Nuclear Many-Body Dynamics Through Barriers
CEA Saclay, DPhN
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Fission with Symmetry-Restored Energy Density Functional

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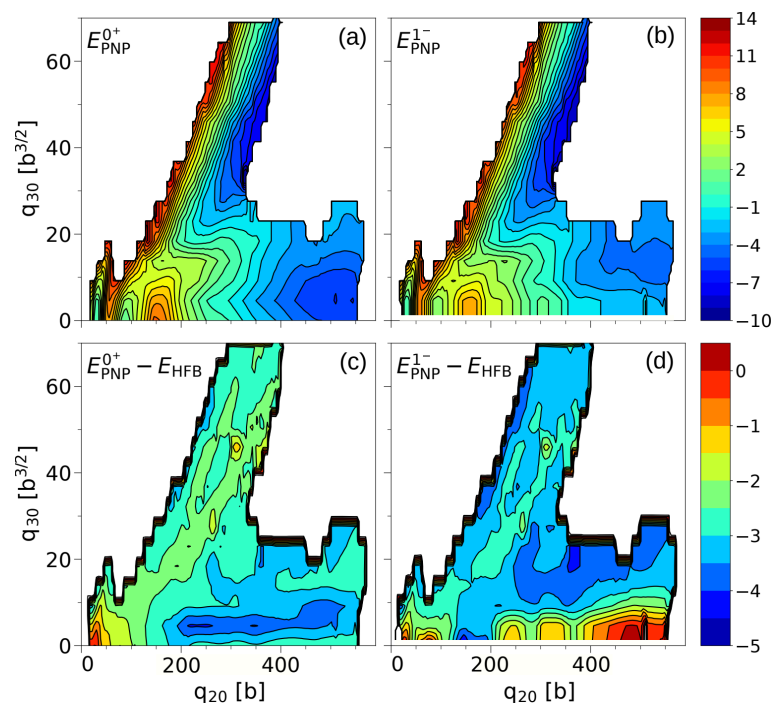
Centre Borelli, ENS Paris-Saclay

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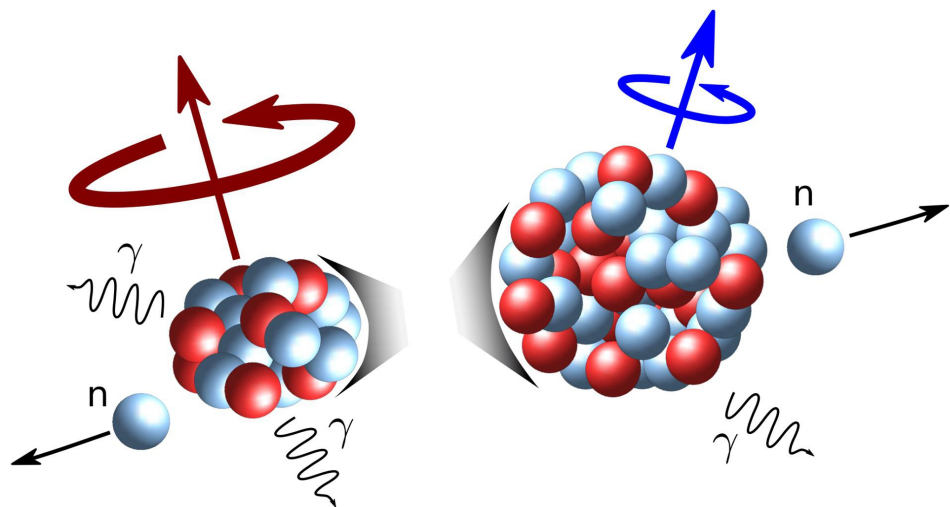PARIS-SACLAY

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Two questions

How to, using symmetry restoration framework, calculate...

... potential energy surfaces for fission studies?

... the angular momentum of the fission fragments?

Outline

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1. Symmetry Restoration and Fission
2. Angular Momentum Projection in Deformed Bases
3. Angular Momentum of Fission Fragments
4. Conclusion

Symmetry Restoration and Fission
Breaking and restoring symmetries in a nutshell

- Basic (mean-field) EDF models are characterized by **symmetry breaking**

Broken Symmetry	Rotational	Particle Number	Reflection	Translational
Due To	Deformation (Any Multipole)	Pairing or Finite T	Deformation (Odd Multipole)	Localization of the Mean-Field
Quantum Numbers	Angular Momentum	Neutron and Proton Number	Parity	Linear Momentum

- In structure models, symmetries are **routinely restored** using the group theory techniques
  - Order parameter $\mathbf{q}=|\mathbf{q}|\exp(i\varphi)$ monitors the level of symmetry breaking
  - We take linear combinations of states $|\Phi(\varphi)\rangle$ with different φ
  - Recovery of **good quantum numbers** of many-body wave functions
  - **Richer wave functions** due to the incorporation of additional correlations

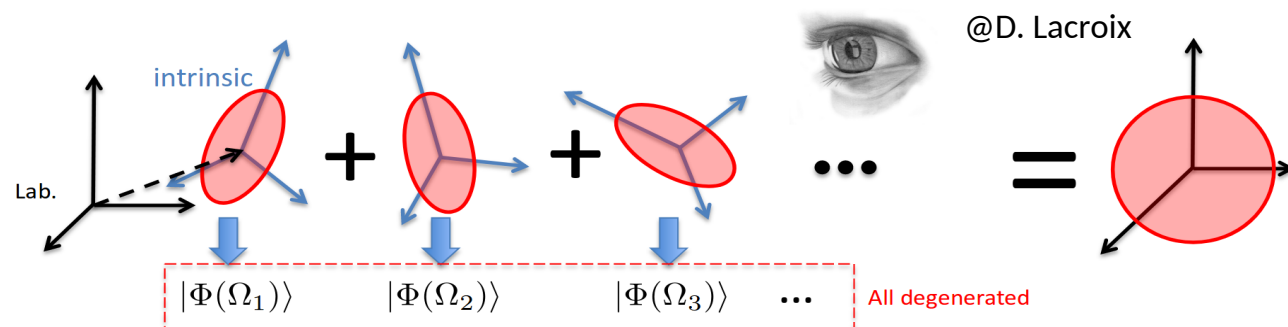*"Symmetry restoration in mean-field approaches"*, J. A. Sheikh *et al.*, J. Phys. G: NPP **48**, 123001 (2021).

@D. Lacroix

intrinsic

Lab.

