ESNT Workshop “Dynamics of Nuclear Fission”
CEA Paris-Saclay, Orme de Merisiers
December 16-19, 2024

Angular momentum distributions in fission fragments from microscopic theory

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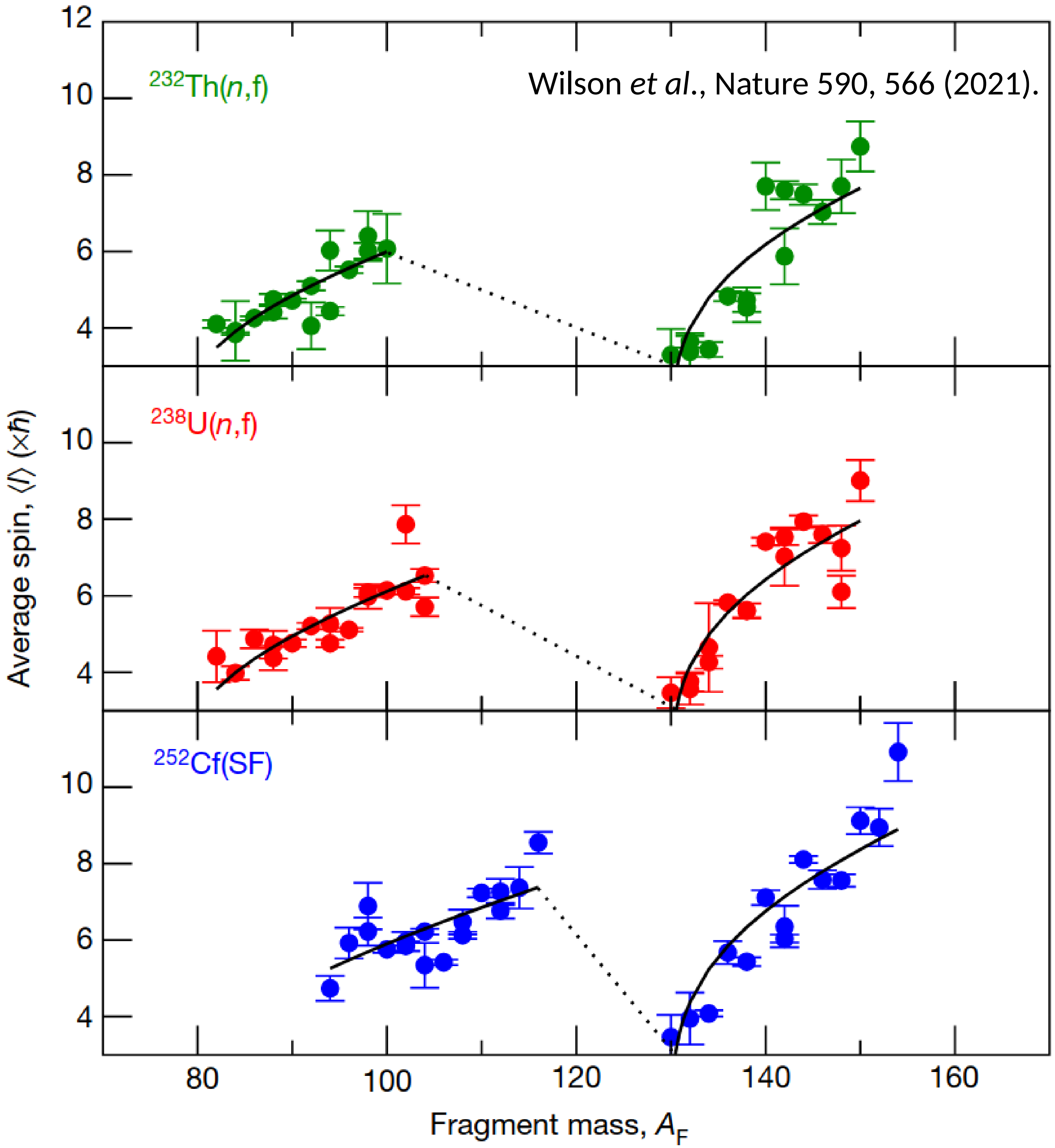
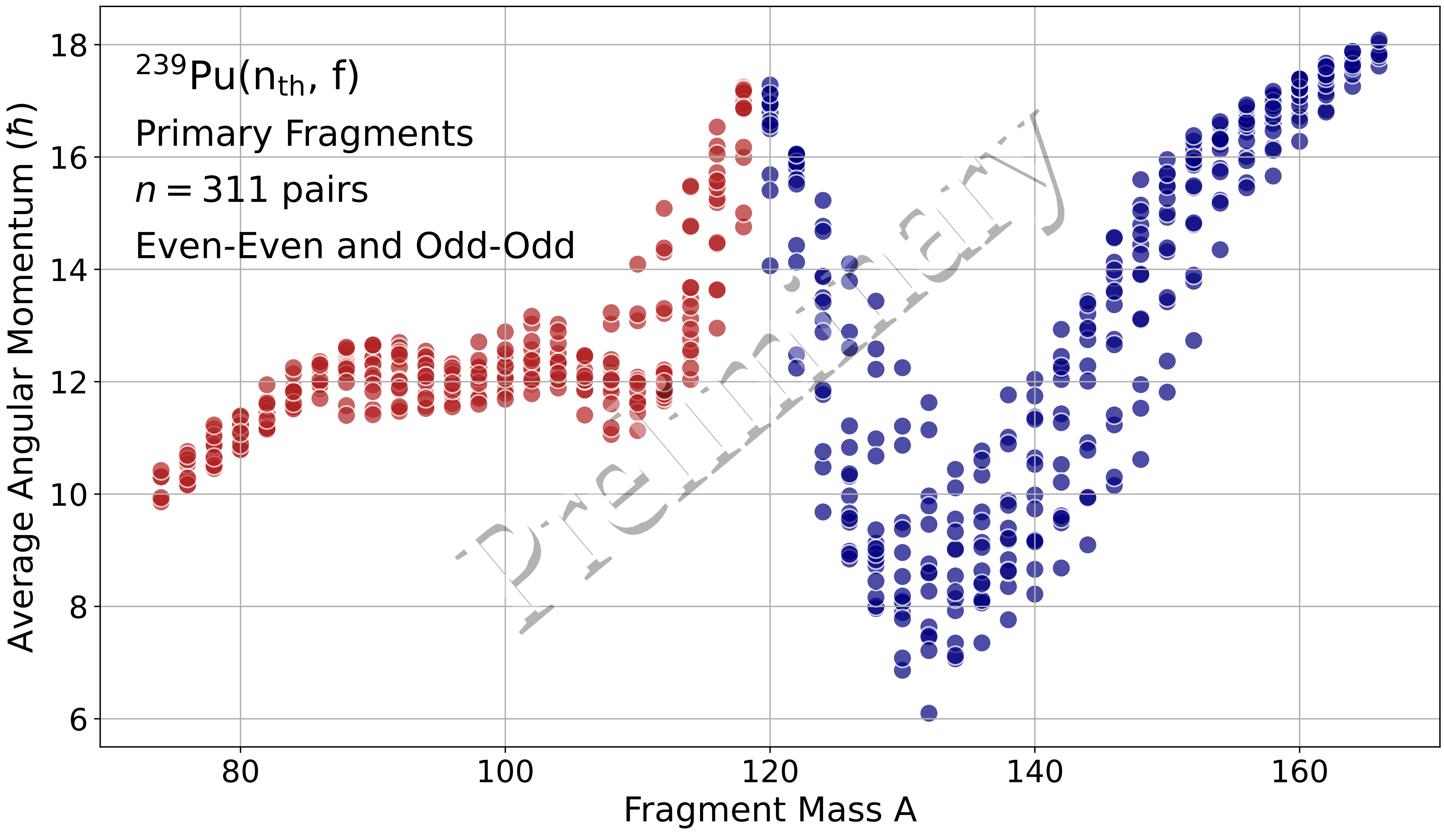
Experiments established a universal sawtooth pattern



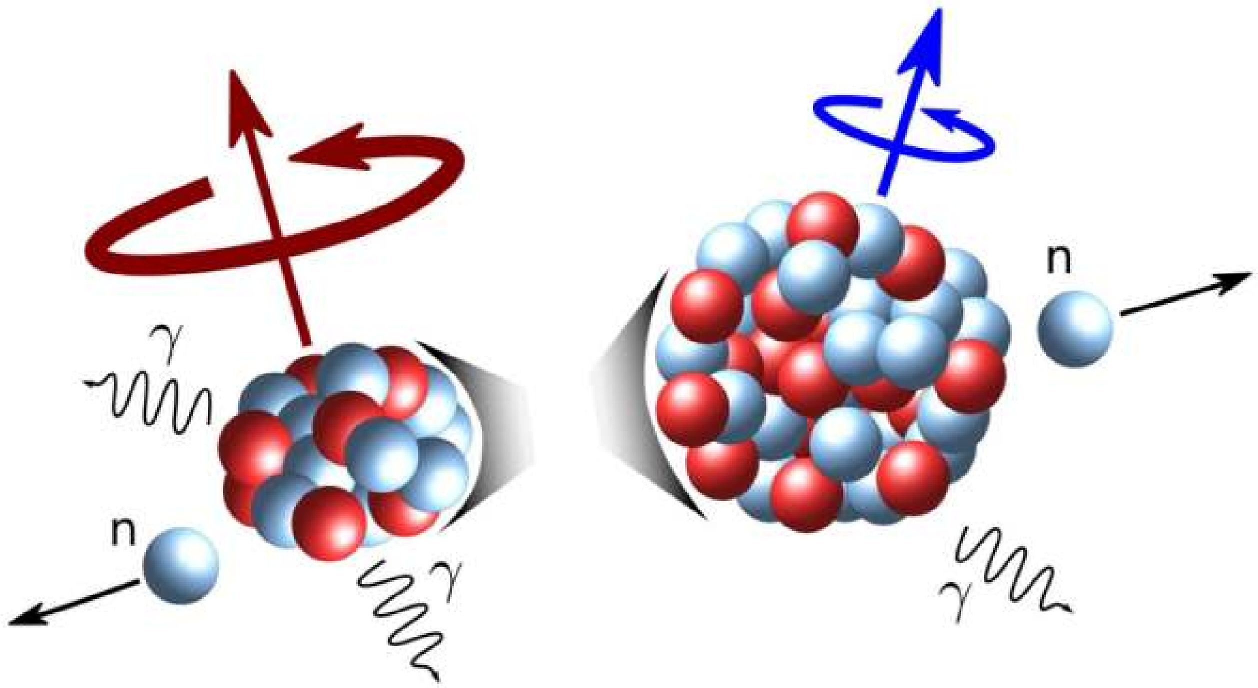
Microscopic calculations predict the sawtooth pattern



