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References: This code of conduct is based heavily on that of the INT and the APS. We are also grateful to Roxanne Springer for valuable discussion and guidance.

Statistical Properties of Actinides from Shell-Model Monte Carlo

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Yale University

Rising Researchers Seminar Series

Institute for Nuclear Theory

May 13, 2025

Yale

Outline

- The configuration-interaction shell model and the shell-model monte Carlo (SMMC)
  - Historical shell model developments
  - Advantages and limitations of the SMMC

- Applying the SMMC to the actinides
  - Model space and interaction

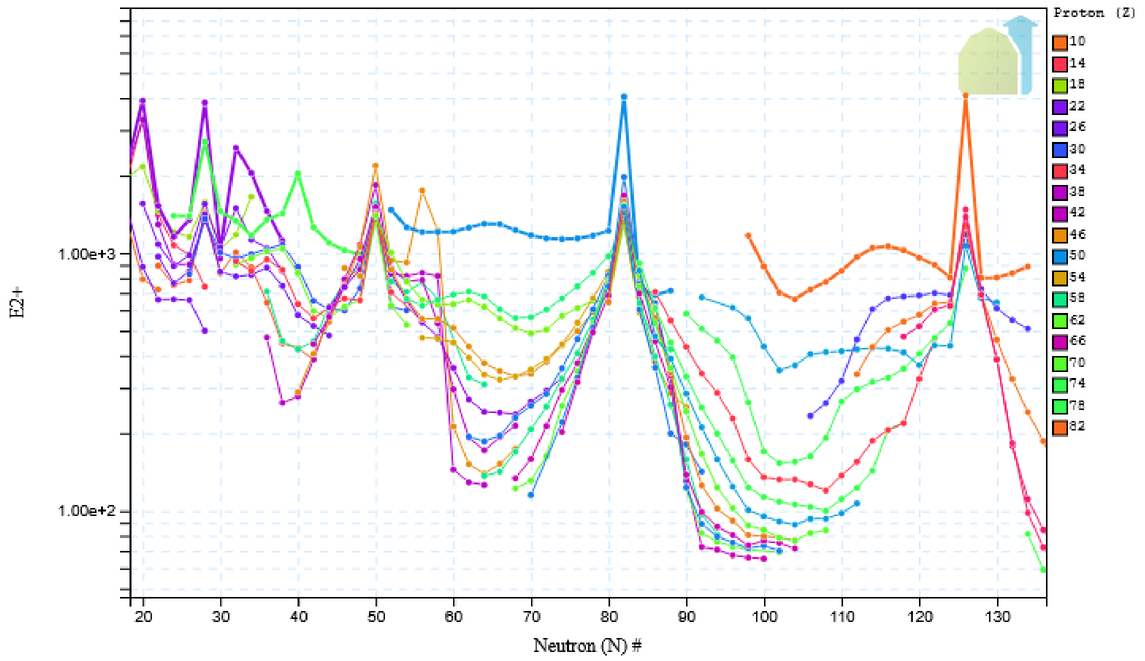
- Statistical properties of the actinides
  - Nuclear level densities and spin distributions
  - γ–ray strength functions
  - Quadrupole shape distributions and their applications (preliminary)

- Outlook and future work

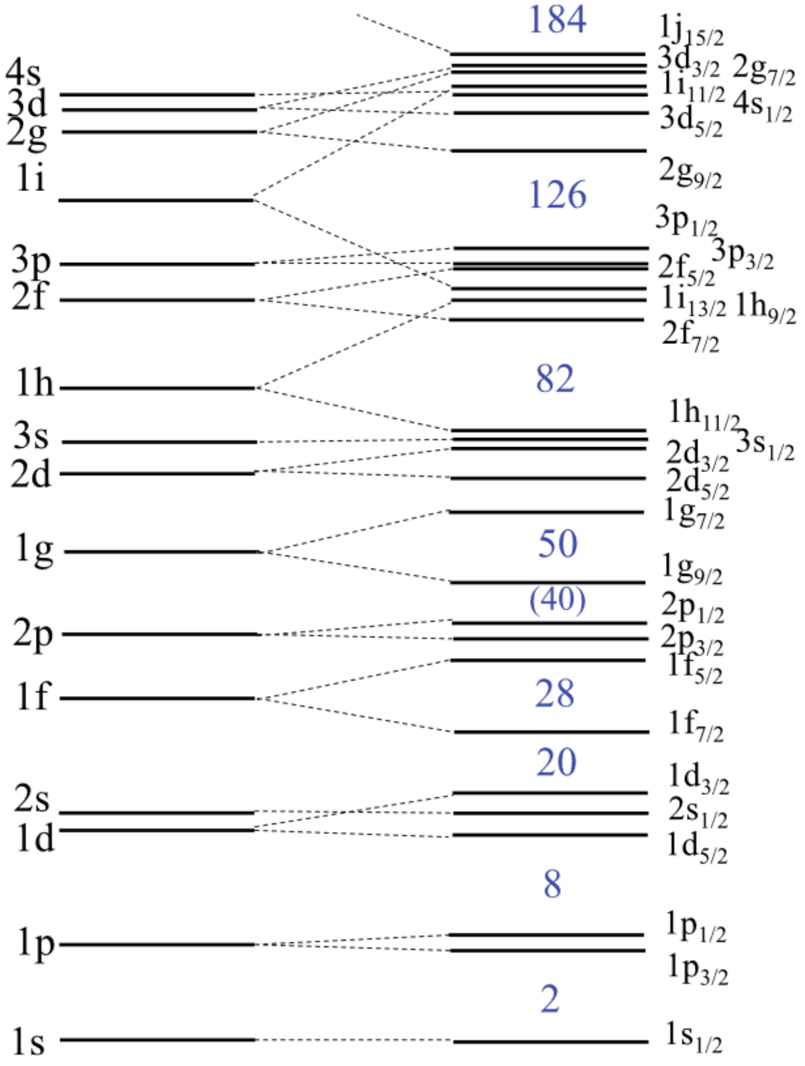
The Nuclear Shell Model

Developed by Goeppert-Mayer, Jensen, and others in 1949

Nucleons in an average one-body potential (harmonic oscillator or Woods-Saxon) with strong spin-orbit coupling explains observed magic numbers



From NuDat 3.0



Spin-orbit coupling ->

Shell Model Calculations

- Configuration-interaction (CI) Hamiltonian with single-particle energies ε_i and residual two- and three-body interactions

$$\hat{H} = \sum_i \varepsilon_i \hat{n}_i + \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k + \sum_{ijklmn} V_{ijklmn}^{(3)} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_m \hat{a}_n + \cdots$$

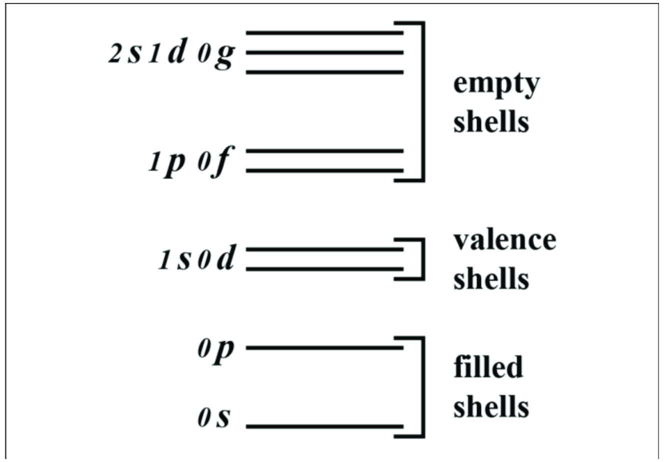
- Solve the many-body Schrodinger equation
  $\hat{H}|\psi\rangle = E|\psi\rangle$, where $|\psi\rangle = \sum_\alpha |\alpha\rangle$ and $|\alpha\rangle$ are Slater determinants

- Many-body basis states are built from single-particle states in a chosen valence space
  - Valence space of active nucleons between an inert core and an excluded region
  - No-core shell model: no inert core, larger model space dimension, limited to lighter nuclei

- Ultimately, this is a huge matrix eigenvector/eigenvalue problem

- Particularly suited for calculating binding energies, excited states, electromagnetic transition strengths, and decay rates

sd-shell space



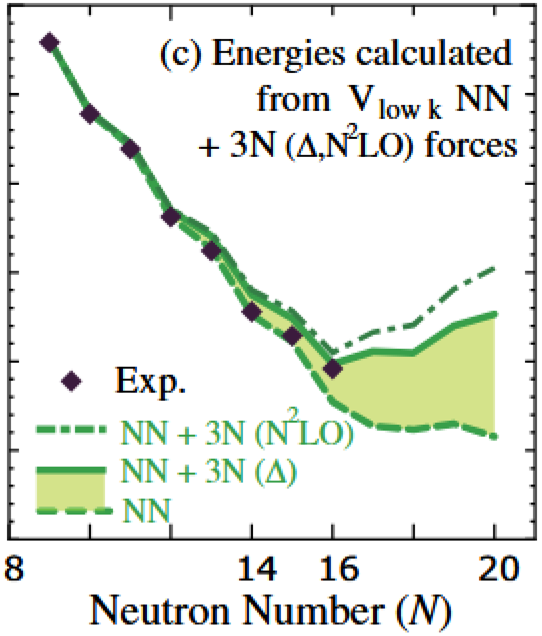
Corragio and Itaco, Front. in Phys. **8** (2020)

Model space dimension grows combinatorially with the number of valence states and valence nucleons.
Largest calculations have dimension around 10^{11} Tsunoda *et al*. PRC **95**, 021304 (2017)

Many state-out-the-art techniques have been developed recently:

- Lanczos-type algorithms for lowest eigenstates in large, sparse matrices
  Shimizu *et al*. Comp. Phys. Comm. **244** 372-384 (2019)
- Two- and three-body forces derived from chiral EFT
  Hebeler *et al*. PRC **83**, 031301 (2011)
- Renormalization group techniques for effective interactions in truncated spaces
  Bogner *et al*. PRL **113**, 142501 (2014), Stroberg *et al*. PRL **118**, 032502 (2017)

g.s. energies of O isotopes



Otsuka *et al*., PRL **105**, 032501 (2010)

Technical challenges:
- Size of the matrix eigenvector problem
- Storage of large number of non-zero matrix elements

The shell-model Monte Carlo (SMMC) method

The SMMC is a *statistical* approach to nuclear structure where we compute a canonical ensemble rather than solving the many-body Schrodinger equation

