Investigating the Validity of Hauser Feshbach Theory in Compound Nuclear Reactions, and Nuclear Fission within Time-Dependent Density Functional Theory

Ibrahim Abdurrahman,
FRIB/MSU

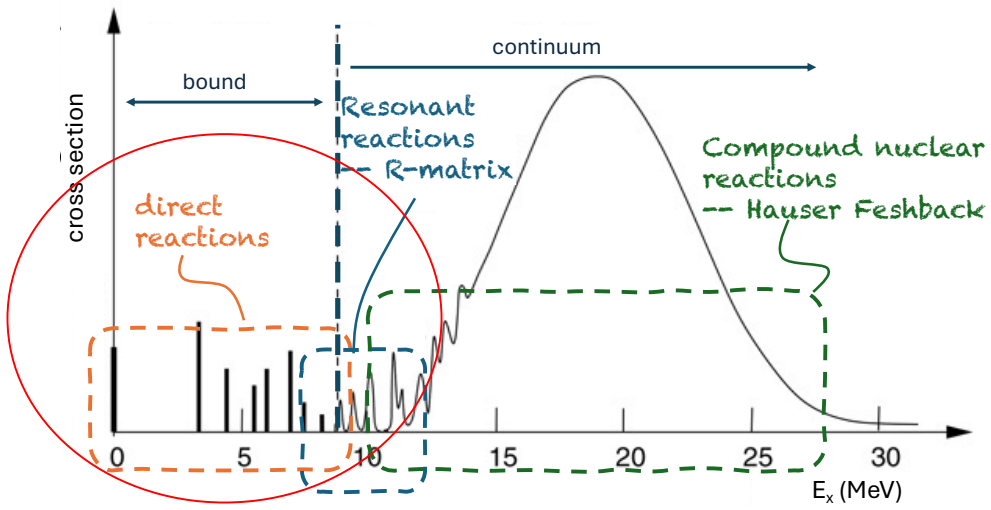




Part 1: Investigating the Validity of Hauser Feshbach Theory in Compound Nuclear Reactions

Motivation

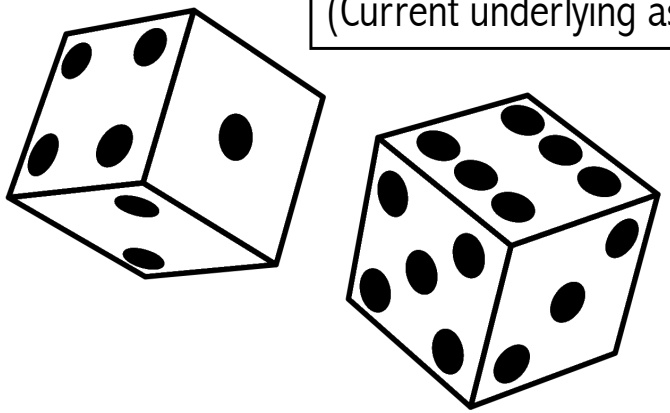
- Hauser Feshbach (HF) theory: statistical framework for compound nuclear reactions.
- Applications:
  1. Energy
  2. Security
  3. Medicine
  4. Basic science
  5. And more



Picture credit: G. Potel.

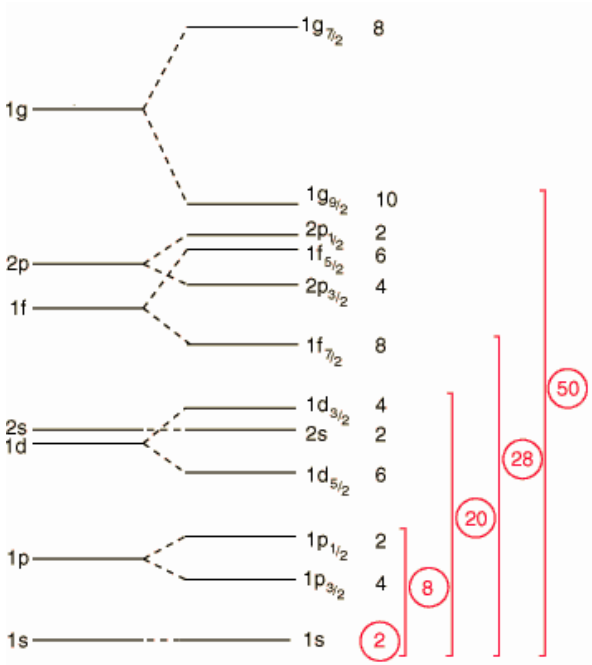
Hauser Feshbach – Random vs Structure

- *Key question: does including information about microscopic structure have an applicable impact on HF theory?*



Random
(Current underlying assumption)

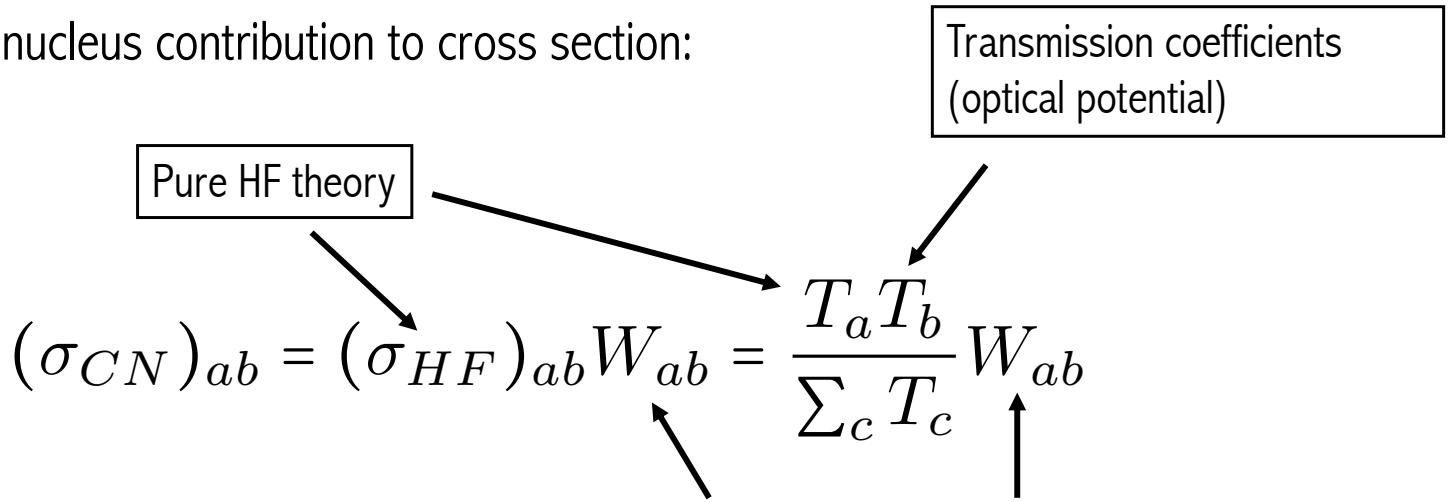
versus



Structure

Hauser Feshbach Basics

- Compound nucleus contribution to cross section:



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

WFCF expressed as ratio

Width Fluctuation Correction Factor

- Arises from energy or ensemble average over S matrix:
  - Related to experimental resolution
  - Non-unitary (energy-averaged) S matrix

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

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

Channel-compound coupling matrices

Member of Gaussian Orthogonal Ensemble (GOE)