$|\Phi(\Omega_1)\rangle$ $|\Phi(\Omega_2)\rangle$ $|\Phi(\Omega_3)\rangle$ ⋯   All degenerated

Illustration: Restoration of Rotational Symmetry

6+

4+

2+

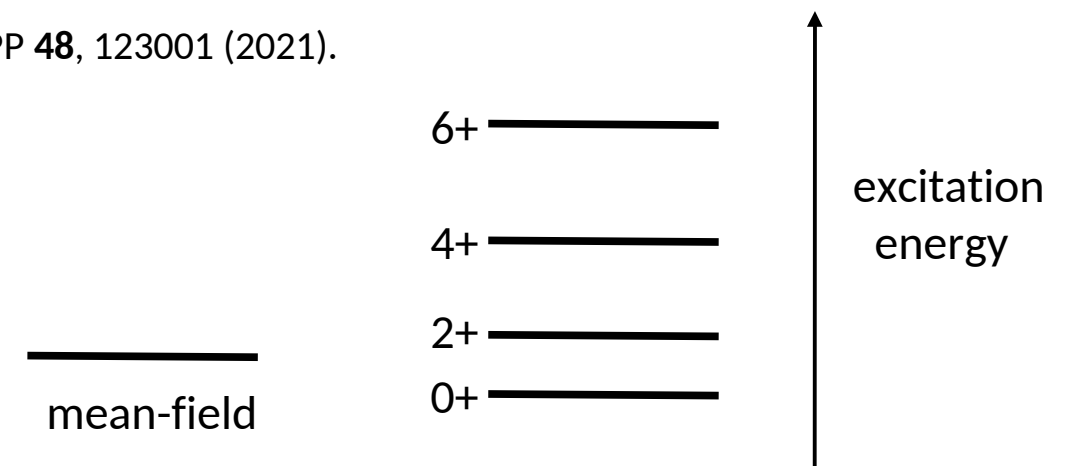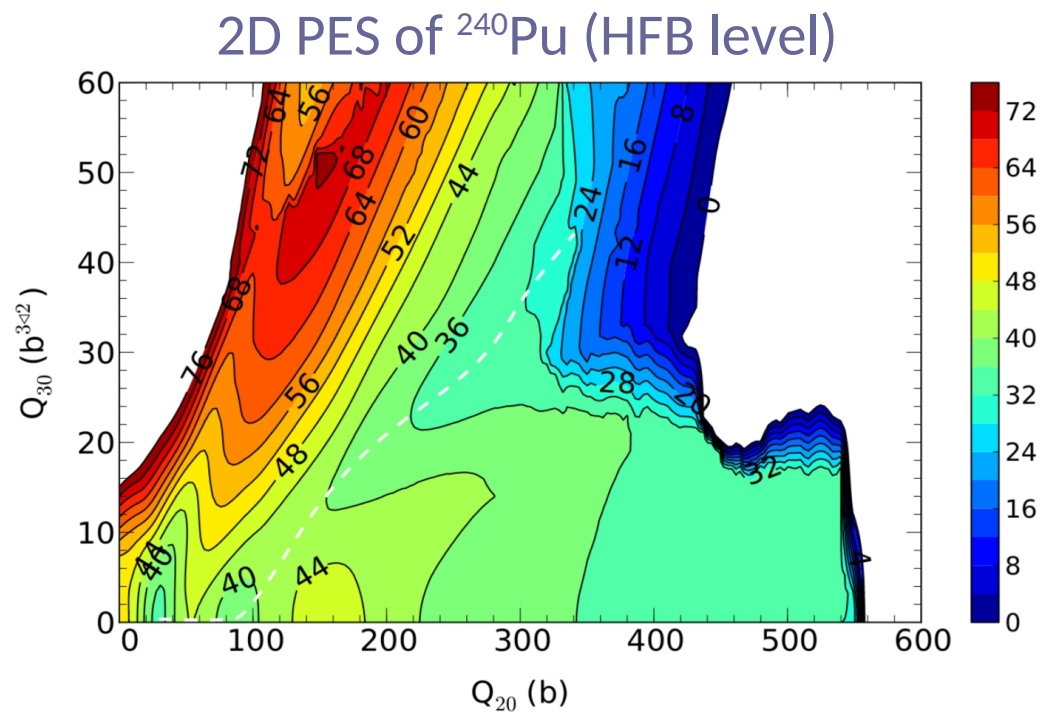0+

excitation energy

mean-field
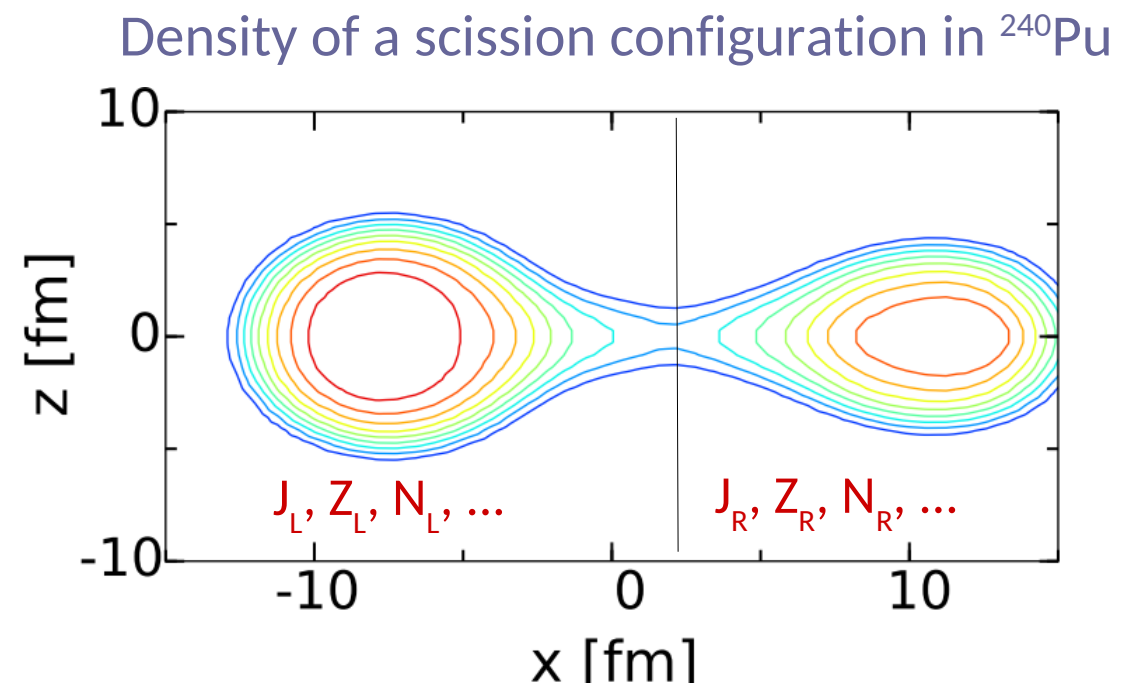
Illustration: Rotational Spectra

Symmetry Restoration and Fission
Restoring symmetries can improve fission models

- Restoring symmetries **can improve fission models** as well

  - Modifying the fission dynamics
  - Modifying the spontaneous fission half-lives
  - Differentiating between entrance channels (e.g., $n+^{235}U$ vs $\gamma+^{236}U$)
  - Determining properties of fission fragments (number of particles, angular momenta, …)

2D PES of ^{240}Pu (HFB level)

Density of a scission configuration in ^{240}Pu

$J_L, Z_L, N_L, …$ $J_R, Z_R, N_R, …$

N. Schunck *et al.*, PRC 90, 054305 (2014).

However, applications of symmetry restoration to fission **have up to recently been very scarce.**

Symmetry Restoration and Fission
Recently, symmetry restoration gained prominence in fission studies

- Pioneering work explored application of symmetry restoration to fission but …
  - ✗ restricted in the range of deformations and/or restored symmetries
  - ✗ no description of fragment properties

  M. Bender, P.-H. Heenen, P. Bonche, PRC **70**, 054304 (2004).
  M. Samyn, S. Goriely, J. Pearson, PRC **72**, 044316 (2005).
  T. V. N. Hao, P. Quentin, L. Bonneau, PRC **86**, 064307 (2012).