Outline

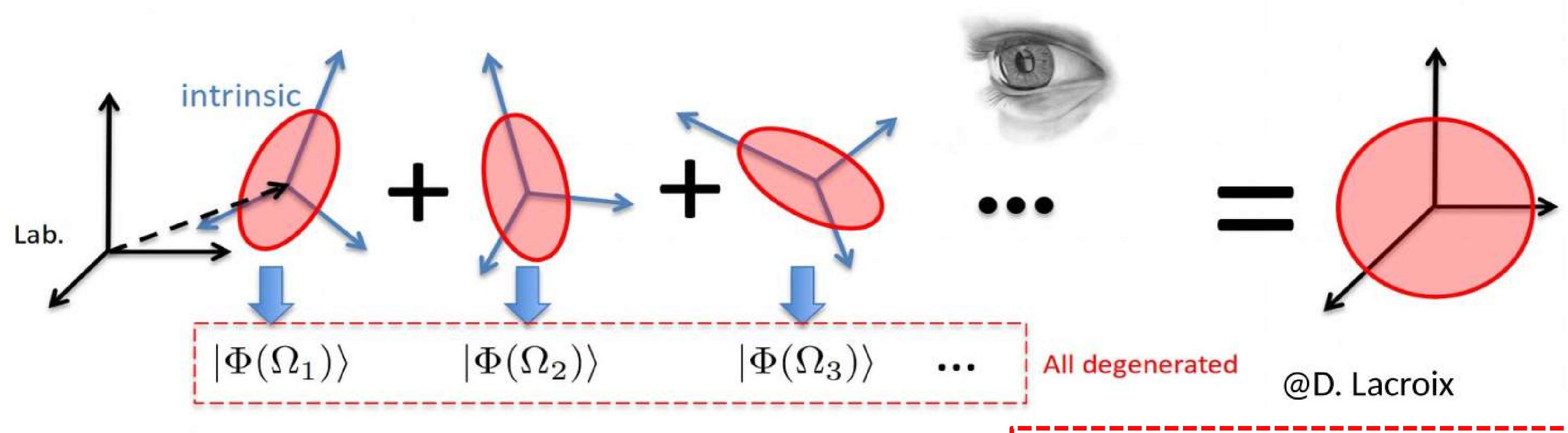
Introduction
Properties of fission fragments

- Fission fragments (FFs) at scission are hot, deformed, and rotating
  - High excitation energy (up to 30 MeV)
  - Large deformation, typically different from the g.s. deformation
  - Distribution of angular momentum (AM)
- Angular momentum of FFs influences the remainder of the process
  - Causes anisotropy in neutron emission
  - Modifies the number of emitted photons and, to a lesser extent, neutrons
  - Impacts population of isomeric states in products
  - Essential ingredient for modeling decay of FFs



Introduction
Angular momentum of fission fragments

- In the past few years, the study of AM of FFs has experienced a *renaissance*
  - High resolution measurements at ALTO confirmed sawtooth-like mass dependence
  - Many theoretical studies by several groups, both microscopic and statistical models
  - Microscopic studies are largely based on applying projection techniques to FFs



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

- Several questions are under discussion

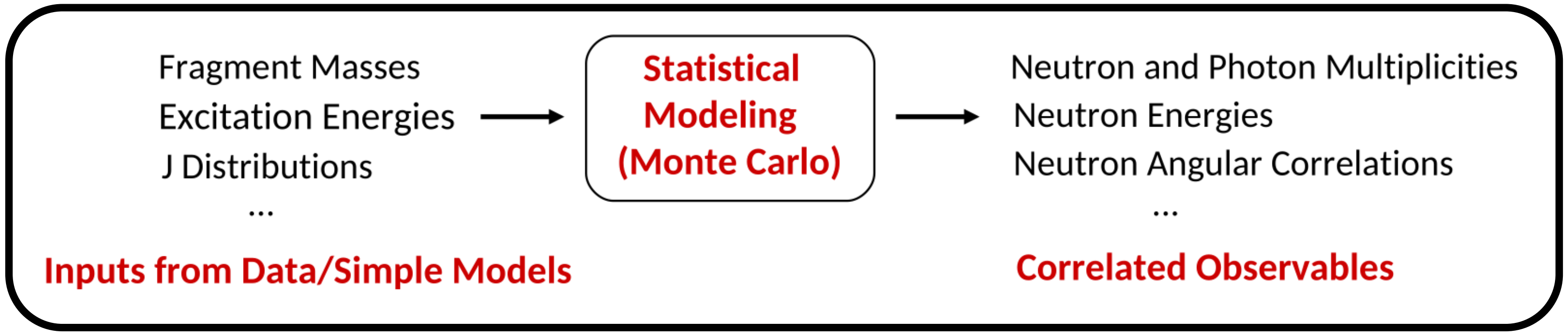
  1) What is the mechanism of generation of AM in FFs?
  2) How are the AM of FFs correlated in magnitude and direction?
  3) How does the sawtooth pattern emerge from (microscopic) theory?
  4) How to obtain (microscopic) distributions for the full range of FFs?

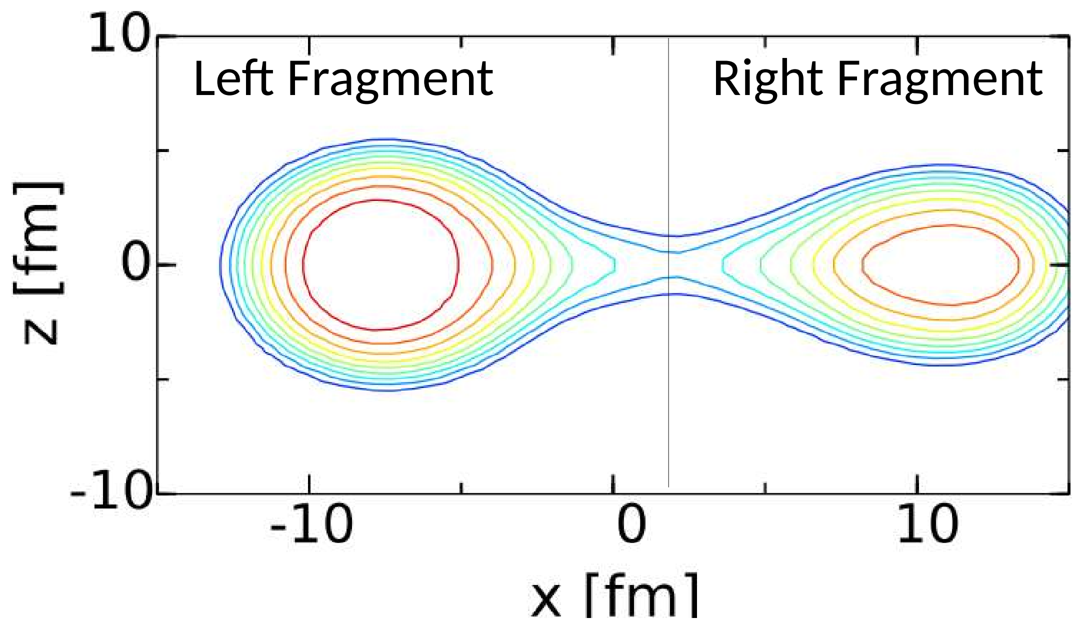
Introduction

The 2021 model in a nutshell

- A microscopic model of how the AM of FFs changes with their mass
  1) Define a set of scission configurations (constrained Hartree-Fock-Bogoliubov)
  2) For each configuration, determine the two FFs via neck position
  3) For each configuration, perform the AM projection in each FF
  4) Use Gaussian process to extract primary FF distributions for integer (N, Z)
  5) Use FREYA to simulate the emission of neutrons and photons

J. Randrup and R. Vogt, PRC 80, 024601 (2009).





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

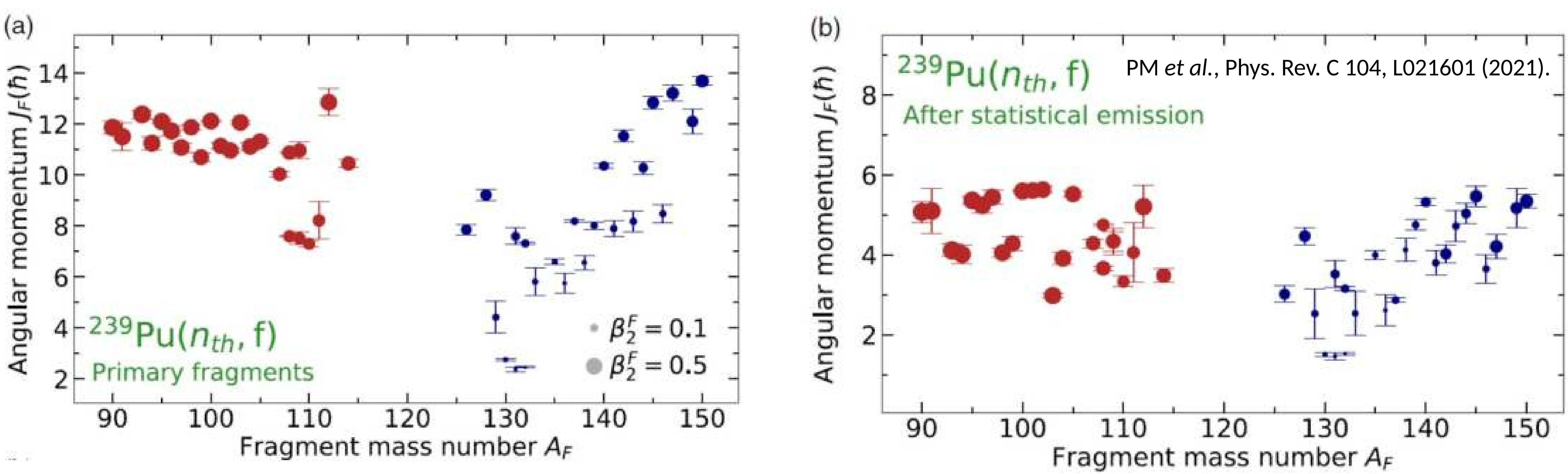
$$\hat{R}_y^F(\beta) = \exp(-i\beta\hat{J}_y^F)$$

PM, N. Schunck, J. Randrup, R. Vogt, PRC 104, L021601 (2021).