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

Compound cross section

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

Gaussian Orthogonal Ensemble

- Random Matrix Theory: E. Wigner and F. Dyson in the 50s and 60s
- Properties:
  - Correct nearest-neighbor spacing distribution
  - Invariant under orthogonal transformations
  - Universal
  - And more
- Maximizes the Shannon information entropy (P. A. Mello and collaborators-1980):
  - Real symmetric matrices (time-reversal invariant systems)
  - Ensemble with minimum information

$$\overline{H_{\mu\nu}^{(GOE)}} = 0$$

$$\overline{H_{\mu\nu}^{(GOE)} H_{\rho\sigma}^{(GOE)}} = \frac{\lambda^2}{N}(\delta_{\mu\rho}\delta_{\nu\sigma} + \delta_{\mu\sigma}\delta_{\nu\rho})$$

$$d = \frac{\pi\lambda}{N}$$

$$I\{P[H]\} = \int d[H]P[H]\log P[H]$$

GOE S Matrix

- WFCF has analytic expression for GOE
  GOE Triple Integral
- Alternative: Monte-Carlo
  - Less computationally demanding
  - Allows for modifications of ensemble
  - First implemented by Kawano, Talou, and Weidenmuller in $\sim$ 2015

$$N = 100$$

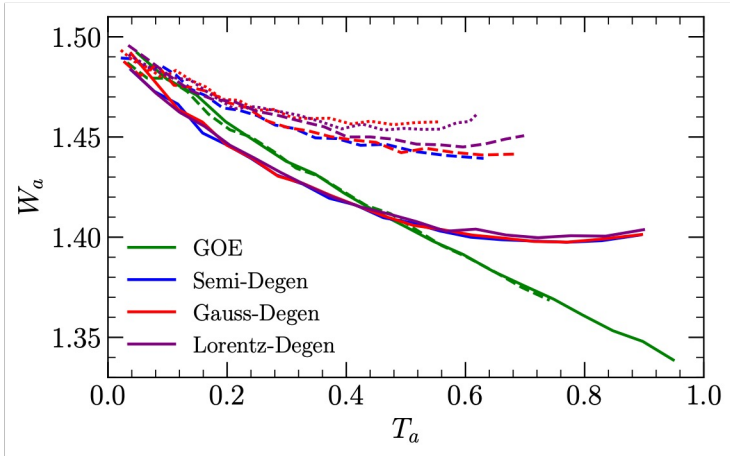
$$N_{\mathrm{samples}} = 1,000,000$$

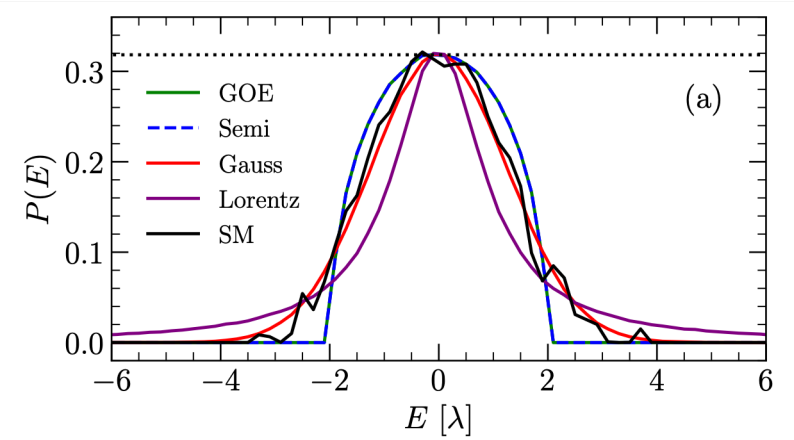
$$\overline{S_{ab}S_{ab}^{*}} - \overline{S_{ab}S_{ab}^{*}} = \frac{1}{8}\int_0^\infty \mathrm{d}\lambda_1 \int_0^\infty \mathrm{d}\lambda_2 \times \int_0^1 \mathrm{d}\lambda \frac{\lambda(1-\lambda)|\lambda_1-\lambda_2|}{\sqrt{\lambda_1(1+\lambda_1)\lambda_2(1+\lambda_2)}(\lambda+\lambda_1)^2(\lambda+\lambda_2)^2}\prod_e \times \frac{1-T_e\lambda}{\sqrt{(1+T_e\lambda_1)(1+T_e\lambda_2)}} \times \left\{\delta_{ab}\delta_{cd}\overline{S_{aa}S_{cc}^{*}}T_aT_c\left(\frac{\lambda_1}{1+T_a\lambda_1}+\frac{\lambda_2}{1+T_a\lambda_2}+\frac{2\lambda}{1-T_a\lambda}\right) \times \left(\frac{\lambda_1}{1+T_c\lambda_1}+\frac{\lambda_2}{1+T_c\lambda_2}+\frac{2\lambda}{1-T_c\lambda}\right) + (\delta_{ac}\delta_{bd}+\delta_{ad}\delta_{bc})T_aT_b\left(\frac{\lambda_1(1+\lambda_1)}{(1+T_a\lambda_1)(1+T_b\lambda_1)} + \frac{\lambda_2(1+\lambda_2)}{(1+T_a\lambda_2)(1+T_b\lambda_2)}+\frac{2\lambda(1-\lambda)}{(1-T_a\lambda)(1-T_b\lambda)}\right)\right\}.$$

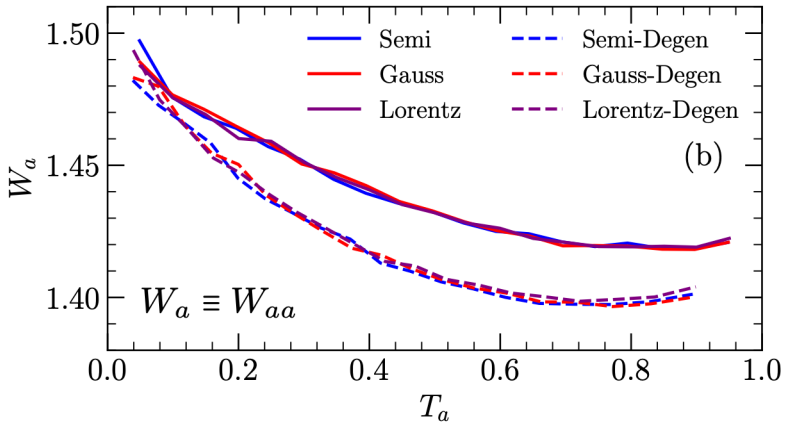
S. Hilaire et al. / Annals of Physics 306 (2003)

Investigation One: Level Density

- Consider degenerate two channel case
- WFCF enhances elastic channel
  Understood in terms of structure and mixing
- Level density has no effect
- True for general WFCF as well







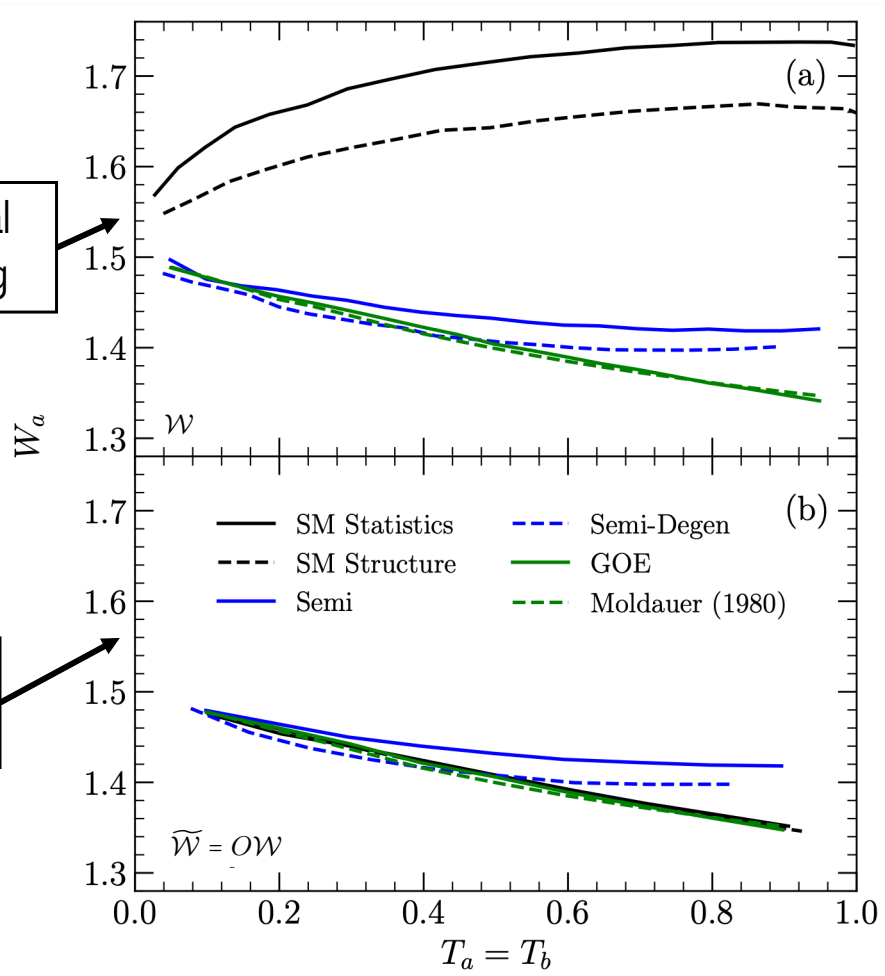
Investigation Two: Structure of Hamiltonian

