Unified Approach to Nuclear Structure and Reactions, and Nuclear Fission within Time-Dependent Density Functional Theory

Ibrahim Abdurrahman,
FRIB/MSU

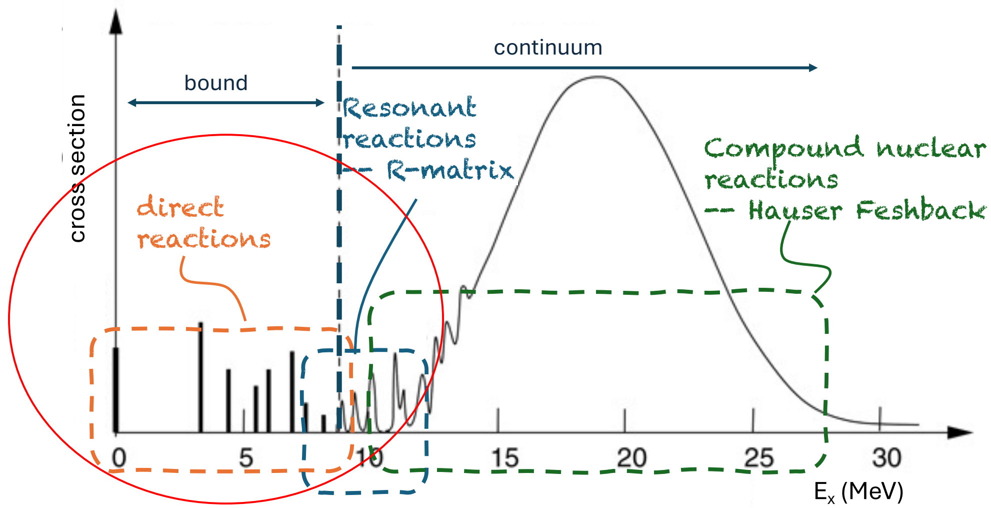
FRIB

MICHIGAN STATE UNIVERSITY

Part 1: Unified Approach to Nuclear Structure and Reactions

Motivation

- Nuclear reaction applications:
    1. Energy
    2. Security
    3. Medicine
    4. Basic science
- Nuclear structure and reactions (typically segregated):
    1. Methods
    2. Fields
    3. Practitioners
- Unification is a hot topic recently:
    Microscopic optical potentials (not the focus here)
- Project was motivated by another investigation (which will be described in the following slides)

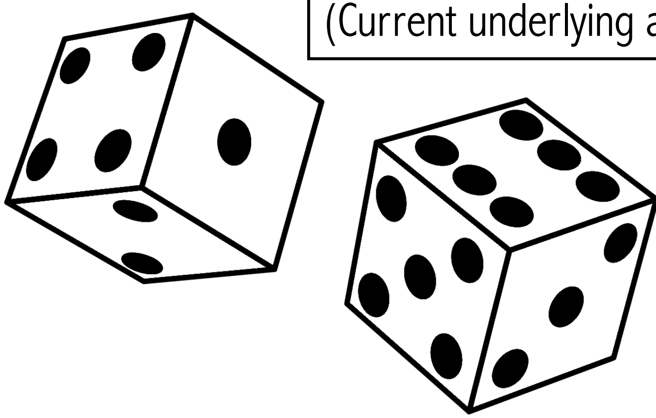


Picture credit: G. Potel.

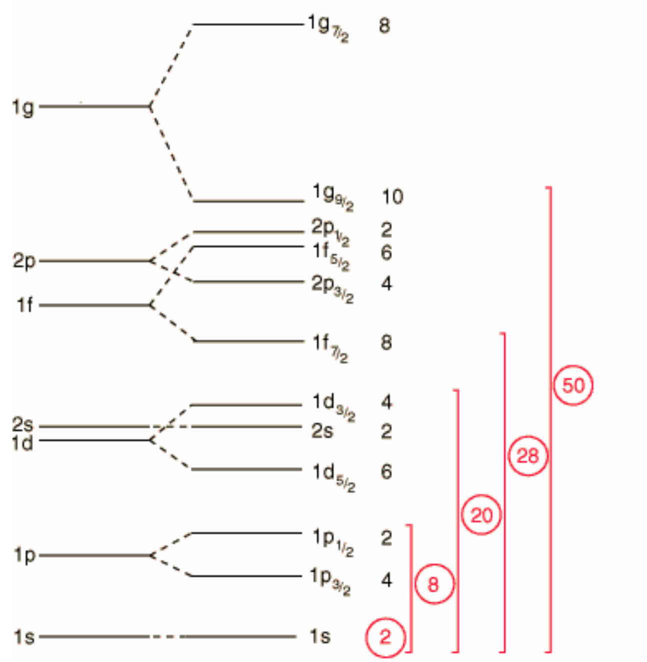
Hauser Feshbach – Random vs Structure

- Hauser Feshbach (HF) theory: statistical framework for compound nuclear reactions
- *Key question: does including microscopic structure information have an applicable impact on HF theory?*

Random
(Current underlying assumption)



versus



Structure

Hauser Feshbach Basics

- Compound nucleus contribution to cross section:

Transmission coefficients (optical potential)

Pure HF theory

$$(\sigma_{CN})_{ab} = (\sigma_{HF})_{ab} W_{ab} = \frac{T_a T_b}{\sum_c T_c} W_{ab}$$

Width Fluctuation Correction Factor (WFCF)

$$W_{ab} = \frac{(\sigma_{CN})_{ab}}{(\sigma_{HF})_{ab}}$$

WFCF expressed as ratio

Width Fluctuation Correction Factor

- Arises from energy average over S matrix:

$$S_{ab}^{(i)} = \delta_{ab} - 2i\pi \sum_{\mu\nu} \mathcal{W}_{a\mu}(D^{-1})_{\mu\nu}\mathcal{W}_{\nu b}$$

$$D_{\mu\nu} = E\delta_{\mu\nu} - H^{(i)}_{\mu\nu} + i\pi \sum_{c} \mathcal{W}_{\mu c}\mathcal{W}_{c\nu}$$

Channel-compound coupling matrices

Member of Gaussian Orthogonal Ensemble (GOE)