Introduction

Lessons and limitations of the 2021 study

- We extracted AM distributions for 26 pairs of FFs
  - Average AM values were consistent with the sawtooth pattern
  - Light FFs are more deformed and on average carry more AM (also Bulgac *et al.*)
  - Statistical photons take away more than 1ħ of AM (also Stetcu *et al.*)
  - Microscopic distributions modify photon multiplicities (FREYA)
- The model had several important limitations
  - Only a narrow window of FF charges (typically one per A_F)
  - Decay was simulated for a small number of FFs
  - No dynamical population of scission configurations, cold FFs

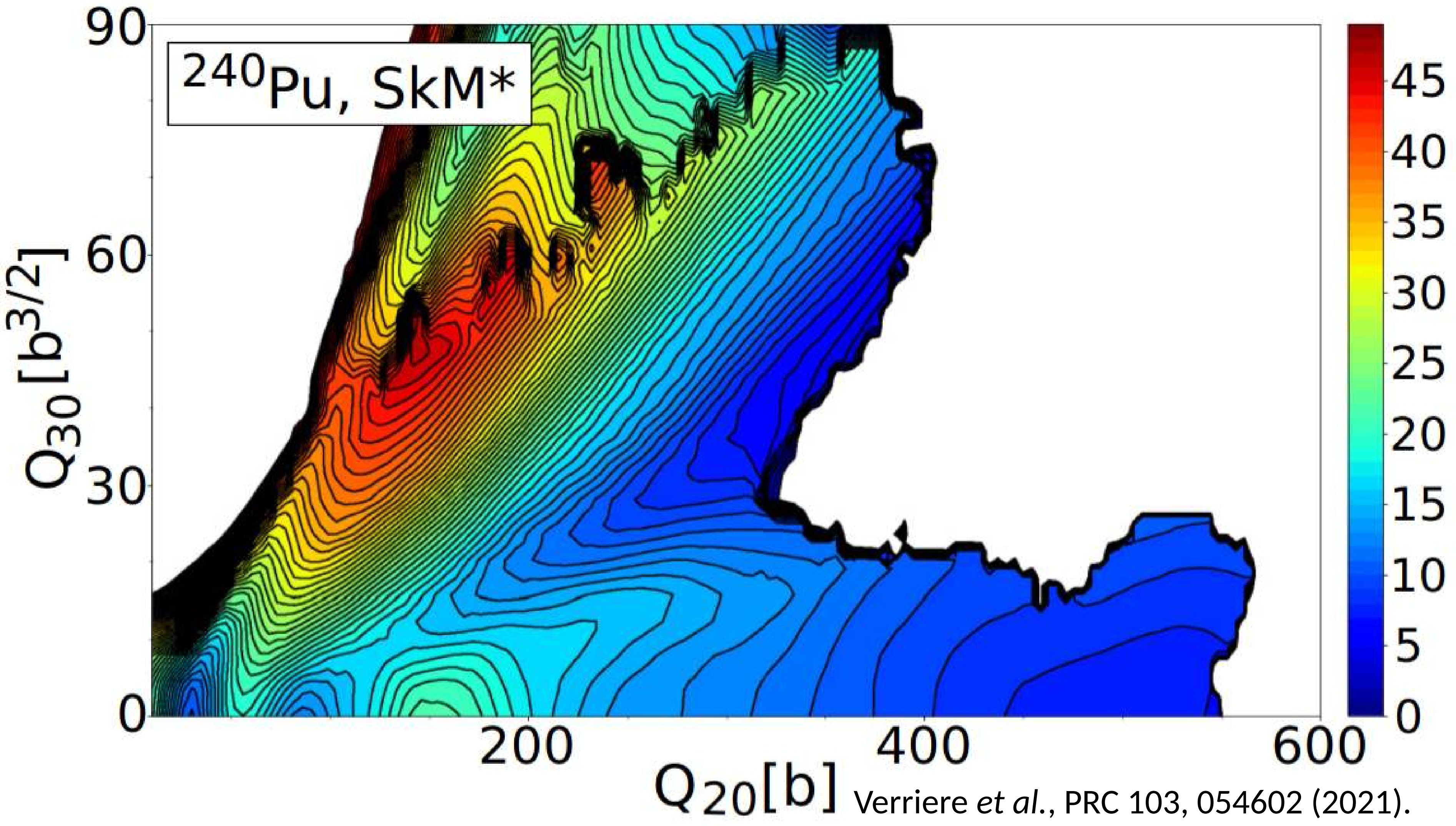


PM *et al.*, Phys. Rev. C 104, L021601 (2021).

Outline

Theoretical Framework
Defining scission configurations

- A set of scission configurations is an essential ingredient of the model
  - Constrained HFB based on global Skyrme EDF, deformed HO basis
  - Axial and time-reversal symmetry are preserved
  - Scission configurations determined through a predefined criterium
  - These are not eigenstates of *J*, *N*, *Z* → projections to obtain distributions



Verriere *et al.*, PRC 103, 054602 (2021).

Theoretical Framework
Quantum number distributions in scission configurations

- AM&PN distributions in configurations are obtained by a quintuple projection
  - Angular momentum projection in FFs
  - Particle number projection in FFs and in the compound nucleus (both isospins)

$$|c_{\boldsymbol{q}}^{J_F;N_F Z_F;NZ}|^2 = \langle \Phi_{\boldsymbol{q}} | \hat{P}^{J_F}_{00} \hat{P}^{N_F} \hat{P}^{Z_F} \hat{P}^{N} \hat{P}^{Z} | \Phi_{\boldsymbol{q}} \rangle$$

  - Projection operators have a standard form, relevant operators redefined in FFs

For example, in AMP: $J_y^F(\boldsymbol{r}, \sigma) = \Theta^{F*}(z - z_N) J_y(\boldsymbol{r}, \sigma) \Theta^F(z - z_N)$

- The result is a probability function at each scission point $\boldsymbol{q}$:

$$|c_{\boldsymbol{q}}^{J_F;N_F Z_F;NZ}|^2 \rightarrow \mathbb{P}(J_F, N_F, Z_F \mid N_0, Z_0, \boldsymbol{q})$$

- The model implies several simplifying assumptions
  - AMP for the compound nucleus and relative motion are neglected
  - Only $K = 0$ excitations are assessed
  - FFs are excited due to deformation, no thermal excitations

Theoretical Framework

Probability of populating scission configurations

- Nuclear dynamics is simulated with the adiabatic TDGCM+GOA
  - Wave function is a superposition of many-body HFB states

$$|\Psi(t)\rangle = \int d\boldsymbol{q}\, f_{\boldsymbol{q}}(t)\, |\Phi_{\boldsymbol{q}}\rangle$$

  - Gaussian overlap approximation (GOA) yields a Schrödinger-like equation

$$i\hbar \frac{\partial}{\partial t} g_{\boldsymbol{q}}(t) = \mathcal{H}^{\text{coll}}_{\boldsymbol{q}}\, g_{\boldsymbol{q}}(t)$$

  - Probability that the wave packet exits through point $\boldsymbol{q}$ is proportional to the time-integrated flux density

$$F(\boldsymbol{q}) = \lim_{t \to \infty} \int_{\tau=0}^{\tau=t} d\tau\, \phi(\boldsymbol{q}, \tau)$$

D. Regnier *et al.*, PRC 93, 054611 (2016).

  - This gives the probability of populating each scission configuration

Theoretical Framework

Obtaining final distributions

- Final distributions in FFs are obtained by folding the two probabilities

$$\mathbb{P}(J_F, N_F, Z_F \mid N_0, Z_0) = \int d\boldsymbol{q} F(\boldsymbol{q}) \mathbb{P}(J_F, N_F, Z_F \mid N_0, Z_0, \boldsymbol{q})$$

  - Distributions are normalized to 1 and cover the full range of N_F and Z_F
  - Fixing (N_F, Z_F) gives the AM distribution in FF
  - Marginalization over J_F can give pre-neutron mass and charge yields

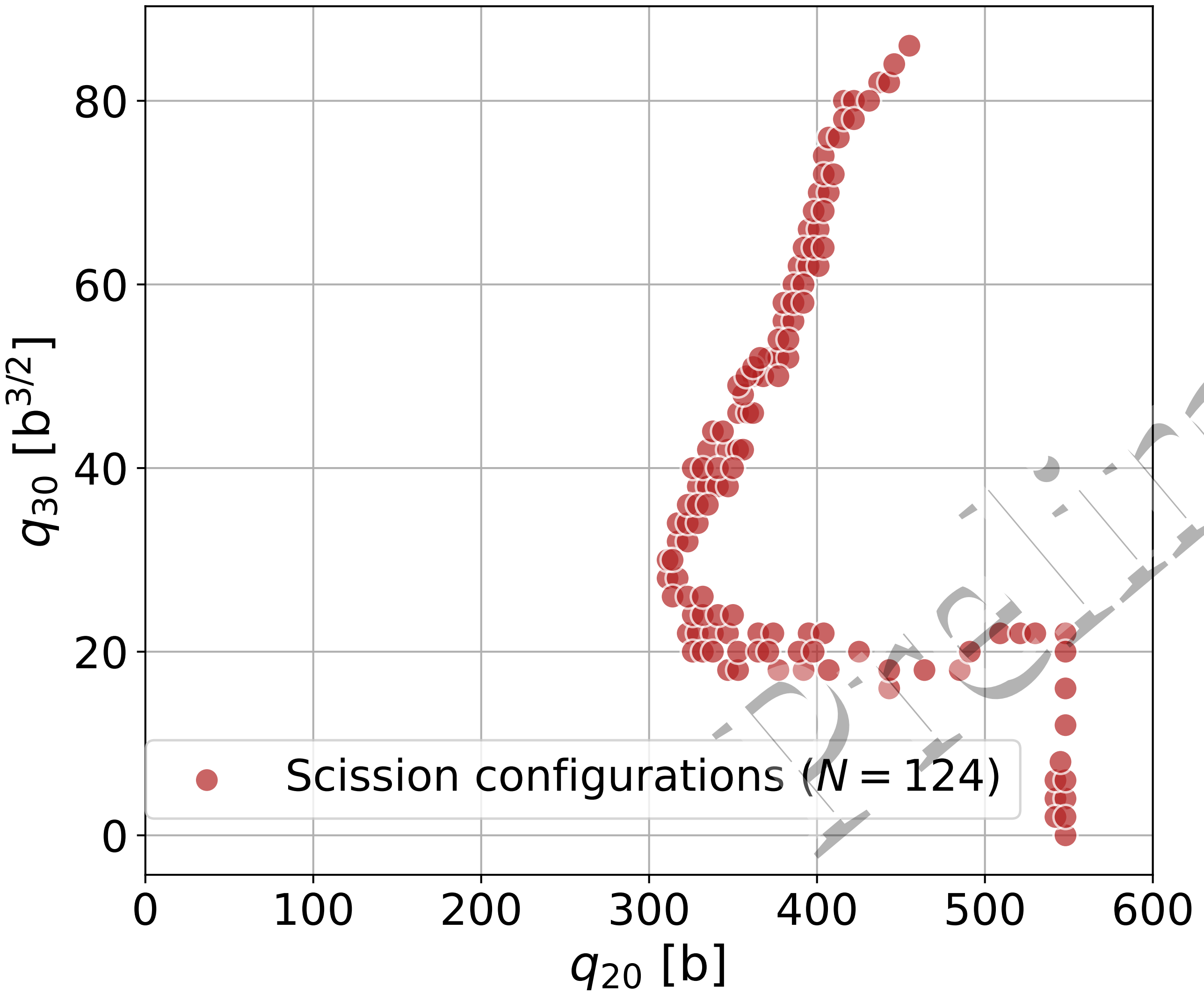
$$\mathbb{P}(N_F, Z_F \mid N_0, Z_0) = \sum_{J_F} \mathbb{P}(J_F, N_F, Z_F \mid N_0, Z_0)$$