- In recent years, symmetry restoration gained prominence in fission studies

  R. Bernard, S. A. Giuliani, L. M. Robledo, PRC **99**, 064301 (2019).
  P. M. and N. Schunck, PRL **125**, 102504 (2020).   Influence on the fission dynamics

  M. Verriere, N. Schunck, T. Kawano, PRC **100**, 024612 (2019).   Number of particles in fragments

  A. Bulgac, *et al.*, PRL **126**, 142502 (2021).
  P. M., *et al.*, PRC **104,** L021601 (2021).   Angular momentum of fragments
  A. Bulgac, *et al.*, PRL **128**, 022501 (2022).

  A. Bulgac, PRC **100,** 034612 (2019).   Formal aspects of symmetry restoration in fragments
  A. Bulgac, PRC **104**, 054601 (2021).

  L. M. Robledo, PRC **105**, L021307 (2022).   Extensions of symmetry restoration formalism
  L. M. Robledo, arXiv:2201.10486 (2022).

Growth in computational resources and theoretical developments **open a new avenue** for fission studies.

Angular Momentum Projection in Deformed Bases

Angular Momentum Projection in Deformed Bases
Problem: Deformed bases are not closed under rotation

- Mean-field (HFB) states are commonly expanded in harmonic oscillator bases

  ✔ General strategy applicable to zero-range and finite-range interactions
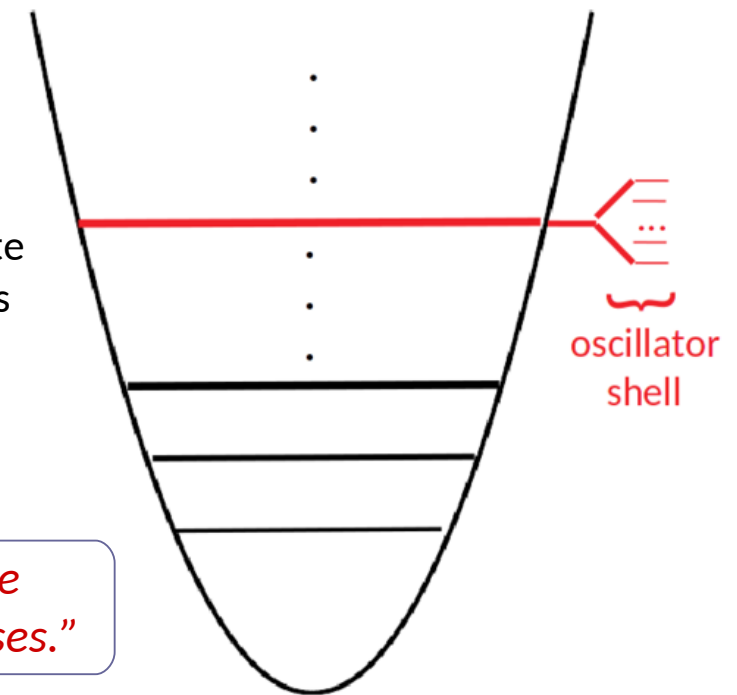 ✔ No additional approximations for symmetry operators (e.g., rotations)

- Angular momentum projection

$$|\Psi^J\rangle = \frac{2J+1}{2} \int_0^\pi d\beta \sin\beta d_{00}^{J*} \hat{R}(\beta) |\Phi\rangle$$

Symmetry-restored state

Integral over rotational angles

Rotation operator

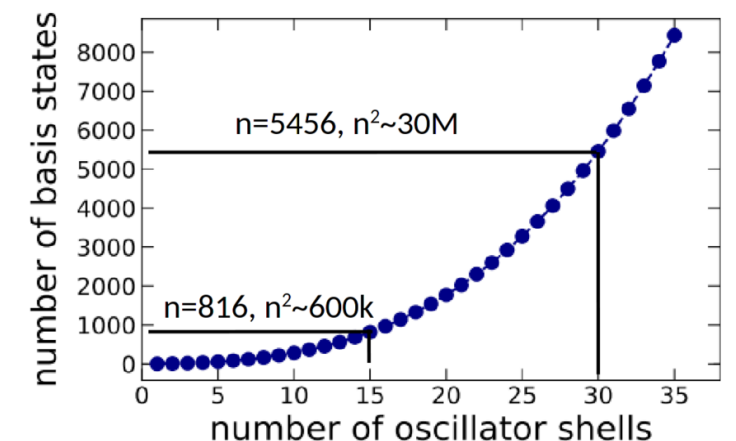Symmetry-breaking state expanded in a HO basis

oscillator shell

- We can just apply the usual strategy, right?

> "This strategy increases the computational cost, *and becomes impractical in some situations like fission, where the large variety of shapes involved would require huge rotationally invariant bases.*"

"Symmetry restoration in mean-field approaches", J. A. Sheikh *et al.*, J. Phys. G: NPP **48**, 123001 (2021).

- All structure models use expansions in bases with **complete shells**…
  … such bases become **too large** in the case of fission

- Size of the basis can be reduced by considering **incomplete shells**…
  … such bases are **not closed under rotation**

Illustration: Size of the oscillator basis

number of basis states

n=5456, n²~30M

n=816, n²~600k

number of oscillator shells

Angular Momentum Projection in Deformed Bases
Solution: Reformulate the Wick theorem

- General problem: Bases of different HFB states **are not connected by unitary transformation**
- Solution: Formally **extend the bases** to an infinite dimension and reapply the Wick theorem

Original work: *L. M. Robledo, PRC* **50**, *2874 (1994).*
Recent upgrades: *L. M. Robledo, PRC* **105**, *L021307 (2022).*
                                  L. M. Robledo, arXiv:2201.10486 (2022).

The basis is initially extended, but all the quantities are finally calculated **in the original basis**.