The two-body interaction term of the Gibbs ensemble $e^{-\beta H}$ at temperature T $(\beta = \frac{1}{T})$ can be rewritten with the Hubbard-Stratonovich transformation:

$$e^{-\frac{1}{2}\Delta\beta V_\alpha \hat{\rho}_\alpha^2} = \sqrt{\frac{\Delta\beta |V_\alpha|}{2\pi}} \int d\sigma_\alpha e^{-\frac{1}{2}\Delta\beta|V_\alpha|\sigma_\alpha^2} \, e^{-\Delta\beta s_\alpha \sigma_\alpha \hat{\rho}_\alpha}$$

Linearizes the exponent; transforms the theory to one of *non-interacting* nucleons moving in time-dependent external fields $\sigma_\alpha(\tau_n)$

$$e^{-\beta H} = \int D[\sigma] \, G_\sigma \hat{U}_\sigma$$

Integral measure

Gaussian weight

One-body propagator

SMMC (continued)

$$\mathrm{Tr}\,\hat{U}_\sigma = \det(\mathbf{1} + \boldsymbol{U}_{\boldsymbol{\sigma}})$$

$\boldsymbol{U}_{\boldsymbol{\sigma}}$ is the matrix that represents the propagator in the single-particle space

- All matrix algebra is done in this space with matrices of dimension ~100 rather than the combinatorially-large many-particle space
- Integration over the set of (up to ~10 million) auxiliary fields $\sigma_\alpha(\tau_n)$ is handled by Monte Carlo
- $\mathrm{Tr}\,\hat{U}_\sigma$ is a grand canonical trace and we use a discrete Fourier transform to project onto specific numbers of protons and neutron to compute a canonical trace for a particular nucleus

$$Tr_A \hat{U}_\sigma = \frac{e^{-\beta\mu A}}{N_s} \sum_{m=1}^{N_s} e^{-i\,\phi_m A} \det(\mathbf{1} + e^{i\phi_m + \beta\mu} \boldsymbol{U}_{\boldsymbol{\sigma}})$$

Ormand, Dean, Johnson, Lang, and Koonin, PRC **49**, 1422 (1994).

The shell-model Monte Carlo (SMMC) enables microscopic calculations in spaces that are many orders of magnitude larger ($>10^{30}$) than those that can be treated by conventional methods ($\sim 10^{11}$).

Early works on the SMMC:

Johnson, Koonin, Lang, and Ormand, PRL **69**, 3157 (1992)
Lang, Johnson, Koonin, and Ormand, PRC **48**, 1518 (1993)
Alhassid, Dean, Koonin, Lang, and Ormand, PRL **72**, 613 (1994)

Recent review:

Y. Alhassid, in *Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling,* ed. K.D. Launey (World Scientific 2017)

SMMC is the state-of-the-art method for the microscopic calculation of statistical properties of nuclei.

Limitations:

- No detailed spectroscopy*
  *Some spectroscopy possible with imaginary time correlation matrices (ITCM)
  Alhassid, Bonett-Matiz, Gilbreth and Vartak PRL 133, 182501 (2024)
- Monte Carlo sign problem, small bad-sign components of interactions can be dealt with using the extrapolation method of Alhassid, Dean, Koonin, Lang, and Ormand, PRL **72**, 613-616 (1994)

Statistical Properties in Heavy Nuclei

Statistical properties of nuclei: level densities, γ–ray strength functions,...

Statistical properties are important input in the Hauser-Feshbach theory of compound nuclear reactions but are not always accessible to direct measurement.

The calculation of statistical properties in the presence of correlations is a challenging many-body problem.

- Mean-field approximations (e.g., Hartree-Fock-Bogoliubov) often miss important correlations and are problematic in the broken symmetry phase.

The configuration-interaction (CI) shell model takes into account correlations beyond the mean-field but the combinatorial increase of the dimensionality of its model space has hindered its applications in heavy nuclei.

SMMC in Heavy Nuclei

- The single-particle Hamiltonian is a Woods-Saxon potential plus spin-orbit coupling,
- Pairing-plus-multipole interaction (quadrupole, octupole, hexadecupole)

$$\hat{H}_{int} = -\sum_{\nu} g_\nu \hat{P}_\nu^\dagger \hat{P}_\nu - \sum_{\lambda} k_\lambda \chi : (\hat{O}_{\lambda,p} + \hat{O}_{\lambda,n}) \cdot (\hat{O}_{\lambda,p} + \hat{O}_{\lambda,n}) :$$

This interaction has a good Monte-Carlo sign and describes the dominant collective components of effective nuclear interactions Dufour and Zuker PRC **54**, 1641 (1996)

Different model space and interaction coefficients for different regions of the nuclear chart

Challenges moving up to actinides:

- Larger single-particle model space
- Lower first excited states -> larger values of β to cool the nucleus to its ground state

Model space for actinides:
- Protons: 82-126 shell plus $1g_{9/2}$
- Neutrons: 126-184 shell plus $1h_{11/2}$

124 total m-scheme single-particle states

Interaction Parameters for Actinides

Used the HFB code HF-SHELL to efficiently test different sets of parameters
Ryssens and Alhassid, EPJA **57**, 76 (2021)

Focused on reproducing odd-even mass staggerings (OES) and nuclear state densities

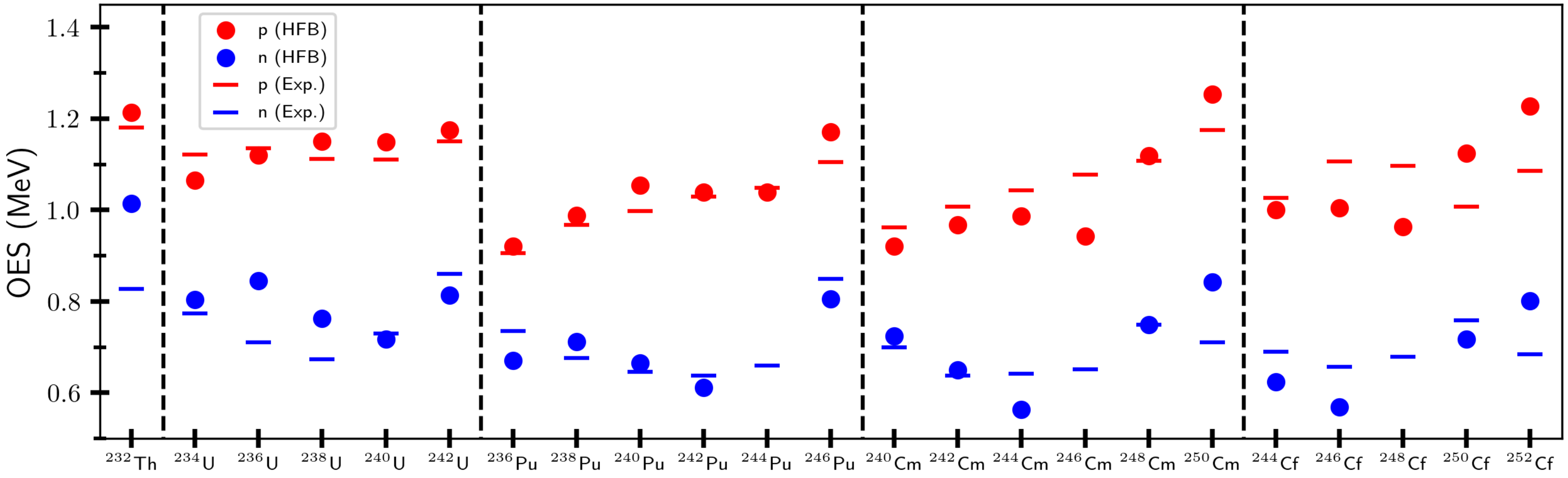
Mean-field values of OES are predicted to reproduce about half of the experimental values
Donati *et al*. J. Phys. G **31**, 295 (2005)

$$g_p = 0.111 + 0.00038(N - 148)$$

$$g_n = 0.0681 + 0.00047(N - 148)^{5/4}$$

$$k_2 = 2.299 - \frac{2.39}{(N-148)^2 + 21.206} - 0.0149(N - 148)$$

$$k_3 = k_4 = 1.0$$



Nuclear State Densities in the SMMC

Partition function:

Calculate the thermal energy $E(\beta) = \langle \hat{H} \rangle$ versus β and integrate $-\frac{\partial \ln Z}{\partial \beta} = E(\beta)$ to find the canonical partition function $Z(\beta)$.

State density:

The state density $\rho(E_x)$ is related to the partition function by an inverse Laplace transform:

$$\rho(E_x) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\beta \, e^{\beta E_x} Z(\beta)$$

- The *average* state density is found from $Z(\beta)$ in the saddle-point approximation:

$$\rho(E_x) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E_x)}$$

S(E) = canonical entropy

$$S(E_x) = \ln Z + \beta E_x$$

C = canonical heat capacity

$$C = -\beta^2 \partial E / \partial \beta$$

Determining Ground-State Energies

Even-even nuclei: ground state energy can be extracted by calculating $\langle \hat{H} \rangle$ at large enough β

Odd-mass nuclei: sign problem exists at low temperatures preventing direct determination of E_0

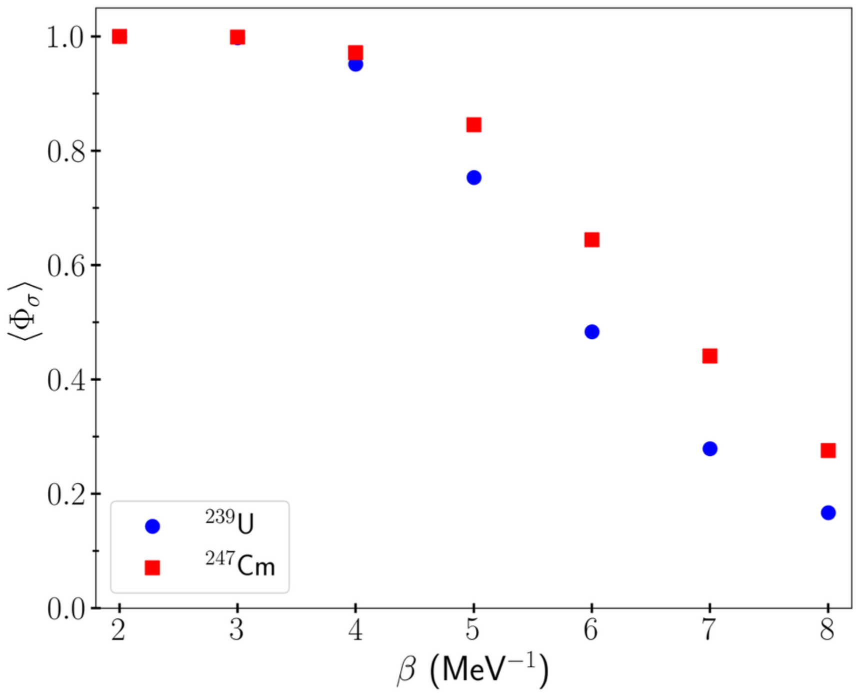
Projection onto an odd number of protons or neutrons introduces a sign problem at low temperatures

