

Level Densities and γ -ray Strength Functions in Heavy Nuclei with Shell-Model Monte Carlo

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The Yale University logo, featuring the word "Yale" in a blue, serif font.

Introduction

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.

The shell-model Monte Carlo (SMMC) enables microscopic calculations in spaces that are many orders of magnitude larger ($\sim 10^{32}$) than those that can be treated by conventional methods ($\sim 10^{11}$).

C. W. Johnson, S. E. Koonin, G. H. Lang, and W. E. Ormand, PRL 69, 3157 (1992)
G.H. Lang, C.W. Johnson, S.E. Koonin, W.E. Ormand, PRC 48, 1518 (1993)
Y. Alhassid, D.J. Dean, S.E. Koonin, G.H. Lang, W.E. Ormand, PRL 72, 613 (1994)

Recent review of SMMC: 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.

The shell-model Monte Carlo (SMMC) method

Gibbs ensemble $e^{-\beta H}$ at temperature T ($\beta = 1/T$) can be written as a superposition of ensembles U_σ of *non-interacting* nucleons moving in time-dependent fields $\sigma(\tau)$

$$e^{-\beta H} = \int D[\sigma] G_\sigma U_\sigma$$

- The integrand reduces to matrix algebra in the single-particle space (of typical dimension 50 – 100)
- The high-dimensional σ integration is evaluated by Monte Carlo methods.
- Calculations are done in the *canonical* ensemble of fixed numbers of protons and neutrons (using exact particle-number projection)

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

SMMC in Heavy Nuclei

- CI Hamiltonian with Woods-Saxon plus spin orbit coupling,
- Pairing-plus-multipole interaction (quadrupole, octupole, hexadecupole)

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

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

Model space for lanthanides:

- Protons: 50-82 shell plus $1f_{7/2}$
- Neutrons: 82-126 shell plus $0h_{11/2}, 1g_{9/2}$

Interaction coefficients in [C. Ozen, Y. Alhassid, H. Nakada PRL 110, 042502 \(2013\)](#)

Model space for actinides:

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

Interaction coefficients in [D.D., Y. Alhassid, \(forthcoming\)](#)