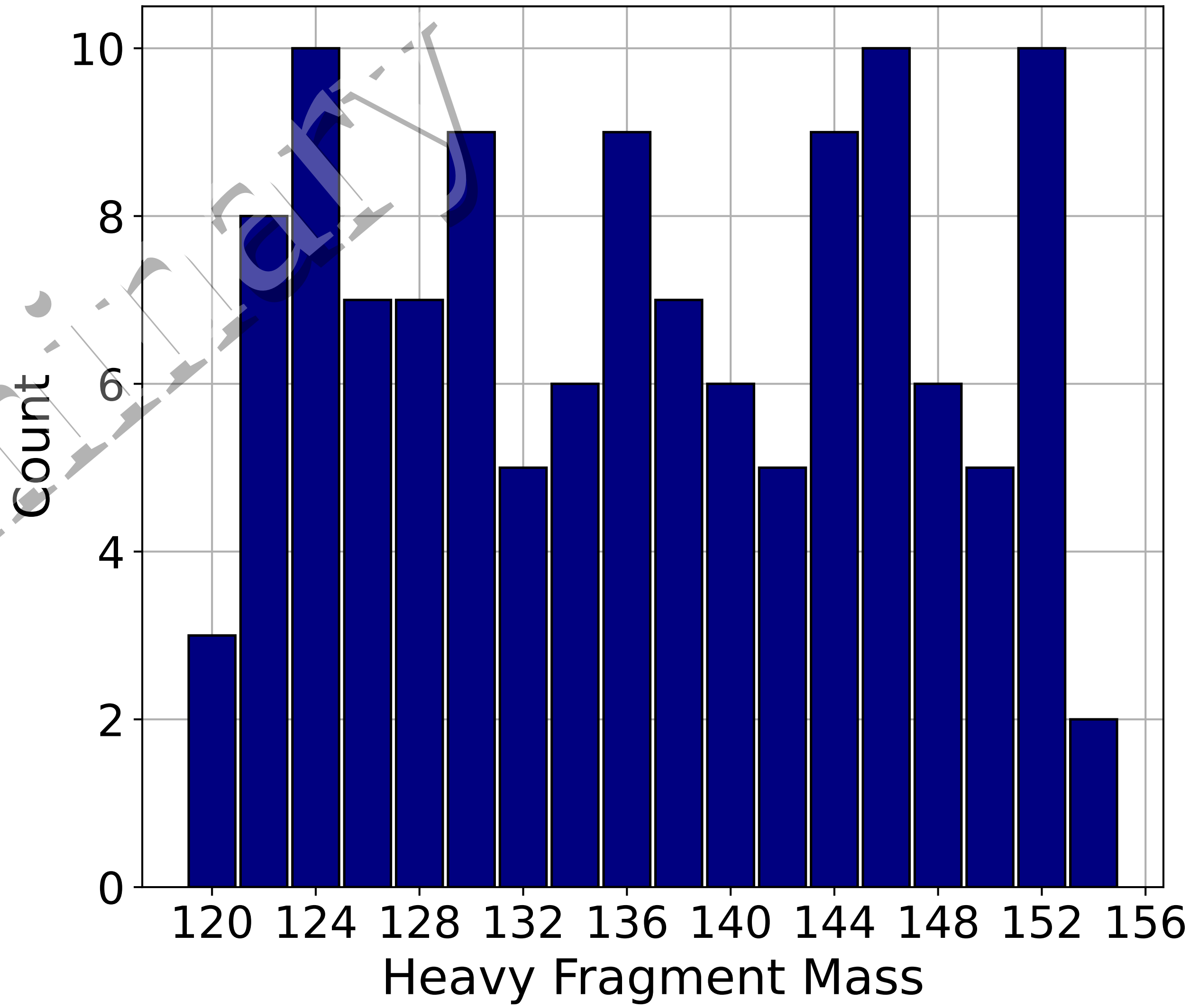
- Properties, extensions and applications of the model
  - Dependence on incident neutron energy by modifying initial conditions
  - Inclusion of intrinsic excitations (finite temperature framework?)
  - Goal: simulating FF decay using consistent microscopic inputs ($Y(A,Z)$, J^{π}, ...)
  - We plan to calculate ^{239}Pu(n_{th},f) and ^{235}U(n_{th},f) and release the data

Outline

Preliminary Results
Calculation parameters

- Calculations were performed using HFBTHO and FELIX programs
  - ^{239}Pu(n_{th}, f), SkM* EDF, deformed HO basis with ~1200 states from 30 shells
  - Preliminary set: 124 scission configurations with a wide range of FF masses
  - AMP with 64 angles, PNP with 31 angles for both isospins
  - TDGCM+GOA in (q_2, q_3) with the initial wave packet energy of 1 MeV above barrier

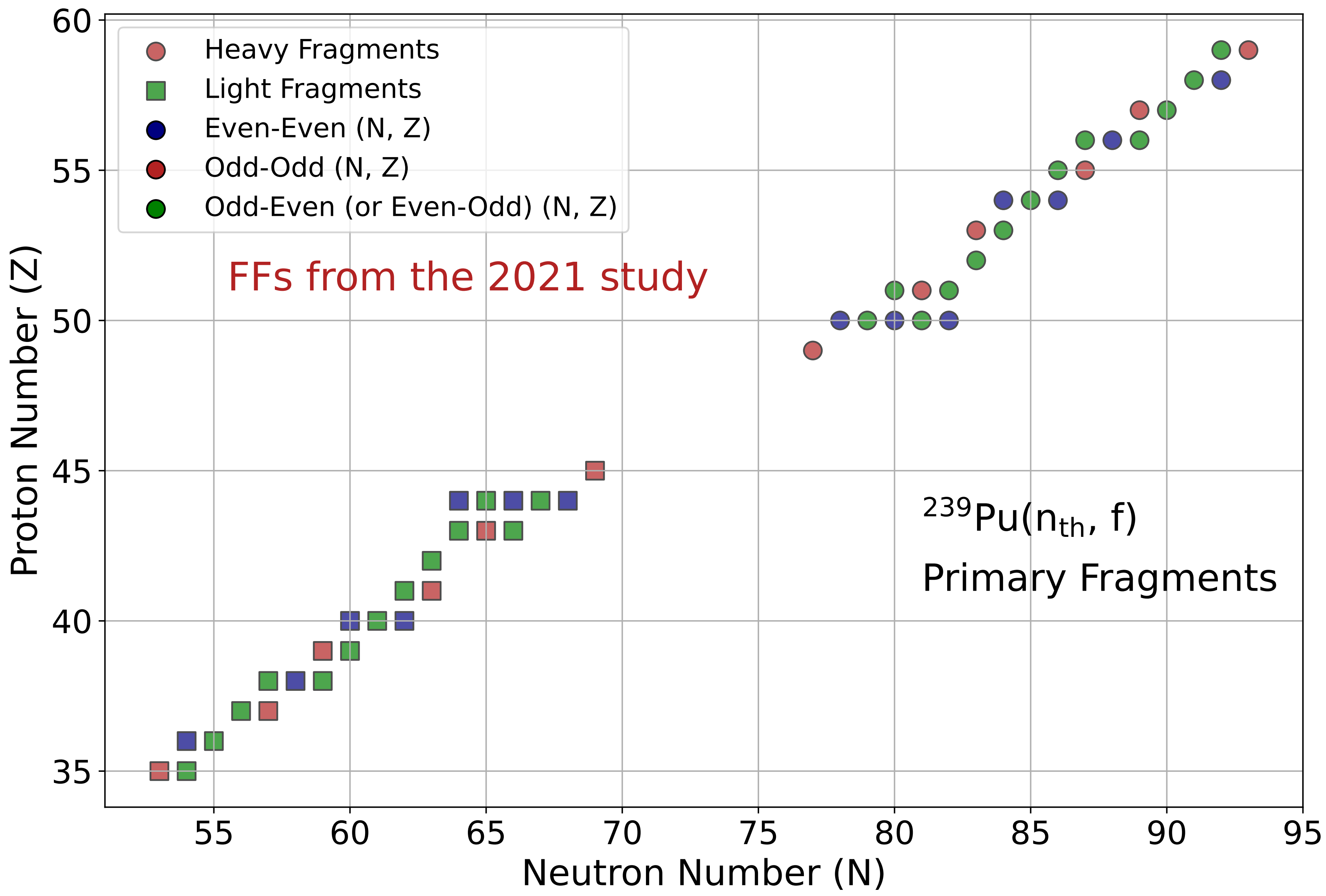




Preliminary Results

Fission fragments in $^{240}Pu^{*}$

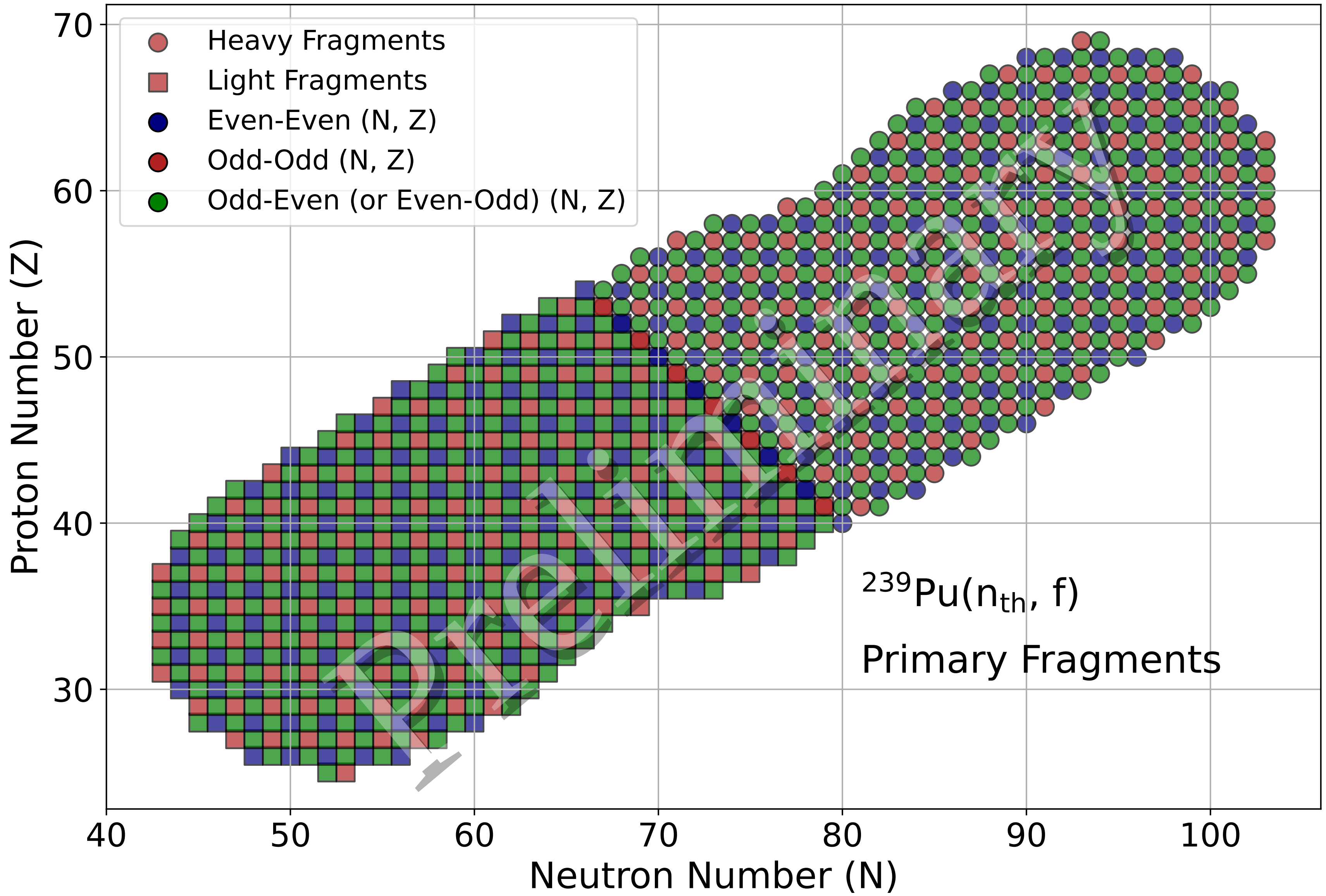
- The result are AM distributions for the full range of FF masses and charges