E.g., calculation of overlaps

$$\mathcal{N}_q^{(\tau)}(\boldsymbol{x}^{(\tau)}) = \sqrt{\det\left[A_q^{(\tau)}(\boldsymbol{x}^{(\tau)})\right]\det\left[R(\boldsymbol{x}^{(\tau)})\right]}$$

$$A_q^{(\tau)}(\boldsymbol{x}^{(\tau)}) = U_q^{(\tau)T}\left[R^T(\boldsymbol{x}^{(\tau)})\right]^{-1}U_q^{(\tau)*} + V_q^{(\tau)T}R(\boldsymbol{x}^{(\tau)})V_q^{(\tau)*}$$

- We implemented the first angular momentum projection model in deformed bases
  - Simultaneous restoration of **rotational, reflection, and particle number** symmetry
  - AMP in deformed bases means **much smaller bases** are needed
  - Computational feasibility: **OMP&MPI** parallelization
  - An access to **arbitrarily heavy and/or deformed** nuclear configurations
  - Limitations: axial shapes, even-even nuclei, T=0, Skyrme interactions
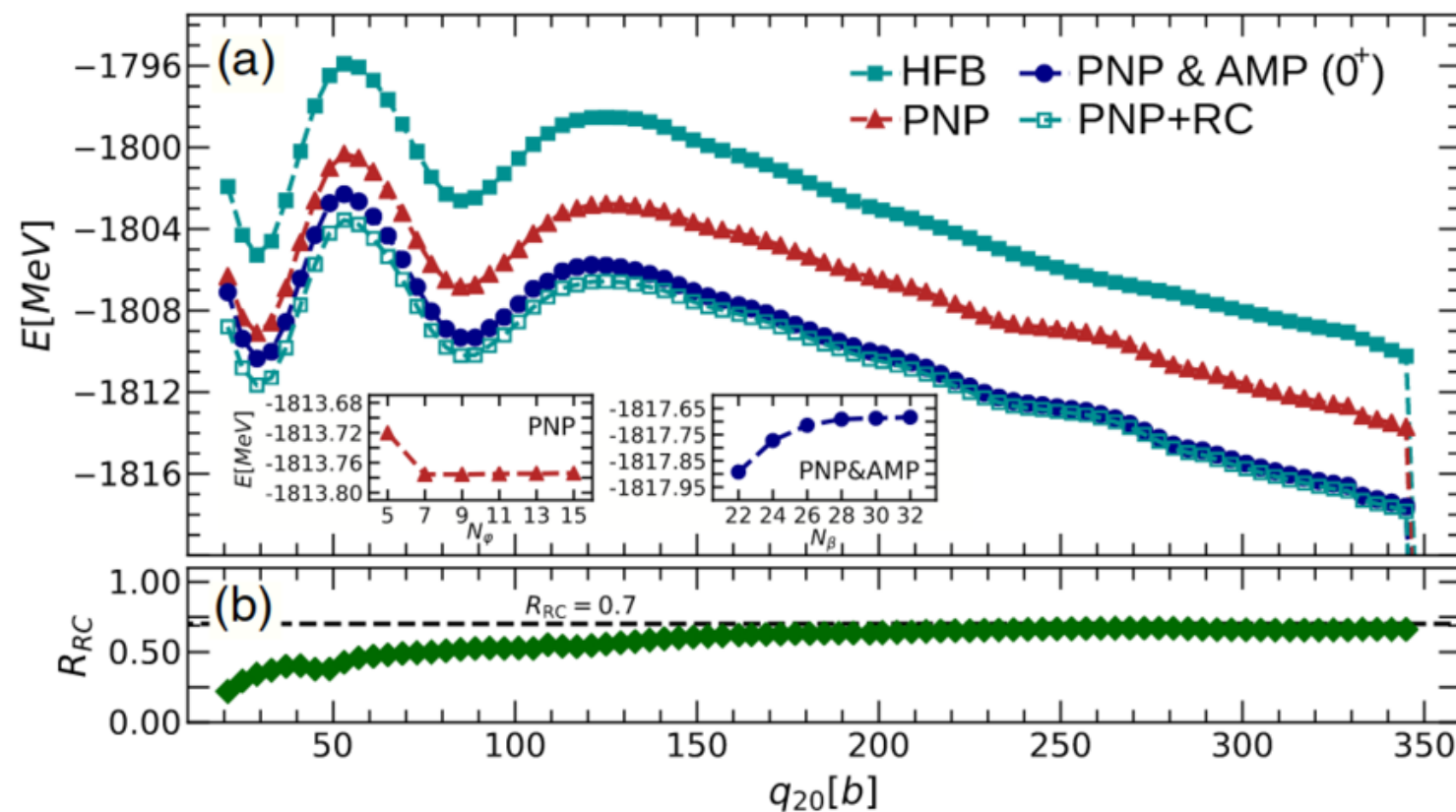 - Made available in the new version of HFBTHO code

P. M. and N. Schunck, PRL **104,** L021601 (2020).
P. M., *et al.*, accepted for publication in CPC (2022).

Angular Momentum Projection in Deformed Bases

Least-energy fission pathway in ^{240}Pu

Least-energy fission pathway of ^{240}Pu

- Impact on the least-energy fission pathway
  - **Lowering** of the fission barriers (1-2 MeV)
  - Pre-scission energy remains **roughly the same**

- Validity of the rotational formula
  - Quenching factor not sufficient for $q_{20} < 150$ b
  - Consequences for observables (SF half-lives, …)

$$E_{RC} = 0.7 \times \underbrace{\left(-\frac{\langle \mathbf{J}^2 \rangle}{2 \mathcal{J}_{PY}^2} \right)}_{E_{PY}}$$

