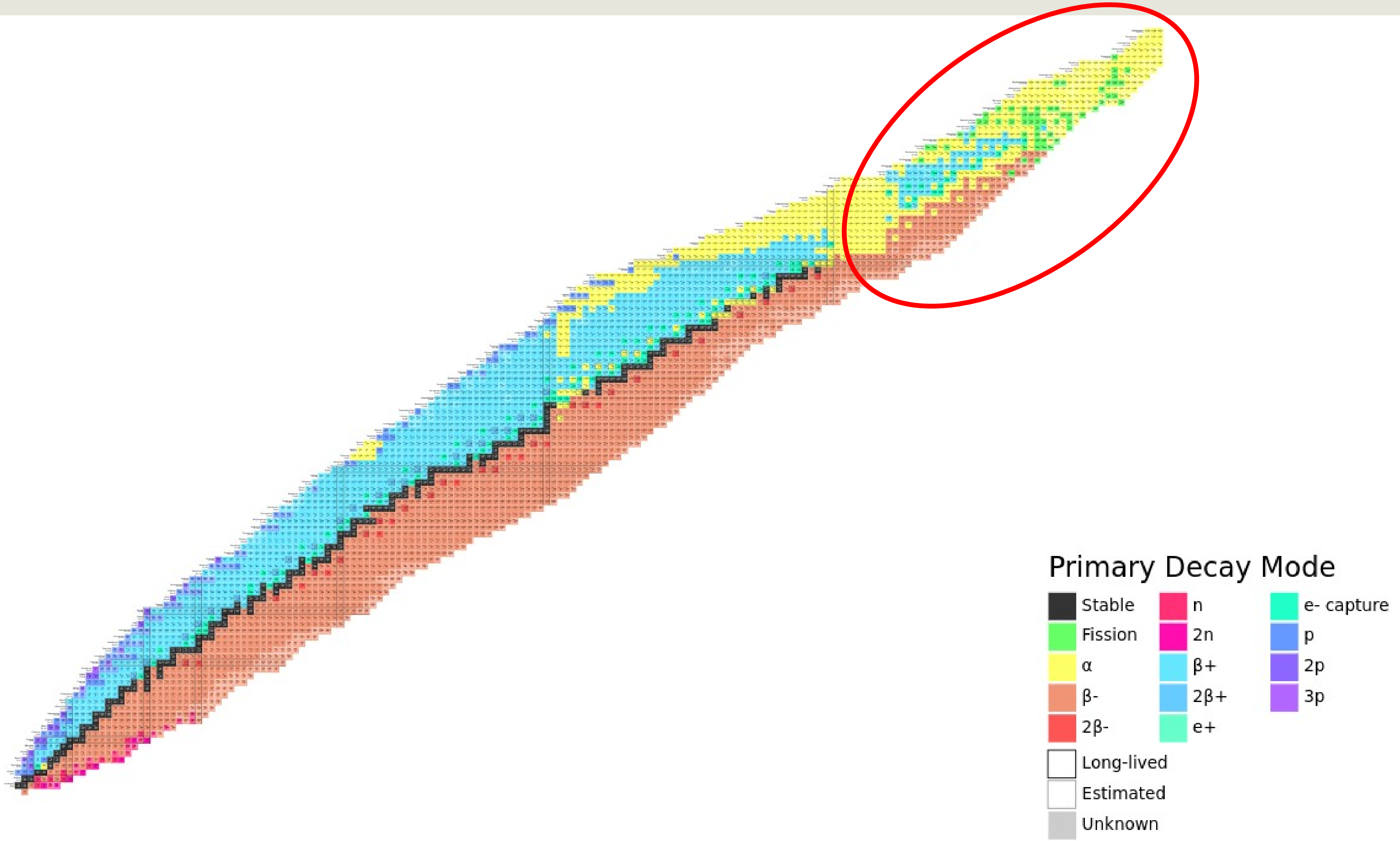
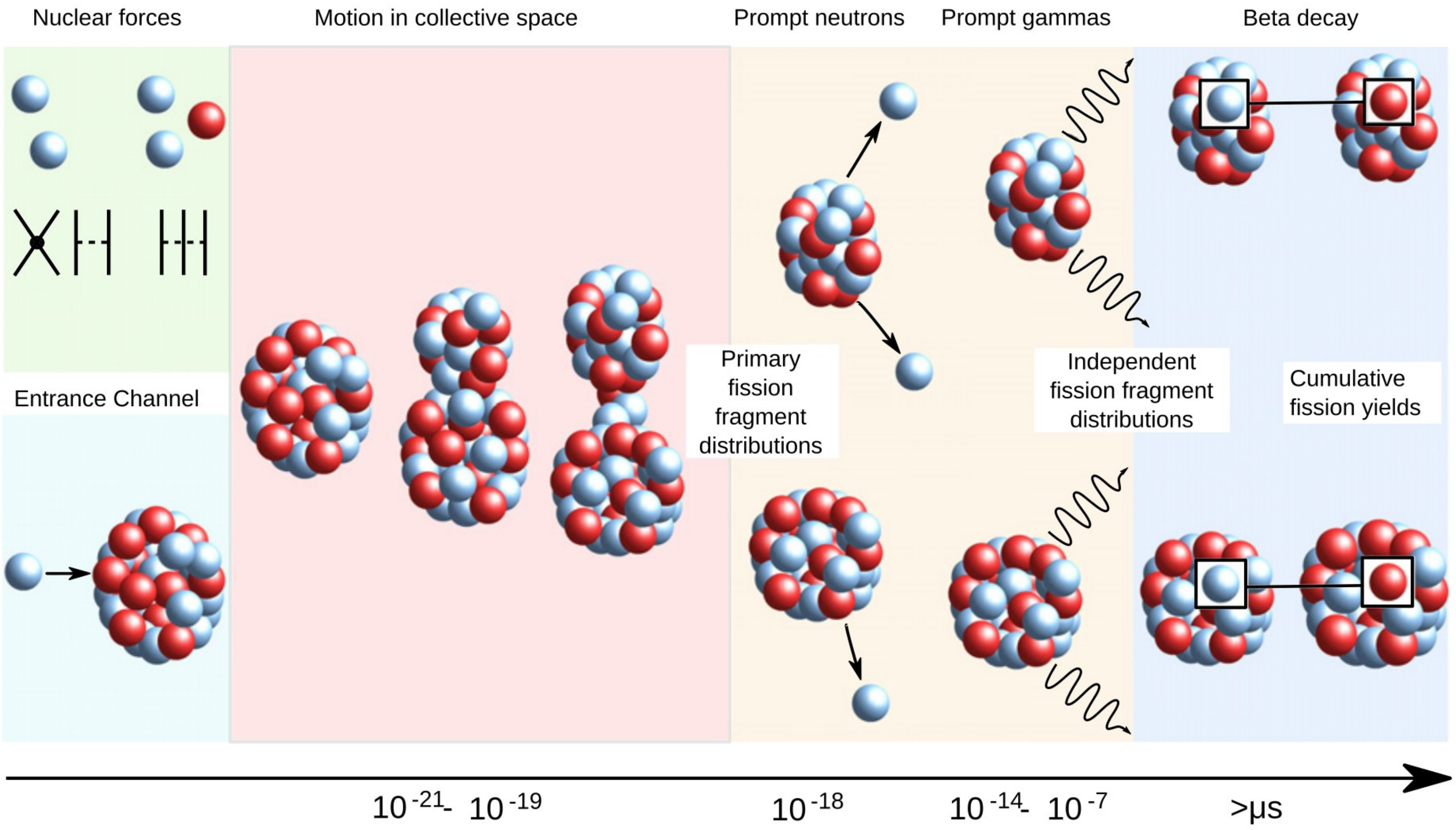
The Landscape