Nuclear State Densities in the SMMC

Partition function

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

State density

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

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

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

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

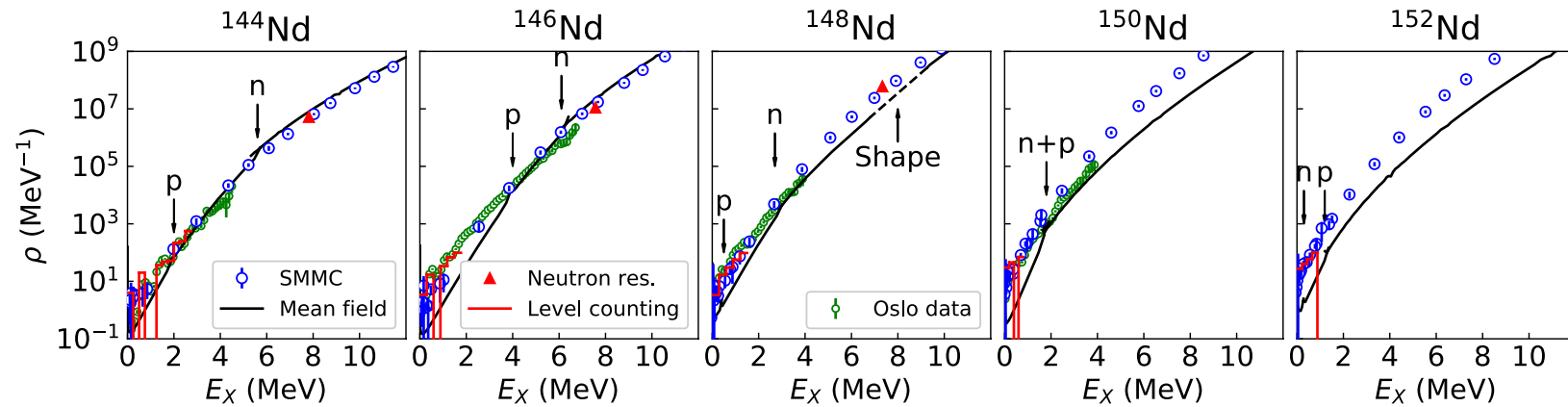
$S(E)$ = canonical entropy

C = canonical heat capacity

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

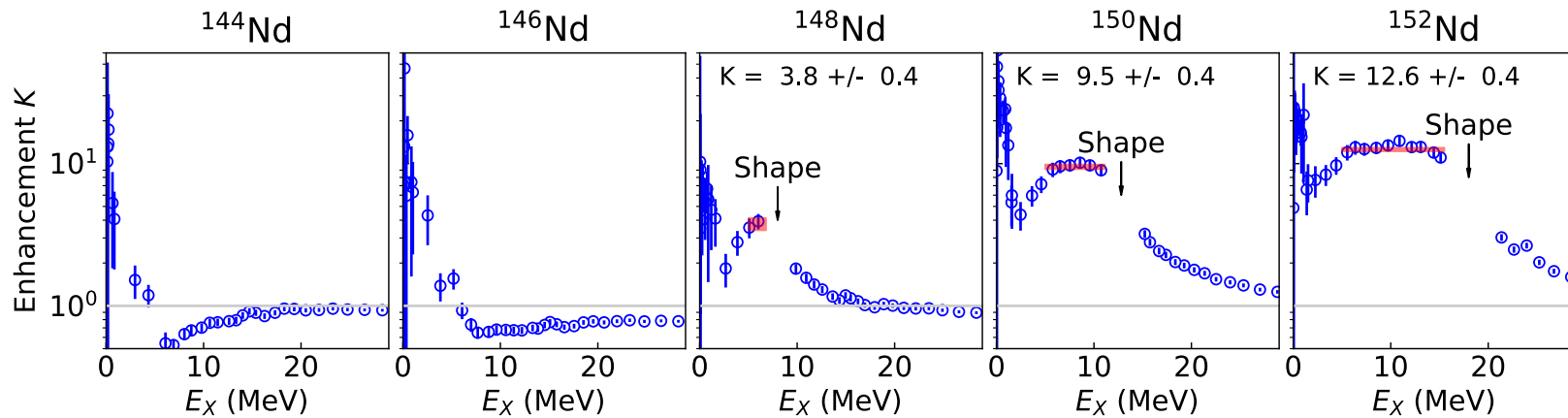
$$C = -\beta^2 \partial E / \partial \beta$$

State densities in Lanthanides



←Spherical

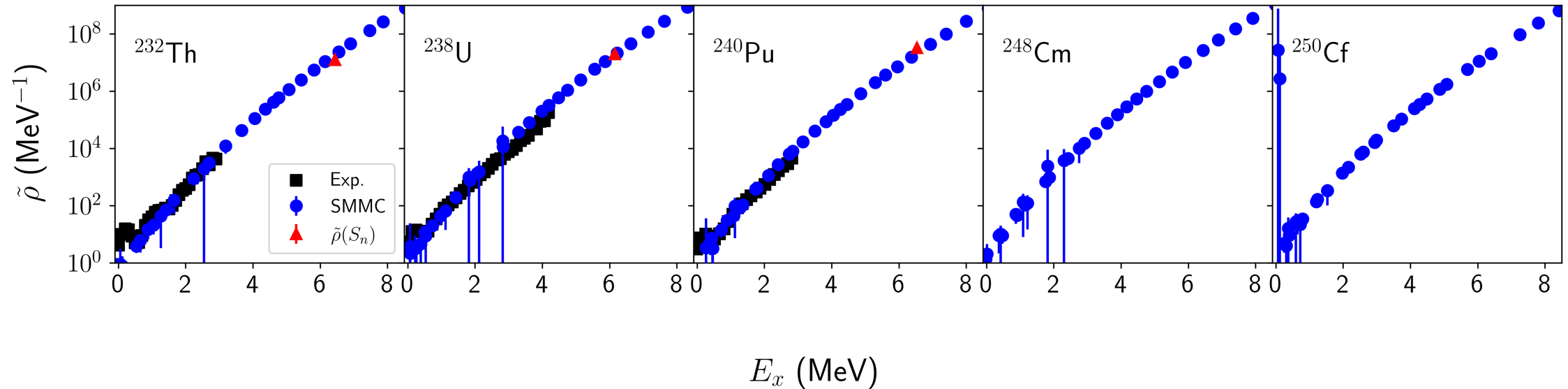
Deformed→



- Enhancement above the mean field values is due to rotation in deformed nuclei and rapidly decreases above the shape transition