Need a method to extract the ground state energy

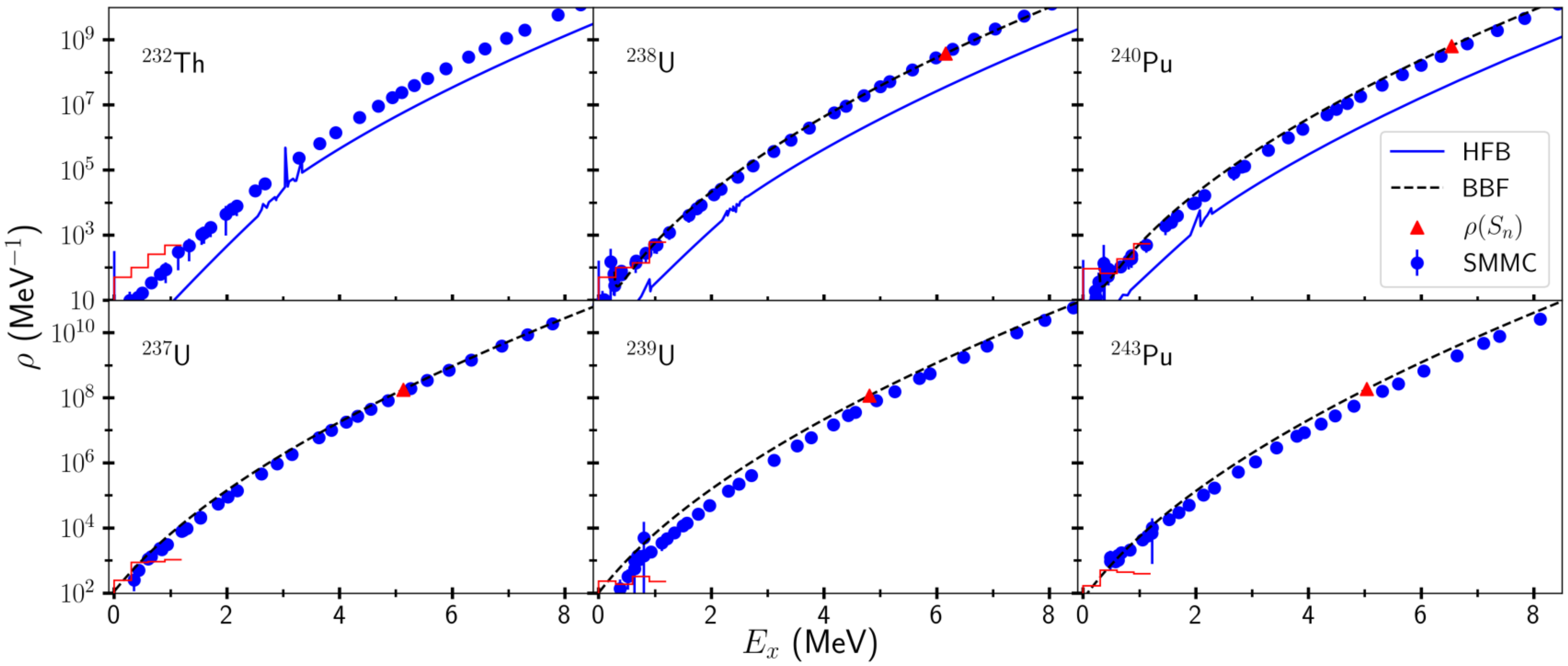
- Could supplement the state density with experimental data on low-lying states
  Ozen, Alhassid, and Nakada, PRC **91**, 034329 (2015).

- Partition function extrapolation method (PFEM) developed to extract ground-state energy without the need for experimental data
  Alhassid, Fanto, and Ozen, PRC **120**, L061303 (2024)

Monte-Carlo sign $\langle \Phi_\sigma \rangle$ vs. β

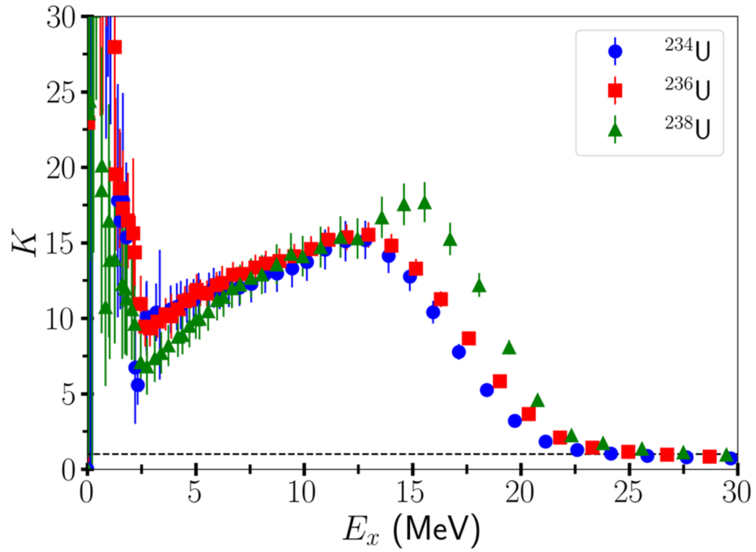


State Densities in Actinides



D.D. and Alhassid (forthcoming)

$$K = \rho_{\mathrm{SMMC}}/\rho_{\mathrm{HFB}}$$



State densities show good agreement with the BBF that is tuned to match with the counting of experimental low-lying states and neutron resonance data

Strong enhancement over mean-field densities due to rotational bands described by the collective enhancement factor K

Nuclear Level Densities and the Spin Projection

- The state density $\rho(E_x)$ counts all 2J+1 degenerate states within each level with spin J. To compute the level density $\tilde{\rho}(E_x)$ we count each level just once.

- We can perform additional projections onto specific values of spin component M

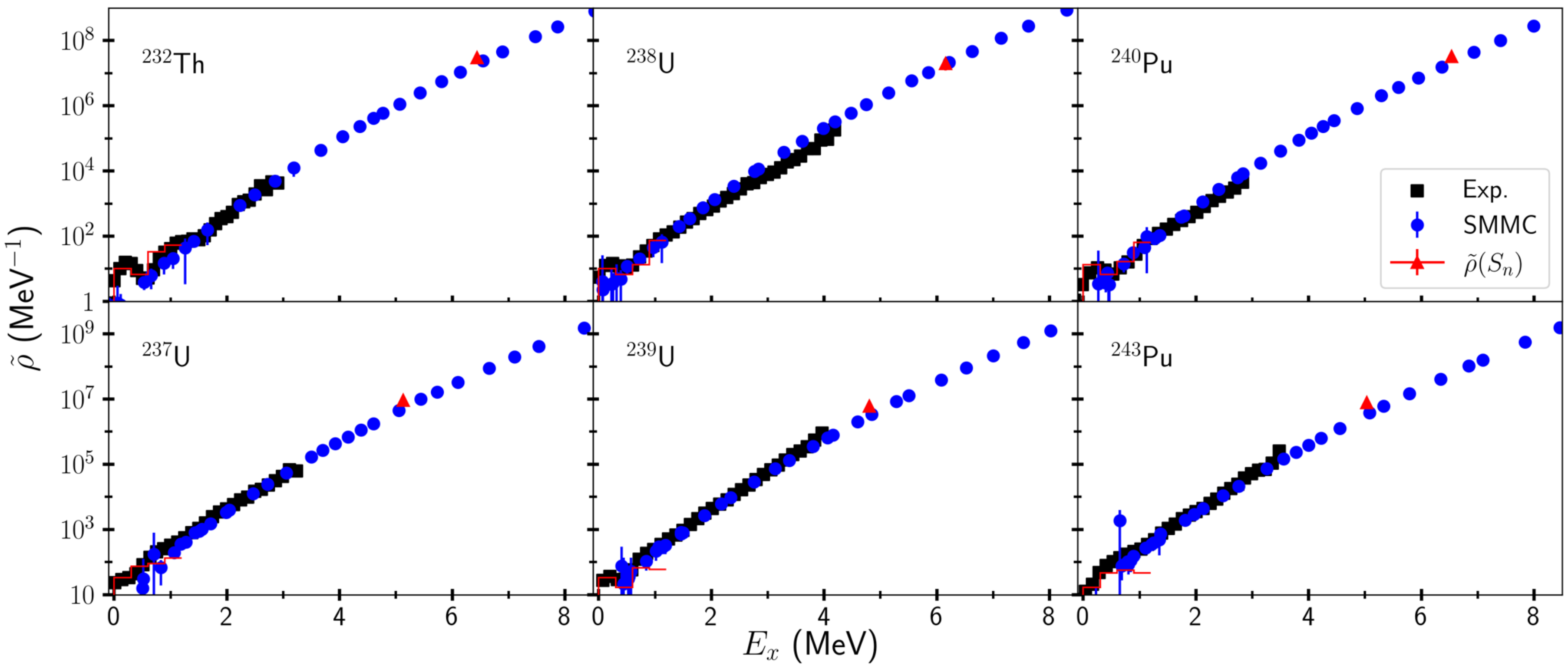
  Alhassid, Liu, and Nakada, PRL **99**, 162504 (2007)

$$\mathrm{Tr}_M \hat{O} = \frac{1}{2J_s+1} \sum_{k=-J_s}^{J_s} e^{i\varphi_k M}\, \mathrm{Tr}(e^{i\varphi_k \hat{J}_z} \hat{O})$$

- By projecting onto $M=0$ (even-mass nuclei) or $M=\frac{1}{2}$ (odd-mass nuclei), only one state from each level is counted, and we obtain $\tilde{\rho}$

- We can also project onto values of total spin J to calculate spin distributions