From Colorful
Nuclear Chart

Time Scales



Bender et. al. , J. Phys. G: Nucl. Part. Phys. 47 (2020) 113002

Stationary Density Functional Theory Approach to Fission

- We use static, constrained HFB density functional theory (DFT).
- The nuclear shape is parameterized by multipole moments in the intrinsic frame.

$$\hat{Q}_{\mu\nu} = \hat{r}^{\mu} Y_{\mu\nu}(\theta, \phi)$$

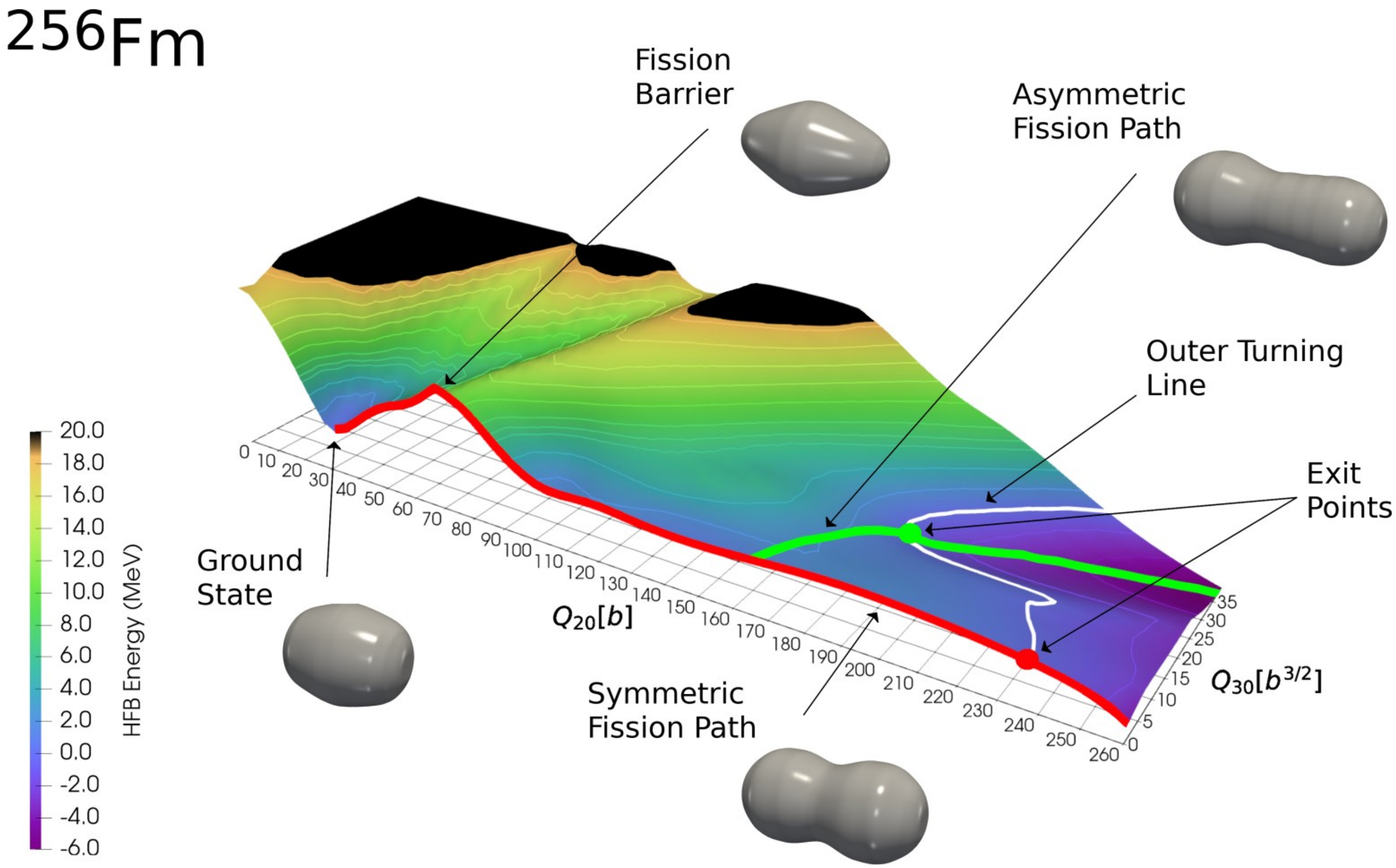
- We calculate the energy of the nucleus by constraining the energy at given multipole moments.

$$E[\rho, \kappa, \kappa^*, Q_{\mu\nu}] = \langle \psi | H - \sum_{\mu\nu} \lambda_{\mu\nu} \hat{Q}_{\mu\nu} | \psi \rangle$$

- Potential energy surfaces (PES) in this work were computed using HFBTHOv3.00 [1] and HFBaxial [2]

[1] Perez, R. Navarro et. al *Computer Physics Communications* 220 (2017): 363-375.
[2] Robledo, Luis M., et. al. *Physical Review C* 84, no. 1 (2011): 014312.

Summary of DFT approach to Fission



Flynn et. al.
Phys. Rev. C
105, 054302

Fission as a Finite Dimensional Tunneling Problem

- **<u>Main Problem</u>: Find the most probable fission pathways in the collective space**
- We can view spontaneous fission as a tunneling problem in a collective space.
- Given a PES, we can solve the collective Schrodinger equation with multidimensional WKB theory:

$$\psi(\vec{q}) \sim e^{-S_0[L]} \quad \text{as} \quad \hbar \longrightarrow 0$$

$$S_0[L] \geq \min \ \frac{1}{\hbar}\int_{s_{\text{in}}}^{s_{\text{out}}} \sqrt{2\mathcal{M}_{\text{eff}}(s)\Big(V_{\text{eff}}(s) - \Delta E\Big)}ds \qquad \begin{aligned} \vec{q}(s_{\text{in}}) &= \vec{q}_{\text{in}} \\ \vec{q}(s_{\text{out}}) &= \vec{q}_{\text{out}} \end{aligned}$$

Effective Inertia ($\mathcal{M}_{\text{eff}}$)

Effective potential (V_{eff})

Zero-point correction to GS (ΔE)