Preliminary Results

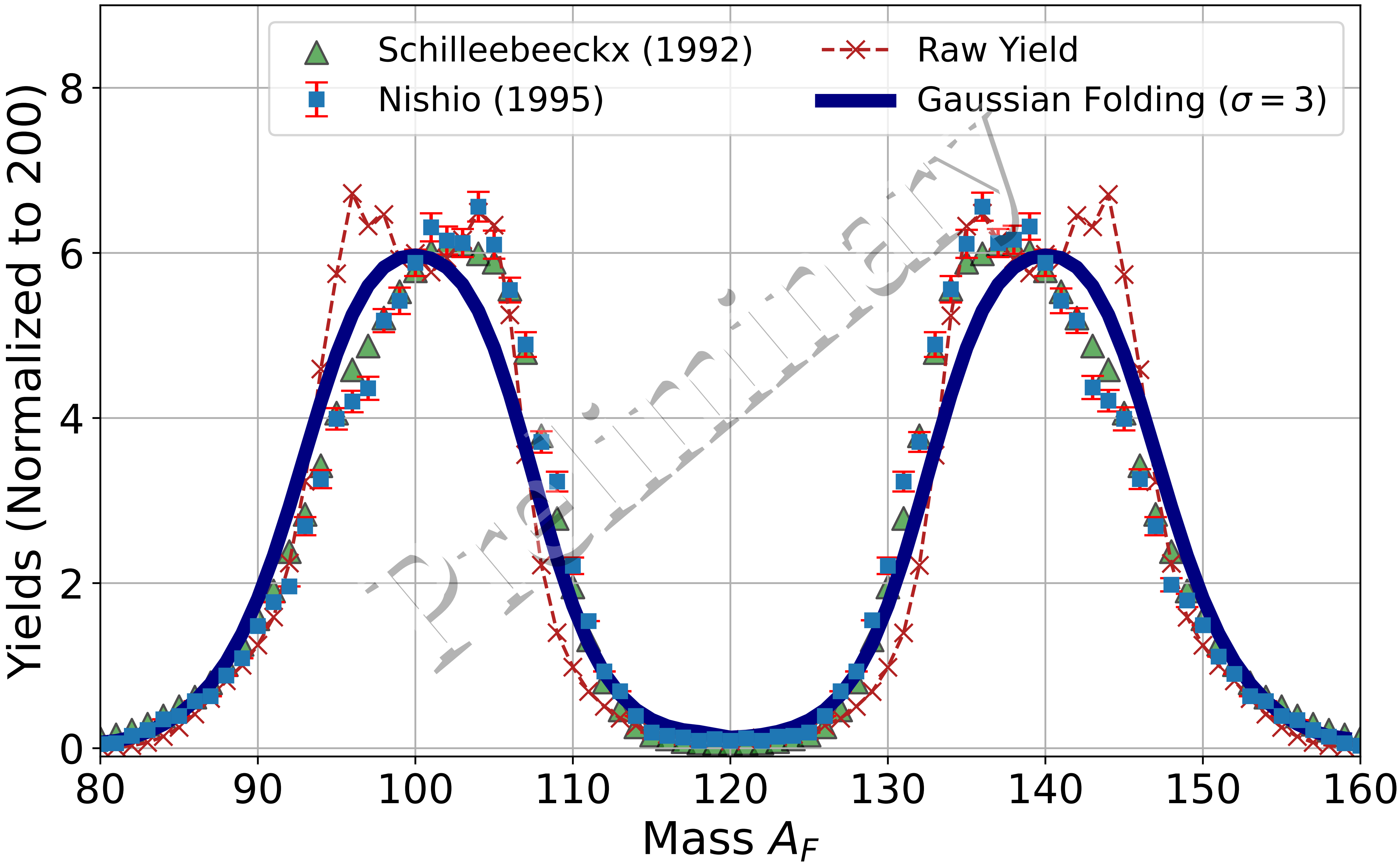
Fission fragments in $^{240}Pu^{*}$

- The result are AM distributions for the full range of FF masses and charges
  - 155 even-even pairs
  - 156 odd-odd pairs
  - 306 odd-even/even-odd pairs



Preliminary Results
Pre-neutron mass yields

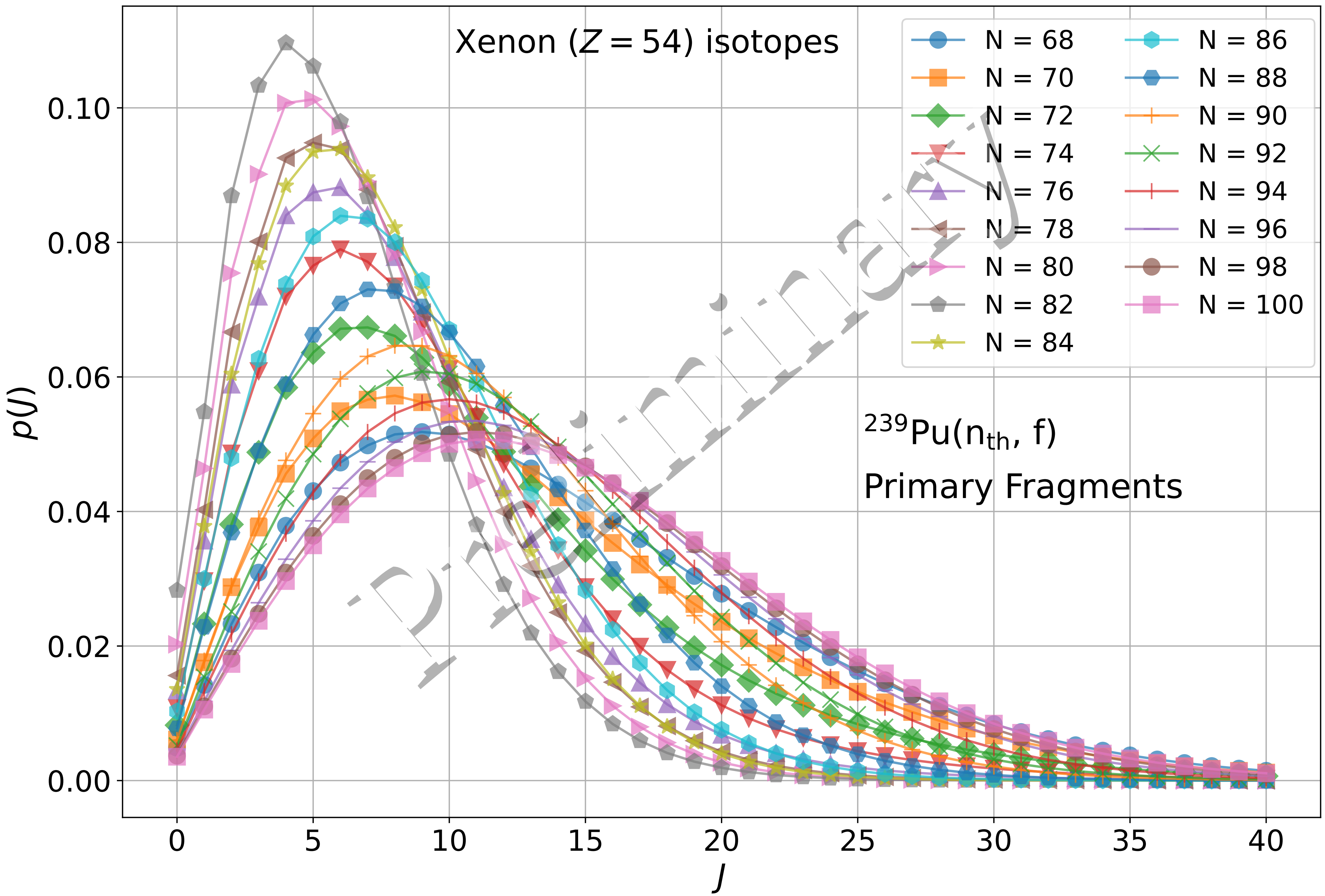
- The model provides pre-neutron mass yields and charge yields