$$R_{RC} = E_{corr.}^{projected} / E_{PY}$$

Angular Momentum Projection in Deformed Bases
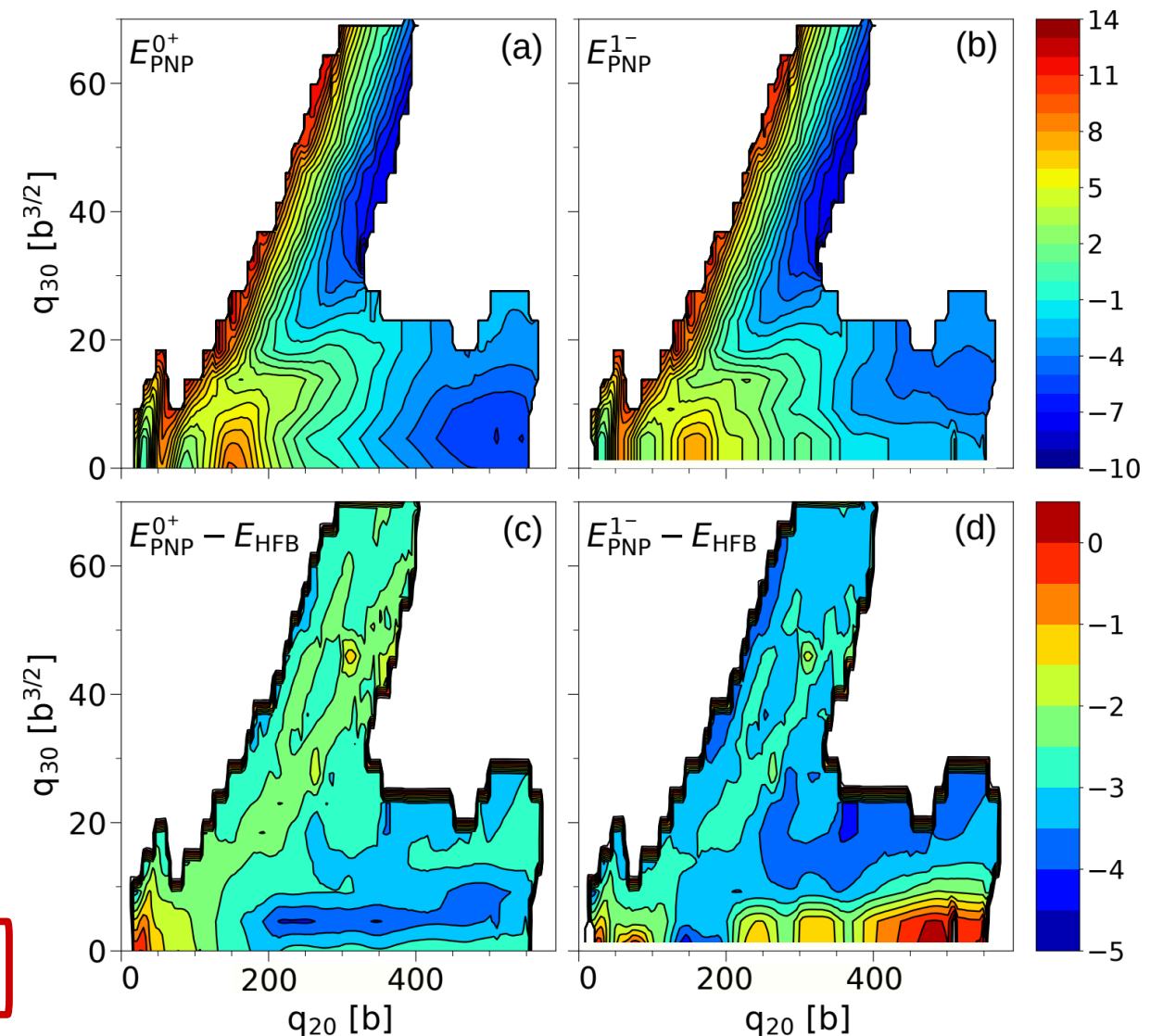## Symmetry-restored 2D potential energy surface

- 2D potential energy surface of ^{240}Pu
  - SkM* interaction, volume-surface contact pairing
  - 1150 configurations, wide range of deformations
  - Basis size reduced drastically (N_{sh}=30, n=1100)
  - Number of angles: $N_\varphi = 9$, $26 \leq N_\beta \leq 30$

- Influence of symmetry restoration on PES
  - Gain at low q_{30} (0^+) …
    … enhancement of symmetric fission?
  - Gain along the least-energy fission path (1^-)…
    … broader fragment distributions?

- PES is an **essential ingredient** of TDGCM (+GOA)

$$i\hbar \frac{\partial g(\mathbf{q},t)}{\partial t} = \hat{H}_{\text{coll}}(\mathbf{q})g(\mathbf{q},t)$$

$$\hat{H}_{\text{coll}}(\mathbf{q}) = -\frac{\hbar^2}{2\gamma^{1/2}(\mathbf{q})}\sum_{ij}\frac{\partial}{\partial q_i}\gamma^{1/2}(\mathbf{q})B_{ij}(\mathbf{q})\frac{\partial}{\partial q_j} + \boxed{V(\mathbf{q})}$$

  - Rigorous justification of GOA in a symmetry-restored framework?
  - Calculation of collective inertia from symmetry-restored framework?

Symmetry-restored 2D PES of ^{240}Pu

Potential energy surfaces are significantly modified by symmetry restoration.

Angular Momentum of Fission Fragments

Angular Momentum of Fission Fragments
Angular momentum of fragments influences the fission process

- AM of FFs influences the fission process
  - Causes anisotropy in neutron emission
  - Modifies the number of emitted neutrons and photons
  - Impacts the population of isomeric states in products

- There remain important **open questions**

  1) How to calculate the AM of FFs from microscopic theory?
  2) How does it depend on the mass of FFs?
  3) What is the mechanism of its generation?

- Over the past year only, answers were suggested by ...
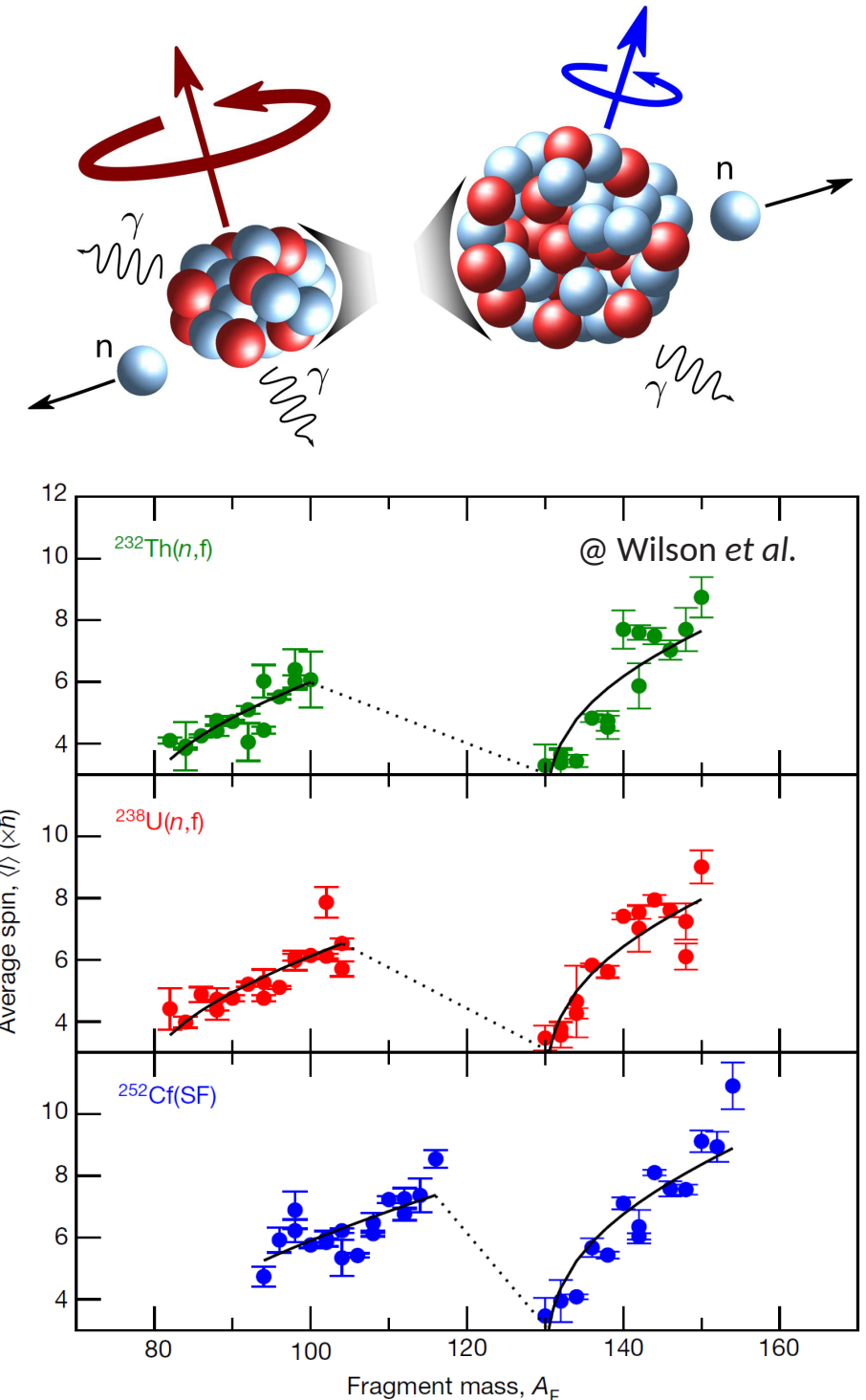
  ... experiments