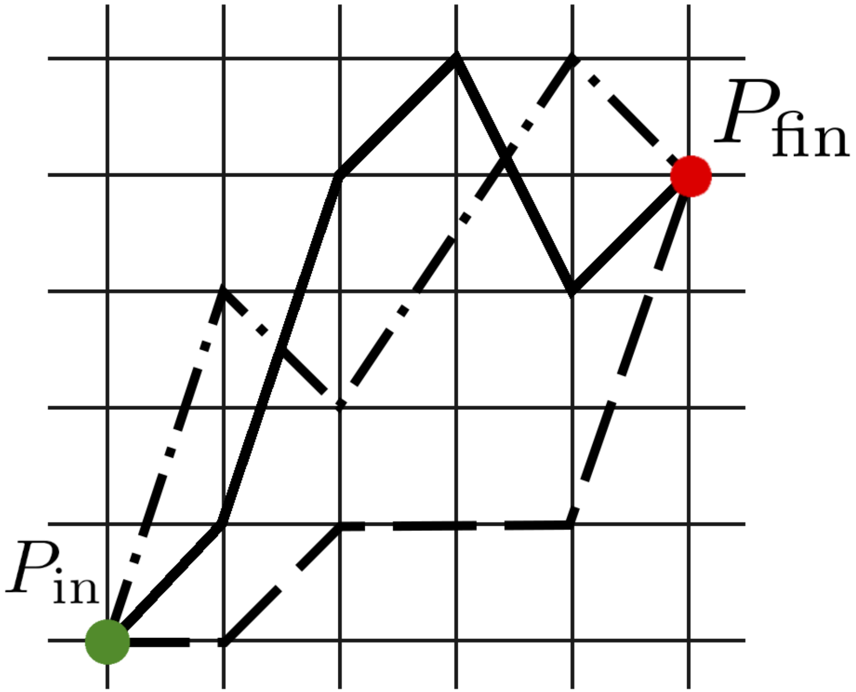
A. Schmid, Ann. Phys. (NY) 170, 333–369 (1986).

Previous Approaches

- **<u>Main Problem</u>: Find the most probable fission pathways in the collective space**
- Previous approaches have used grid-based methods to find least action paths (LAPs)
- Baran et. al. (1981) [1] used Dynamic Programming Method (DPM) to search for the LAP for fixed initial and final positions.

<u>Drawbacks of grid-based methods</u>

- Path is restricted to a grid.
- Can only find global minimum.
- Doesn't scale well with respect to dimension and grid size.



Flynn et. al.
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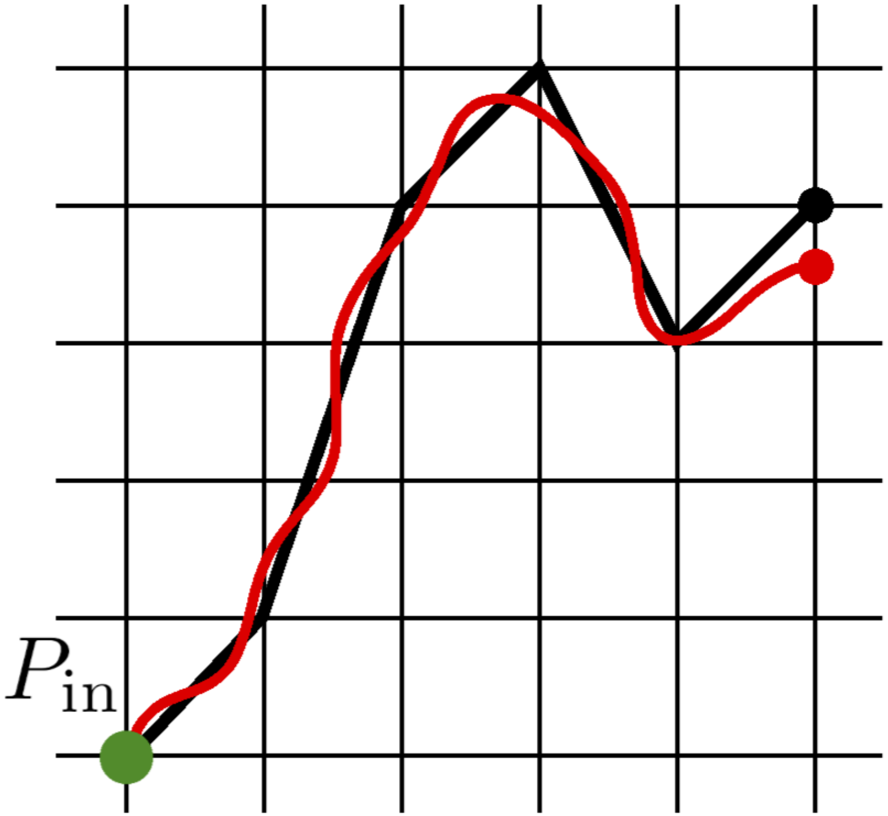
105, 054302

[1] Baran, A. et. al., Nucl. Phys. A 361, 83 (1981).

The Nudged Elastic Band (NEB) Method

- The nudged elastic band method (NEB) was introduced in molecular chemistry by Henkelman et. al [1,2]
  - Originally used to find minimum energy paths (MEPs)
  - Later extended to LAPs.
- Requires local evaluations of an interpolation function
- Scales well with grid size and dimension compared to grid-based methods