Level Densities in Actinides



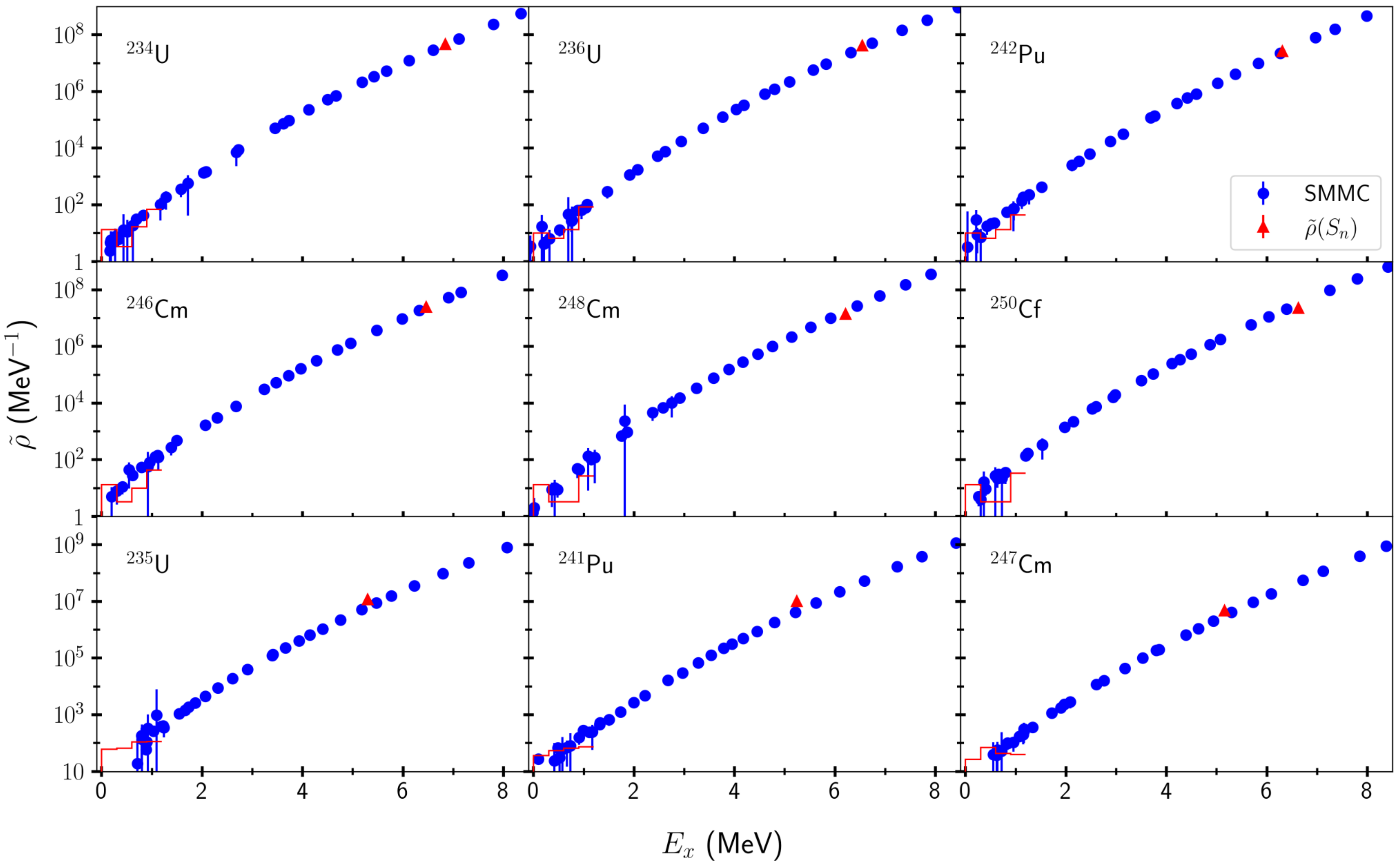
SMMC shows excellent agreement with Oslo experiments

Experimental Results:

^{232}Th, $^{237\text{-}239}$U: Guttormsen *et al.*, PRC **88** 024307 (2013)

^{240}Pu: Zeiser *et al.*, PRC **100** 024305 (2019)

^{243}Pu: Laplace *et al.*, PRC **93** 014323 (2016)



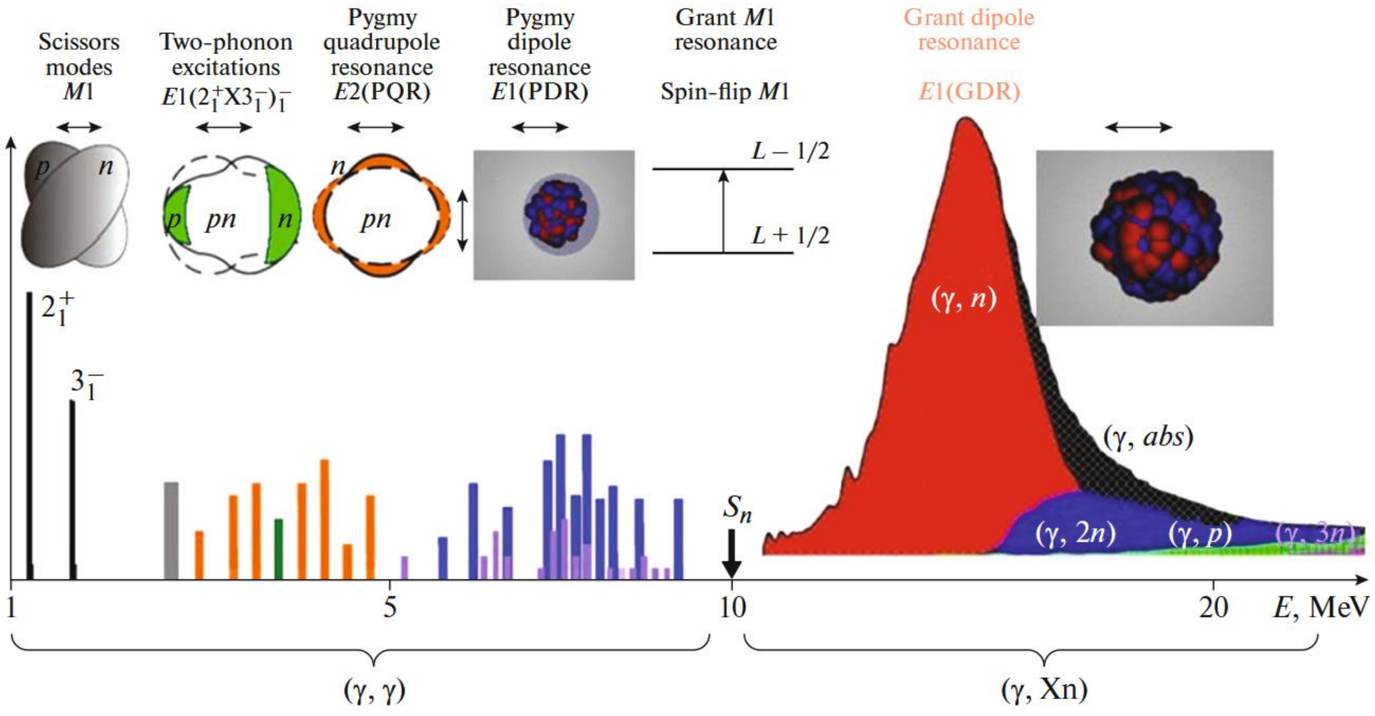
More level densities for nuclei where Oslo data is not available

γ-ray Strength Functions (γSF)

Gamma-ray strength function:

$$f_{XL}(E_\gamma; E_i, J_i^\pi) = \frac{\Gamma_i^{XL}(E_\gamma)\widetilde{\rho}(E_i, J_i^\pi)}{E_\gamma^{2L+1}}$$ where Γ_i is the partial decay width

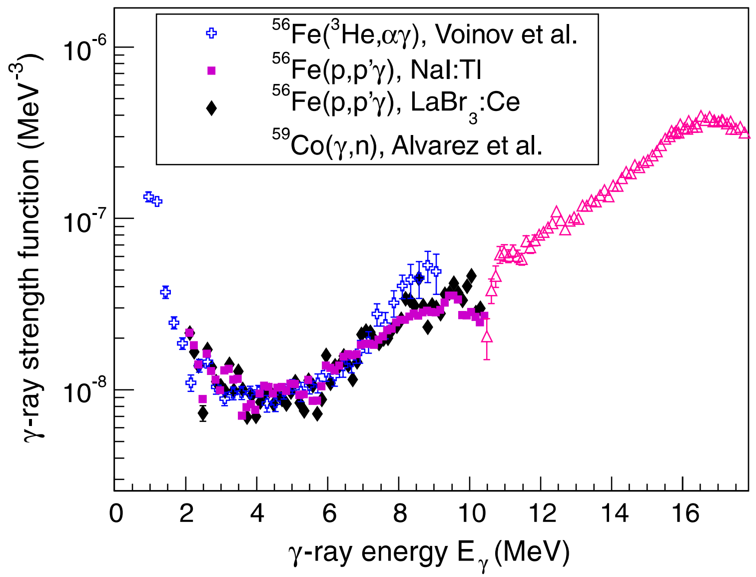
- The γSF contains important information about collective structures in nuclei
- Important input for compound nucleus reactions codes
- Measured with photo-excitation from ground state or decay from excited states (Oslo method)



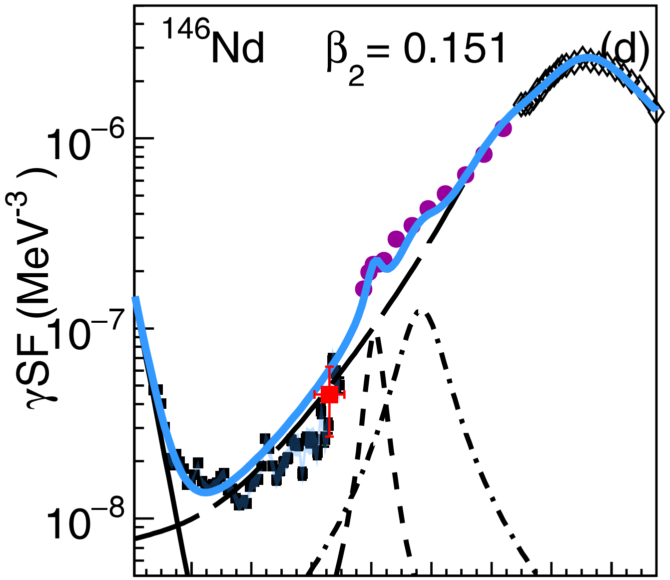
Kamerdzhiev and Shitov, Moscow Univ. Phys. **79**, 191-199 (2024)

The Low-Energy Enhancement (LEE)

In recent years, a low-energy enhancement (LEE) was observed in the γSF of mid-mass nuclei and in a few rare-earth nuclei



Larsen *et al.*, PRL **111**, 242504 (2013)



Guttormsen *et al.*, PRC **106**, 034314 (2022)

If the LEE persists in heavy neutron-rich nuclei, it can have significant effects on r-process nucleosynthesis by enhancing radiative neutron capture rates near the neutron drip line. Larsen and Goriely, PRC **82**, 014318 (2010)

Theoretical Calculations of γ-ray Strength Functions

The calculation of strength functions in the presence of correlations is a challenging many-body problem and microscopic approaches are limited:

- Quasiparticle random-phase approximation (QRPA) strength functions can often miss important correlations and require empirical modifications.
- QRPA does not produce the LEE
- Conventional CI shell model studies have attributed the LEE to the M1 γSF but they are limited to light and medium-mass nuclei.