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

$$\mathcal{W}_{a\mu} = \begin{bmatrix} \nu_1 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & \nu_2 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & \nu_3 & \dots & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & \dots & \nu_\Lambda & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}_{\Lambda \times N} \qquad \widetilde{\mathcal{W}} = O\mathcal{W}$$

Diagonal Coupling

Random Coupling



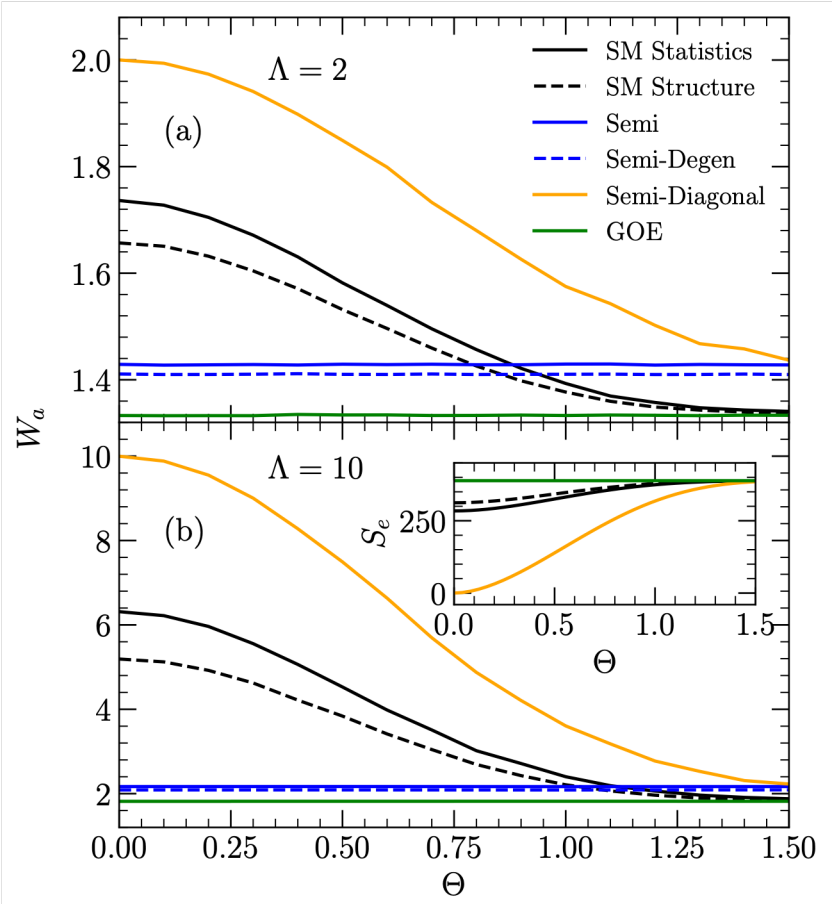
Insight gained from Entropy

- 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
- Entropy as measure of deviation from GOE

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.



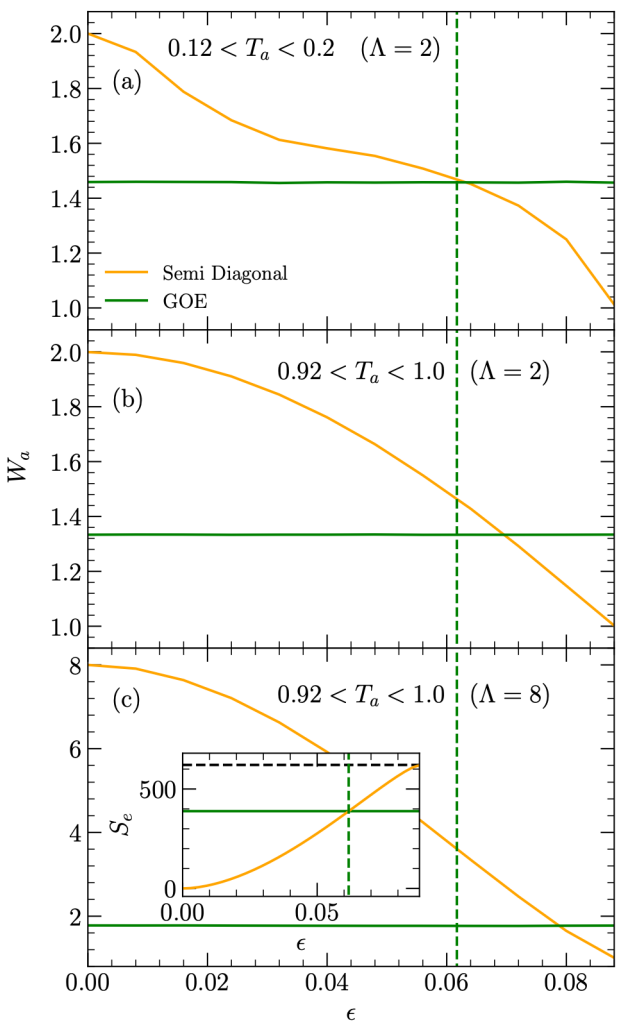
Aside: Pure HF Theory

- Hamiltonian:

$$H = H_{Had}^{T} E H_{Had}$$

$$H_{Had} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

- Physical interpretation:
  - High temperature compound
  - Pure pairing Hamiltonian
- Maximizes local entropy
- Cannot be realized in all dimensions



Part 1b: Unified Approach to Nuclear Reactions and Structure

Motivation

- 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)
- Help investigate validity of GOE in HF theory (and other investigations)

Building a 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:

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

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

- 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

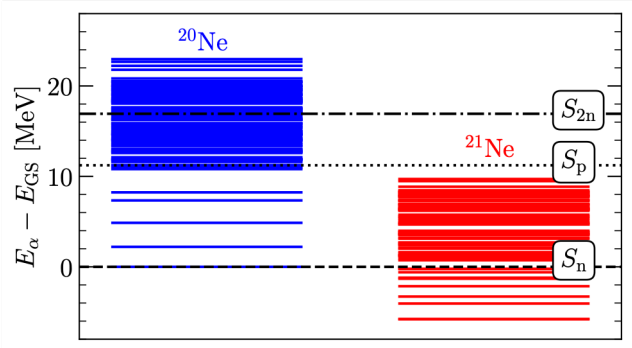
$$\Gamma_{\mu c}^{(1/2)} = A_{\mu c} \Gamma_{\mu c}^{(1/2)(sp)}$$