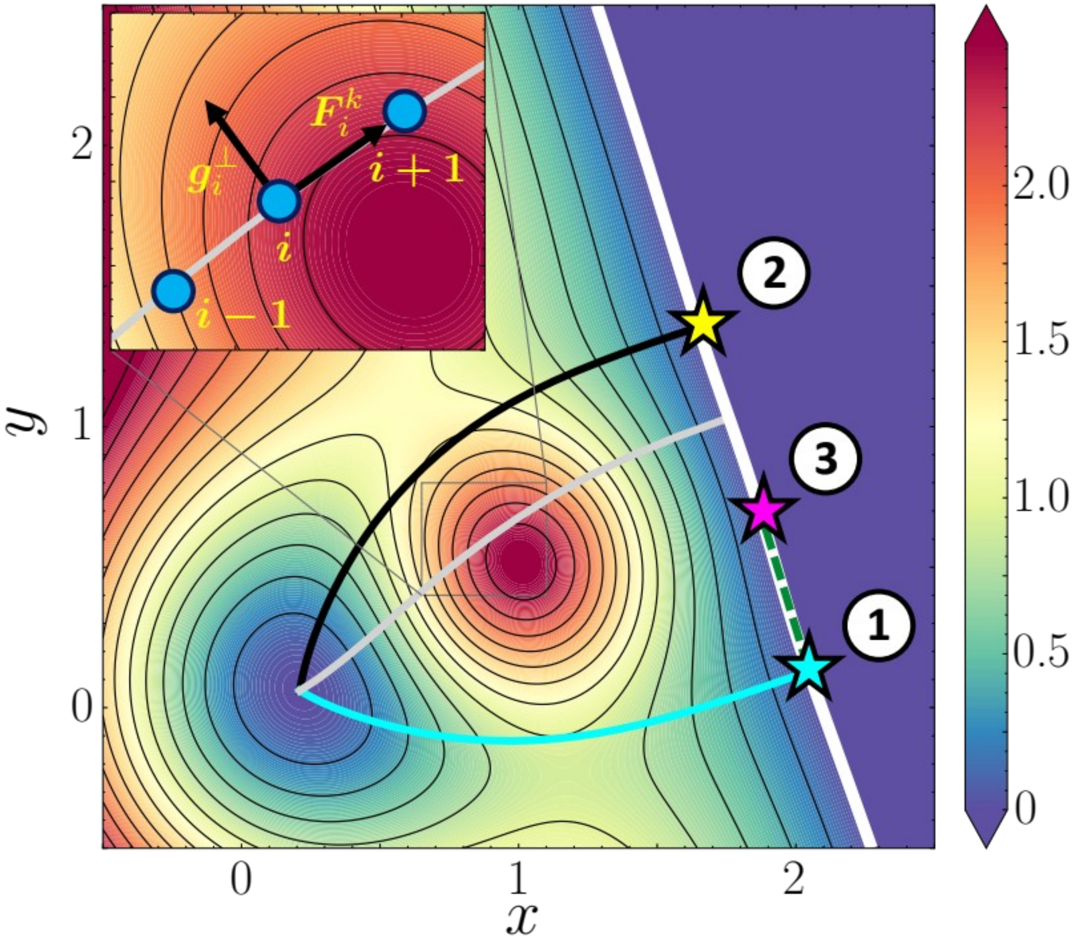


[1] Henkelman, Graeme, and Hannes Jónsson. The Journal of chemical physics 113, no. 22 (2000): 9978-9985.
[2] Henkelman, Graeme, Blas P. Uberuaga, and Hannes Jónsson. The Journal of chemical physics 113, no. 22 (2000): 9901-9904.

The Nudged Elastic Band (NEB) Method

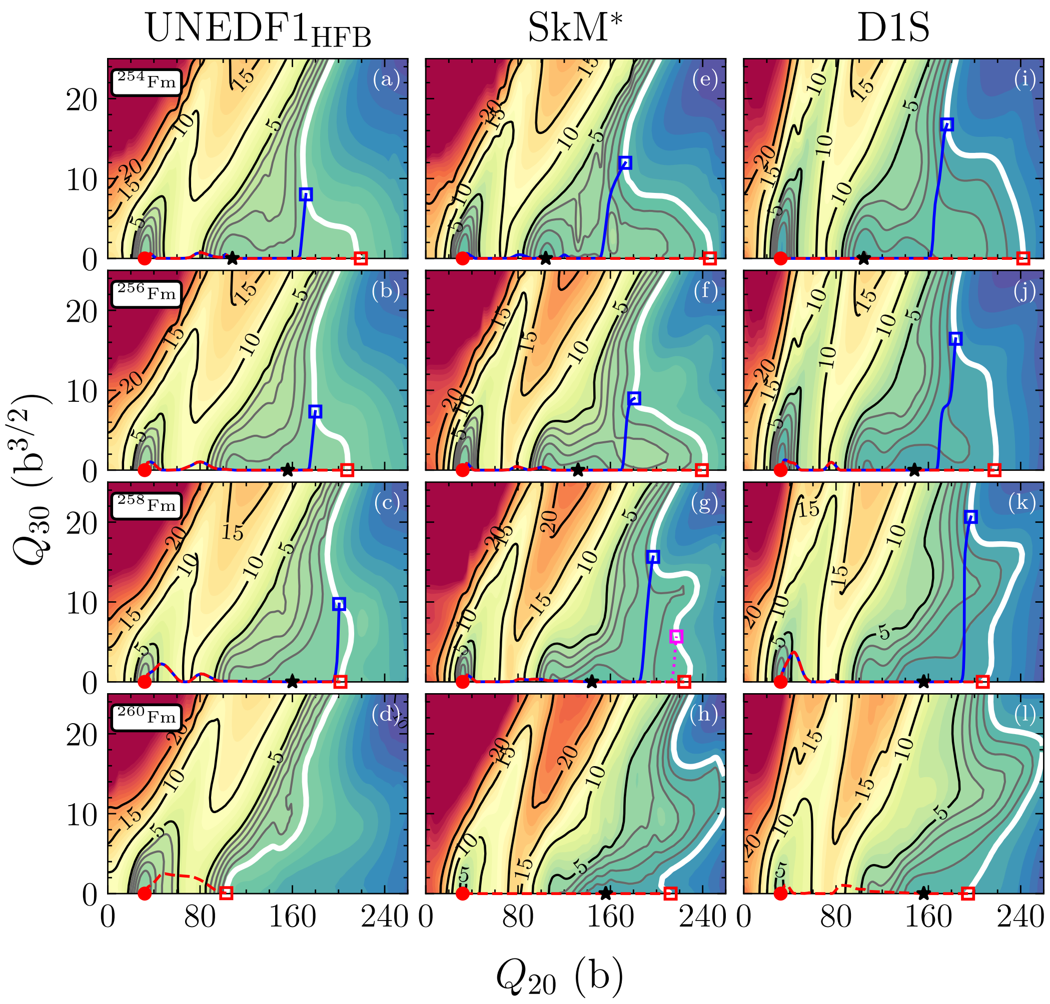
- Uses a string of "particles" with mass in a potential (the PES), connected by springs.
- Given an initial guess pathway, the particles adjust their positions according to the gradient a net force.
  - Net force is the sum of the spring force $\vec{F}_i^k$ and the gradient of the action $\vec{\nabla} S_i$.
- The particles are updated locally
  - Can find local minima easily so it can be applied to multi-modal fission.
- Harmonic force is applied to constrain the end point to an energy contour.

• **Demo:** Www.pyneb.dev/



Flynn, Eric, Daniel Lay, at. el. Physical Review C 105, no. 5 (2022): 054302.