Preliminary Results

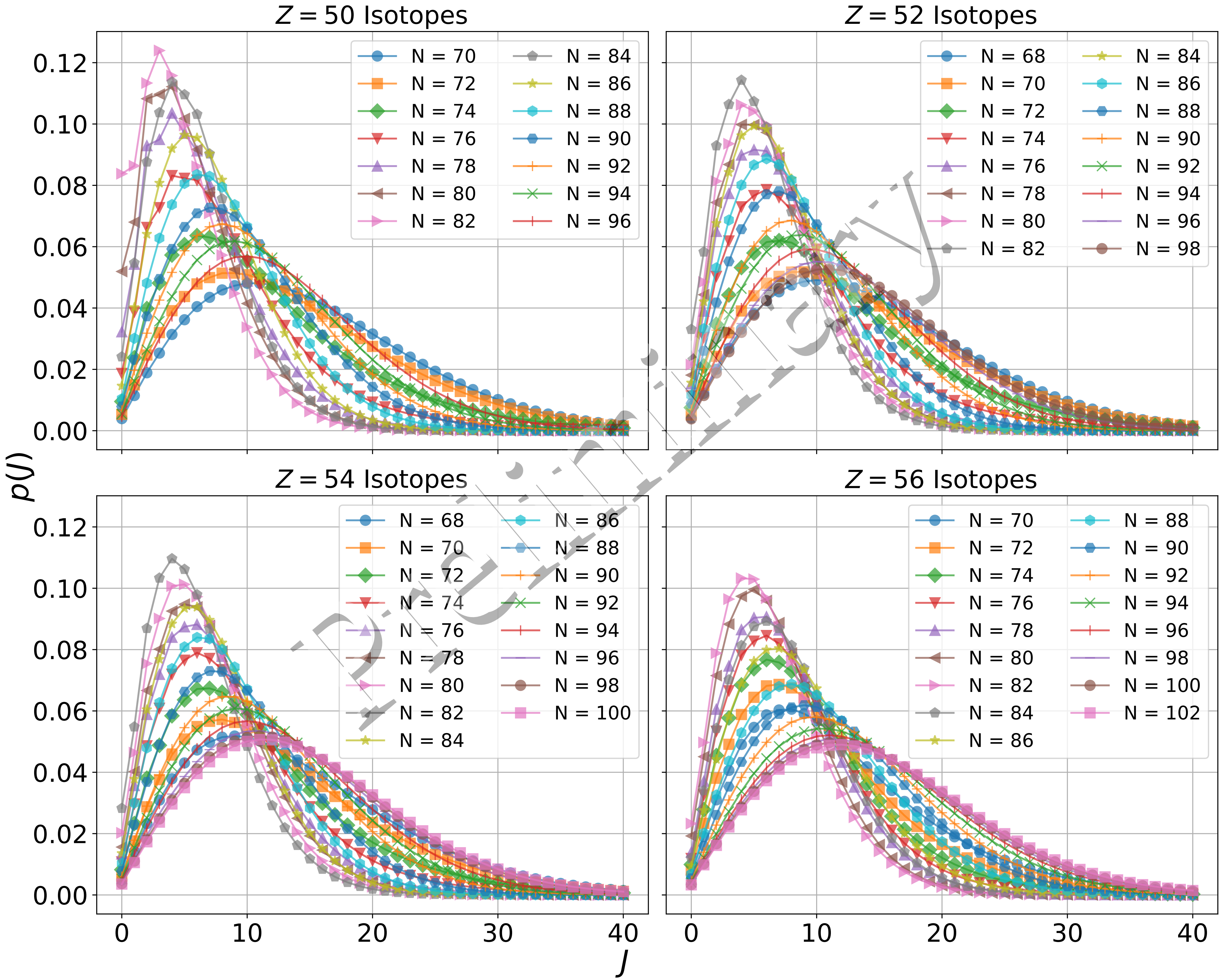
Angular momentum distributions of selected isotopic chains