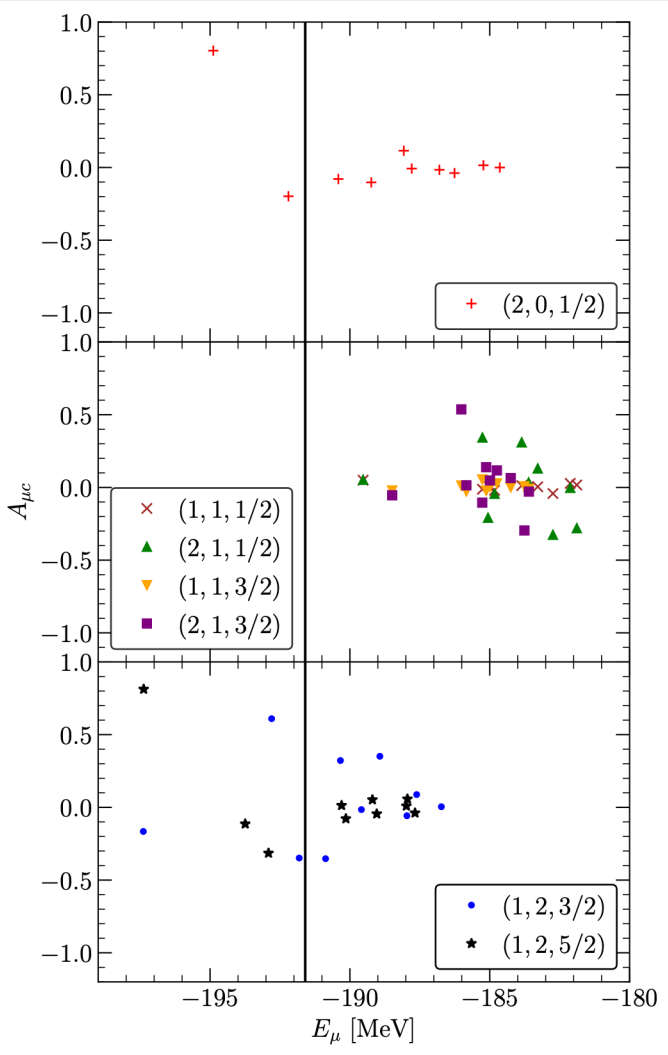
Spectroscopic Amplitude

Single particle partial width

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



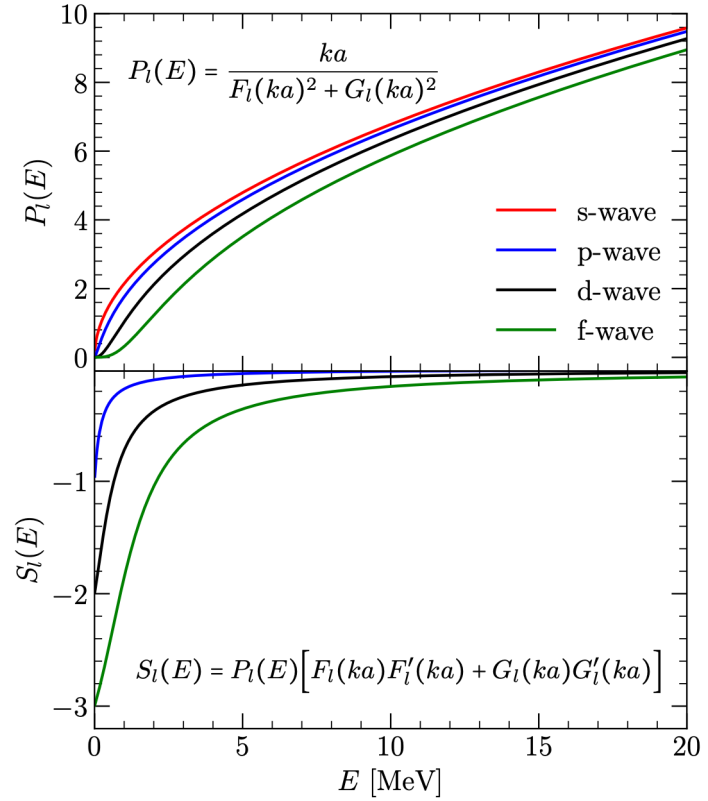


Single Particle Quantities and R Matrix Theory

- 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:

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

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

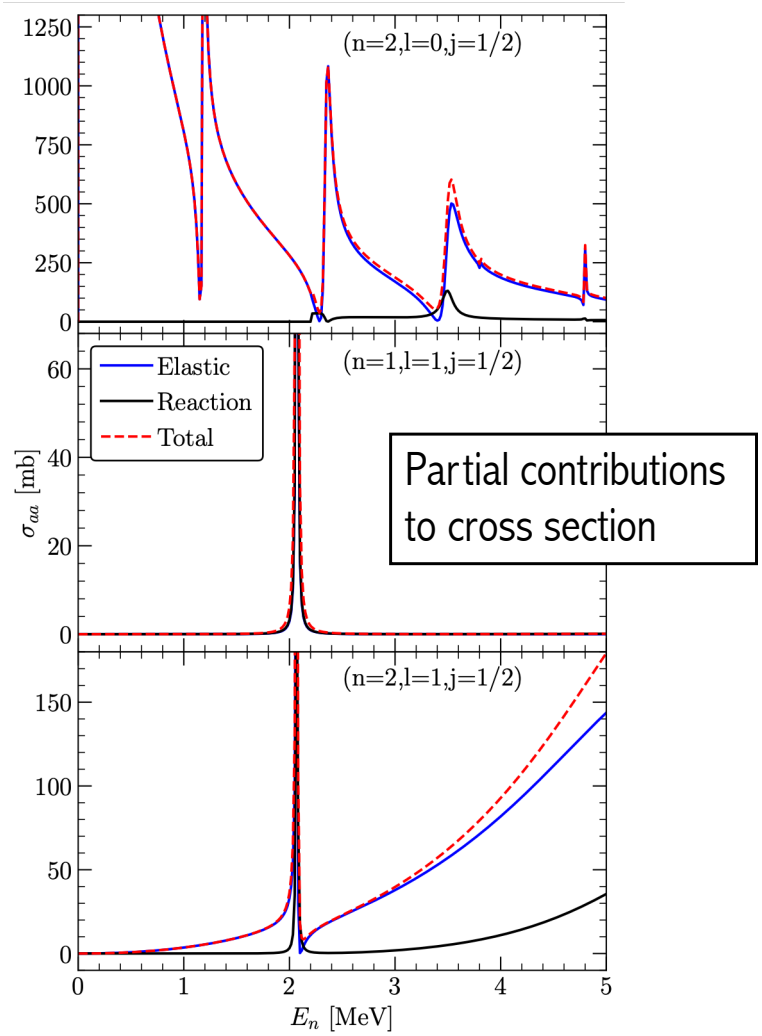
$$(\sigma_r)_{ab} = \delta_{ab} - |S_{ab}|^2$$

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

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

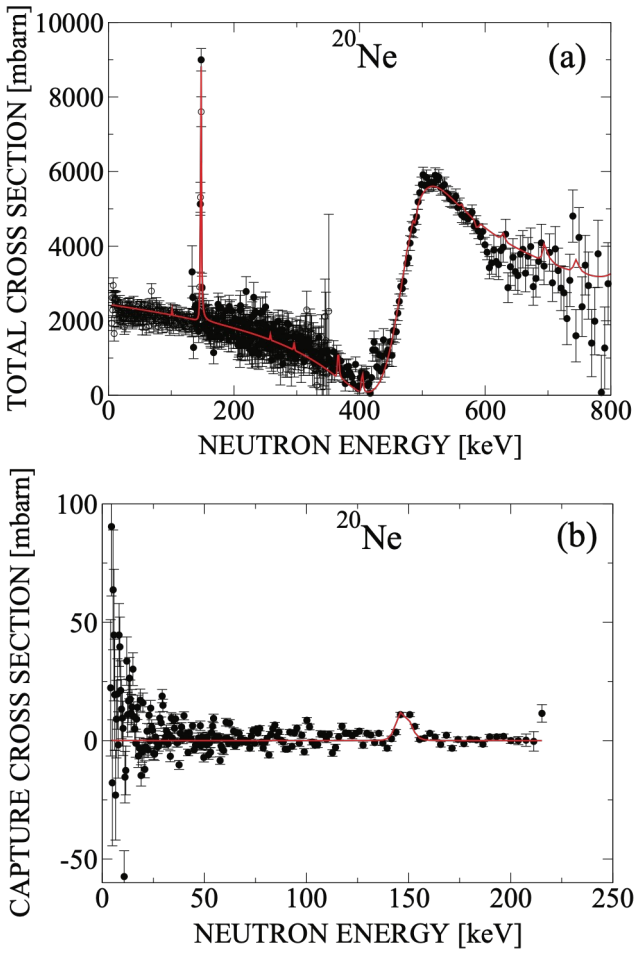
$$(\sigma_{CN})_{ab} = \langle |S_{ab}|^2 \rangle - \langle |S_{ab}| \rangle^2$$

- Can obtain differential cross sections as well



Much Work Remains

- Outlook:
  1. Finish treatment of neutron channels
  2. Improve treatment of single particle quantities
  3. Include proton, gamma, alpha, and other channels (fission might be too difficult)
  4. Investigate more systems
  5. Investigate more microscopic models
- *Confront results with experiment*