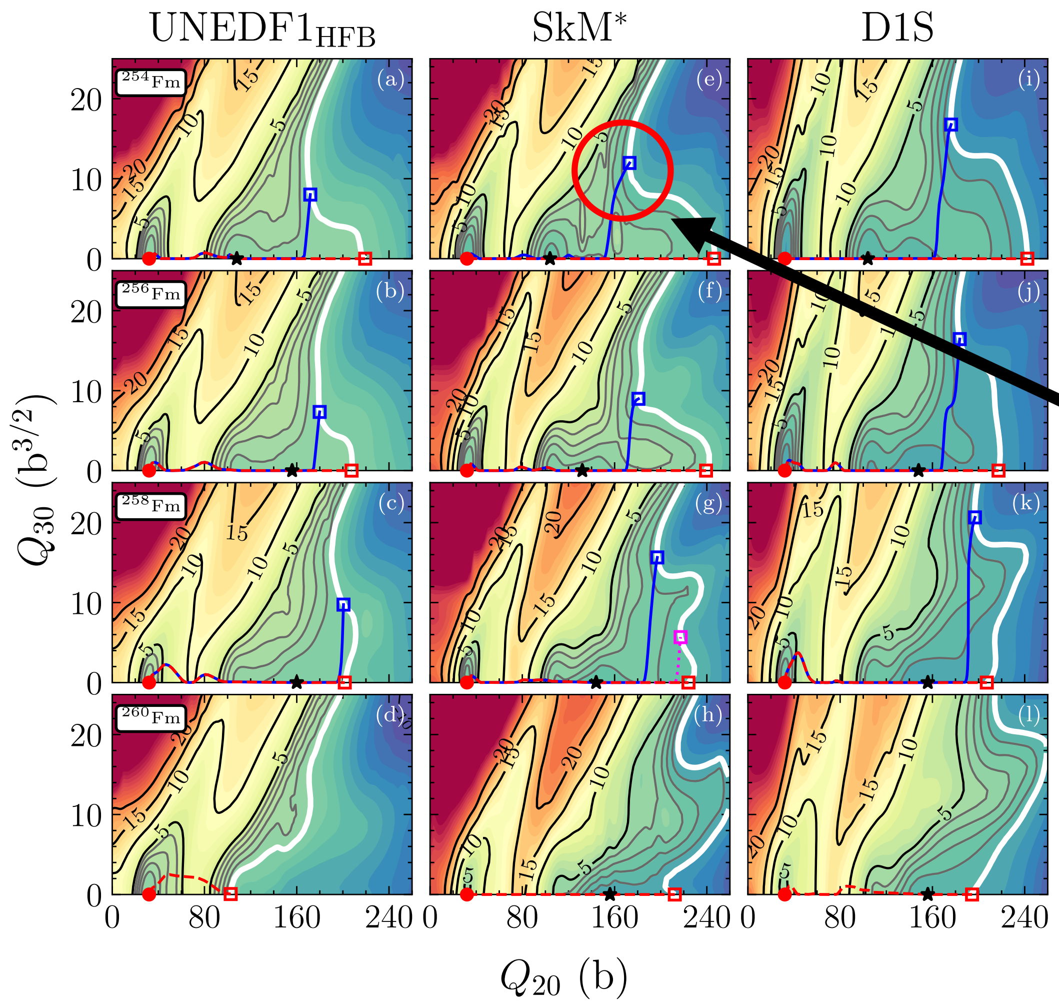
Results: Fermium Isotope Chain Pathways



- At the exit points (square points on left), we identify a pre-scission configuration using a nucleon localization function.
- We use the hybrid approach developed by Sadhukhan et al. Phys. Rev. C 101, 065803 2020.

Lay, Daniel, Eric Flynn, et. al. Physical Review C 109, no. 4 (2024): 044306.

Results: Fermium Isotope Chain Pathways



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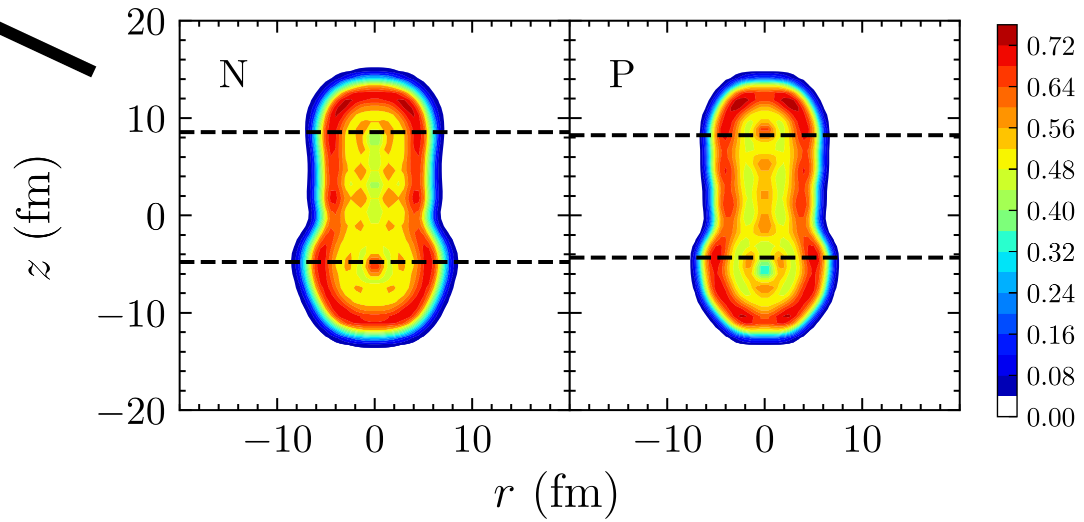
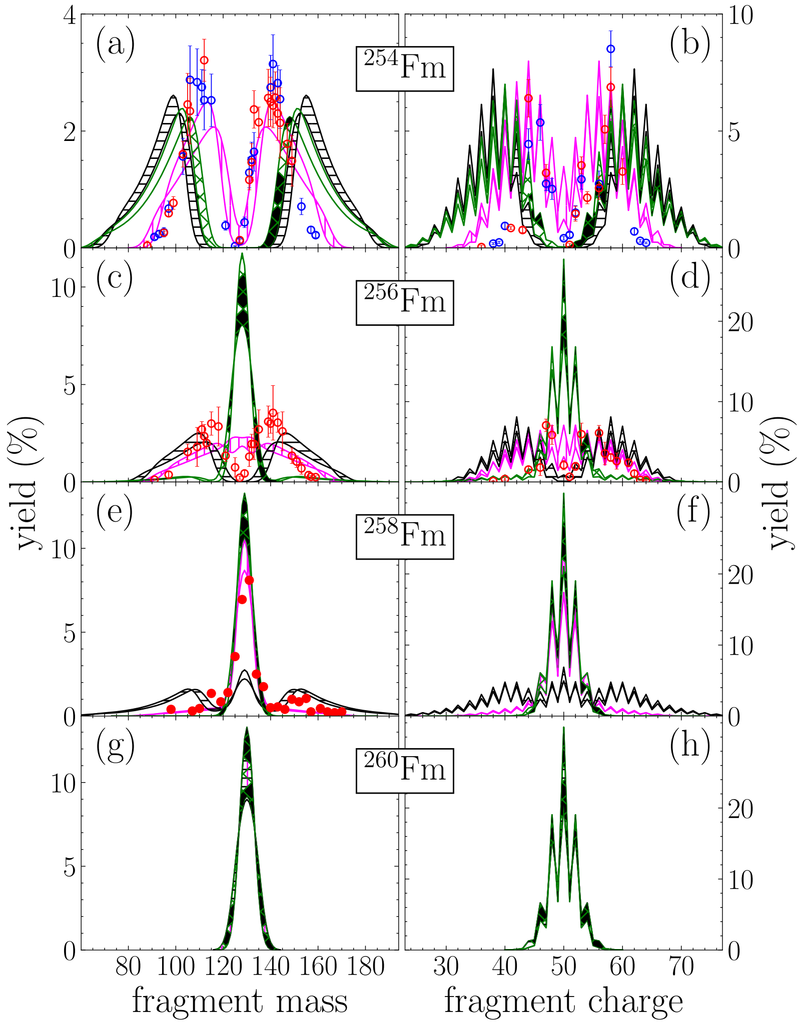


Lay, Daniel, Eric Flynn, et. al. Physical Review C 109, no. 4 (2024): 044306.