Guttormsen, Alhassid, Ryssens et al., PLB 816, 136206 (2021)

Level Densities in Actinides



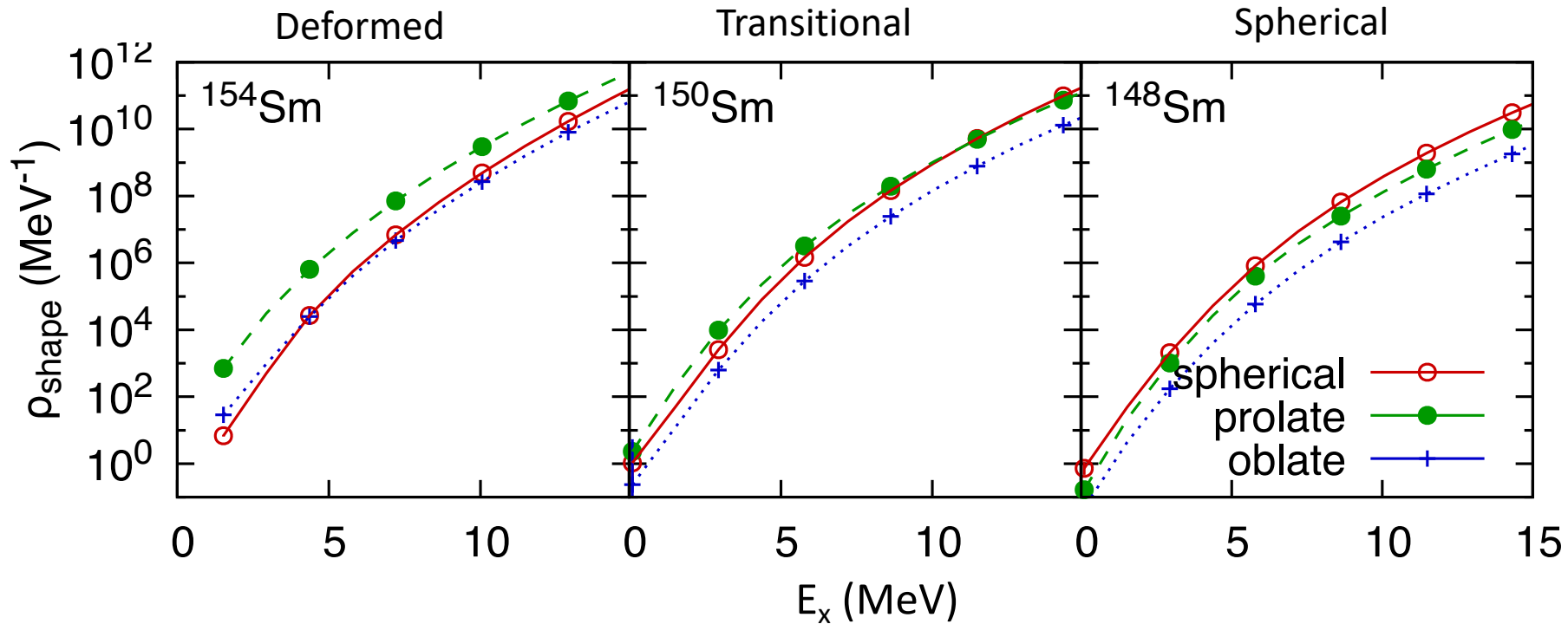
- Actinides: Larger single-particle model space, requires larger β to calculate ground-state energy
- SMMC shows excellent agreement with Oslo experiments

Experimental Results:

^{232}Th , ^{238}U : [M. Guttormsen et al, PRC 88 024307 \(2013\)](#)

^{240}Pu : [F. Zeiser et al, PRC 100 024305 \(2019\)](#)

Shape Dependence of State Densities



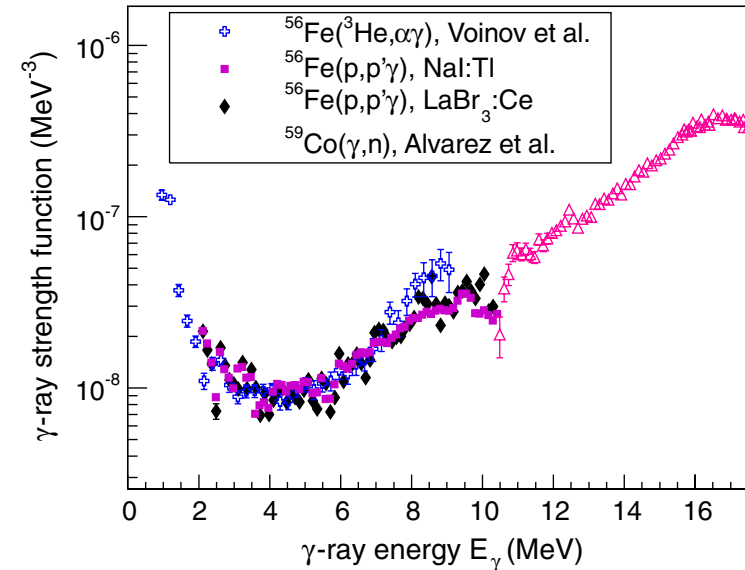
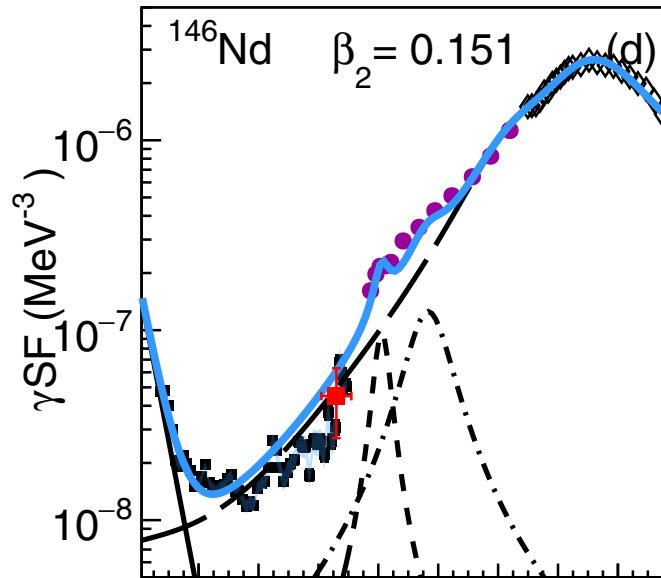
Mustonen, Gilbreth, Alhassid, and Bertsch, PRC 98, 034317 (2018)

Shape dependence is determined by projecting on the mass quadrupole

- In strongly deformed nuclei, the contributions from prolate shapes dominate the state density below the shape transition energy.
- In spherical nuclei, both spherical and prolate shapes make significant contributions.

γ -ray Strength Functions (γ SF)

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



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

A.C. Larsen et al., PRL 111, 242504 (2013)

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.

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:

- 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 γ SF 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