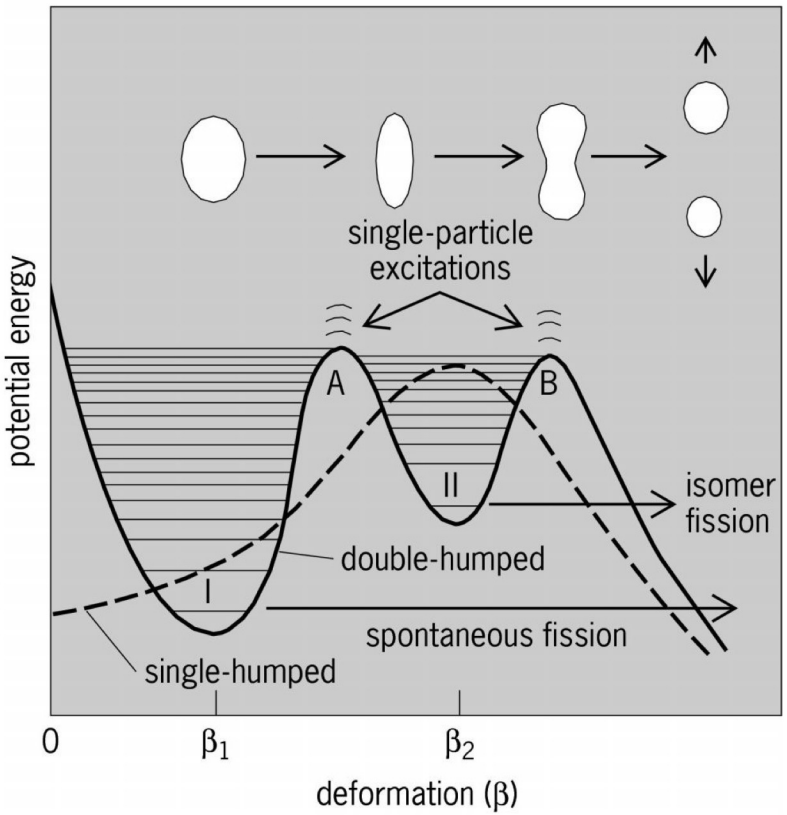
Source: M. Heil, el al, Phys. Rev. C 90, 045804 (2014)

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

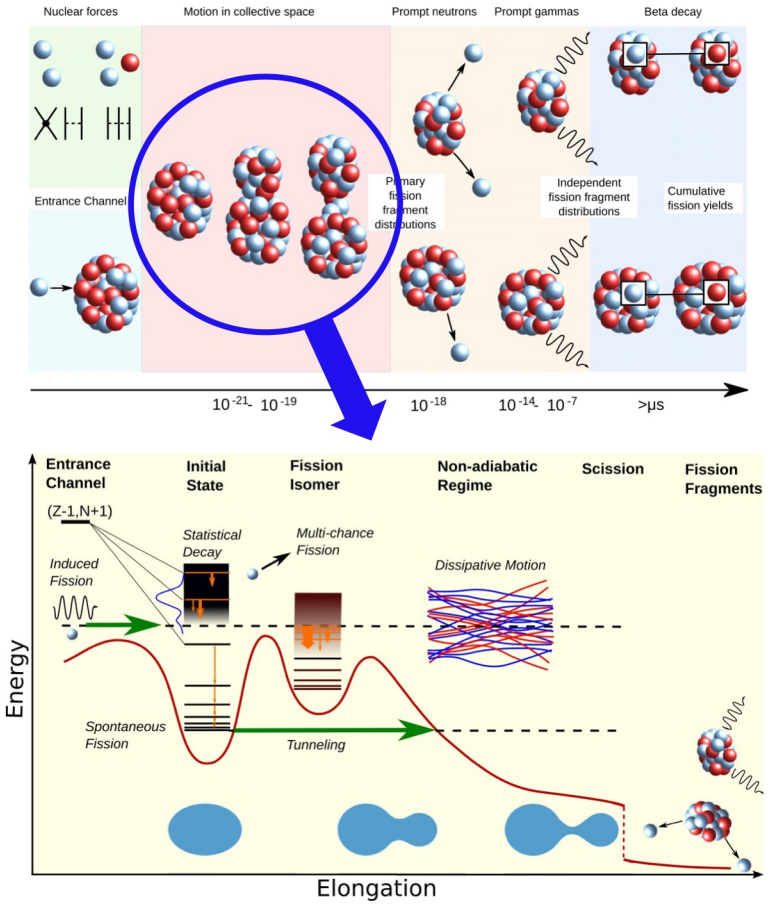


Source: J. R. Huizenga, Science, 168:1405–1413, (1979).

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

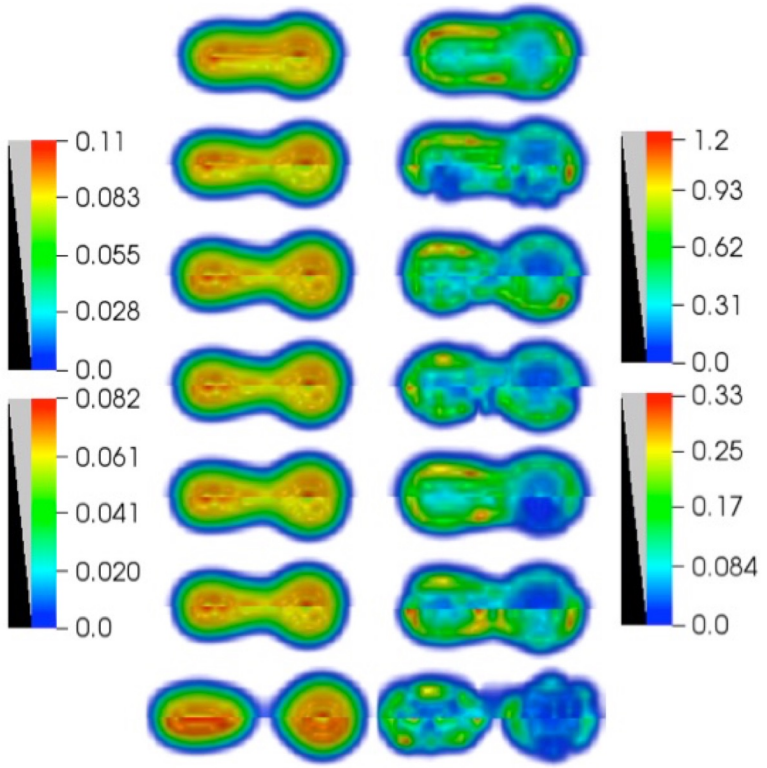
  Source: F. Gönnenwein FIESTA lecture notes (2014).
- Main goal - unified microscopic theory



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



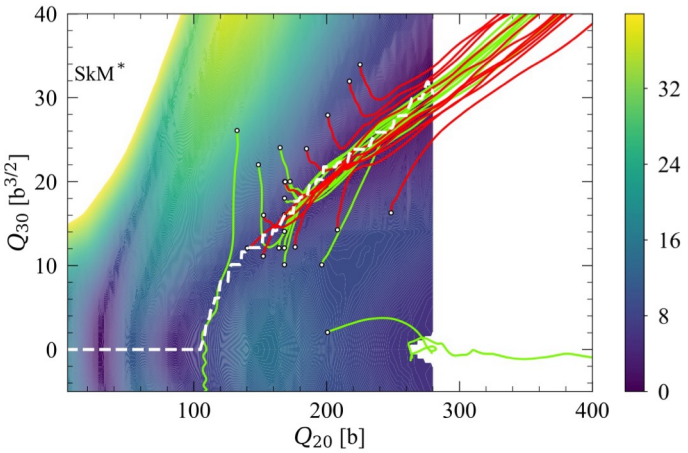
A. Bulgac, P. Magierski, K. J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