$$(\sigma_{CN})_{ab} = \overline{|S_{ab}|^2} - |\overline{S_{ab}}|^2$$

Compound cross section

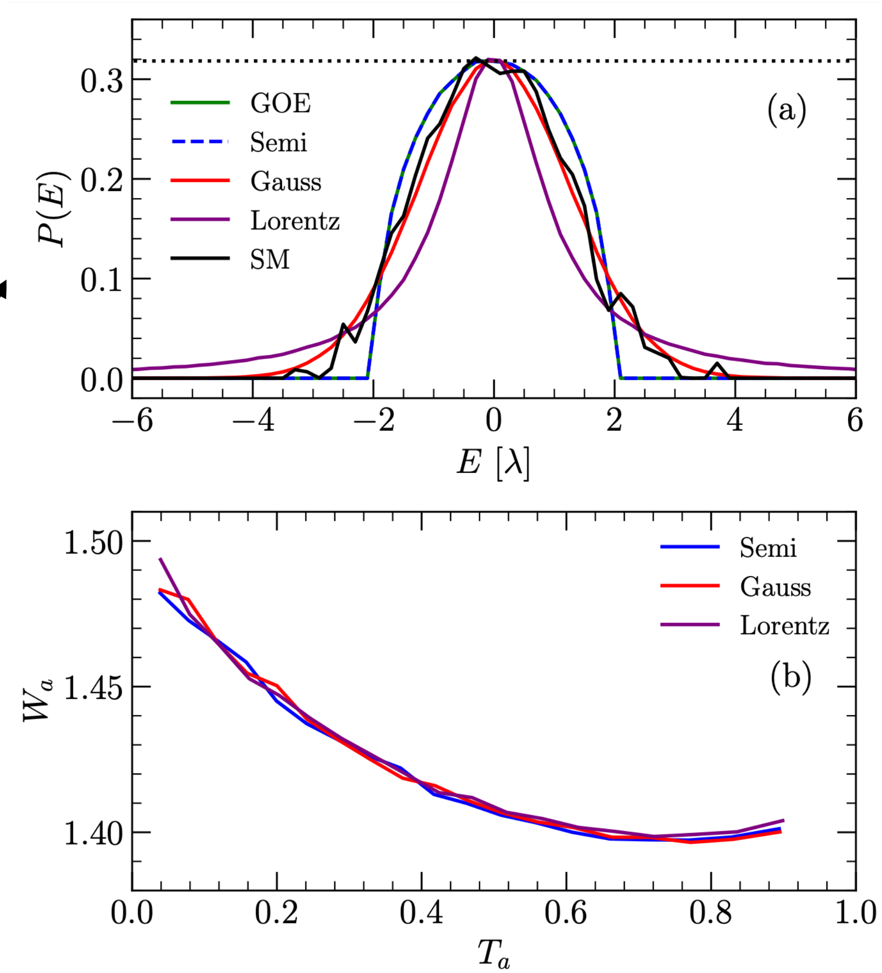
$$T_a = 1 - |\overline{S_{aa}}|^2$$

Effect of Level Density

- WFCF enhances elastic channel
- Understood in terms of structure and mixing
- Level density has no effect

Level density

Elastic enhancement factor

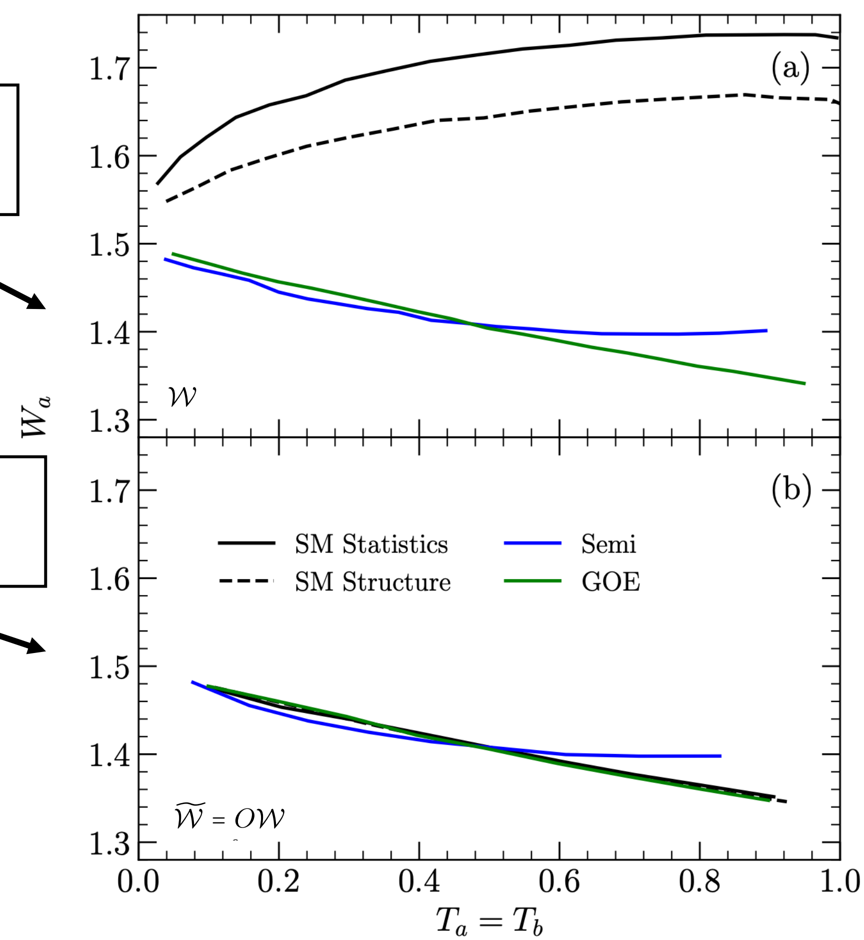


Effect of Structure of Hamiltonian

- Consider two ensembles inspired from nuclear shell model
- Structure has significant effect
- Caveat: no longer basis independent

Diagonal coupling

Random coupling



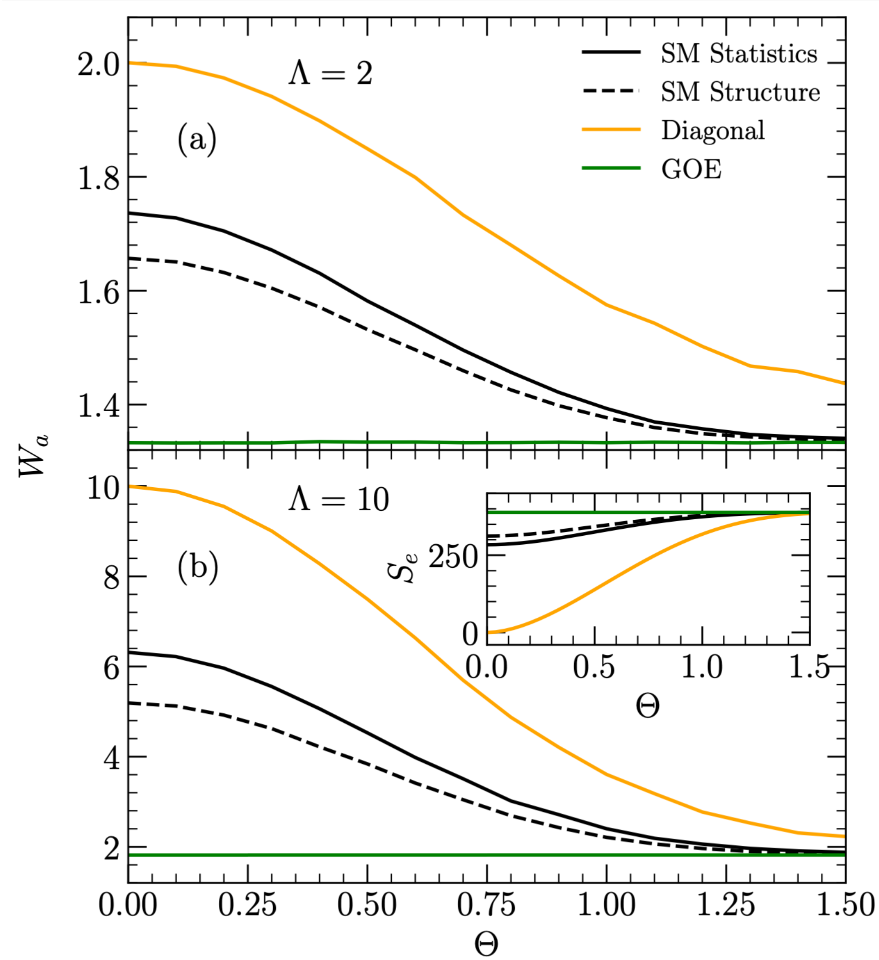
Insight gained from Entropy

- Shannon information entropy:

$$S_e^{(i)} = -2 \sum_{i,j=1}^{N} |M_{ij}^{(i)}|^2 \log(|M_{ij}^{(i)}|)$$

- Maximal ensemble entropy: GOE
- Minimal local entropy: elastic scattering
- Maximal local entropy: pure HF

The structure of the Hamiltonian is not enough to determine the effects of microscopic information of Hauser Feshbach theory. Both the compound Hamiltonian and channel – state couplings must be chosen consistently.