  J. N. Wilson *et al.*, Nature **590**, 566 (2021).
  M. Travar *et al.*, PLB **817**, 136293 (2021).

  ... theoretical modeling

  A. Bulgac *et al.*, PRL **126**, 142502 (2021).
  P. M. *et al.*, PRC **104,** L021601 (2021).
  J. Randrup and R. Vogt, PRL **127,** 062502 (2021).
  I. Stetcu *et al.*, PRL **127**, 222502 (2021).
  A. Bulgac *et al.*, PRL **128**, 022501 (2022).

- Experiments suggest a **universal sawtooth-like pattern**

- Goal: a microscopic model describing the physics of scission **without adjustable parameters**

Angular Momentum of Fission Fragments
A new model describing the mass-dependence of AM of FFs

We developed a microscopic model of how the AM of FFs changes with mass.

1) Define a set of scission configurations through constrained (q_{20}, q_{30}, q_N) HFB calculations

2) In each configuration, determine the two FFs via neck position

3) In each configuration, perform the angular momentum projection in each FF

$$\left| a_J^F(\boldsymbol{q}) \right|^2 = \int_\beta \langle \Phi(\boldsymbol{q}) | \hat{R}_y^F(\beta) | \Phi(\boldsymbol{q}) \rangle \qquad \hat{R}_y^F(\beta) = \exp(-i\beta \hat{J}_y^F)$$

$$J_y^F(\boldsymbol{r}, \sigma) = \Theta^{F*}(z - z_N) J_y(\boldsymbol{r}, \sigma) \Theta^F(z - z_N)$$

4) Use Gaussian Process to extract primary fragment distributions for integer A, Z

5) Use FREYA to simulate the emission of neutrons and photons
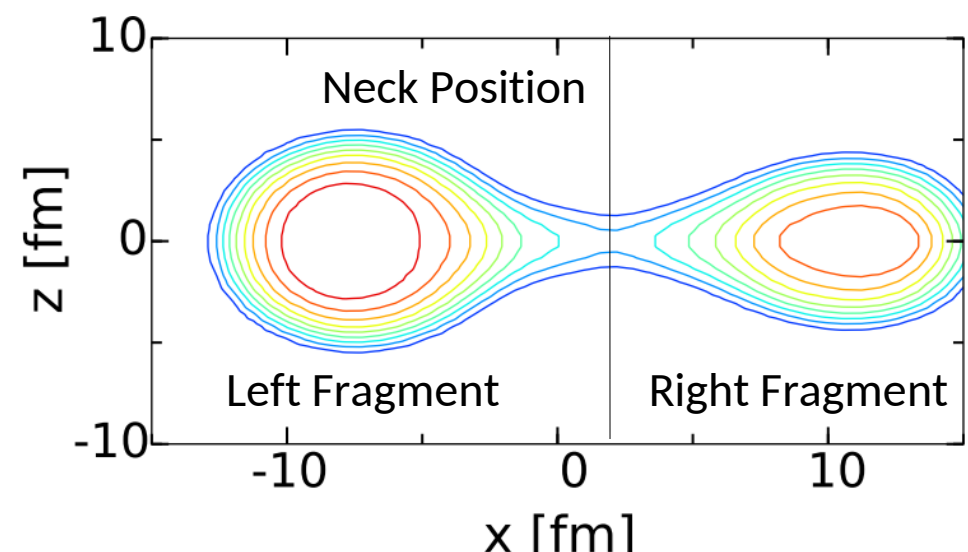
J. Randrup and R. Vogt, PRC **80**, 024601 (2009).

Illustration: Density of a scission configuration

Pros

✔ Based on microscopic theory
✔ FF deformations fixed by var. principle
✔ Predictions for a wide range of FF masses

Cons

✗ A and Z of FFs not integers
✗ FFs not excited
✗ FFs not fully separated

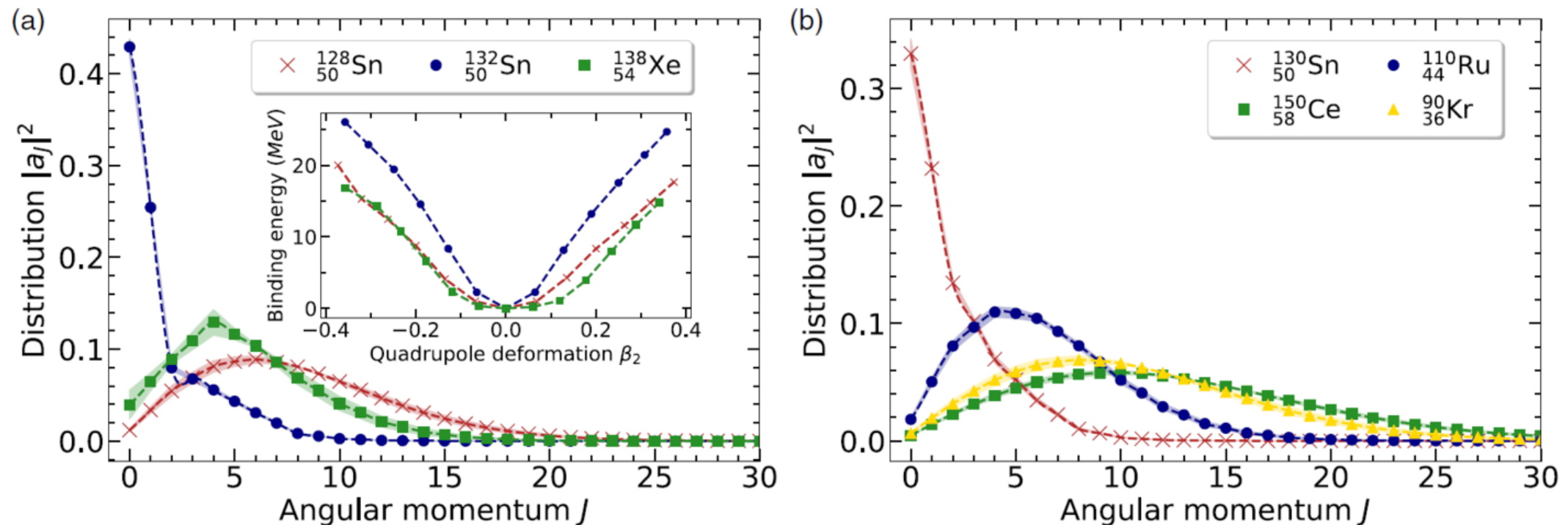P. M., N. Schunck, J. Randrup, R. Vogt PRC **104,** L021601 (2021).