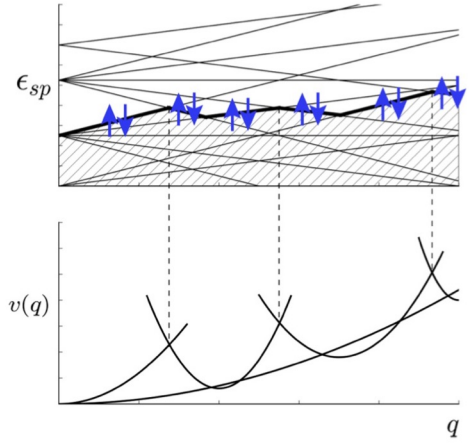
Role of Pairing

- 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



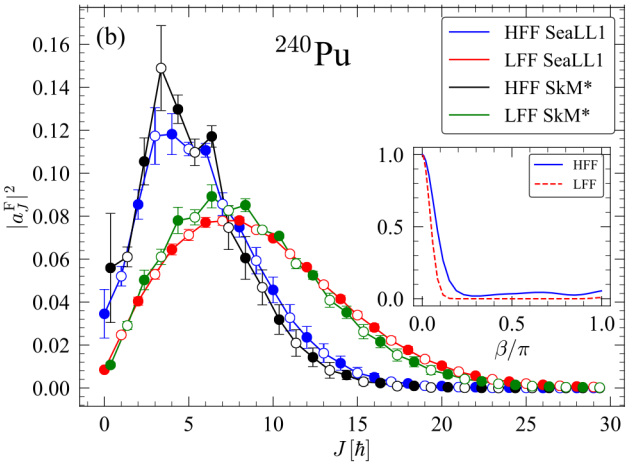


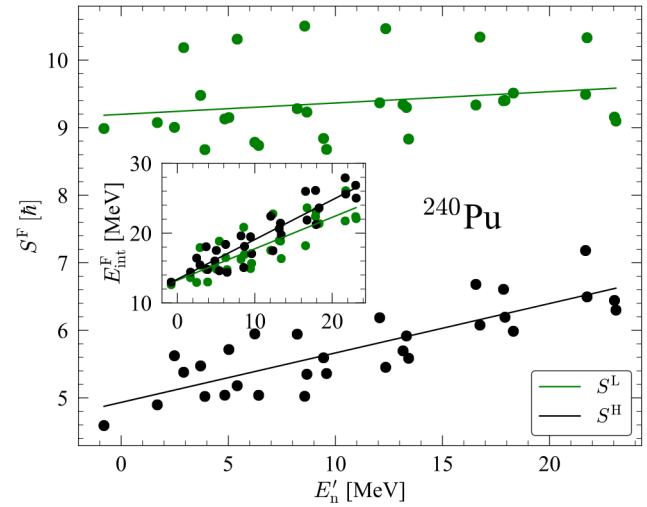
A. Bulgac, S. Jin, K. J. Roche, N. Schunck, and I. Stetcu, Phys. Rev. C 100, 034615 (2019)

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

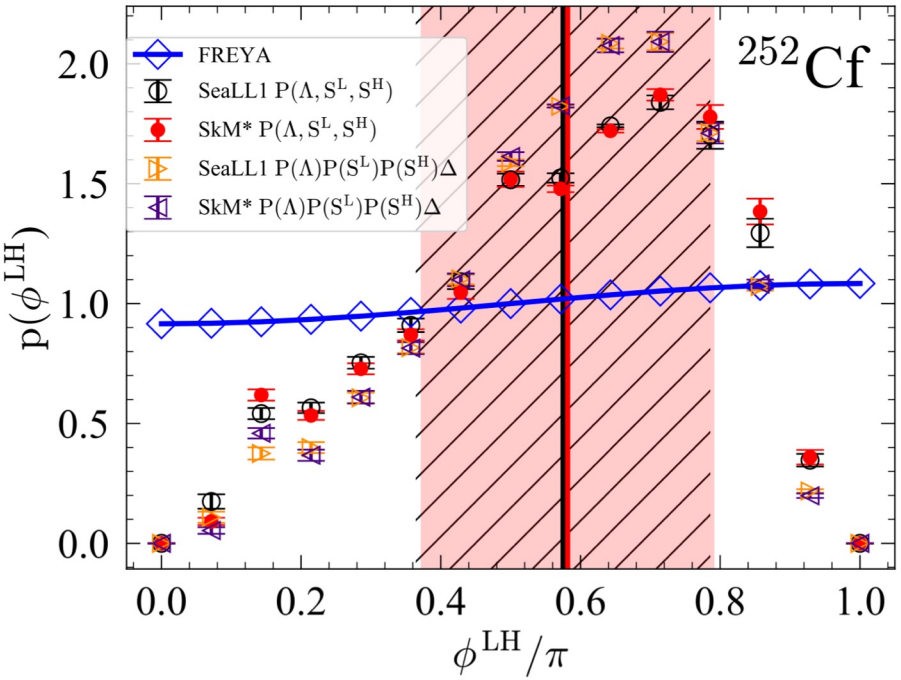




Source: A. Bulgac, I. Abdurrahman, S. Jin, K. Godbey, N. Schunck, and I. Stetcu, Phys. Rev. Lett. 126, 142502 (2021)

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),

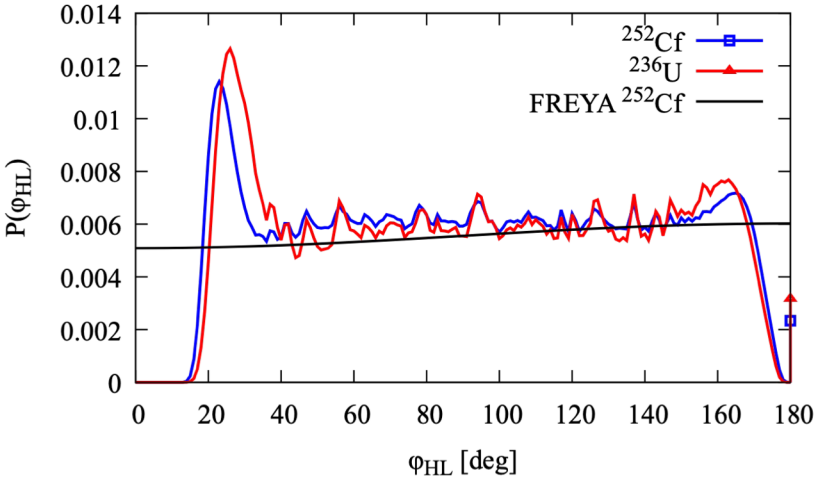
J. Randrup and R. Vogt, Phys. Rev. Lett. 127, 062502 (2021)

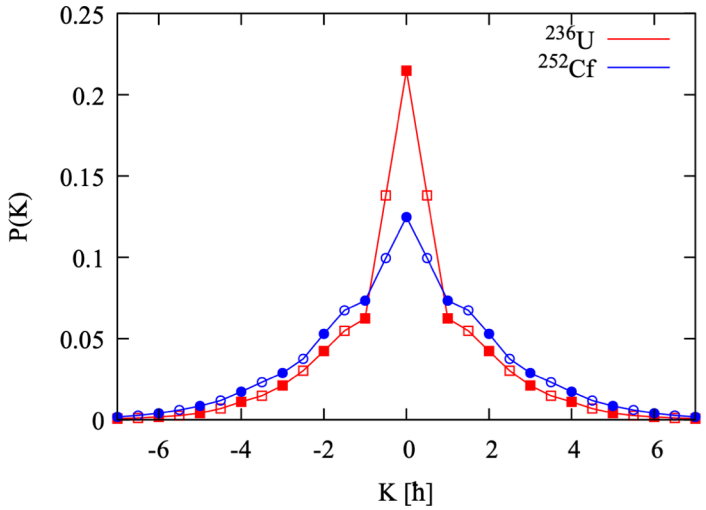
FF Angular Momenta Vector Correlations - Continued

- 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

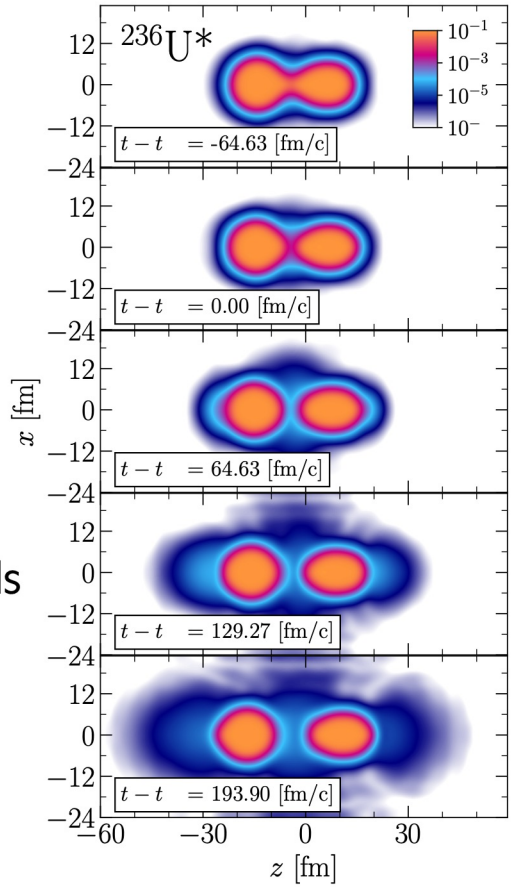
Source: G. Scamps, I. Abdurrahman, M. Kafker, I. Stetcu, and A. Bulgac, Phys. Rev. C 108, L061602 (2023)