Part 1b: Building Microscopic Framework in a More Rigorous Manner

- Method suggested in 60s:
    1. C. Mahaux and H. A. Weidenmuller, "Shell Model Approach to Nuclear Reactions" (1969)
    2. Unified approach for structure and reactions
    3. Modern computing makes problem computationally feasible
- Similar to previous S matrix:

$$H_{\mu\nu} \to E_\mu \delta_{\mu\nu}$$

$$\mathcal{W}_{\mu c} \to \frac{1}{\sqrt{2\pi}} \Gamma_{\mu c}^{(1/2)}$$

- Method includes shift function
- Method is agnostic to microscopic model
- Currently no direct channel – channel coupling

S Matrix

$$S_{ab}(E) = \Omega_a \Omega_b \Big[\delta_{ab} + i \sum_{\mu\nu} D_{\mu\nu}(E) \Gamma_{\mu a}^{1/2}(E) \Gamma_{\mu b}^{1/2}(E) \Big]$$

$$(D^{-1})_{\mu\nu}(E) = (E_\mu - E)\delta_{\mu\nu} + \Delta_{\mu\nu}(E) - \frac{i}{2} \sum_c \Gamma_{\mu c}^{1/2}(E) \Gamma_{\nu c}^{1/2}(E)$$

Resonance Width

$$\Gamma_{\mu c}^{(1/2)} = A_{\mu c} \Gamma_{\mu c}^{(1/2)(sp)}$$

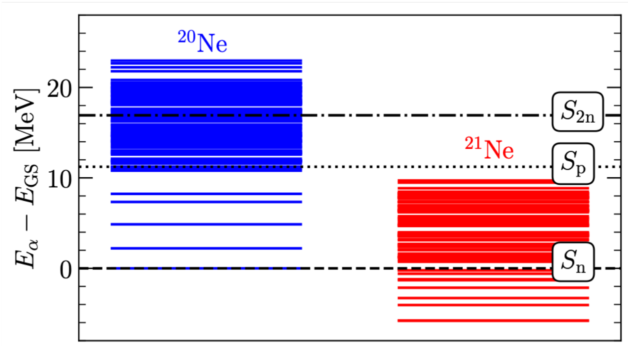
Spectroscopic Amplitude ($A_{\mu c}$)

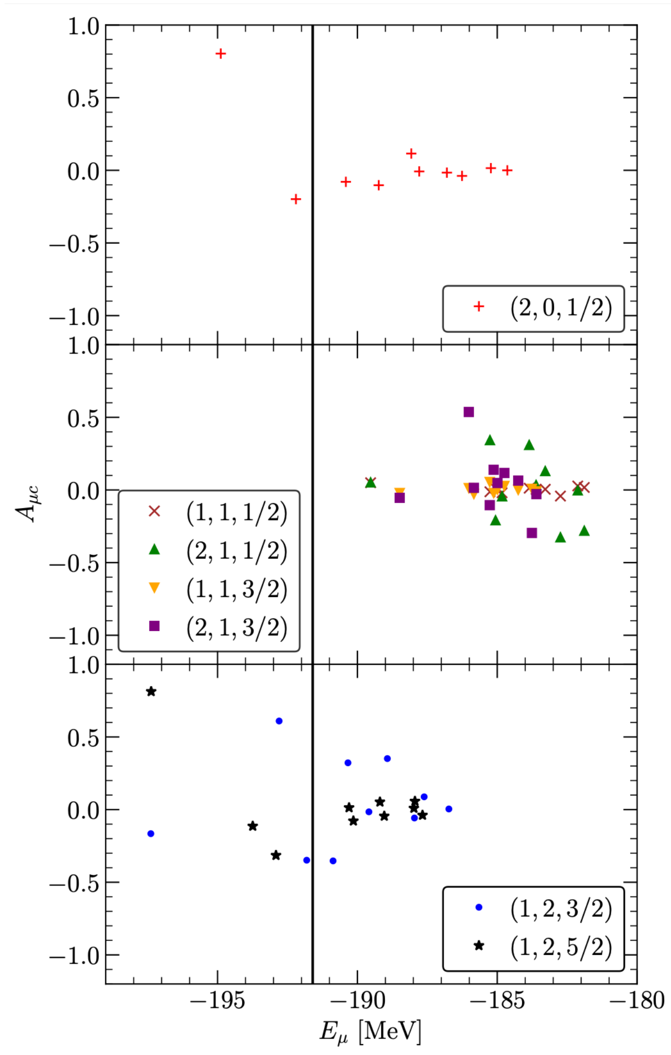
Single particle partial width ($\Gamma_{\mu c}^{(1/2)(sp)}$)

Spectroscopic Amplitudes

- Contains structure information
- Obtained from Nuclear Shell Model

  Also works for other microscopic methods
- Details:
  1. Program: NuShellX
  2. Valence space shell model
  3. spsdpf model space
  4. 1 hbar omega cross shell excitations



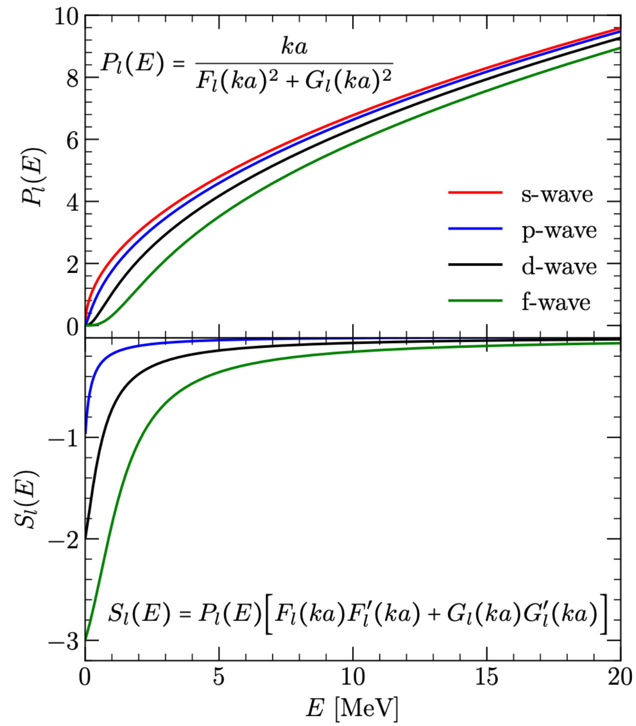


Single Particle Quantities and R Matrix Theory

- Reference: P. Descouvemont and D. Baye 2010 Rep. Prog. Phys. 73 036301 (2010)
- Shell Model contains incorrect asymptotic behavior
  - Harmonic oscillator basis
- Resonant widths extracted from adjustable Wood-Saxon
- Bound states influence shift function
  1. Exact treatment still unclear
  2. Should depend on asymptotic renormalization coefficients (ANCs)
- Important check: no channel radius dependence

$$\Gamma^{(sp)}_{\mu\nu,c} = 2P_c(E)\gamma^{(sp)}_{\mu c}\gamma^{(sp)}_{\nu c}$$

$$\Delta^{(sp)}_{\mu\nu,c} = -\mathcal{L}_c(E)\gamma^{(sp)}_{\mu c}\gamma^{(sp)}_{\nu c}$$



Cross Sections

- Experimental observable.
- Cross section from S matrix:

$$(\sigma_{el})_{aa} = |1 - S_{aa}|^2$$

$$(\sigma_{inel})_{ab} = |S_{ab}|^2$$

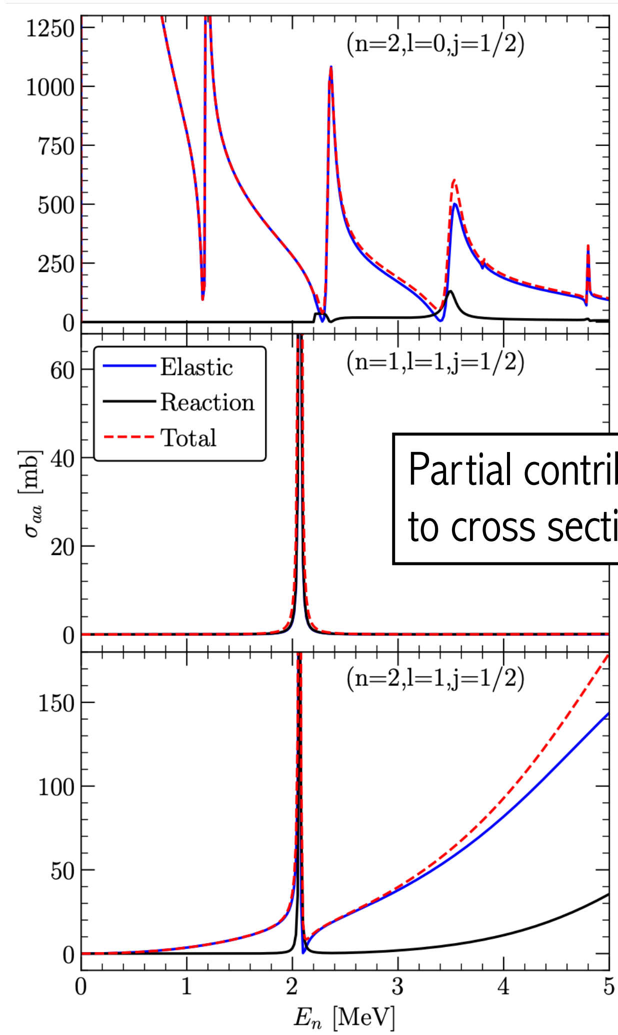
$$(\sigma_r)_{ab} = \delta_{ab} - |S_{ab}|^2$$