SMMC enables exact (up to statistical errors) calculations in heavy nuclei!

The finite-temperature strength function of a transition operator $\hat{O}$ (e.g., E1,M1,...) is

$$S_0(\omega) = \sum_{i,f} \frac{e^{-\beta E_i}}{Z} |\langle f|\hat{O}|i\rangle|^2 \delta(\omega - (E_f - E_i))$$

In SMMC, it is only possible to calculate imaginary-time response functions

$$R_0(\tau) = \langle \hat{O}(\tau)\hat{O}(0) \rangle$$

The response function $R_0(\tau)$ is the Laplace transform of the strength function

$$R_0(\tau) = \int_{-\infty}^{\infty} d\omega\, e^{-\tau\omega} S_0(\omega)$$

The inversion requires analytic continuation to real time and is numerically ill-defined (no unique solution)

We use the maximum entropy method (MEM): fitting to the SMMC response function while staying “sufficiently close” to a prior strength function

The success of the method depends on a good choice for a prior strength function
➡ we use the static path approximation, where the strength function can be calculated directly (includes large-amplitude static fluctuations of the mean field)

M1 Strength Functions

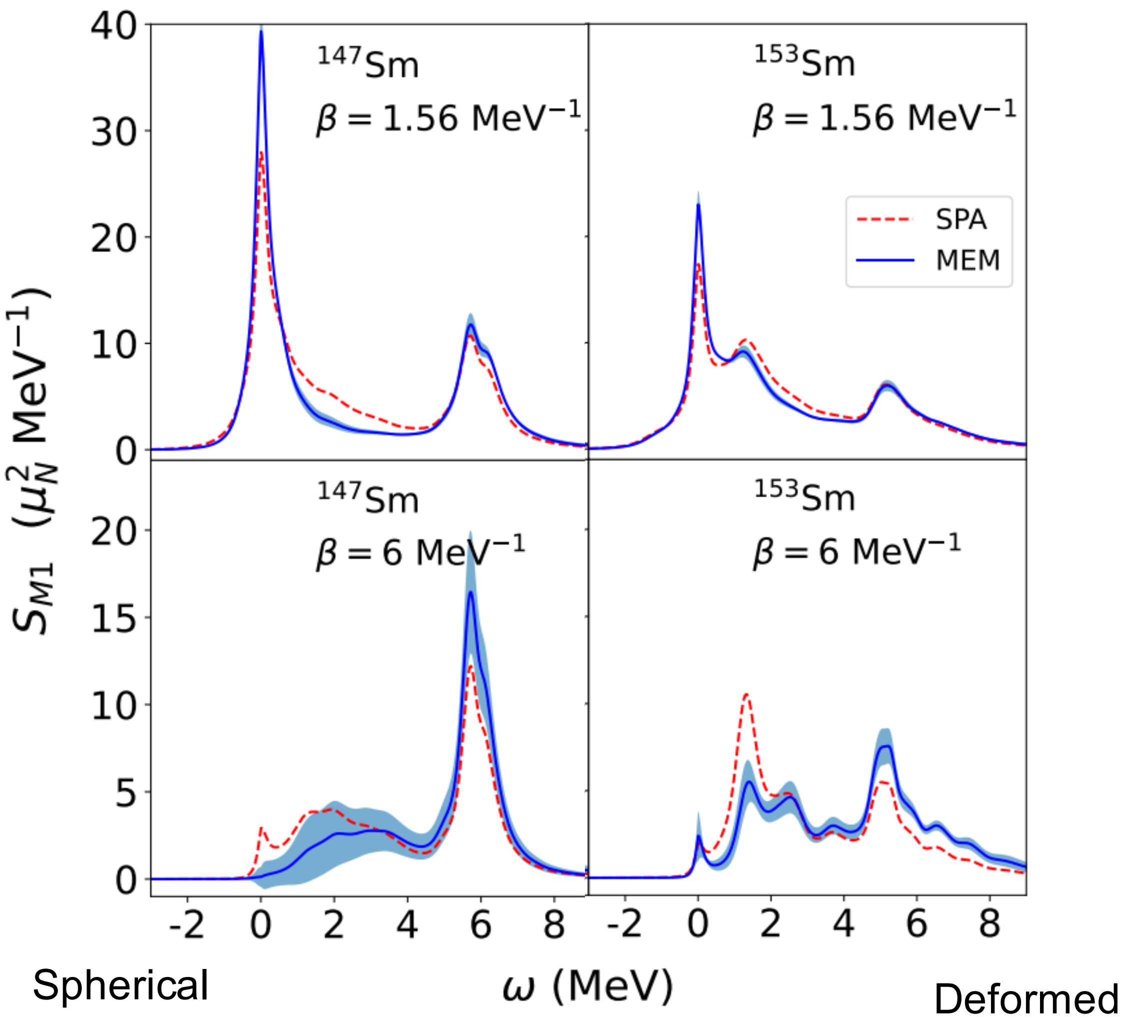
Several collective structures can be identified in the M1 strength functions

- LEE – Large peak near $\omega = 0$, seen at finite temperature, but not in the ground state

  - Experimentally seen in Oslo method in the deexcitation strength but not in photo-excitation strength

- Scissor mode – Broad peak near $\omega = 2$ MeV in deformed nuclei

- Spin-flip mode – Sharp peak near $\omega = 5 - 6$ MeV seen in all nuclei



D.D., Alhassid, PRC **111**, 034315 (2025)

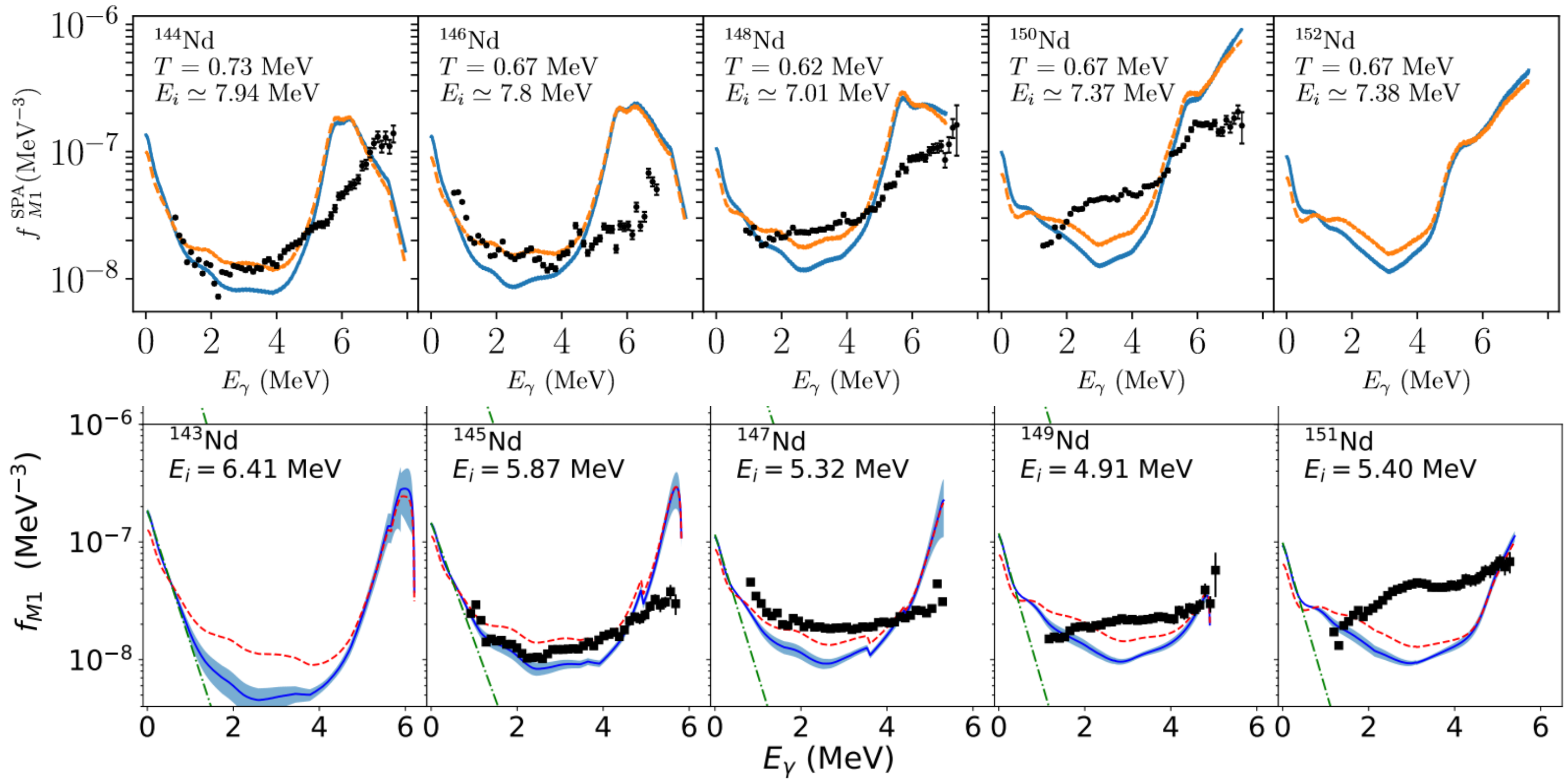
M1 γSFs in Lanthanides

$$f_{M1}(E_\gamma) = \frac{a\tilde{\rho}(E_i)}{3\tilde{\rho}(E_i - E_\gamma)} S_{M1}(-E_\gamma)$$

LEE is seen in all nuclei, magnitude and slope only weakly vary with N – good agreement with experiment