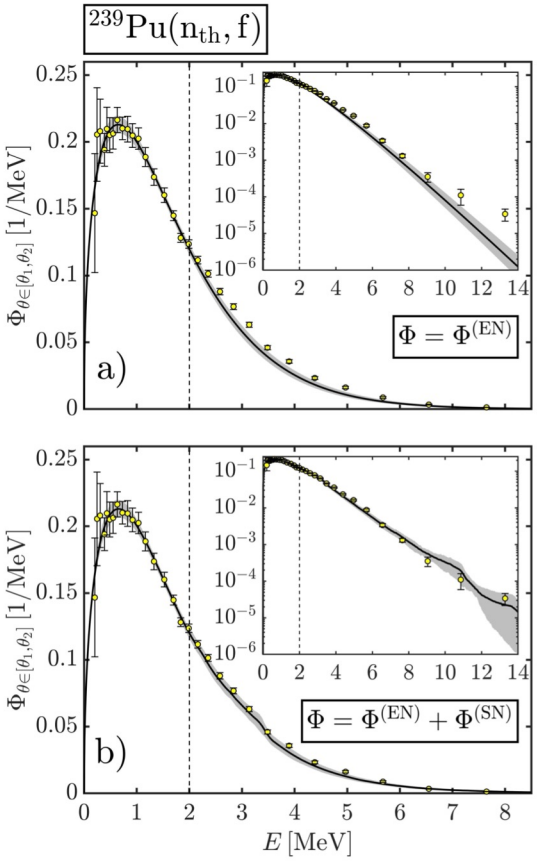


Scission Neutrons

- 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



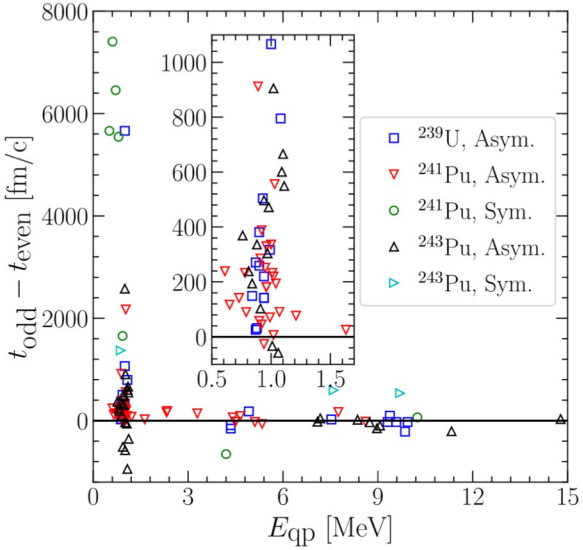
Source: I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, Phys. Rev. Lett. 132, 242501 (2024)



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

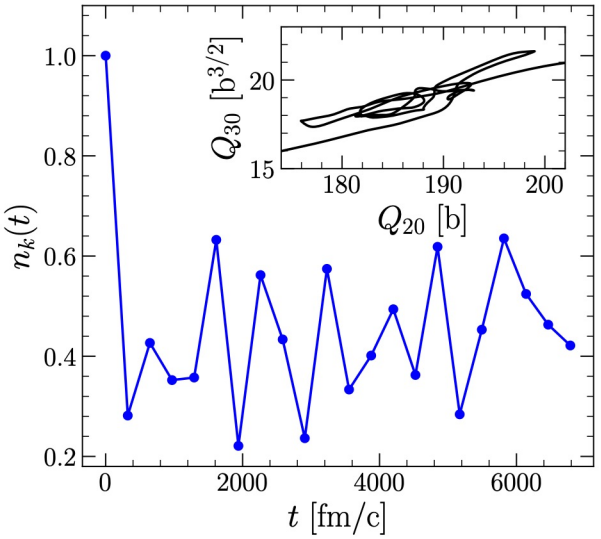
Odd Nuclei

- 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

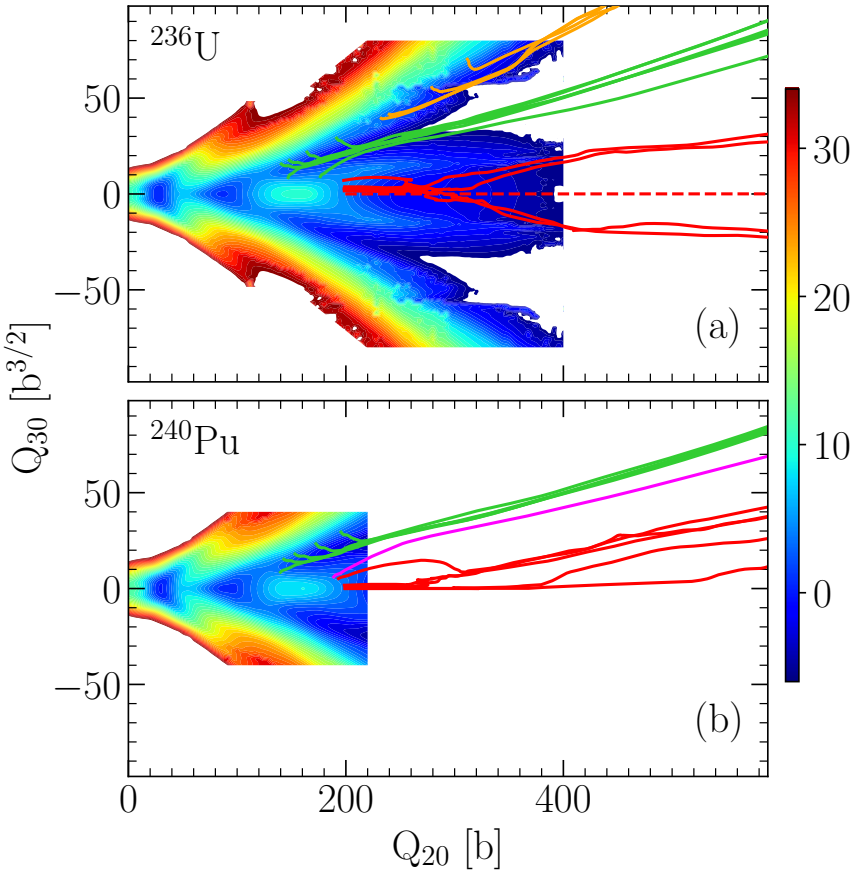
$$|\Phi\rangle = a_i^\dagger \prod_{k\neq i} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)\,|-\rangle$$



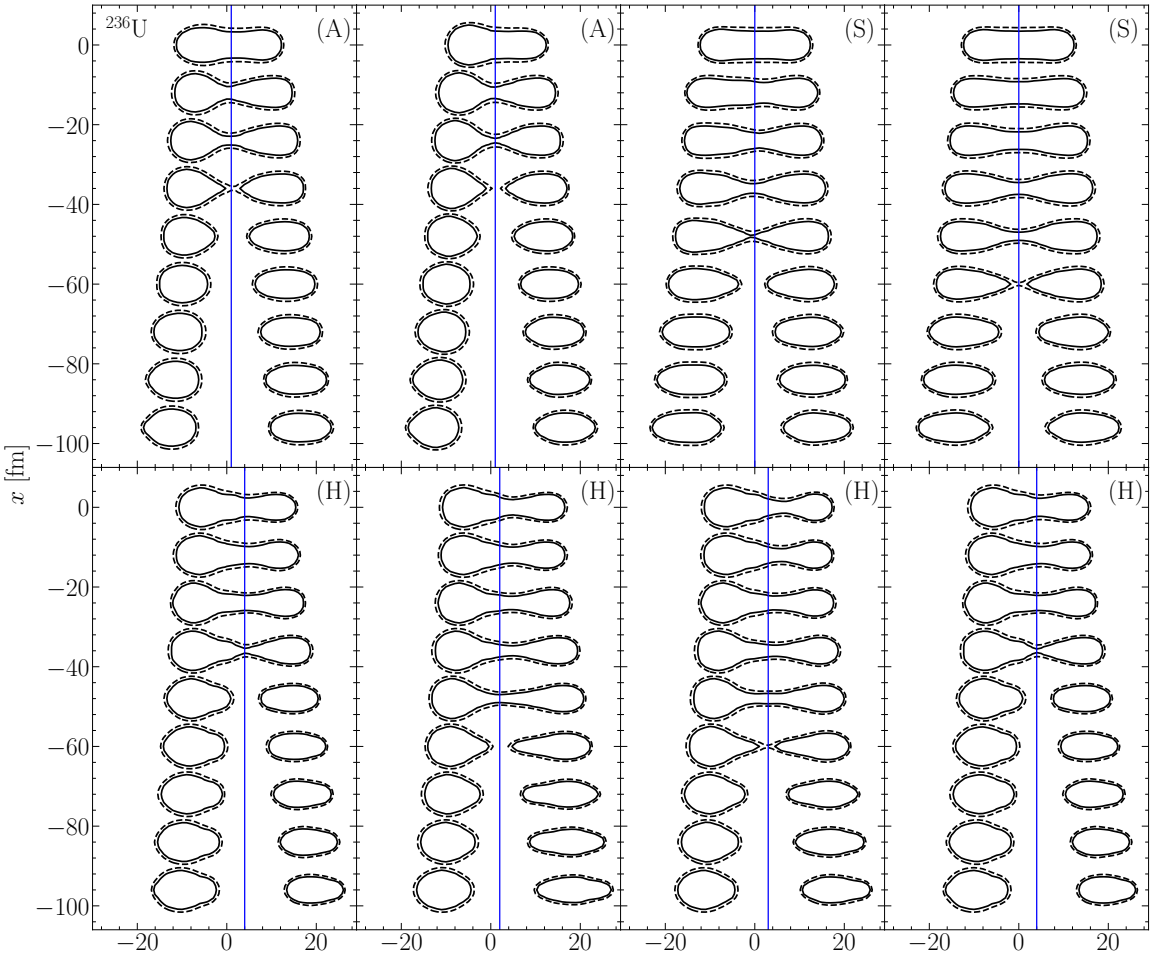
Source: A. Bulgac, I. Abdurrahman, M. Kafker, and I. Stetcu,, Phys. Rev. Lett. 135, 062501 (2025).