- The model provides AM distributions for full isotopic chains



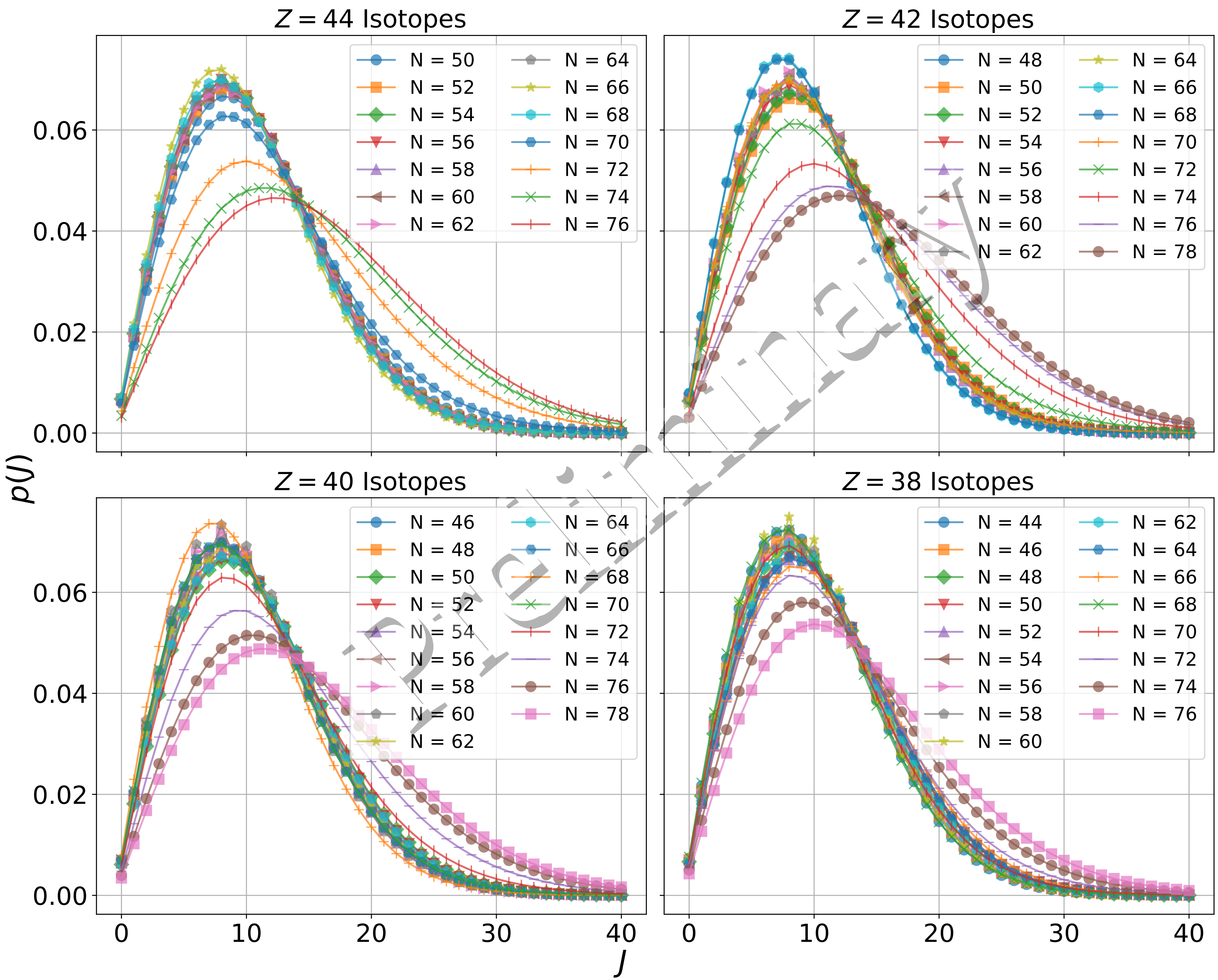
Preliminary Results

Angular momentum distributions of selected isotopic chains



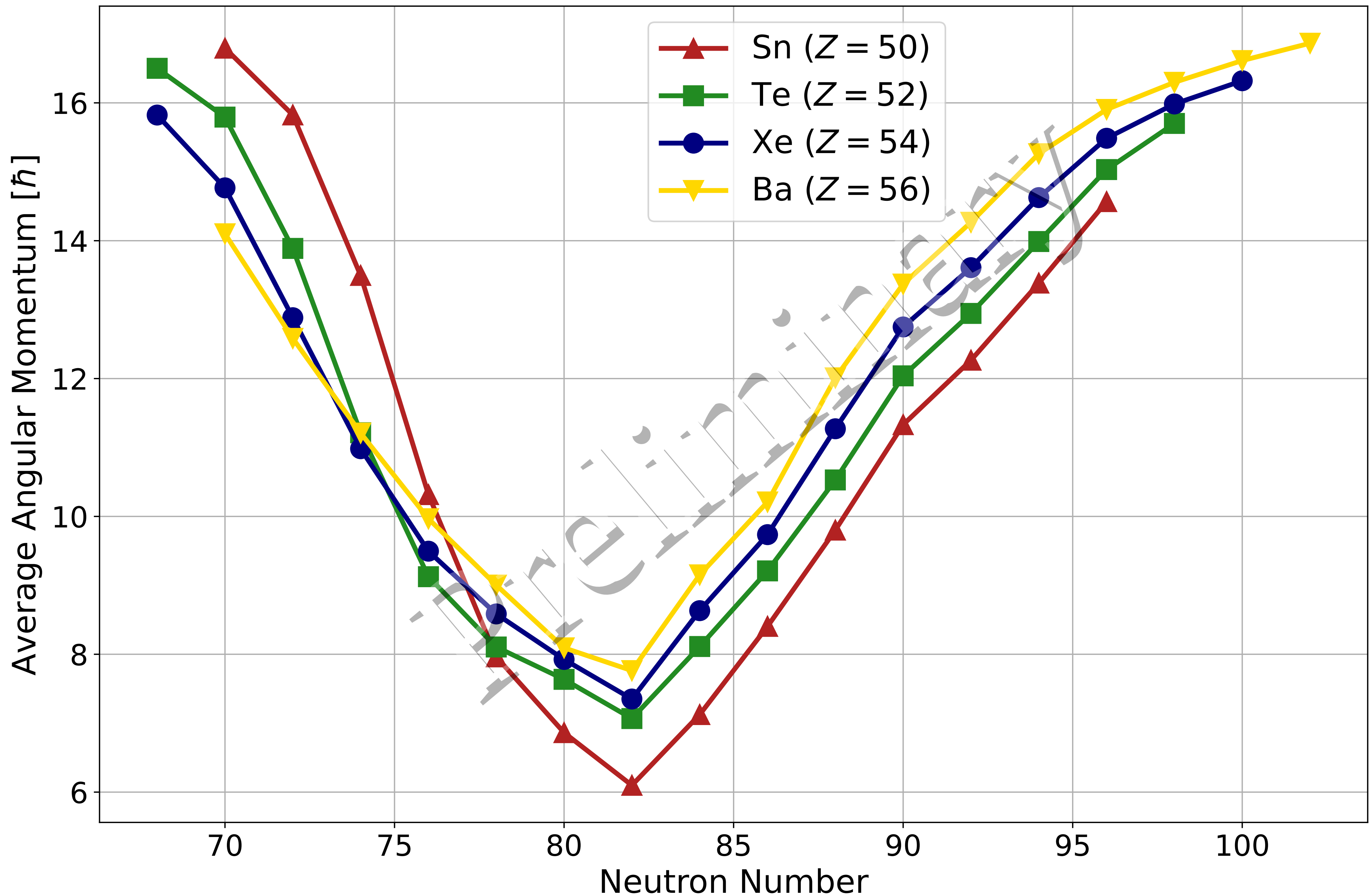
Preliminary Results

Angular momentum distributions of selected isotopic chains



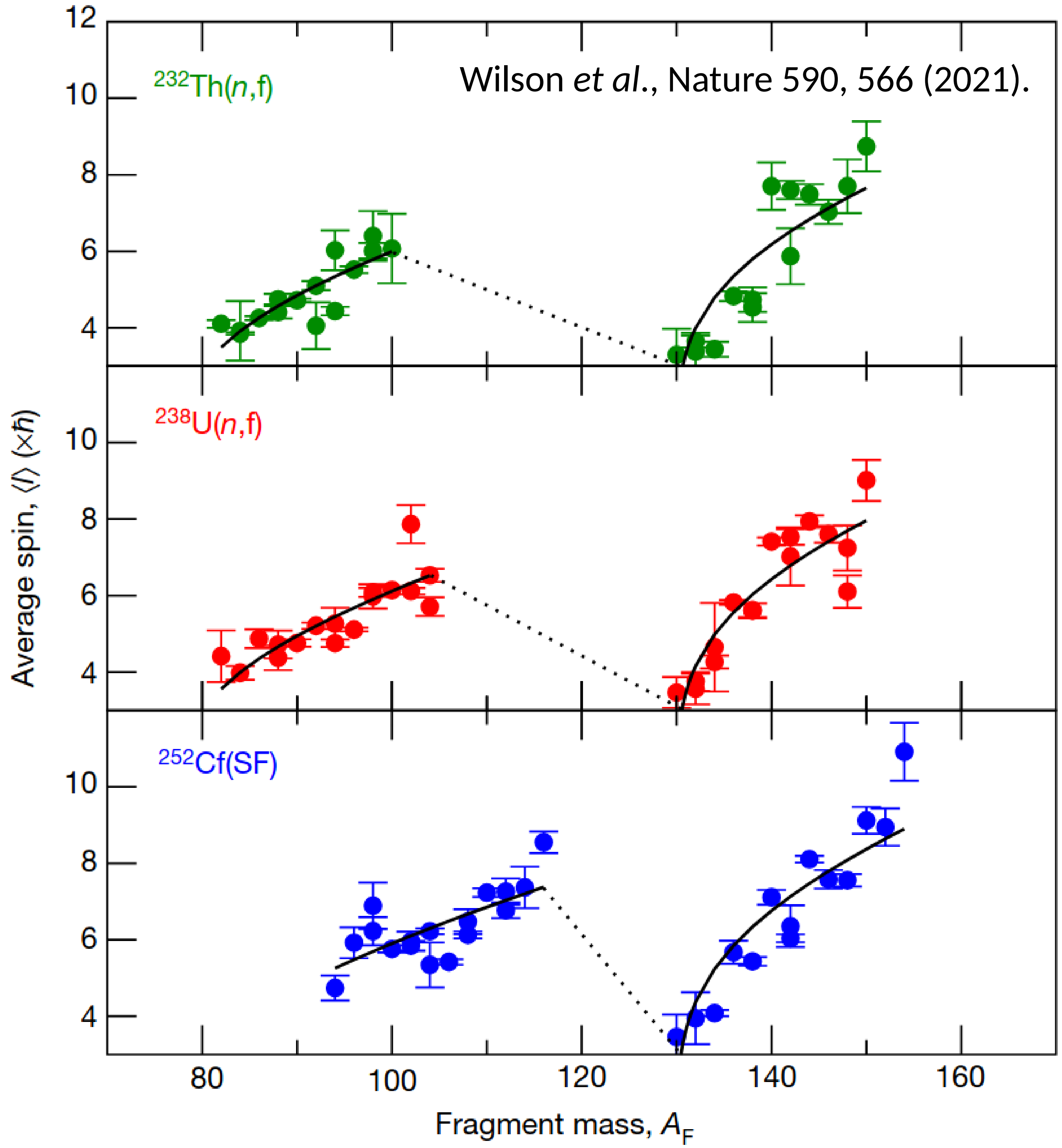
Preliminary Results
Shell effects in average angular momentum values

- The average value is minimal at the N = 82 magic number (shell effects)



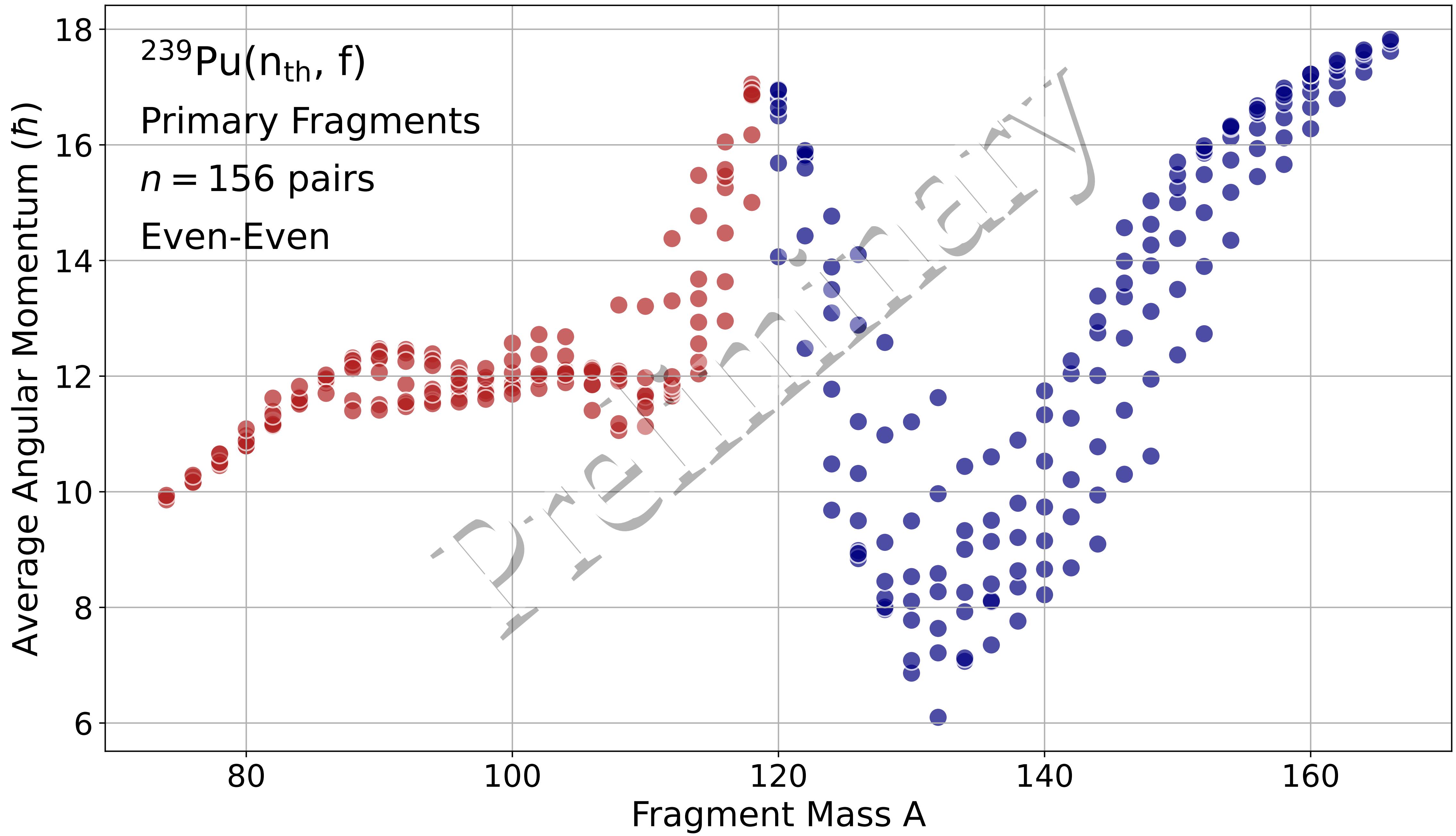
Preliminary Results
The sawtooth pattern

- The experiment established a sawtooth mass dependence (after the neutron emission)



Preliminary Results
The sawtooth pattern

- The model predicts a sawtooth pattern already for the primary FFs
  (Caution: calculated AM are not directly comparable to experimentally inferred values)