$$(\sigma_{tot})_{ab} = \delta_{ab} - \mathrm{Re}[S_{ab}]$$

$$T_a = 1 - \langle |S_{aa}| \rangle^2$$

$$(\sigma_{CN})_{ab} = \langle |S_{ab}|^2 \rangle - \langle |S_{ab}| \rangle^2$$

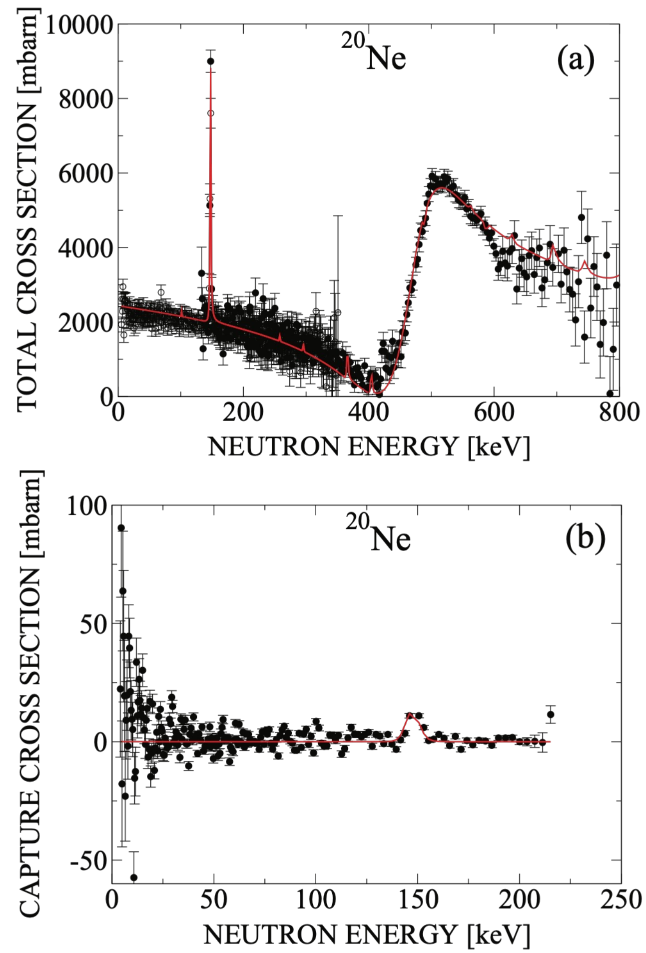
- Can obtain differential cross sections as well.



Partial contributions to cross section

Significant Work Remains

- Still to do:
    1. Finish treatment of neutron channels
    2. Include proton, gamma, alpha, and other channels
    3. Investigate more systems
    4. Investigate more microscopic models
- *Confront results with experiment*



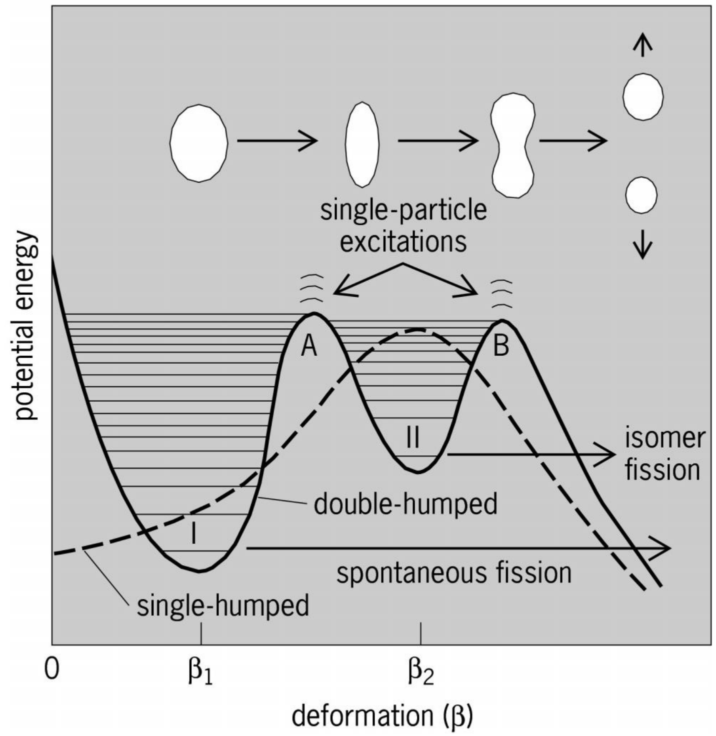
Source: M. Heil, el al, Phys. Rev. C 90, 045804 (2014)

Part 2: Nuclear Fission within Time-Dependent Density Functional Theory

Motivation

- Applications for:
  1. Nuclear energy
  2. Security
  3. Basic science (R-process Nucleosynthesis)
- Long standing quantum many body problem:
  1. (Experiment) Otto Hahn and Fritz Strassmann: December 1938
  2. (Theory) Lise Meitner and Otto Frisch: January 1939

     Coulomb energy vs surface tension
  3. (Fission Isomer) Strutinsky: April 1967

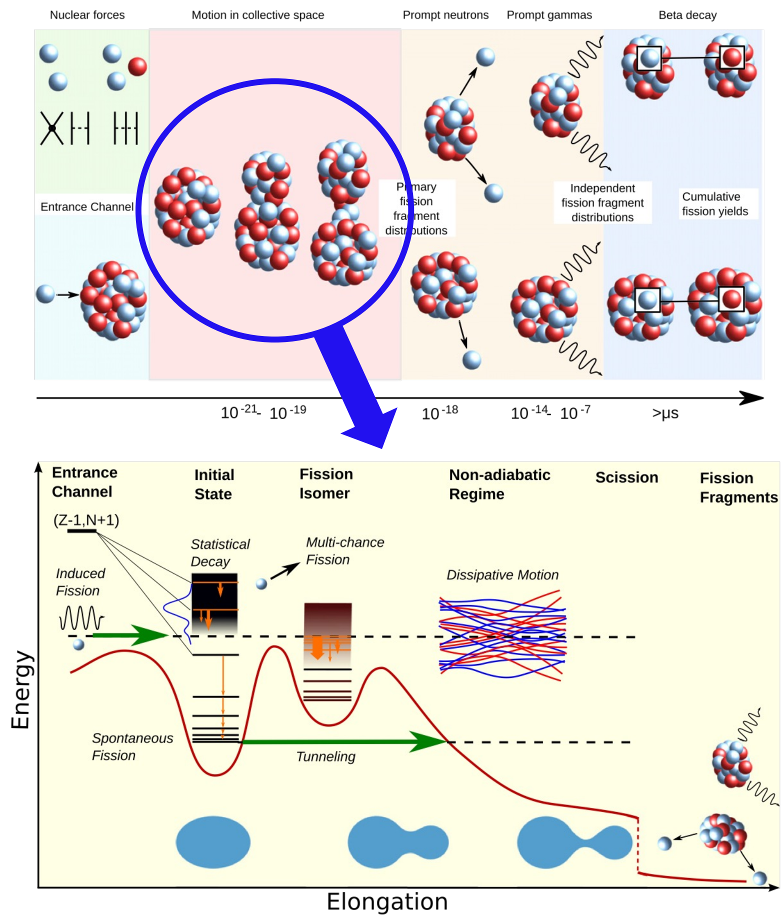


Source: J. R. Huizenga, Science, 168:1405–1413, (1979).