Angular Momentum of Fission Fragments
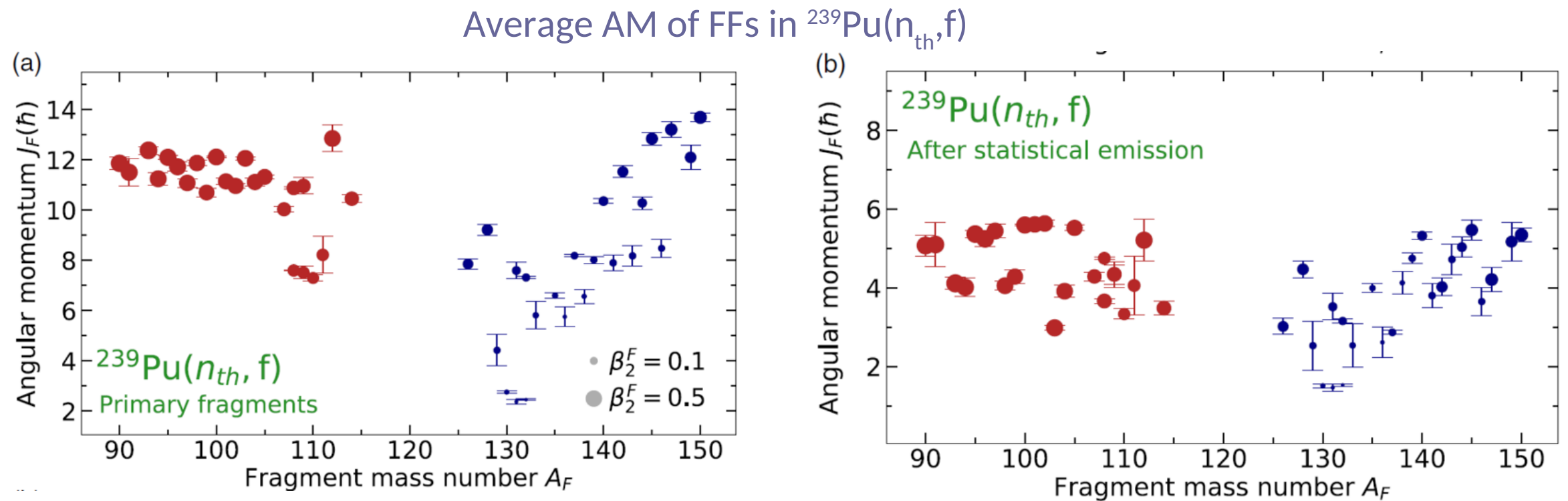Predictions are possible for a wide range of fragment masses

AM distributions of primary FFs in ^{239}Pu(n$_{th}$,f)

- The model has a **predictive capability**

  - FFs can have different distributions even when the g.s. deformations coincide
  - Angular momenta can be **highly asymmetric** between the FF partners

- For the most likely fragmentation, very good agreement with TDHFB (Bulgac *et al.*)

  $J_H/J_L = 5.8(0.4)\hbar/11.1(0.2)\hbar$ [This work]

  $J_H/J_L = 5.8(0.5)\hbar/9.4(0.4)\hbar$ [TDHFB]   <u>Warning</u>: Theoretical uncertainties aren't full nor equivalent

Angular Momentum of Fission Fragments
Average AM are consistent with a sawtooth pattern

Average AM of FFs in ^{239}Pu(n_{th},f)

- AM and deformation of FFs **at scission** are correlated
  - Heavy FFs display a wide range of AM
  - **Shell effects** at scission determine the AM of FFs, hindering their values around ^{132}Sn
  - Light FFs are more deformed and typically carry **more** AM
  - This is at odds with phenomenological models (FREYA, CGMF) that have $I_H > I_L \rightarrow J_H > J_L$
- Microscopic distributions can be used as inputs to FREYA simulator
  - Statistical photons carry away much more than 1$\hbar$
  - Distributions are **consistent with a sawtooth pattern**
  - Neutron and photon multiplicities are modified in comparison to default FREYA distributions
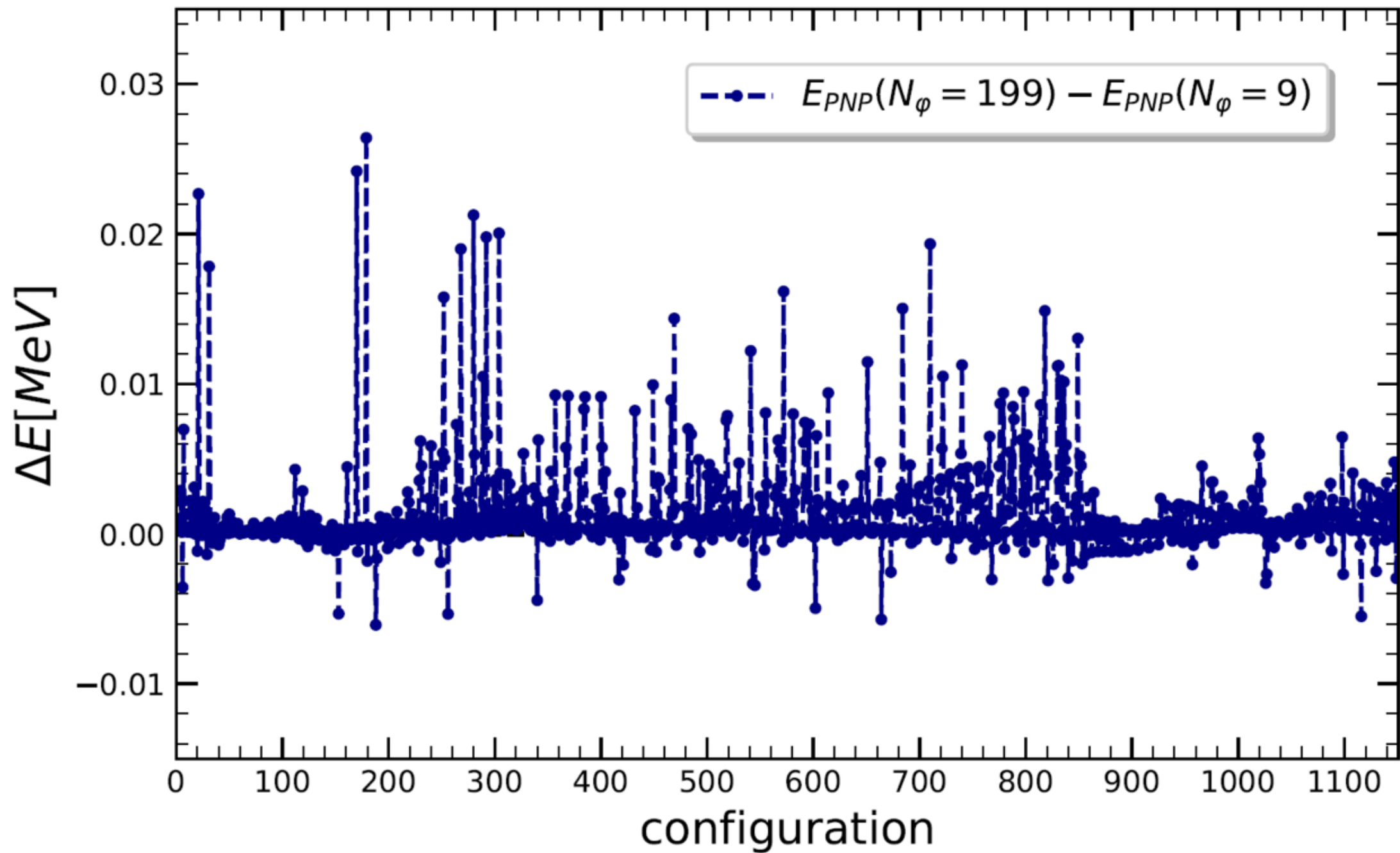
Conclusion