Results: Fermium Isotope Chain Yields

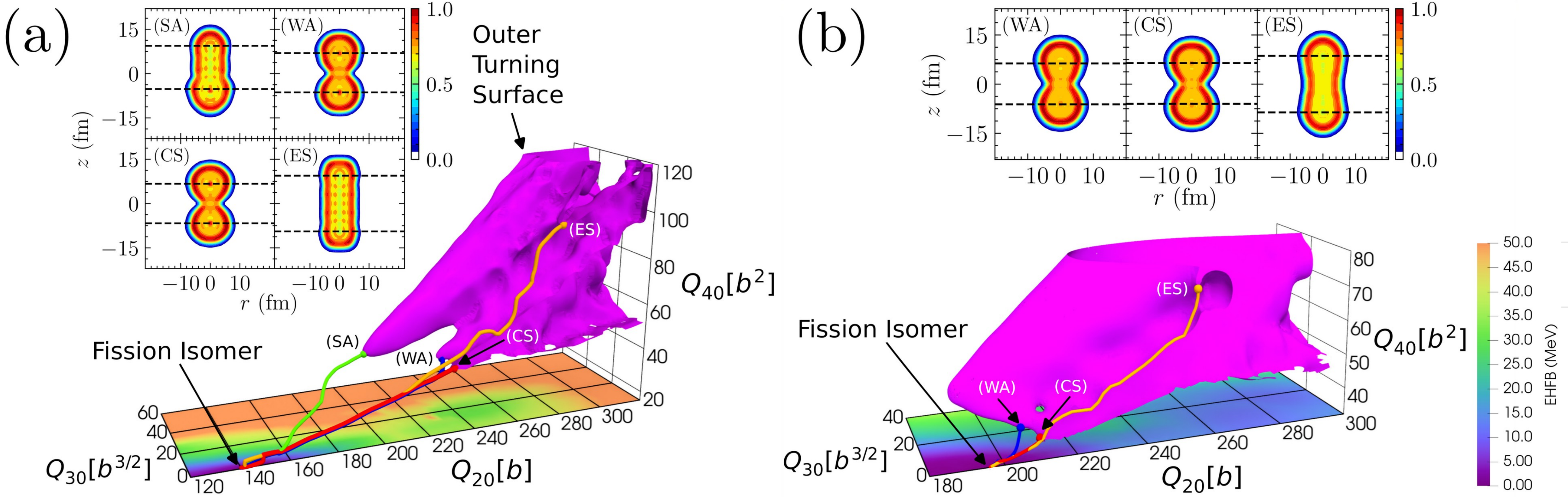


Black = SkM*, Magenta = UNEDF1$_{HFB}$, Green = D1S

- Weighting each mode by it's respective action, we can estimate the total yield.
- The asymmetric mode becomes less significant.
- Observed shift from asymmetric dominant fission to symmetric dominant in the Fermium chain.
  - This is due to the shell closure at ^{132}Sn
- PyNEB can identify multiple modes of fission and classify them based on the action.

Lay, Daniel, Eric Flynn, et. al. Physical Review C 109, no. 4 (2024): 044306.

Results: ^{258}Fm in 3-D

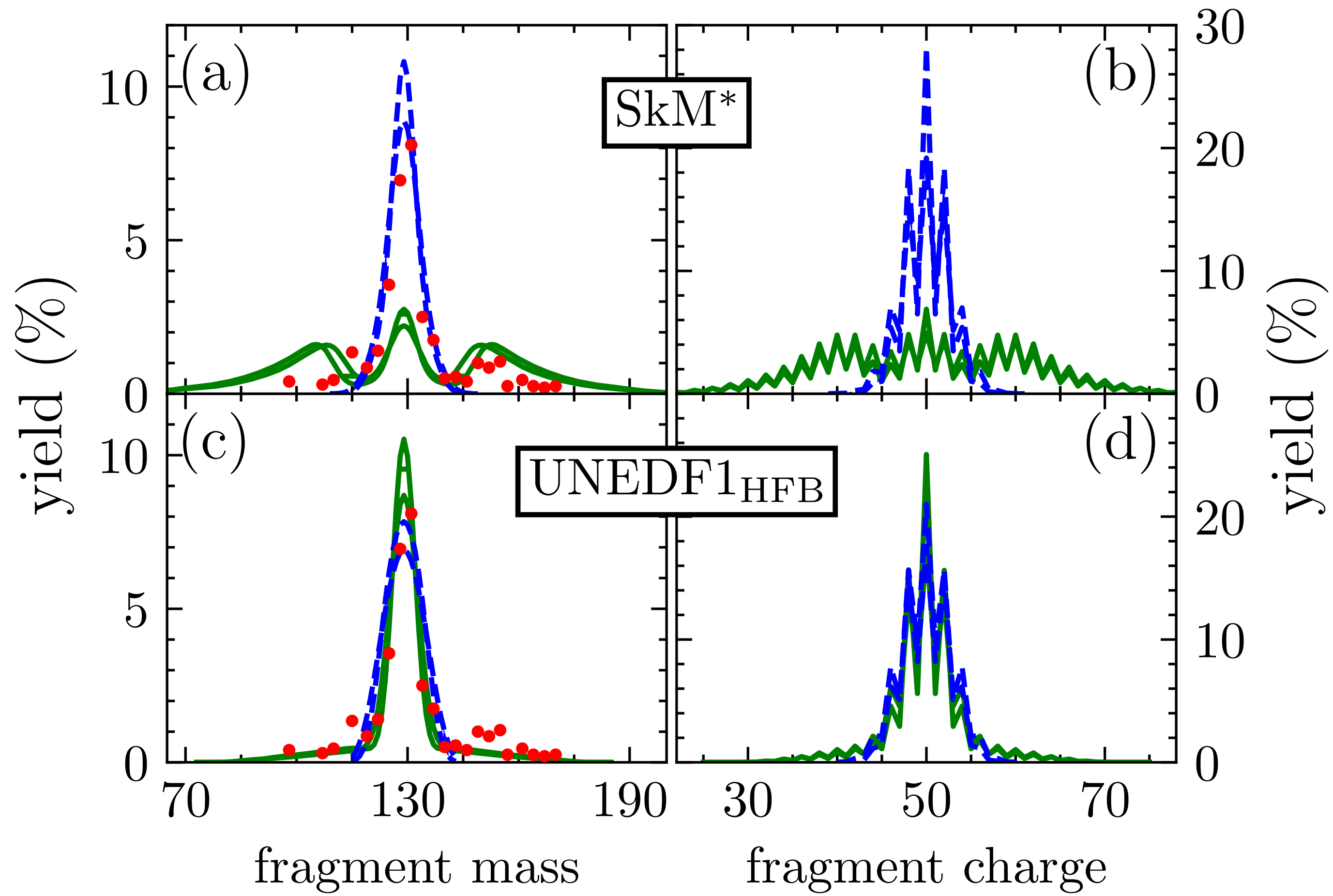


SkM*

UNEDF1$_{HFB}$

Lay, Daniel, Eric Flynn, et. al. Physical Review C 109, no. 4 (2024): 044306.

Results: ^{258}Fm 2D vs 3D



Lay, Daniel, Eric Flynn, et. al. Physical Review C 109, no. 4 (2024): 044306.