Detailed Overview

- Fission - highly complex quantum many body phenomena:
    1. Entrance channel, typical neutron induced or spontaneous fission.
    2. Evolution to saddle ~ 5 x 10^{-15} s
    3. Saddle to scission ~ 5 x 10^{-21} s
    4. Neck rupture ~ 10^{-22} s
    5. Acceleration of fragments ~ 5 x 10^{-21} s
    6. Emission of prompt neutrons ~ 10^{-18} s to 10^{-14} s
    7. Emission of prompt gammas ~ 10^{-14} s to 10^{-3} s
    8. Beta decay ~ 10^{-3} s to billions of years

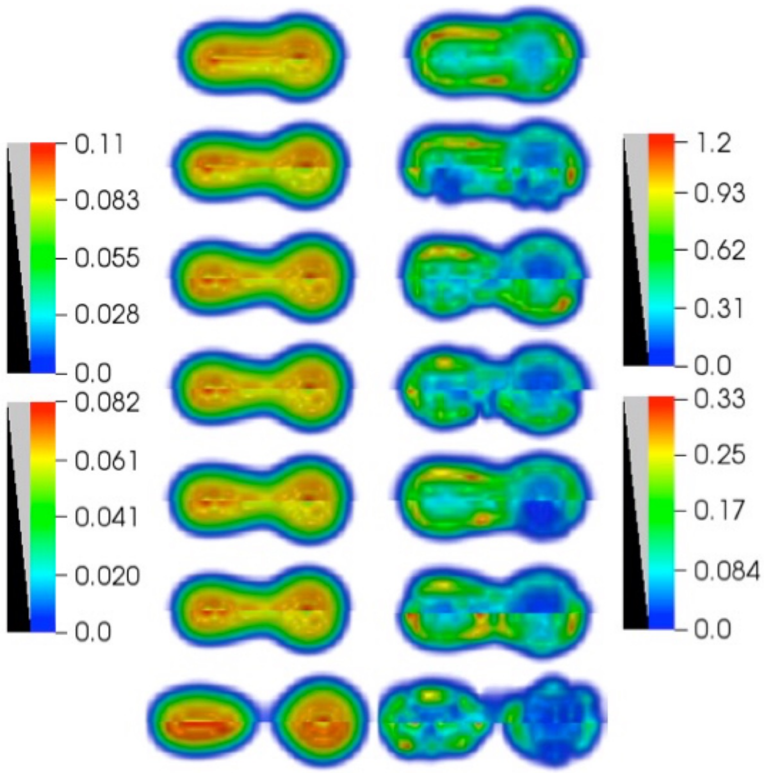
    Source: F. Gönnenwein FIESTA lecture notes (2014).
- Main goal - unified microscopic theory



Source: M. Bender, et al. Journal of Physics G: Nuclear and Particle Physics 47, 113002 (2020).

Real time evolution

- TDDFT w/ pairing
- First fully microscopic time-dependent simulation from saddle to scission (2016)
    1. Realistic deformations
    2. Realistic excitation energies
- Ground state to saddle - remains to be done
- Key insight: pairing is critical for fission



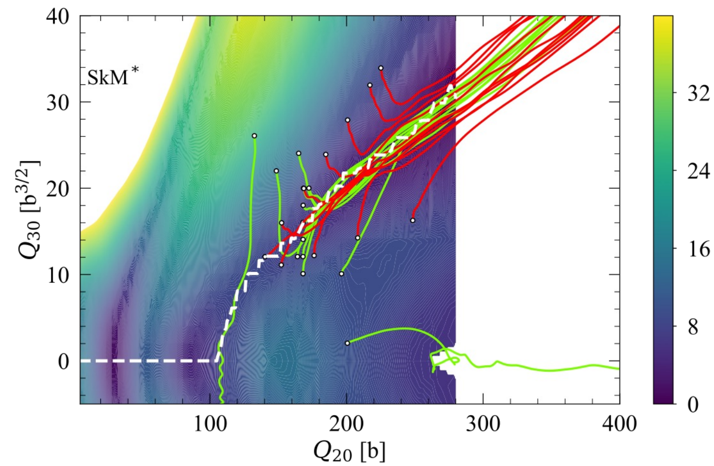
A. Bulgac, P. Magierski, K. J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

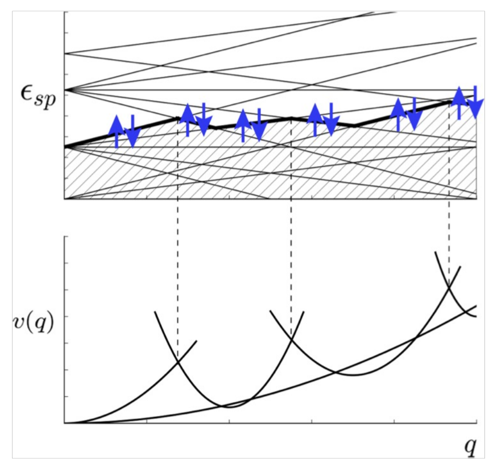
Role of Pairing

- Nucleus as 3D infinite square well – (Hill and Wheeler 1953)

$$E(n_x, n_y, n_z) \sim \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}$$

- Bose enhancement at level crossings
- Enhanced dynamic deformability
- Other key lessons:
    1. Constant collective flow energy
    2. Strong dissipation
    3. Compound heats up

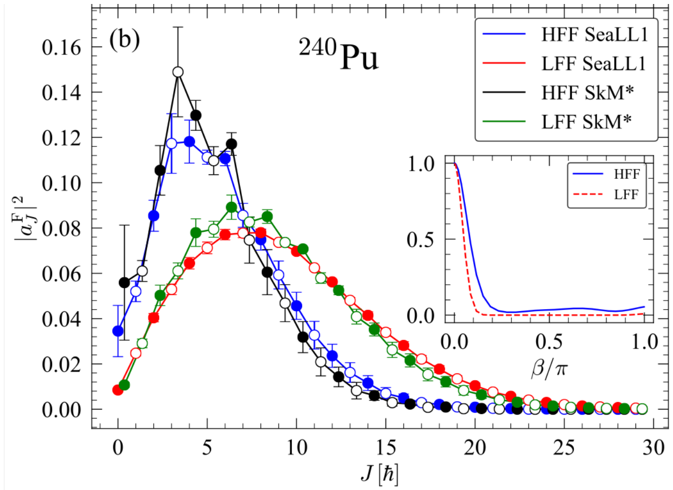


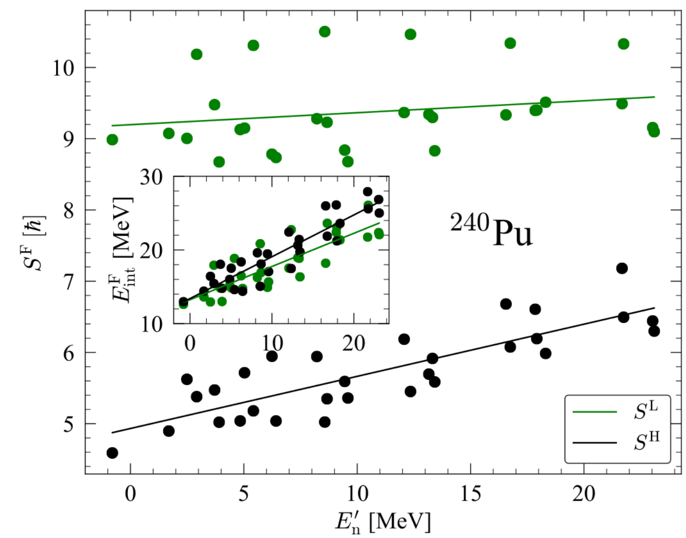


A. Bulgac, S. Jin, K. J. Roche, N. Schunck, and I. Stetcu, Phys. Rev. C 100, 034615 (2019)

FF Spins

- Joined group
- Hot topic recently:
  See Workshop on Fission Fragment Angular Momenta (2022)
- First microscopic extraction of FF spin distributions
- Predict higher FF spins than seen in experiment
- Weak energy dependence
  1. Caveat: on average
  2. Weighing of initial conditions unaccounted for