Preliminary Results
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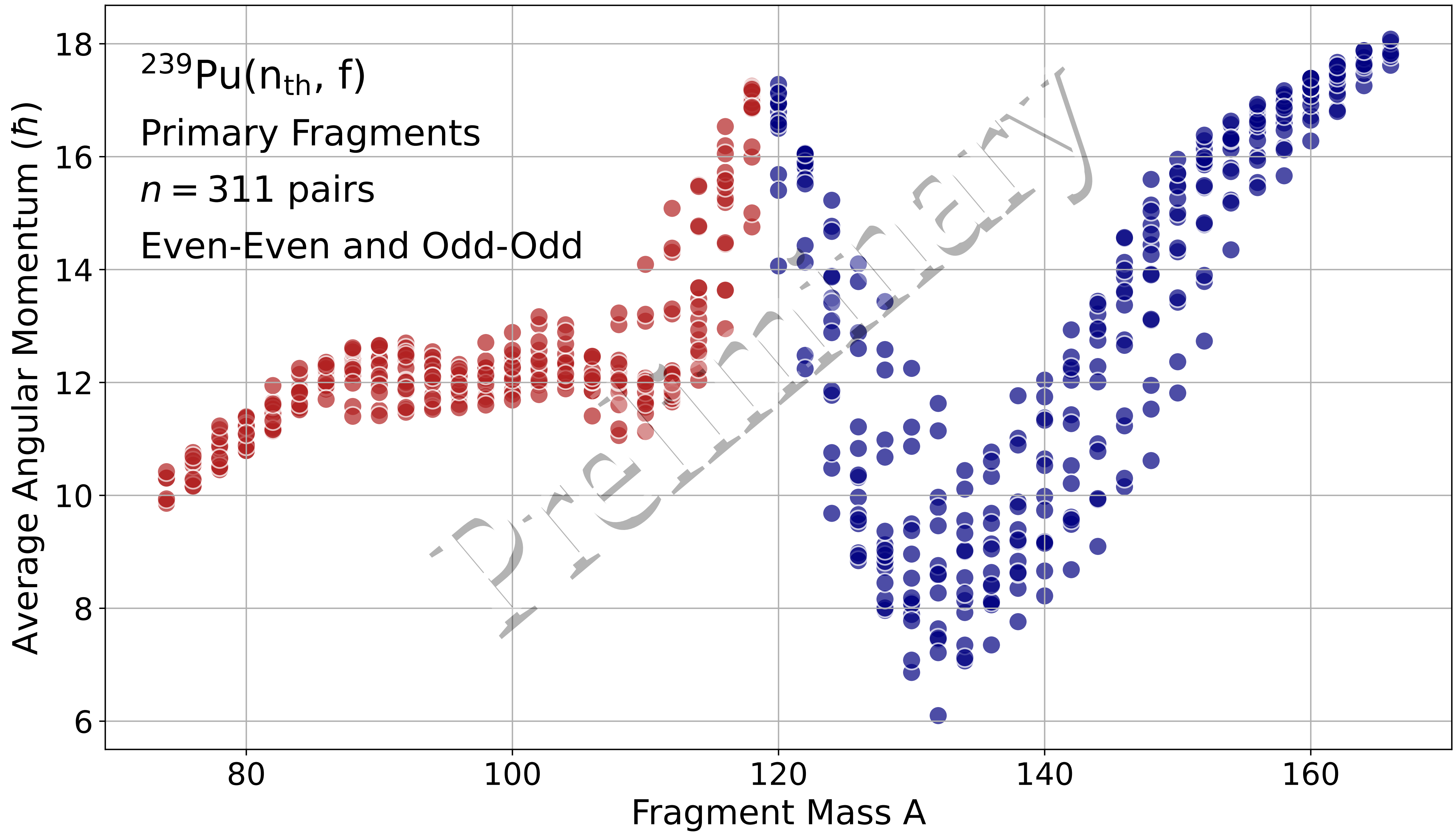
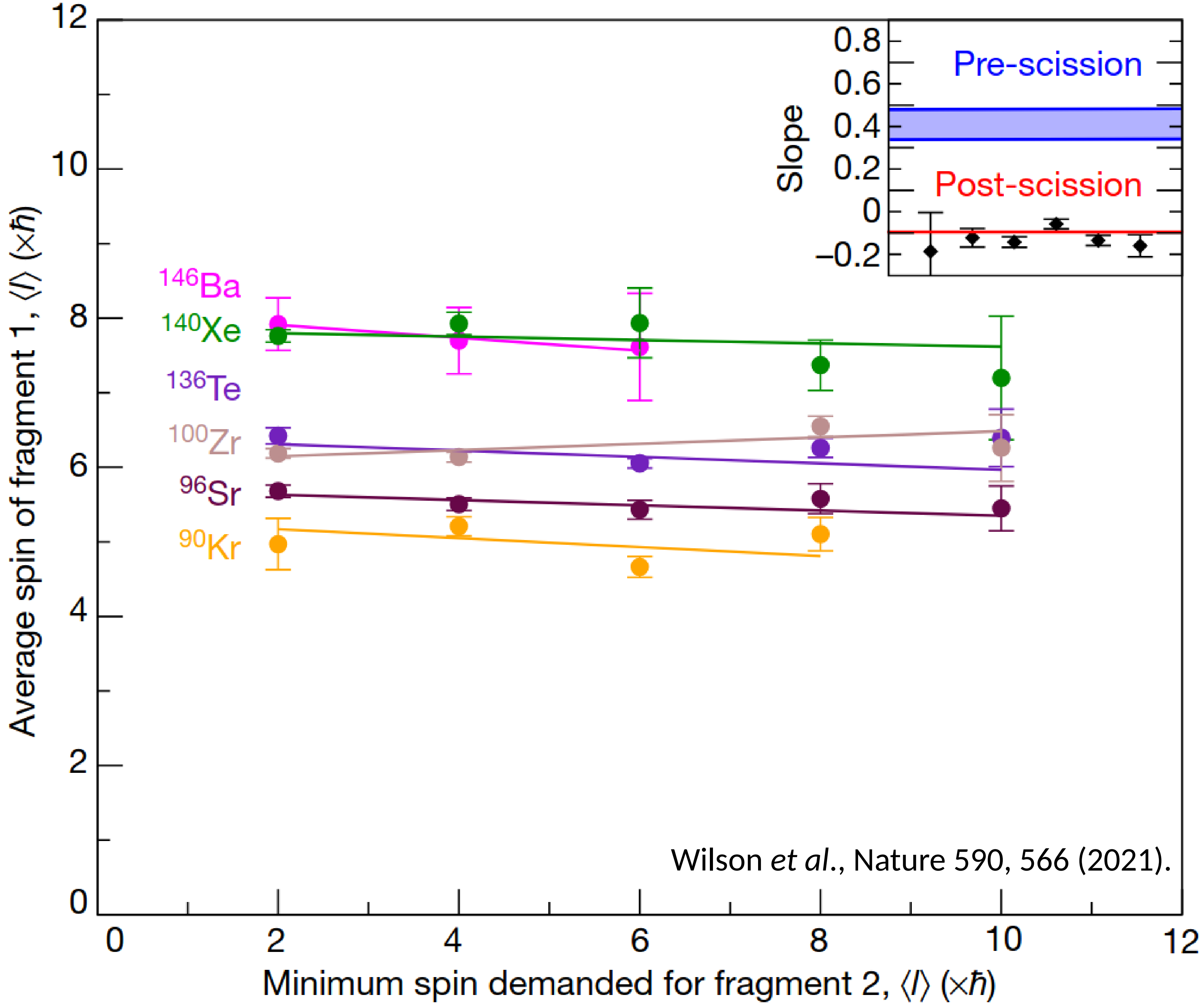


Preliminary Results

Correlation between fragments’ angular momenta

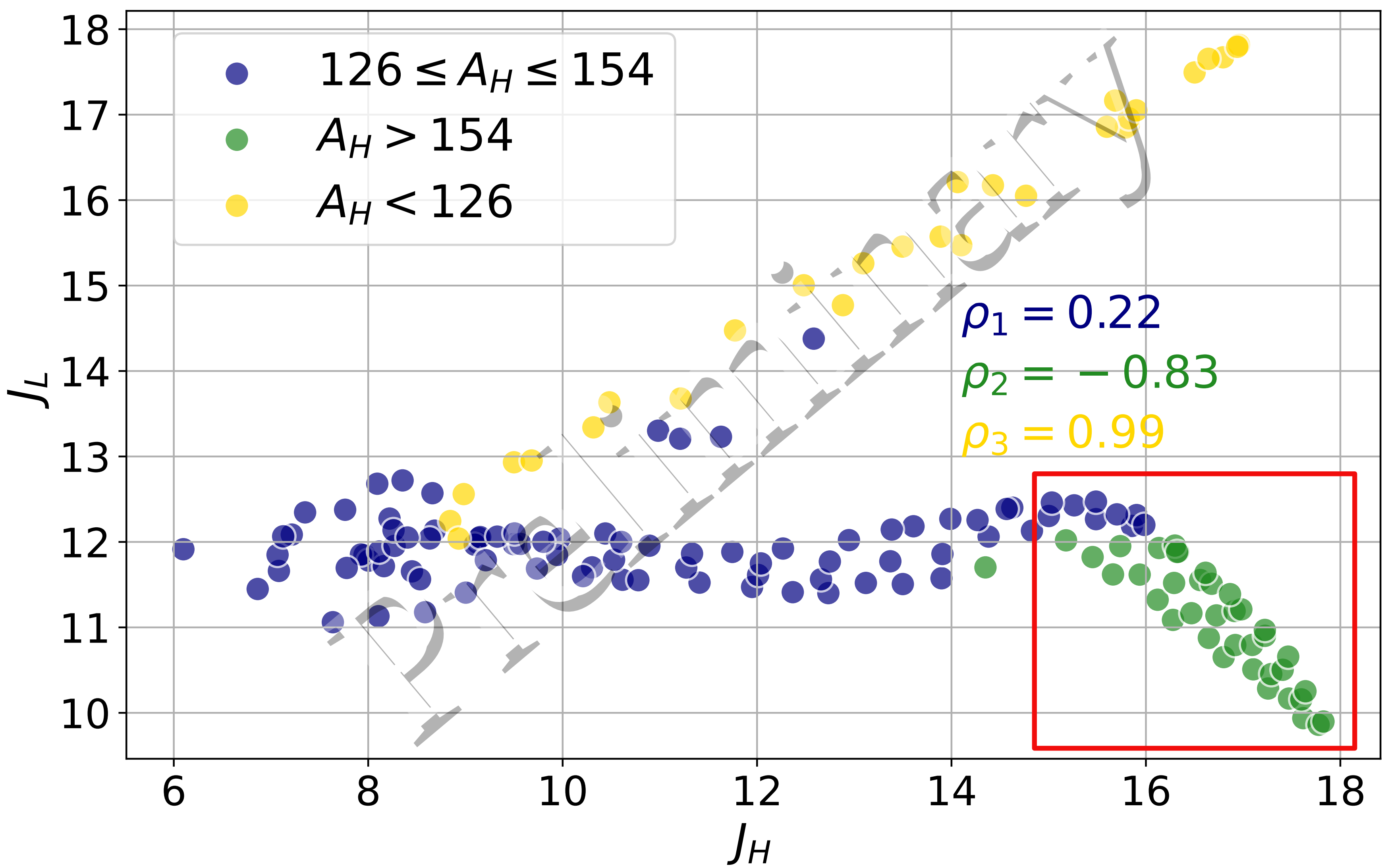
- The experiment observed no correlation in magnitude for “*most strongly populated FFs*”

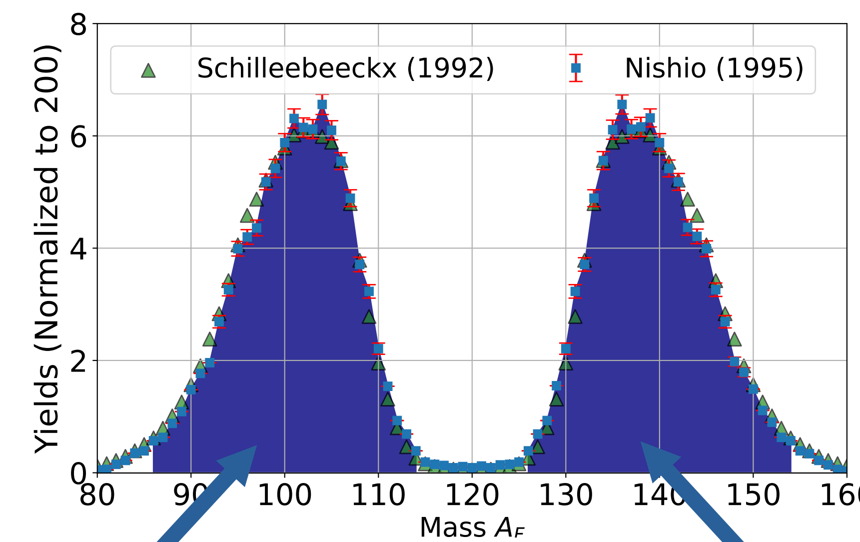


Wilson *et al.*, Nature 590, 566 (2021).

Preliminary Results

Correlation between fragments' angular momenta





"most strongly populated FFs"

Due to the initial set of scission configurations?

- Very weak correlation for the most strongly populated primary FFs
- Strong correlation for configurations approaching A_H = *120*
- Deexcitation is likely to further decorrelate FF angular momenta

Outline

1. Introduction
2. Theoretical Framework
3. Preliminary Results
4. **Conclusion**

Conclusion

1) AMP&PNP + TDGCM is a powerful tool for predicting AM of FFs

2) The preliminary results are encouraging

- AM distributions for the full range of FF masses and charges
- Sawtooth pattern for mass dependence of average AM in primary FFs
- Weak correlation in magnitudes of primary FF angular momenta

3) Further developments are under way

- Including the effect of nuclear excitation (neutron energy, thermal excitation)
- Calculating AM in FFs for ^{239}Pu(n_{th}, f) and ^{235}U(n_{th}, f), releasing the data
- Toward fission modeling based on inputs from microscopic theory

Thank you!

This work was funded by the EU through MSCA-PF 2023