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

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

$$R_o(\tau) = \langle O(\tau) O(0) \rangle$$

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

$$R_o(\tau) = \int_{-\infty}^{\infty} d\omega e^{-\tau\omega} S_o(\omega)$$

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

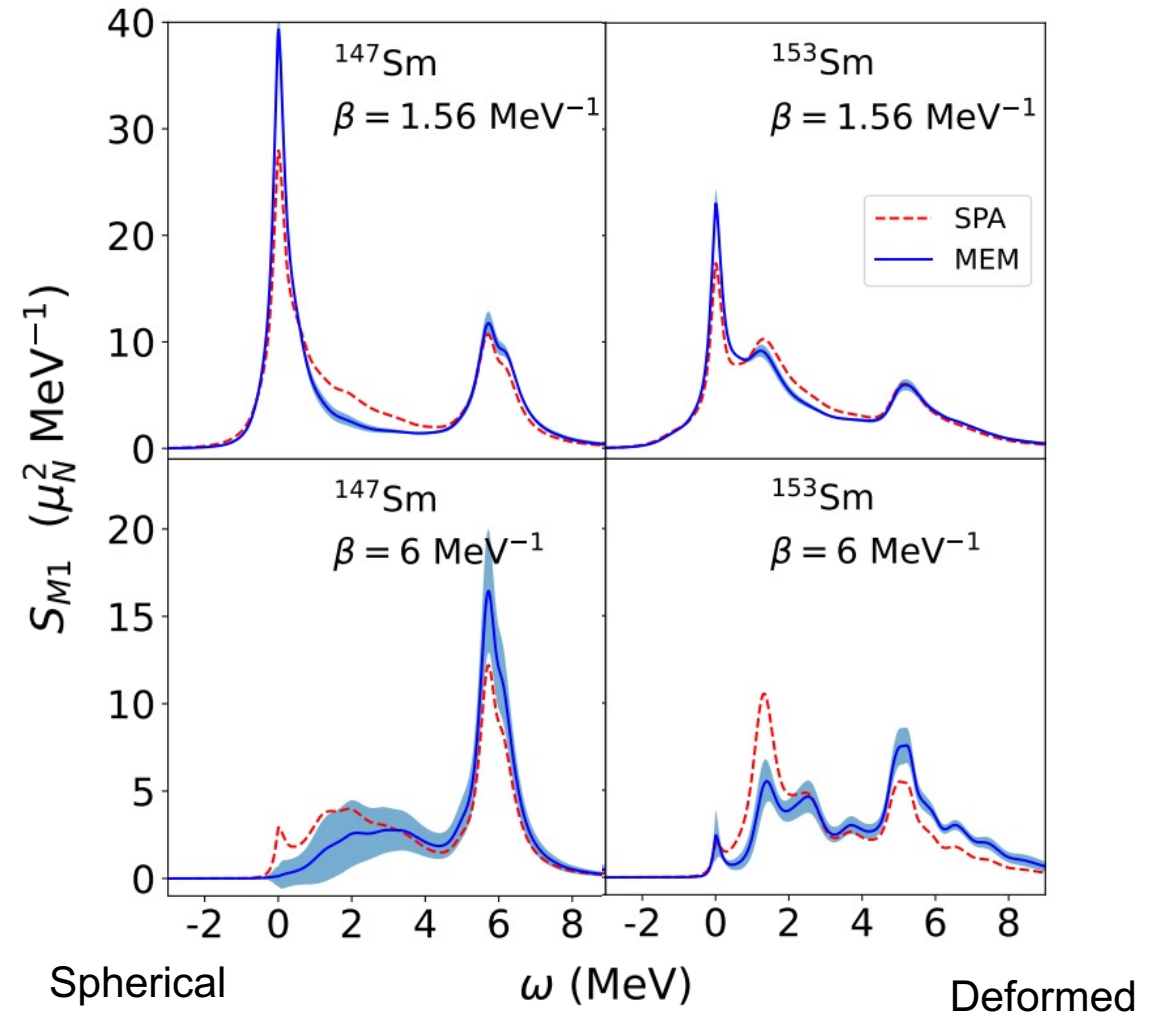
The success of the method depends on a good choice for a prior strength function

→ we use the static path approximation (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., Y. Alhassid (forthcoming)