Scissors mode built on excited states emerges as deformation increases

Experimental strength function contains both M1 and E1



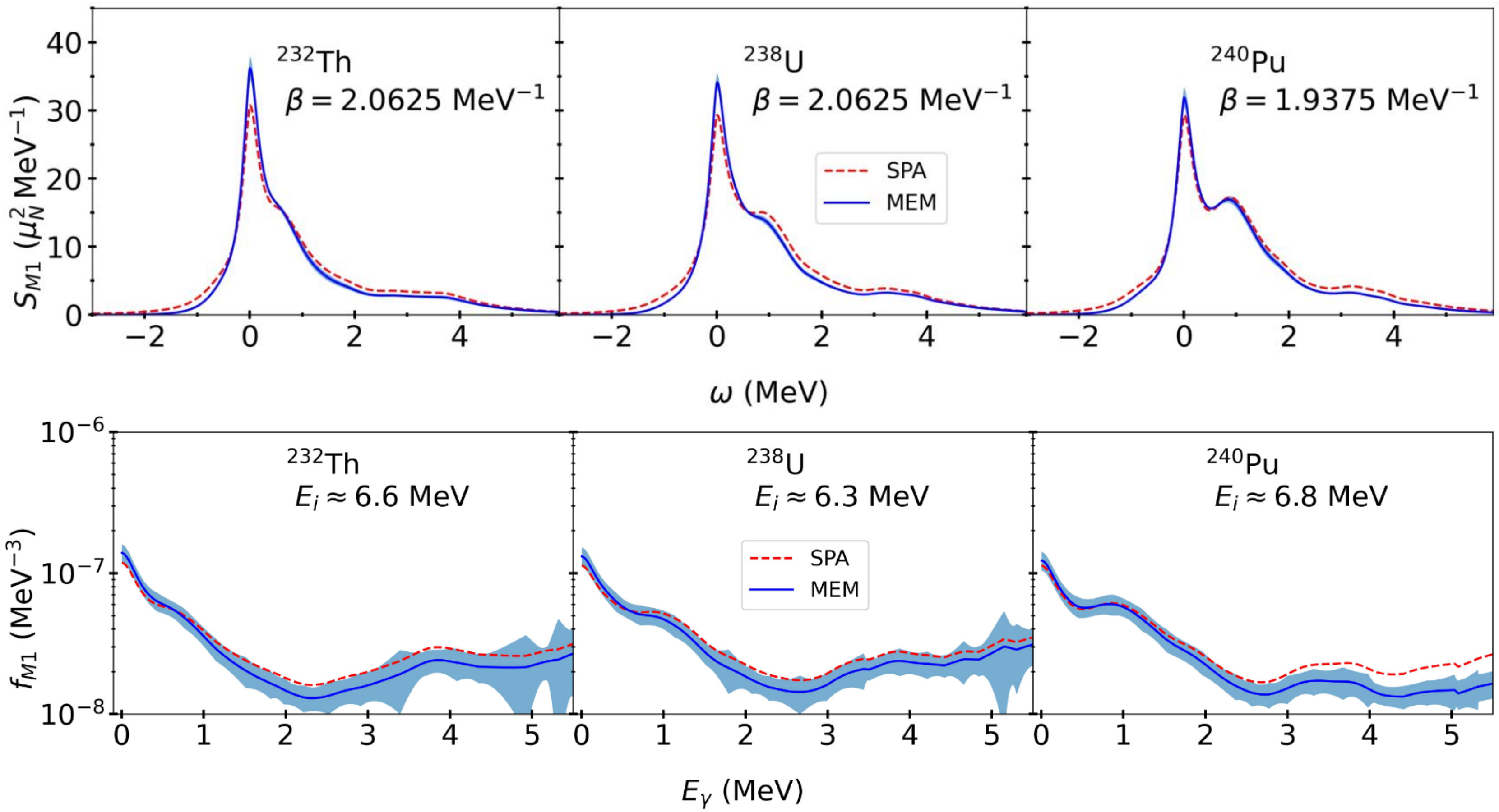
Even mass: Mercenne, Fanto, Ryssens, and Alhassid, PRC **110**, 054313 (2024)
Odd mass: D.D., Alhassid, PRC **111**, 034315 (2025)

M1 γSFs in Actinides

LEE and scissors mode seen in all of these deformed actinides

Weaker spin-flip mode than the one seen in the lanthanides

First prediction that the LEE persists in the actinides



Rodgers, D.D., and Alhassid (forthcoming)

Applications of Nuclear Shapes in Actinides

Nuclear Fission:

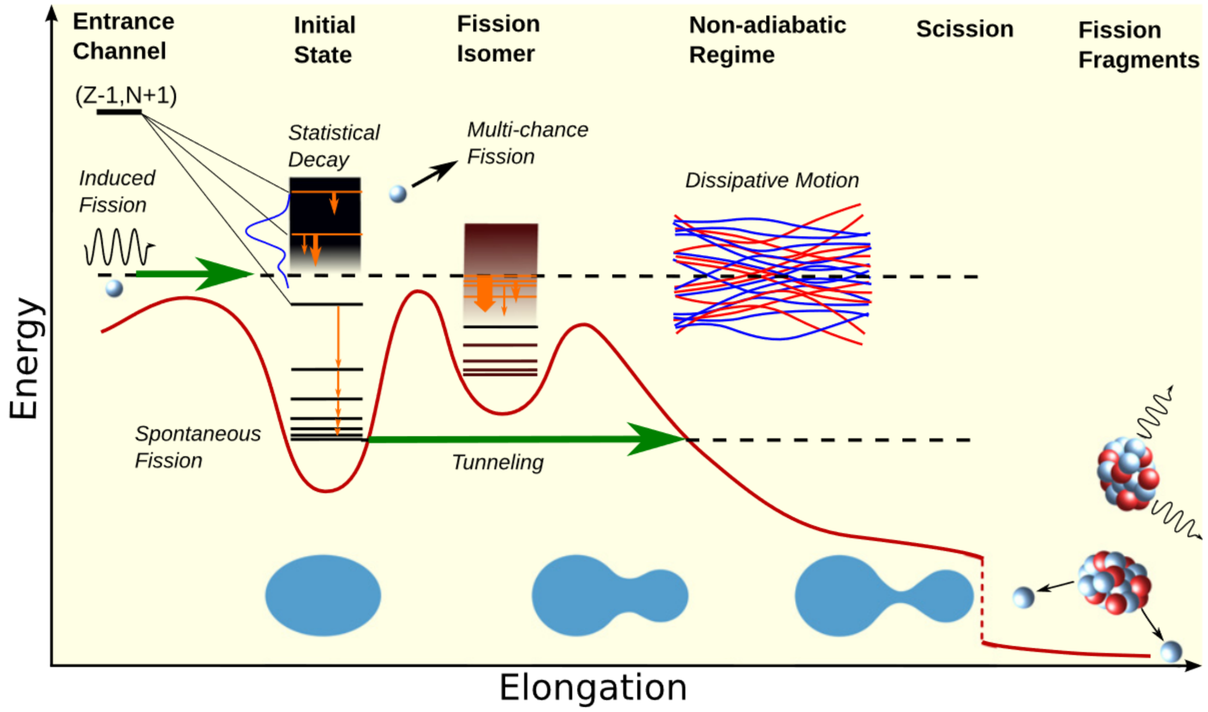
Dynamical real-time evolution of strongly correlated nucleonic system

Density functional methods are widely used
Bulgac, Jin, Roche, Schunck, and Stetcu, PRC **100**, 034615 (2019)
Marevic and Schunck, PRL **125,** 102504 (2020)

SMMC can now be used to calculate relevant statistical properties:

- Potential energy surface $E(\beta_2, \gamma, \dots)$
- Shape-dependent state densities $\rho(E_x, \beta_2, \gamma, \dots)$

Both properties play an important role in the modeling of fission



Bender *et al.*, J. Phys. G **47**, 113002 (2020)

Nuclei undergo extreme deformation as they fission

Applications of Nuclear Shapes in Actinides

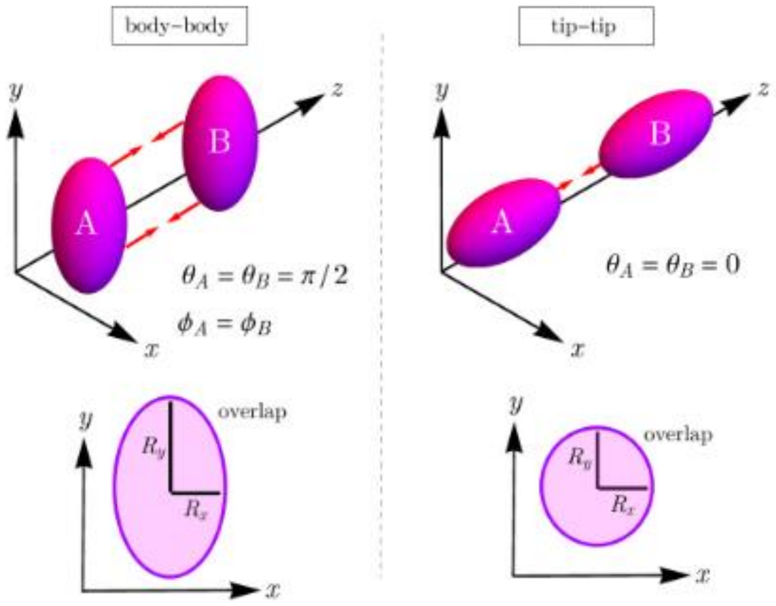
Nuclear deformation has an impact on flow observables in relativistic heavy-ion collisions
Adamczyk *et al.*, PRL **115**, 222301 (2015), Magdy, Eur. Phys. J. A **59**, 64 (2023)

1. Initial nucleon configuration is sampled from a Woods-Saxon potential (requires β_2, β_3, β_4, γ etc. as input)

2. Initial conditions of QGP which then evolves hydrodynamically

3. Particle correlations, momentum distributions, etc.

Giacalone, PRC **102**, 024901 (2020)



Fluctuations in the nuclear shape also have an impact
Dimri, Bhatta, and Jia, Eur. Phys. J. A **59**, 45 (2023)

^{238}U is the largest and most deformed nucleus collided at RHIC

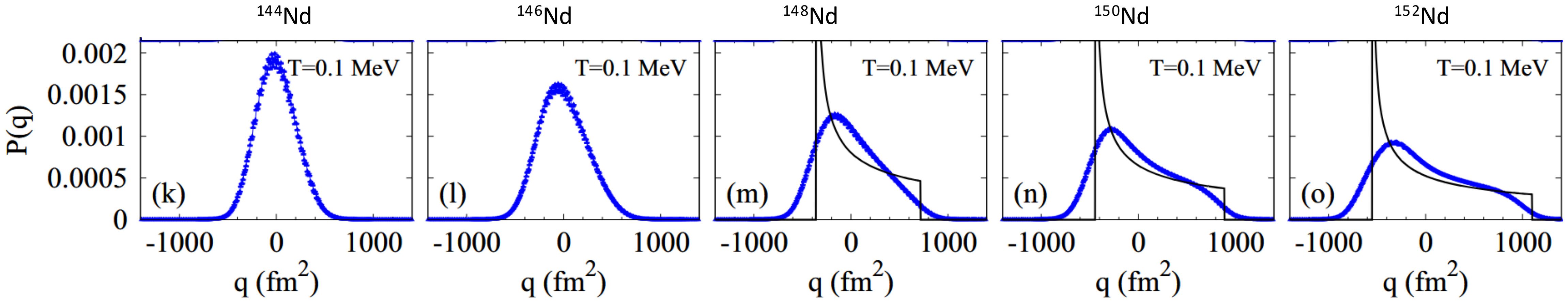
Quadrupole Shape Distribution in the CI Shell Model

Probability distribution of axial quadrupole *q* can be computed with a quadrupole projection

$$\mathrm{Tr}[\delta(\hat{Q}_{20} - q)\hat{U}_\sigma] \approx \frac{1}{2q_{\max}} \sum_{k=-M}^{M} e^{-i\varphi_k q}\ \mathrm{Tr}(e^{i\varphi_k \hat{Q}_{20}}\hat{U}_\sigma)$$

This determines the distribution in the *laboratory frame.*

<-Spherical Deformed->



Gilbreth, Alhassid, and Bertsch, PRC **97**, 014315 (2018)

We want to extract distributions of β and γ, which are defined in the *intrinsic frame* of the nucleus.