Future Directions: Instantons

- PES and inertia calculations become difficult problem as dimension increases.
- We can instead look for mean-field instantons using framework developed by Levit, Negele, et. al Phys. Rev. C 22, 1979 and H. Reinhardt Nucl. Phys. A, Volume 367, Issue 2, 1981
- By conservation of effort, we exchange the curse of dimensionality for a more tricky numerical problem.

$$\mathrm{Tr}_N\left(\frac{1}{\hat{H}-E}\right) = i\int_\gamma e^{-E\beta}\mathrm{Tr}_N\left(e^{-\beta\hat{H}}\right)d\beta$$

$$Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \int\prod_{rs} D\sigma_{rs}e^{-S_{eff}[\sigma]}$$

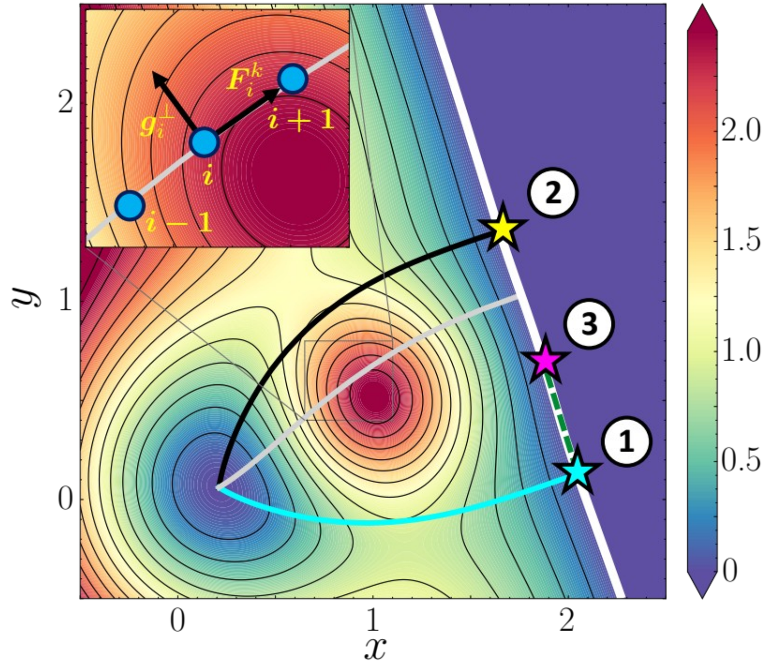
Future Directions: Instantons

$$\delta S[\sigma] = 0$$

- Analytic expressions for the saddle points are two coupled partial differential equations: forward propagating and backward propagating imaginary time equations.
- Solutions must be periodic in imaginary time.
- Numerically unstable and resistant to standard self-consistent mean-field theory methods.
- Saddle points are generically complex.
- **Idea:** Use the holomorphic gradient flow technique used by Scott Lawrence and Yukari Yamauchi Phys. Rev. D 103, 114509 2021 to find saddle points of the functional integral representation of the partition function.

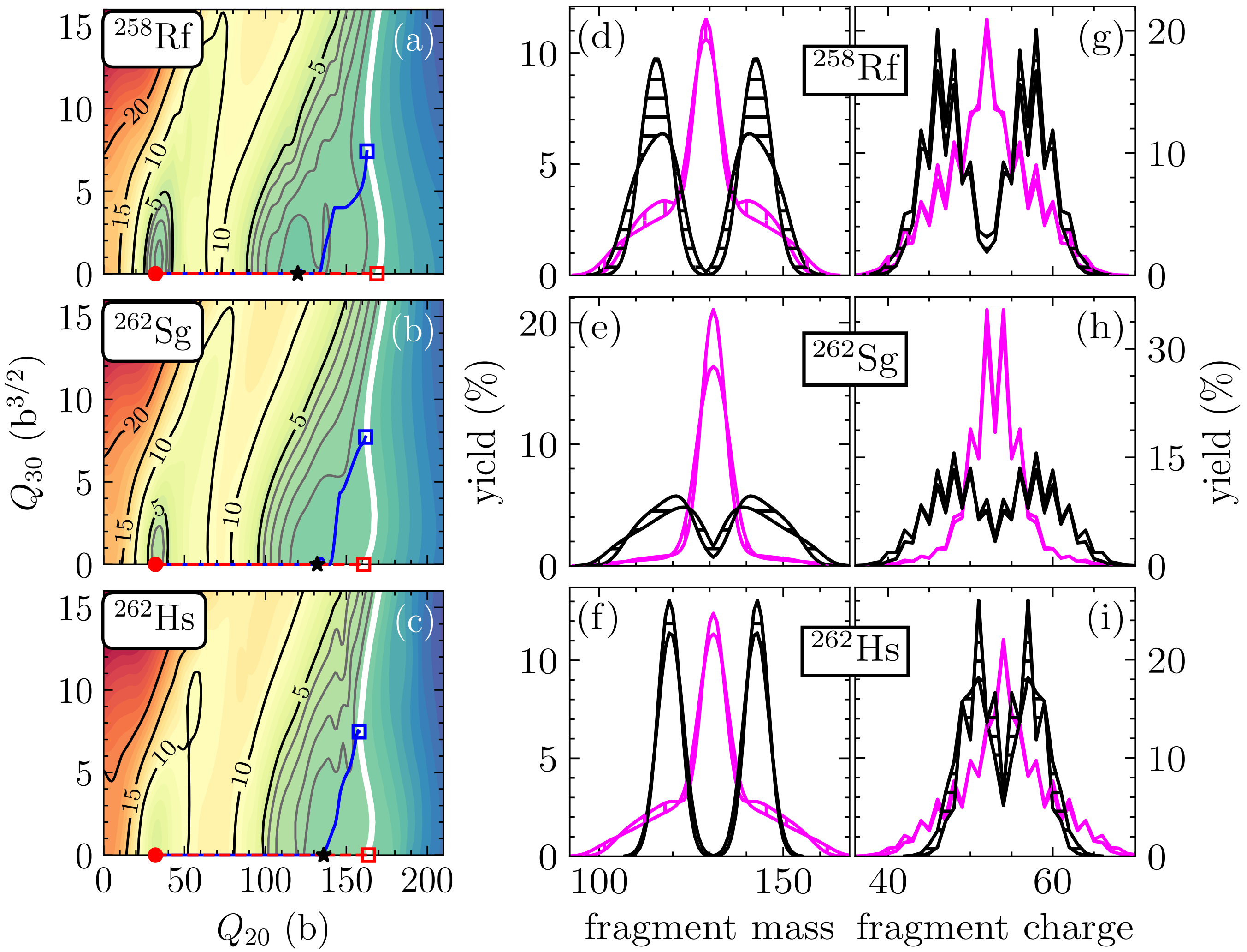
Conclusions

- NEB can efficiently classify different modes of fission in 2 and 3 dimensions.
- NEB overcomes limitations of grid-based algorithms.
- Combined with the micro-canonical hybrid model, NEB can efficiently predict fission yields and potentially predict realistic fission lifetimes.
- Mean-field instantons?
- Thanks to all collaborators and group members: Sylvester Agbemava, Samuel Giuliani, Kyle Godbey, Daniel Lay, Witek Nazarewicz, Jhilam Sadhukhan
- Thanks to Yukari Yamauchi and Scott Lawrence for helpful discussions