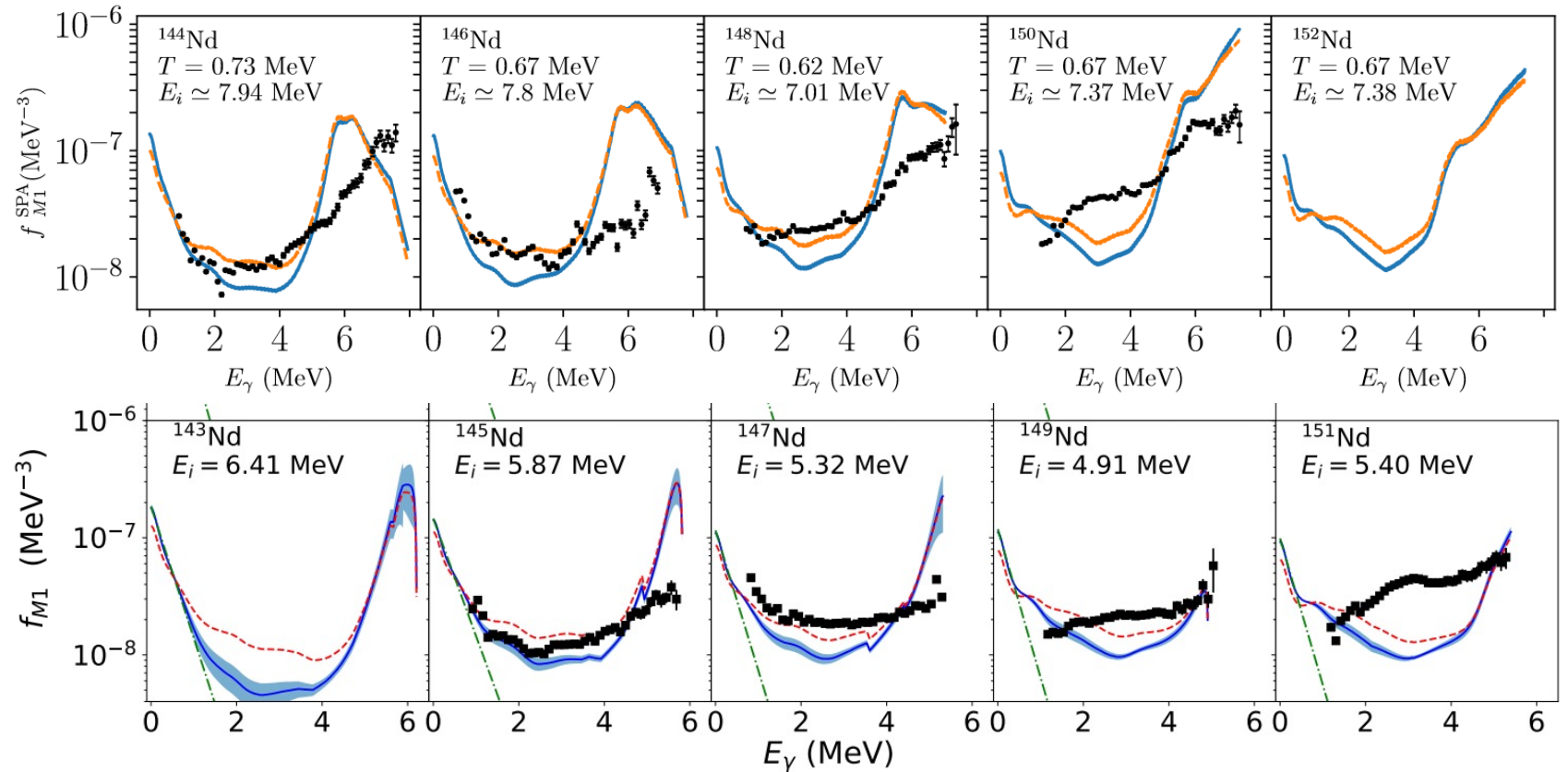
M1 De-excitation Strength Functions

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

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, Alhassid, arXiv:2407.06161](https://arxiv.org/abs/2407.06161)

Conclusions:

- SMMC enables microscopic computations in very large model spaces such as those required for the lanthanides and actinides
- Nuclear level densities from SMMC show excellent agreement with experimental data
- γ SFs can be computed in the SMMC using the MEM with the SPA strength as a prior
- The LEE is observed theoretically (and experimentally) in heavy nuclei

Prospects:

- Further computations of NLDs in actinides, including odd-A nuclei
- First calculations of the γ SFs in actinides; Does the LEE persist?
- Shape dependent state densities in actinides - relevant for fission