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.



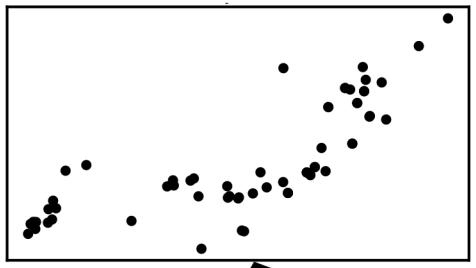
Source: Manuscript in preparation.

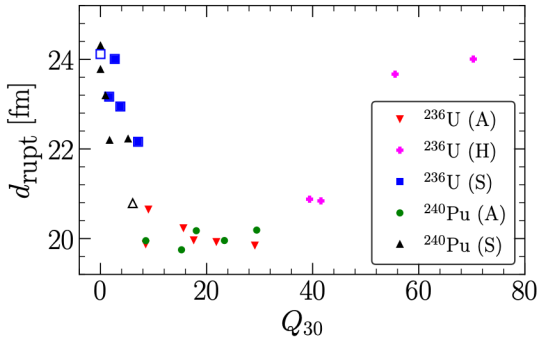
Partition of Energy between Fragments

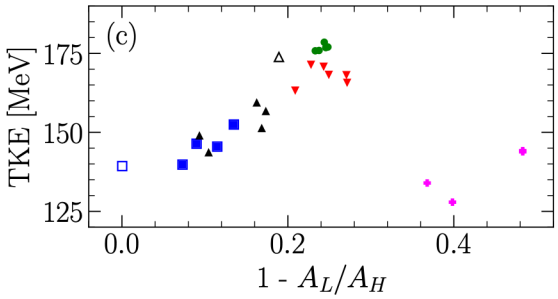
- Larger rupture distances for near-symmetric and highly-asymmetric modes
- Leads to lower TKE:

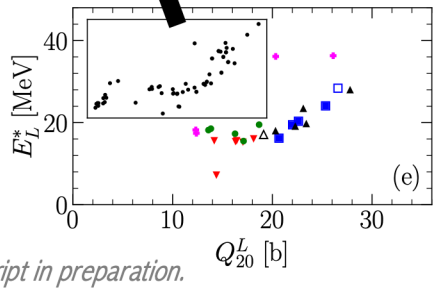
$$TKE \approx \frac{e^2 Z_L Z_H}{d_{\mathrm{rupt}}} + K_{\mathrm{rupt}}$$

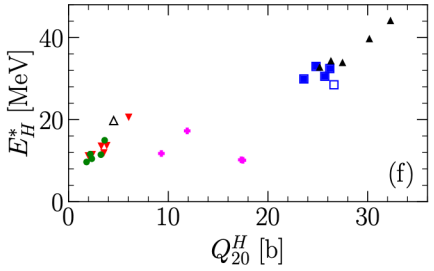
- Exotic modes populated more as initial energy increases
- Beyond certain threshold, energy goes into deformation
- Theory overestimates excitation energy:
  1. Too much dissipation
  2. Missing triaxial (and other) shapes
  3. Beyond mean field effects
  4. All of the above







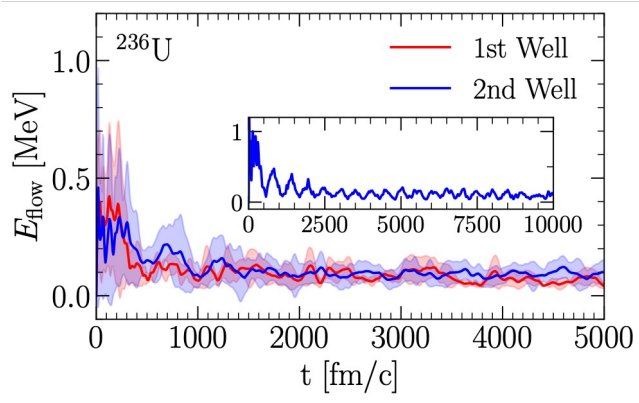


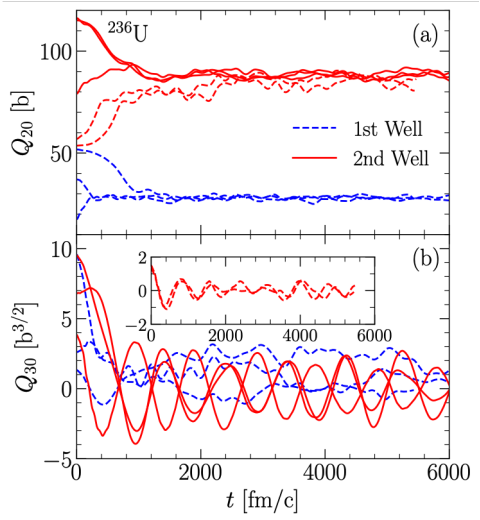


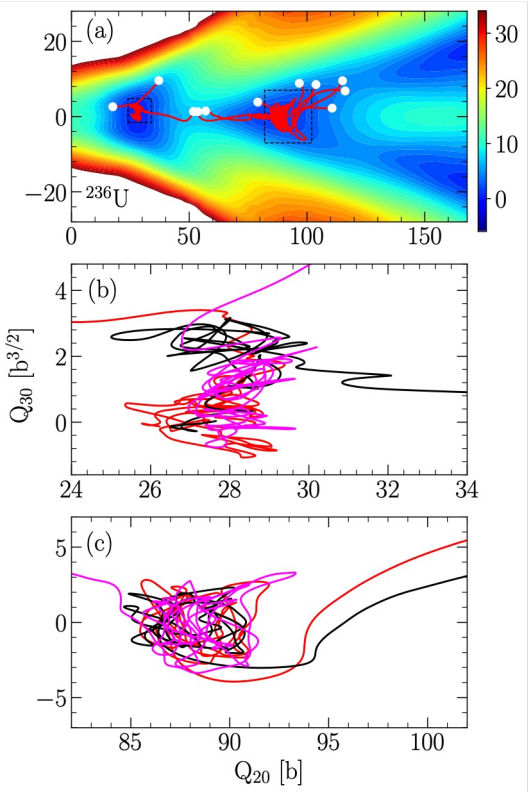
Source: Manuscript in preparation.

Dynamics Inside Ground State and Isomeric Wells

- Bohr's Hypothesis:
  - No memory of formation
  - Dynamics are strongly dissipative
- Emergence of period shape fluctuations in isomer well
- Probe of strength of fluctuations: Ratio of symmetric to asymmetric fission







Source: Manuscript in Preparation.

Thank you for your time!
Any questions?