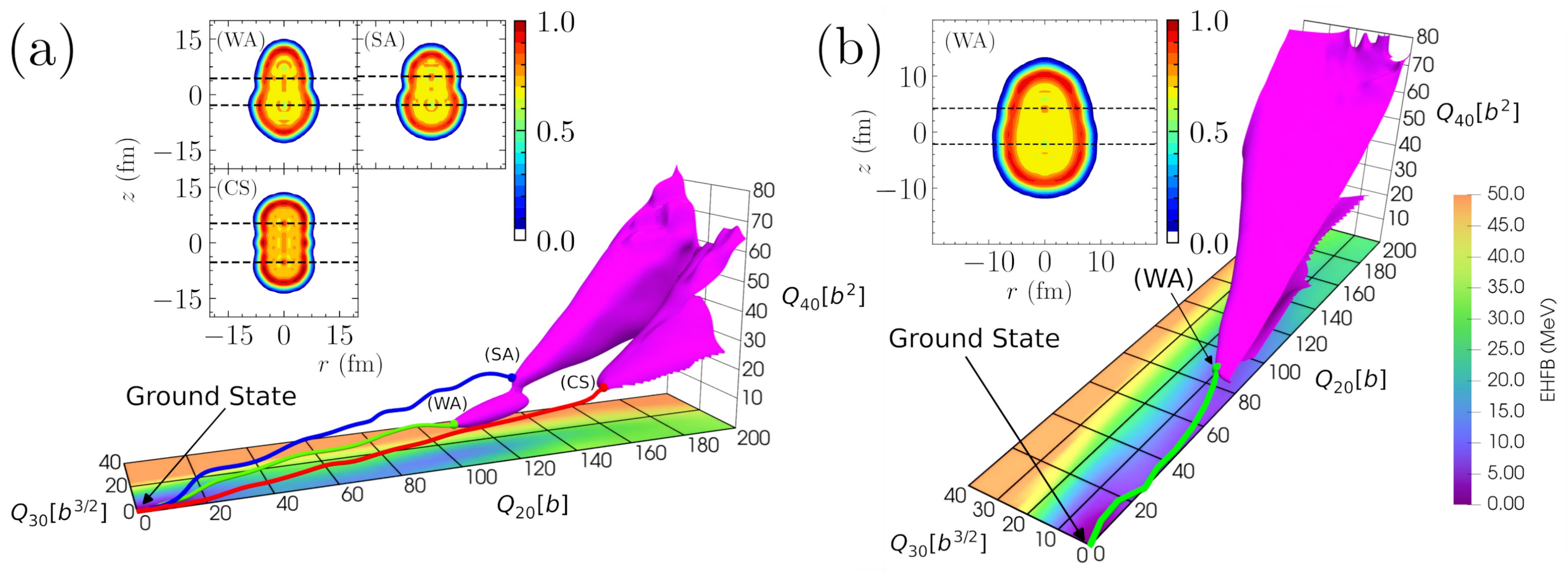


Additional Slides

Superheavy Results



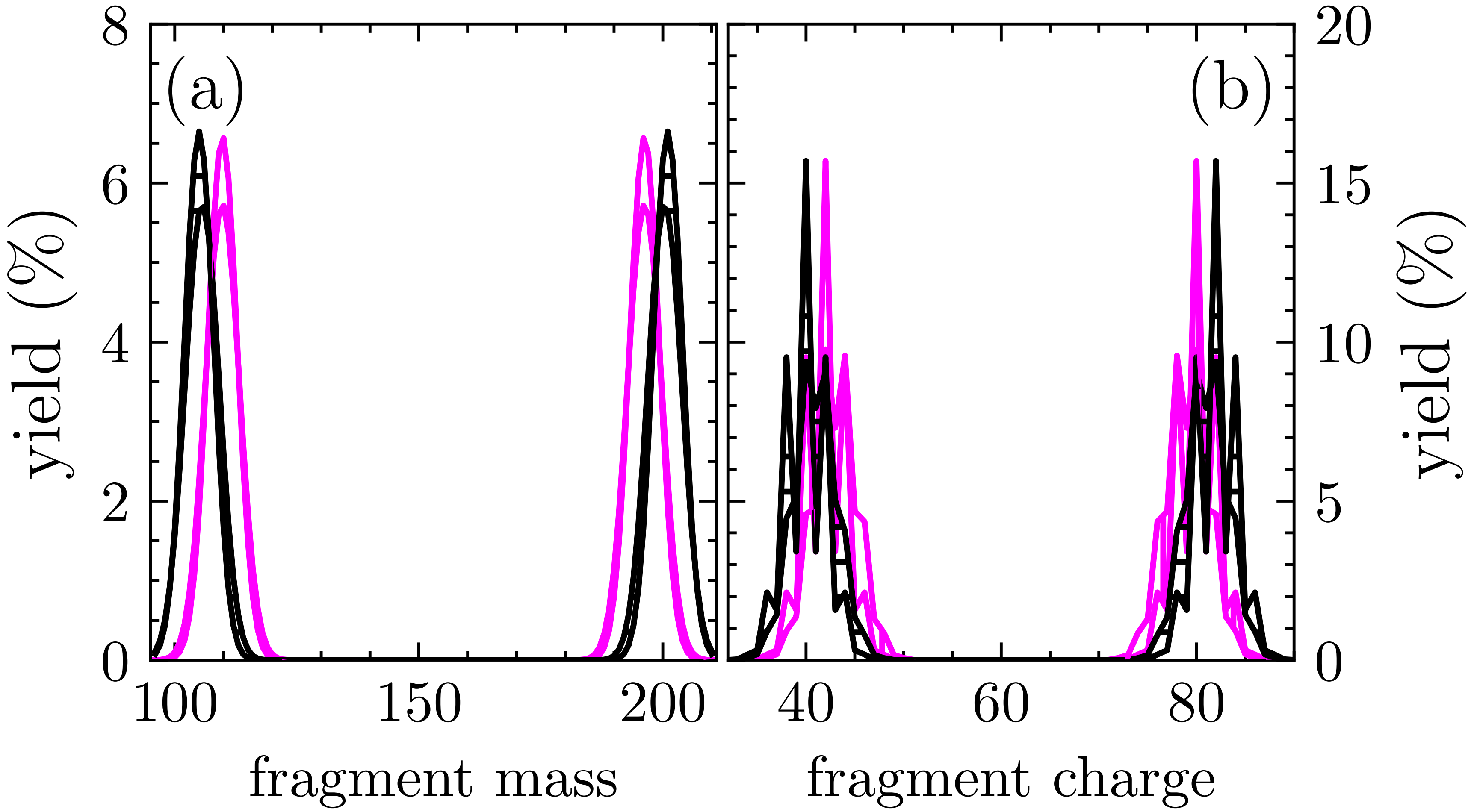
^{306}122 in 3-D



SkM*

UNEDF1

^{306}122 Yields



Future Directions: Instantons

$$\left(-\hbar\frac{\partial}{\partial\beta} - h[\sigma]\right)\phi_{p_k}(x,\beta) = \varepsilon_{p_k}[\sigma,\beta_T]\phi_{p_k}(x,\beta)$$

$$\left(\hbar\frac{\partial}{\partial\beta} - h[\sigma]\right)\phi_{p_k}(x,-\beta) = \overline{\varepsilon}_{p_k}[\sigma,\beta_T]\phi_{p_k}(x,-\beta)$$