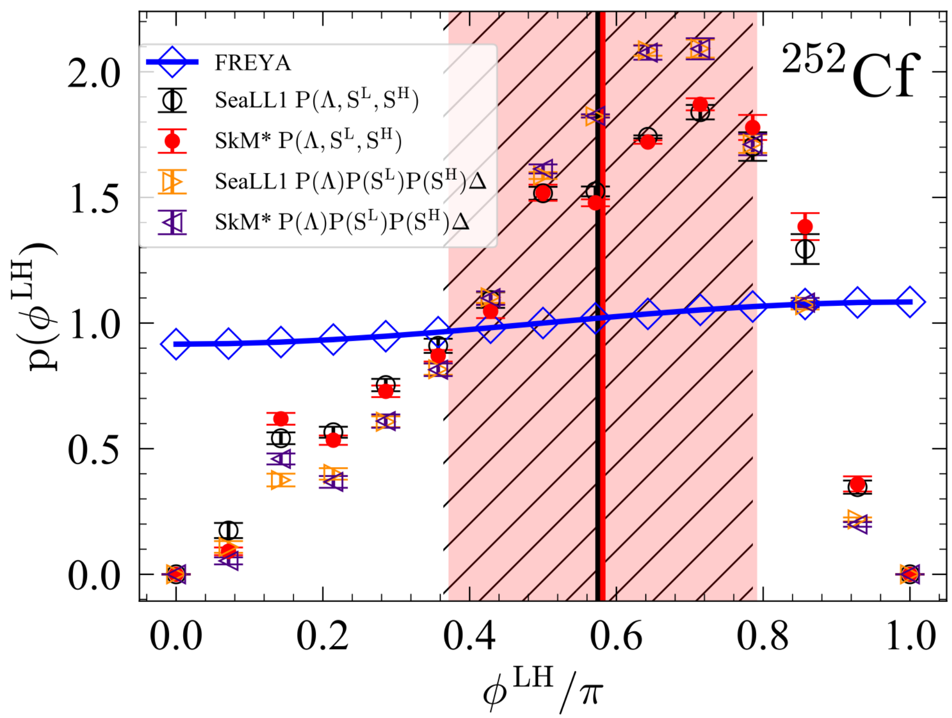




Source: A. Bulgac, I. Abdurrahman, S. Jin, K. Godbey, N. Schunck, and I. Stetcu, Phys. Rev. Lett. 126, 142502 (2021)

FF Angular Momenta Vector Correlations

- Magnitude of FF angular momenta vectors are uncorrelated
- Striking disagreement between two theories
- Disagreement between two models:
  - Unconstrained 2D vs 3D character
  - Twisting collective angular momenta mode



Sources: A. Bulgac, I. Abdurrahman, K. Godbey, and I. Stetcu, Phys. Rev. Lett. 128, 022501 (2022),

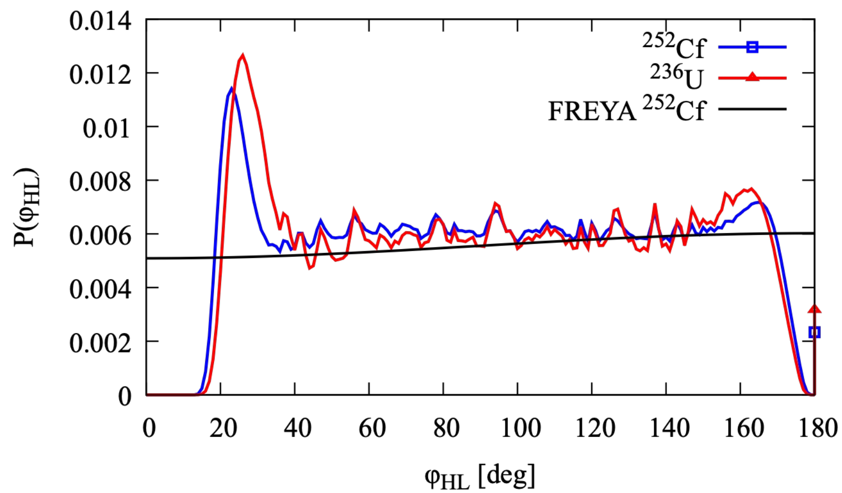
J. Randrup and R. Vogt, Phys. Rev. Lett. 127, 062502 (2021)

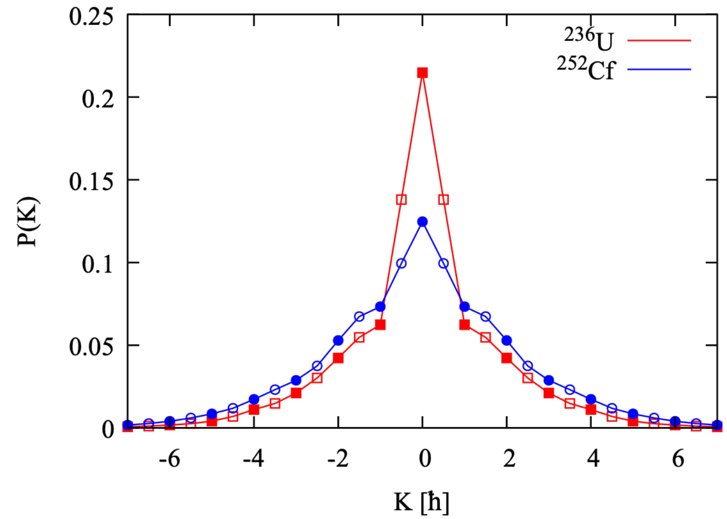
FF Angular Momenta Vector Correlations - Continued

- More exact extraction of FF spin distributions:
  1. Possible with canonical representation
  2. Still see non-zero K modes
  3. New character: 2.5 D
- George Bertsch: non-zero K modes related to pair breaking

  Related to FF excitation energy
- 17th Nuclear Reaction Mechanisms conference: J. Wilson and S. Marin suggest experiment might soon have answers

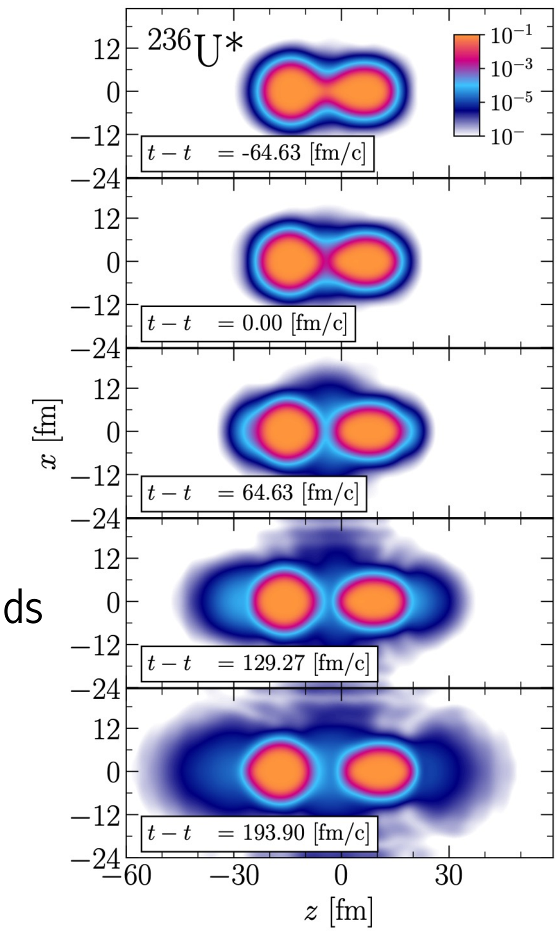
Source: G. Scamps, I. Abdurrahman, M. Kafker, I. Stetcu, and A. Bulgac, Phys. Rev. C 108, L061602 (2023)