Quadrupole Shape Distribution in the Intrinsic Frame

Relate quadrupole invariants to moments of the distribution of $\hat{Q}_{20}$ in the lab frame Kumar, PRL **28**, 249 (1972)

$$\langle \hat{Q}\cdot\hat{Q}\rangle = 5\langle \hat{Q}_{20}^2\rangle = \chi^2\langle\beta^2\rangle_L$$

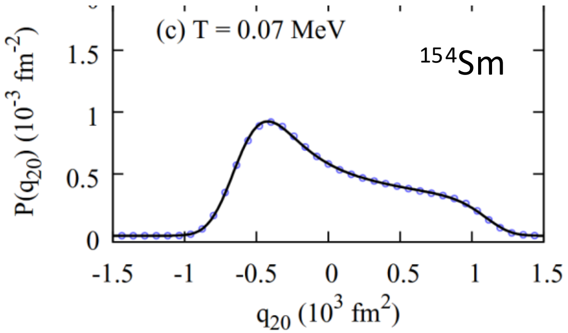
$$\langle [\hat{Q} x \hat{Q}]_2\cdot\hat{Q}\rangle = -5\sqrt{\frac{7}{2}}\langle \hat{Q}_{20}^3\rangle = \chi^3\langle\beta^3\cos 3\gamma\rangle_L$$

$$\left\langle (\hat{Q}\cdot\hat{Q})^2\right\rangle = \frac{35}{3}\langle \hat{Q}_{20}^4\rangle = \chi^4\langle\beta^4\rangle_L$$

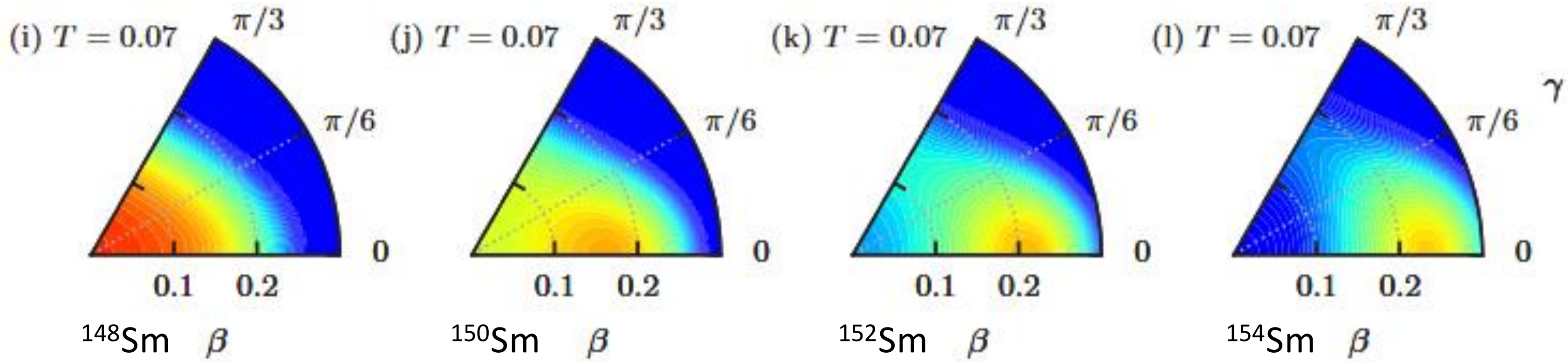
where $\chi = \frac{1}{\sqrt{5\pi}} r_0^2 A^{5/3}$

We expand the log of the probability distribution in quadrupole invariants à la Landau theory

$$P(T,\beta,\gamma) = N(T)\, e^{-a(T)\beta^2 - b(T)\beta^3\cos 3\gamma - c(T)\beta^4}$$



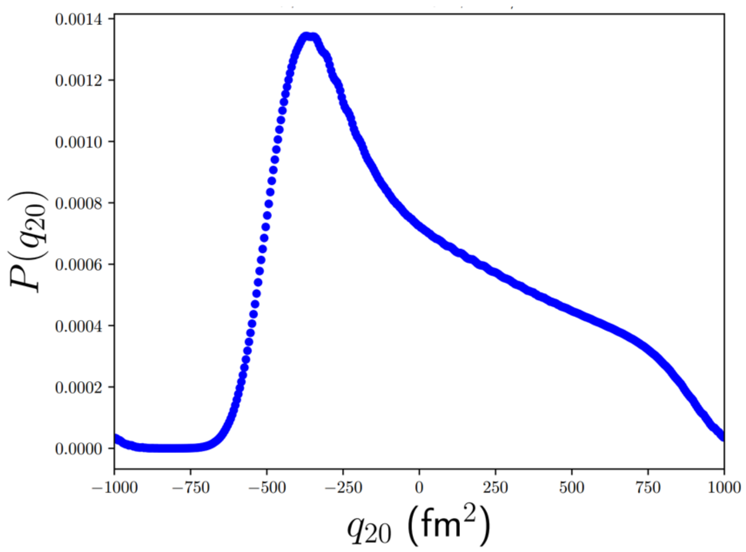
Intrinsic distribution in the (β,γ)-plane



Mustonen, Gilbreth, Alhassid, and Bertsch, PRC **98**, 034317 (2018)

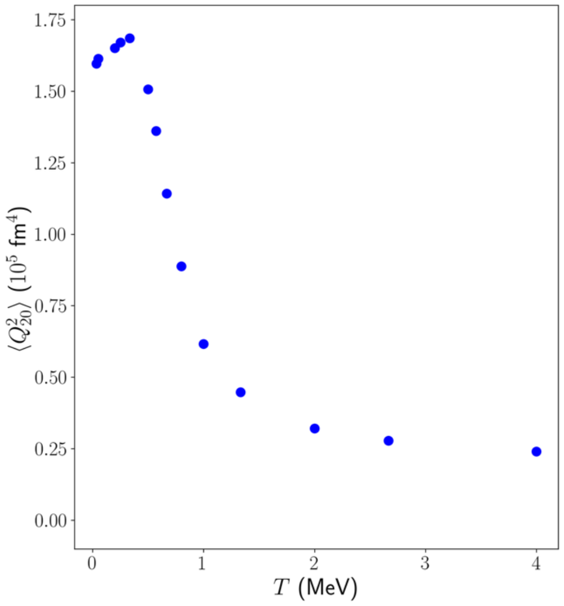
Some Preliminary Results in ^{240}Pu

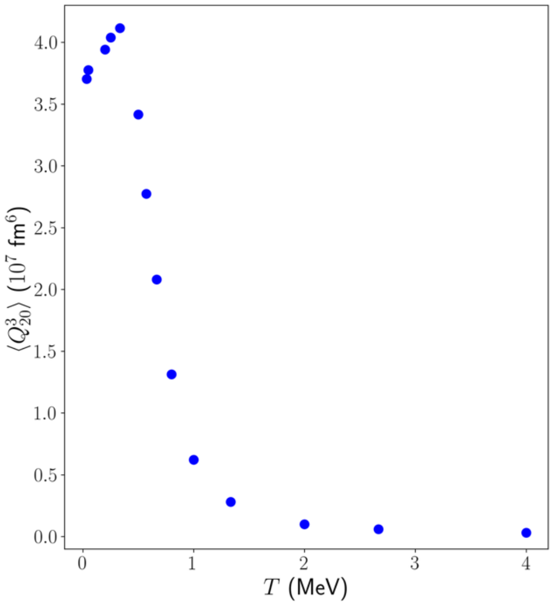
T=0.05 MeV

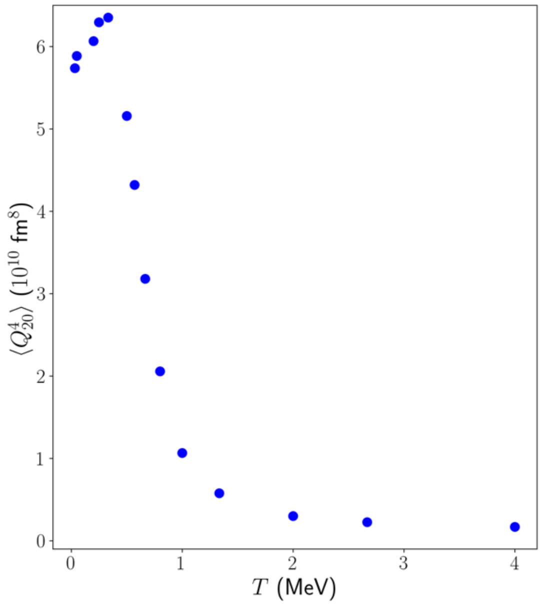


Same characteristic distribution of a deformed nucleus seen near the ground state

Evolution of distribution and moments of $\hat{Q}_{20}$ suggest a shape transition near T ≈ 1 MeV