Conclusion

- Symmetry restoration is a promising tool for extending fission models
  - ✔ Symmetry-preserving surfaces for an entire range of collective coordinates
  - ✔ Angular momentum of fission fragments from microscopic theory
  - ✔ Number of particles in fission fragments from microscopic theory

- Some open questions and perspectives:

  1) Applicability of the GOA in a symmetry-restored framework?
  2) Calculation of collective inertia from symmetry-restored framework?
  3) The influence on observables (mass/charge distributions, SF half-lives, …)?
  4) The influence of EDF vs Hamiltonian distinction and possible divergences?
  5) A proper definition of scission configurations?
  6) Dynamical extension of the static HFB model of AM in FFs (TDGCM+GOA)?
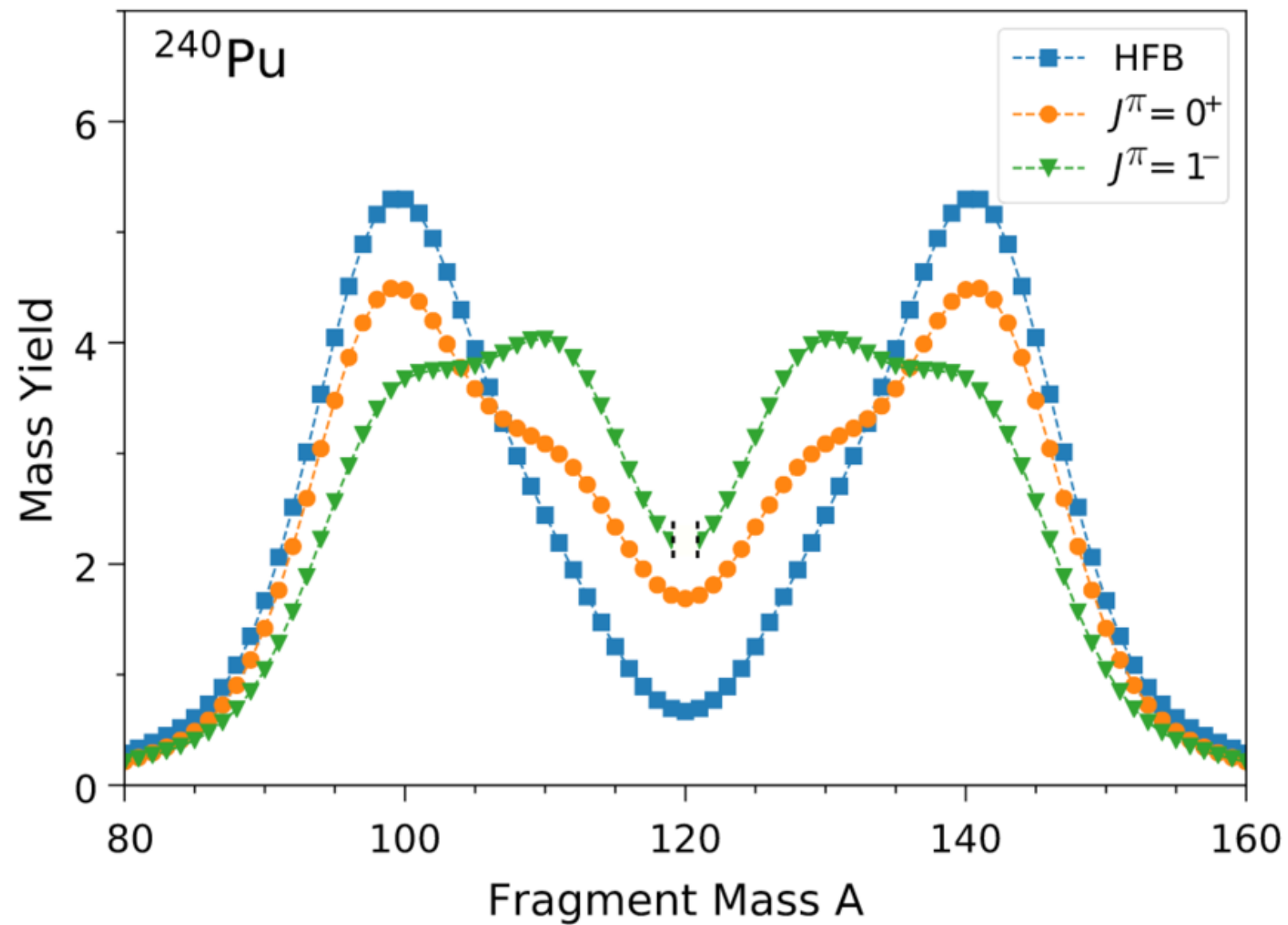 7) Extension of the TDHFB model to other fragmentations?
      … ?

Backup

Convergence of PNP energies

Fragment mass distributions from different PES