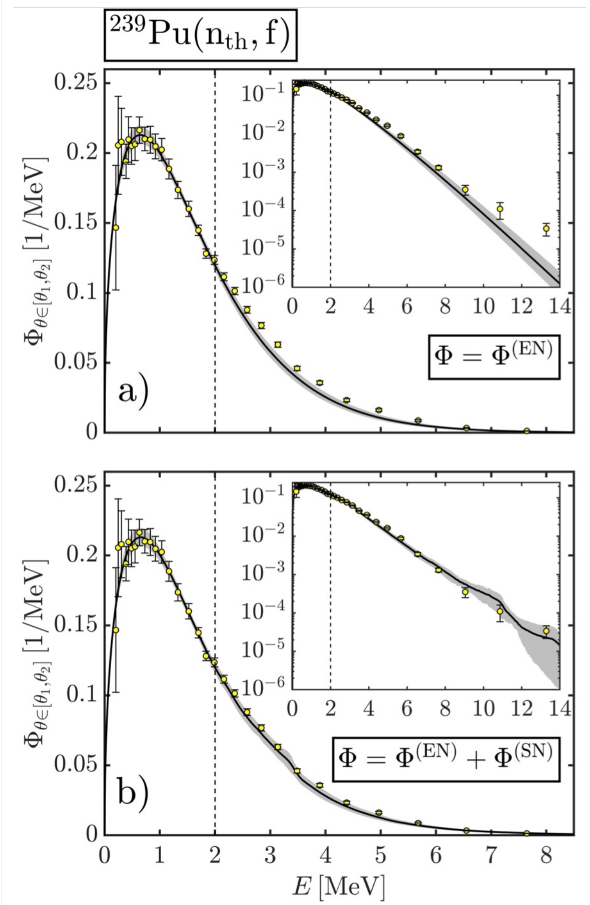


Scission Neutrons

- Bohr and Wheeler (1939)
- Contentious topic
- Isotropic emission hypothesis (current standard)
- Microscopic theory predicts scission neutrons (SNs)
- Universal signal: 3 neutron clouds
- Catapult mechanism (Mädler 1984)
- SNs probe neck dynamics
- Claim: signal already present in data
- Future: larger lattices



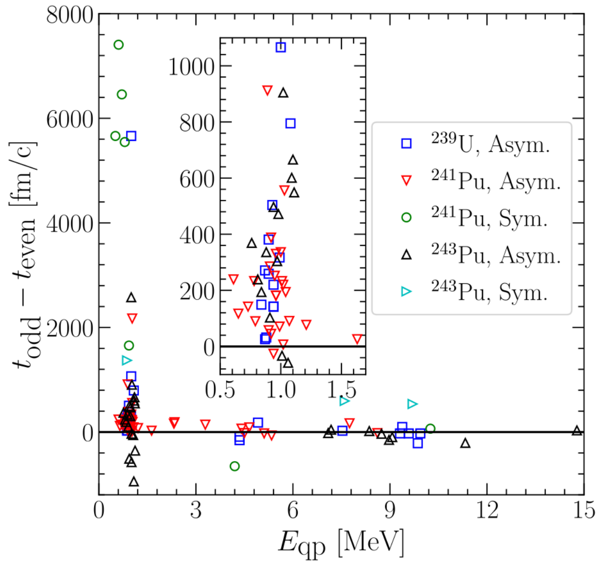
Source: I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, Phys. Rev. Lett. 132, 242501 (2024)



Source: A. Bjelčić, , I. Abdurrahman, K. Godbey, arXiv: 2606.09656 (2026)

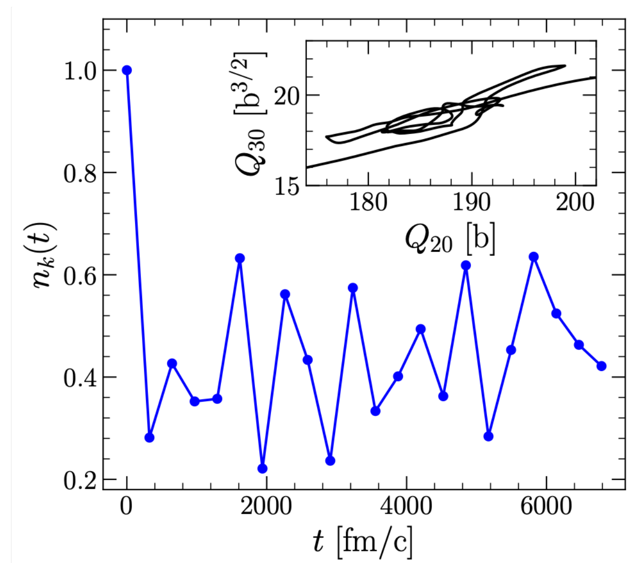
Odd Nuclei

- Investigated initial excitation energy simultaneously
- Unpaired nucleon leads to longer saddle to scission times



- Evolution to scission is more convoluted
- Pauli approximation does not hold for dynamics

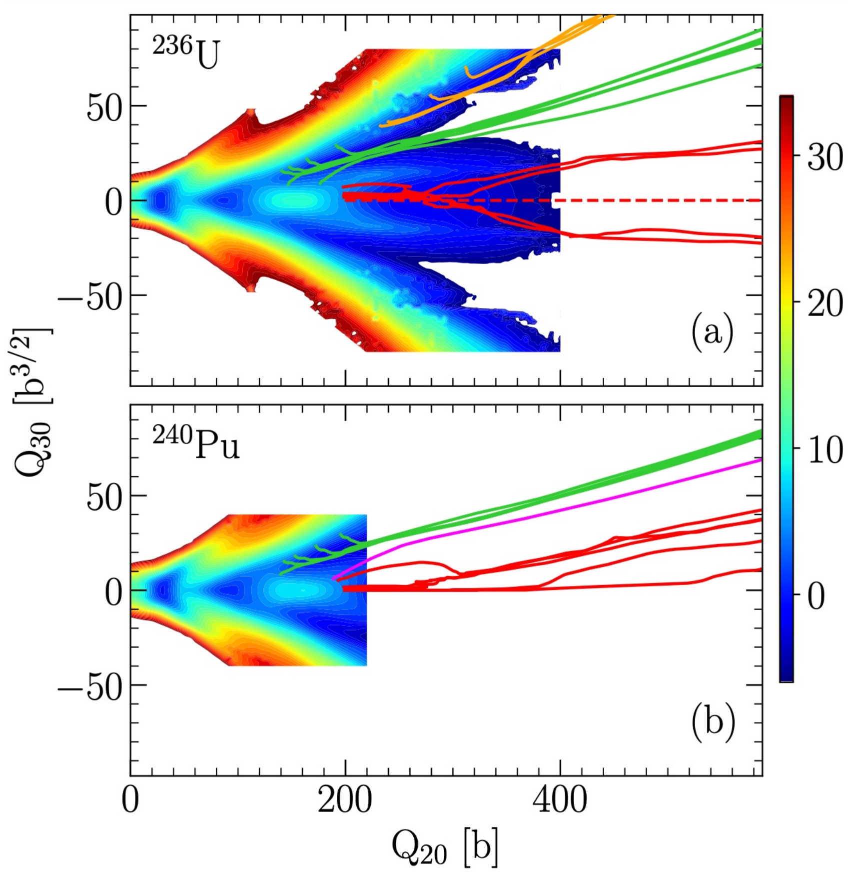
$$|\Phi\rangle = a_i^\dagger \prod_{k\neq i} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)\,|-\rangle$$