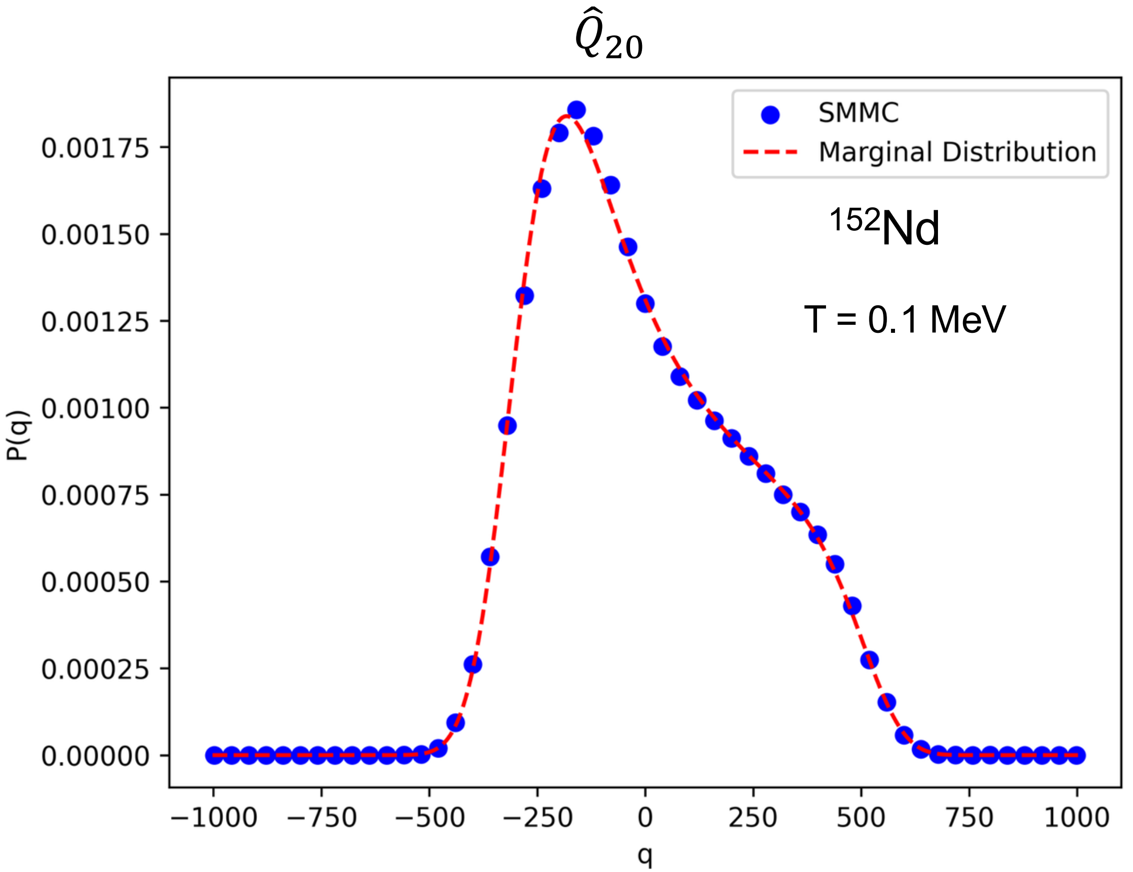


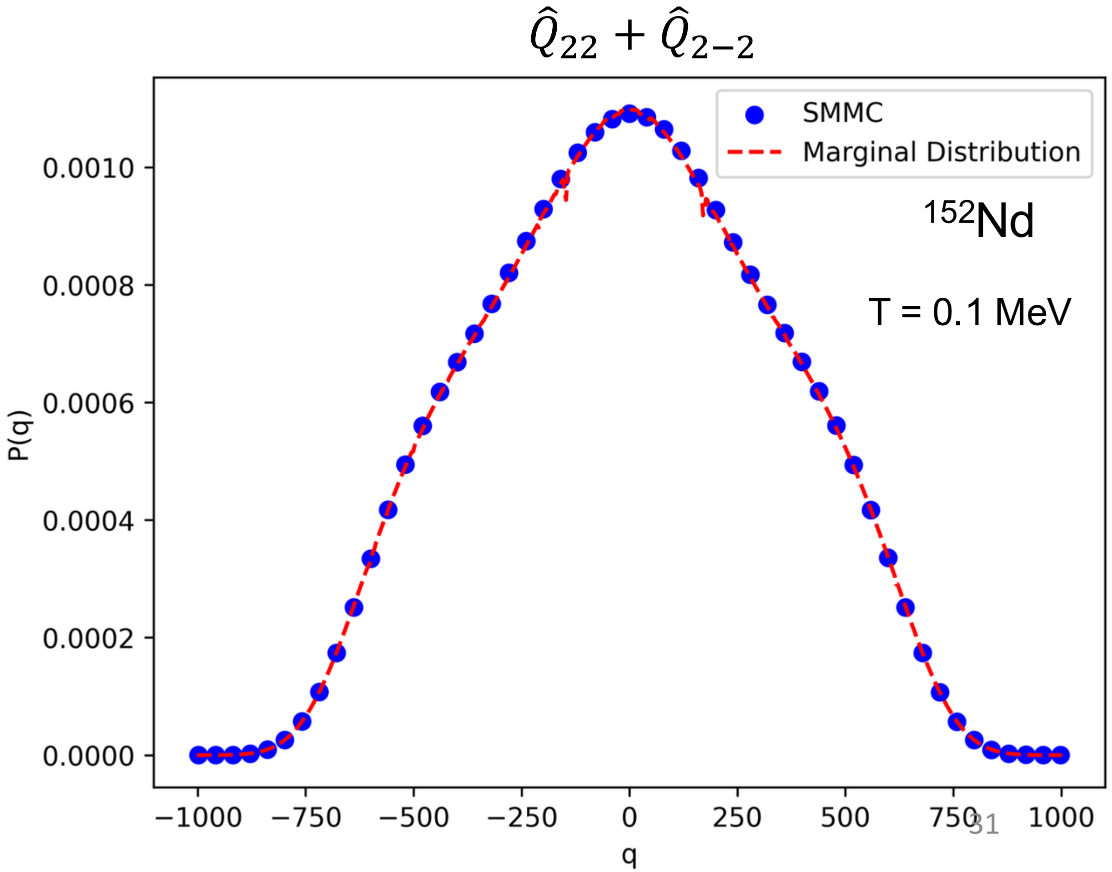


Distributions of Other Components of the Quadrupole Operator in the Lab Frame

$$\hat{Q}_{22} + \hat{Q}_{2-2} \propto r_\perp^2 \cos 2\varphi\,, \qquad i(\hat{Q}_{22} - \hat{Q}_{2-2}) \propto r_\perp^2 \sin 2\varphi$$

Distribution of one component of the quadrupole operator can accurately predict distributions of other components





Conclusions:

- SMMC enables microscopic computations in very large model spaces such as those required for the lanthanides and actinides
- Nuclear level densities from SMMC are in excellent agreement with experimental data – for both even- and odd-mass actinides
- γ-ray strength functions can be computed in the SMMC using the maximum entropy method with the SPA strength as a prior
- This novel method for calculating γ-ray strength functions is the only one that can reproduce the low-energy enhancement (LEE) in heavy nuclei
- The LEE is predicted to persist in the actinides

Outlook:

- Microscopic calculations of shape-dependent properties of actinides in the CI shell model are now possible and various applications are currently being investigated

Thank you!

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Collaborators

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The Partition Function Extrapolation Method (PFEM)

Fits the low-temperature partition function to a parameterized form of the state density (backshifted Bethe formula (BBF))

$$\rho_{BBF} = \frac{\sqrt{\pi} e^{2\sqrt{a(E_x - \Delta)}}}{12 a^{1/4} (E_x - \Delta)^{5/4}}$$

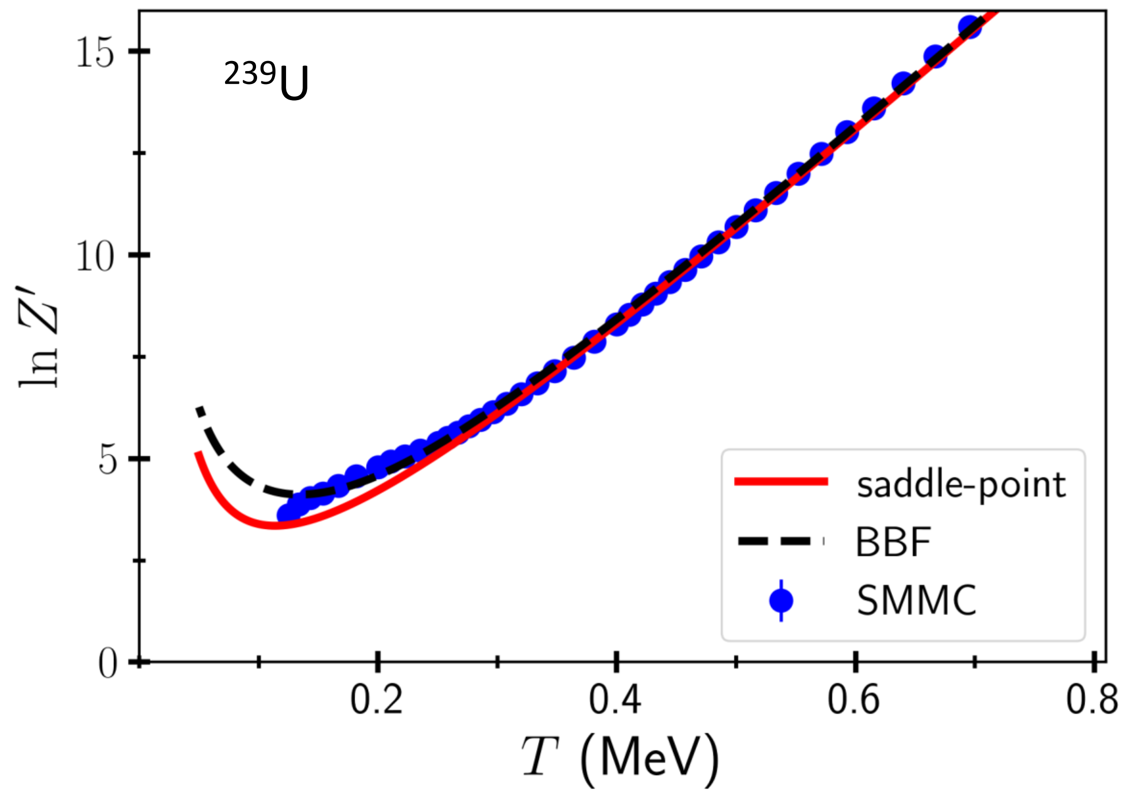
Define a partition function relative to some E_{ref}

$$\ln Z'(\beta; E_{\text{ref}}) = \ln Z'(\beta; E_0) - \beta(E_0 - E_{\text{ref}})$$

Two step fit:

Fit $\ln Z'$ to a saddle-point approximation of the BBF state density to determine BBF parameters

Numerical fit to the full BBF at low temperatures to determine E_0



Uncertainties in E_0:

Even-even: ~ 40-50 keV

Odd-mass: ~ 100-150 keV