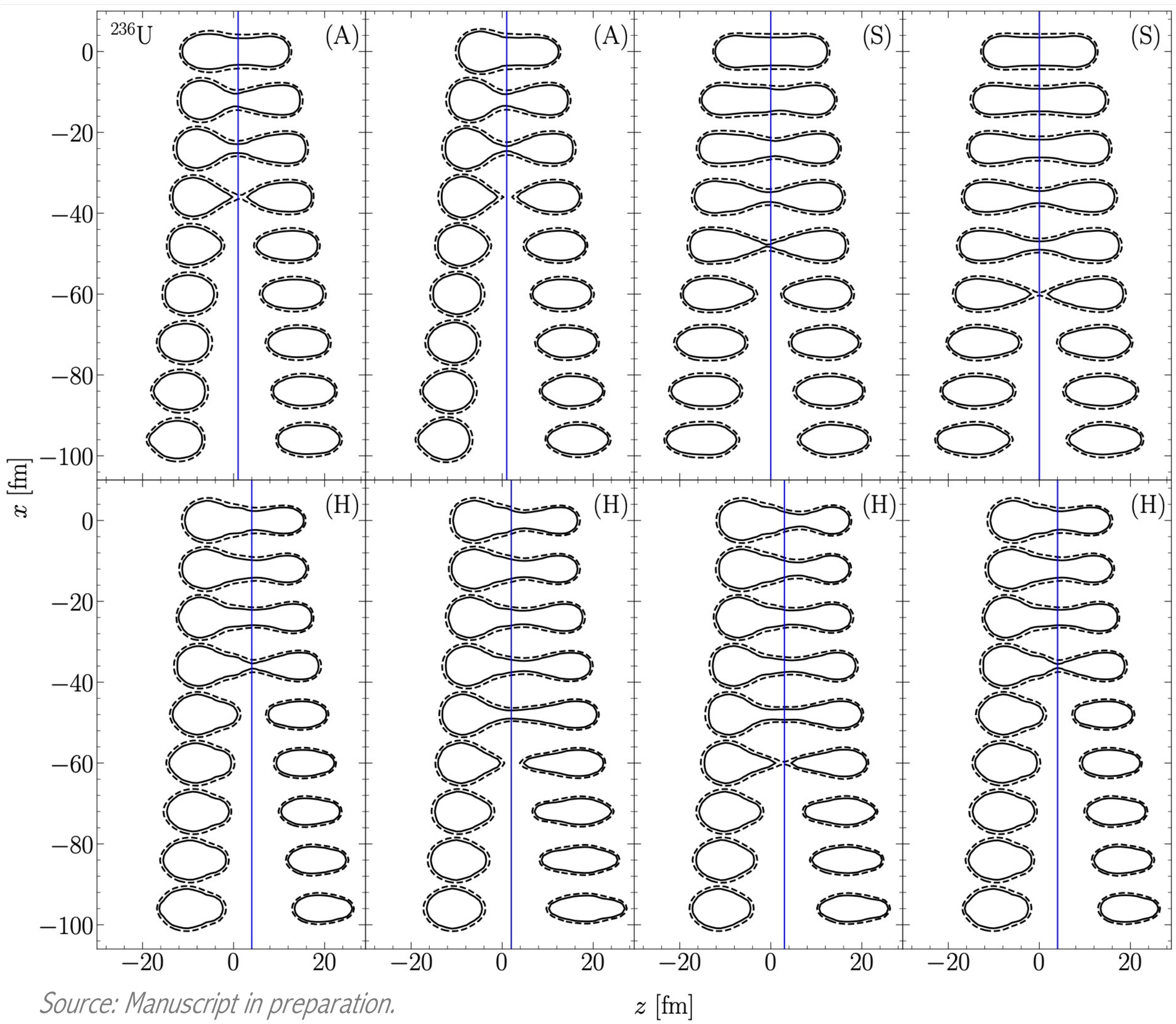
Source: A. Bulgac, I. Abdurrahman, M. Kafker, and I. Stetcu,, Phys. Rev. Lett. 135, 062501 (2025).

Influence of Exit Channel

- Initial weights are currently absent in dynamical methods
- Consider different fission modes (from outer saddle):
  1. Asymmetric (typical)
  2. Near-symmetric or exactly symmetric
  3. Highly-asymmetric
- Major question: why does TKE decrease as a function of the initial excitation energy of the compound nucleus?



Source: Manuscript in preparation.



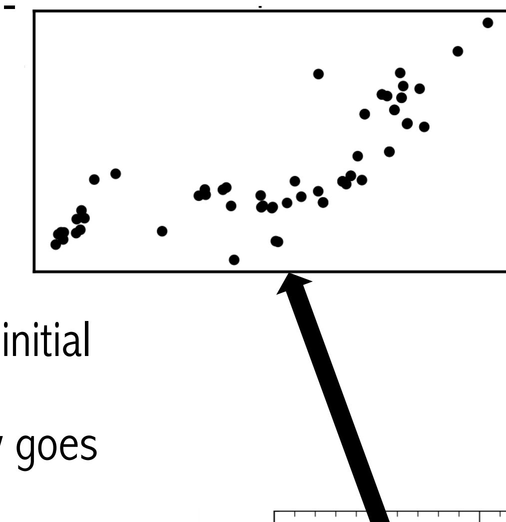
Source: Manuscript in preparation.

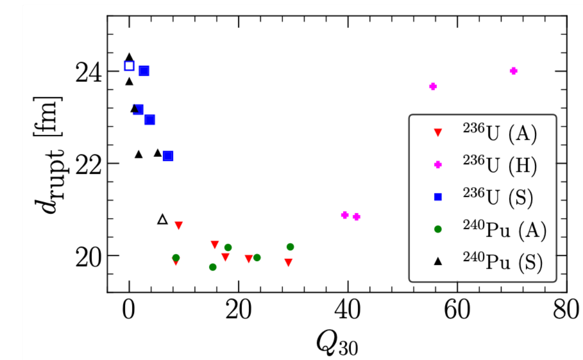
Partition of Energy between Fragments

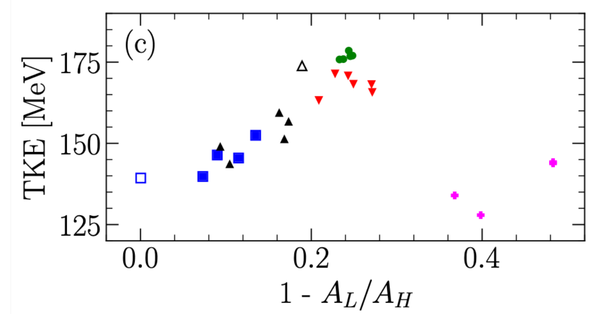
- Larger rupture distances for near-symmetric and highly-asymmetric modes
- Leads to lower TKE:

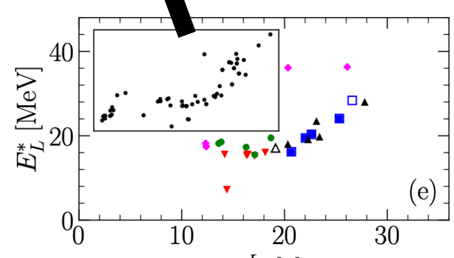
$$TKE \approx \frac{e^2 Z_L Z_H}{d_{\rm rupt}} + K_{\rm rupt}$$

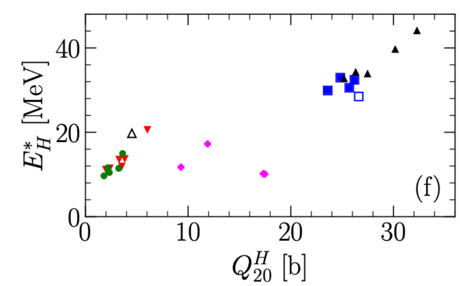
- Exotic modes populated more as initial energy increases
- Beyond certain threshold, energy goes into deformation
- Theory overestimates excitation energy:
  1. Too much dissipation
  2. Missing triaxial (and other) shapes
  3. Beyond mean field effects
  4. All of the above











Source: Manuscript in preparation.

Thank you for your time!
Any questions?