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

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Symposium Celebrating 75 Years of the Nuclear Shell Model and Maria Goeppert-Mayer

Argonne National Laboratory

July 21, 2024

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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)

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

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:

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

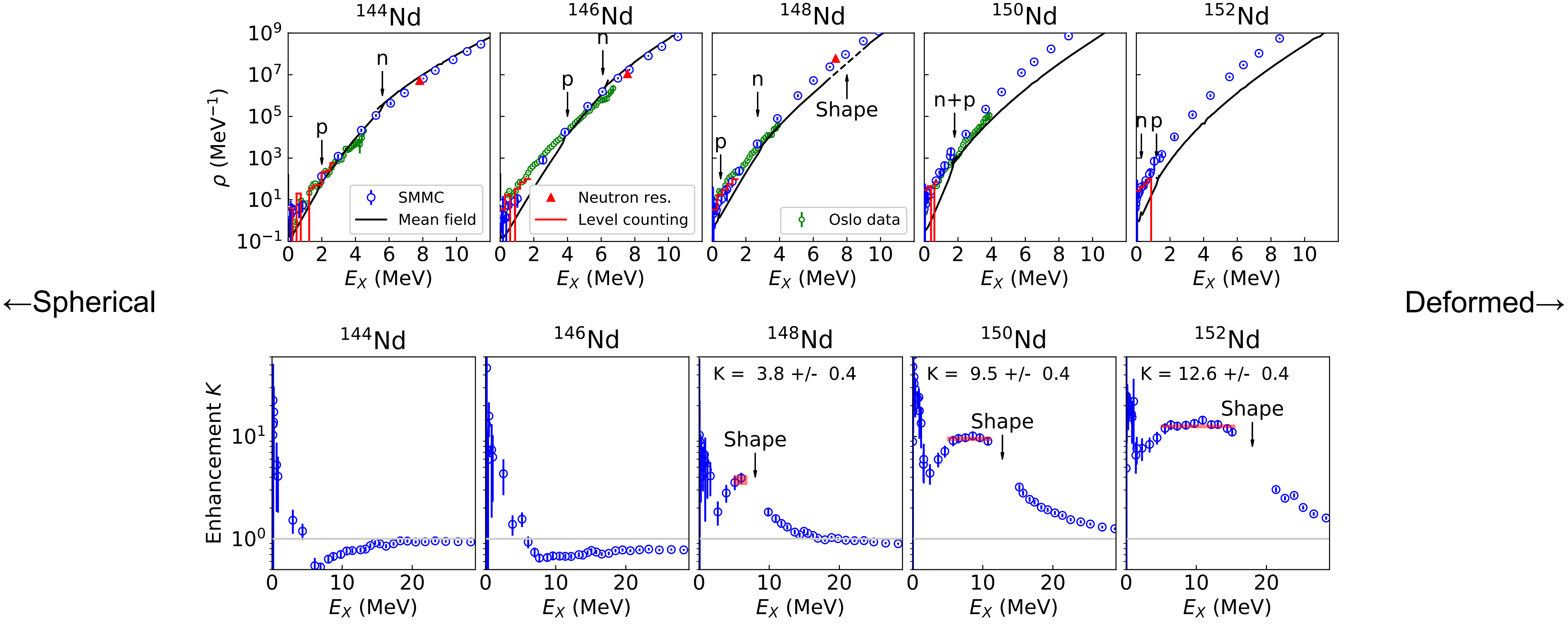
S(E) = canonical entropy

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

C = canonical heat capacity

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

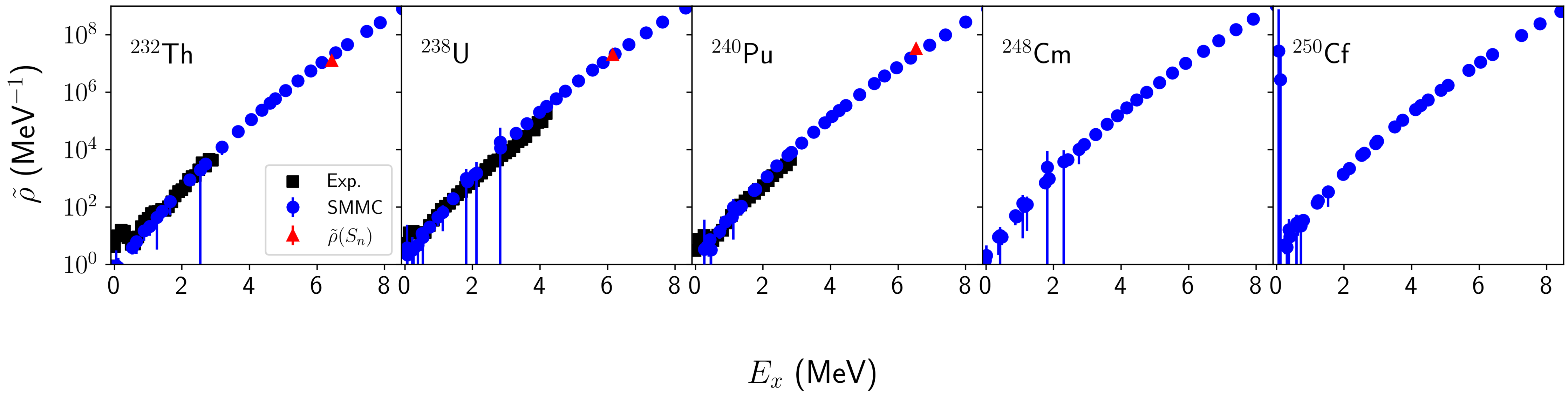
State densities in Lanthanides



- 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

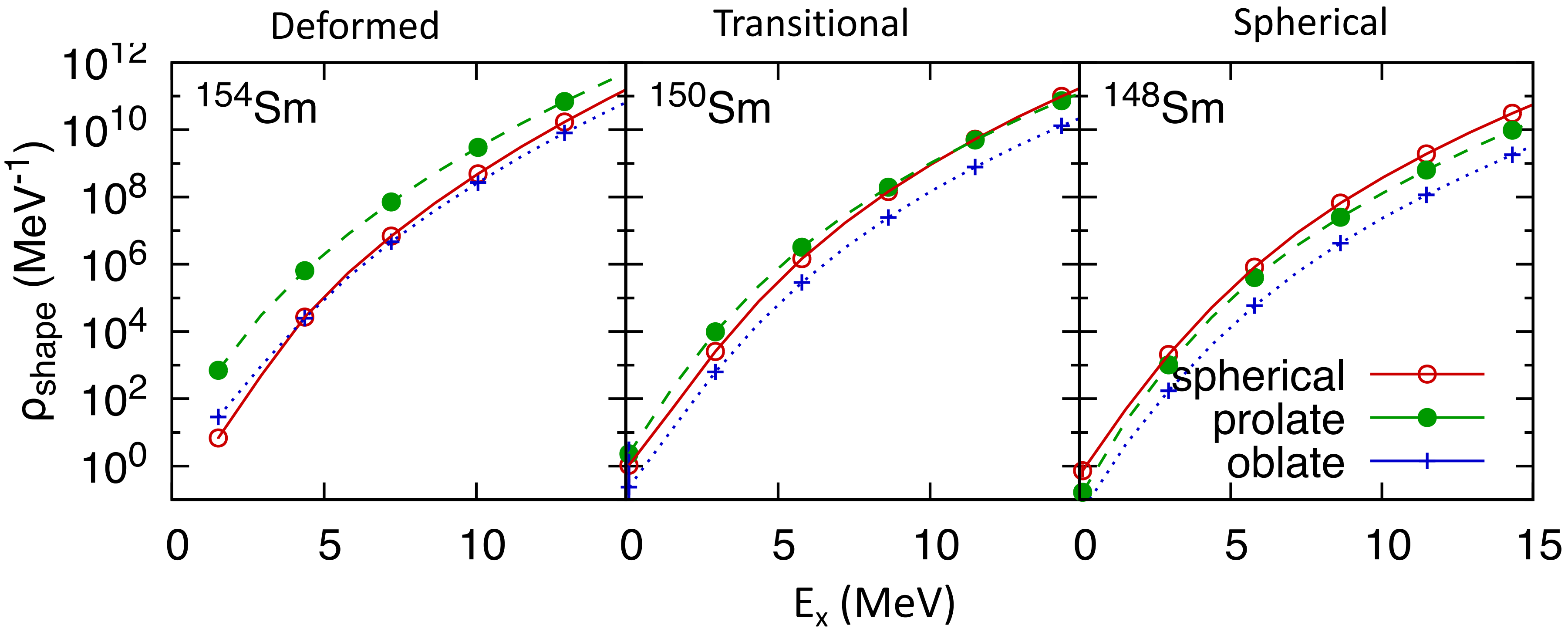


- Actinides: Larger single-particle model space, requires larger β to calculate ground-state energy

- 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



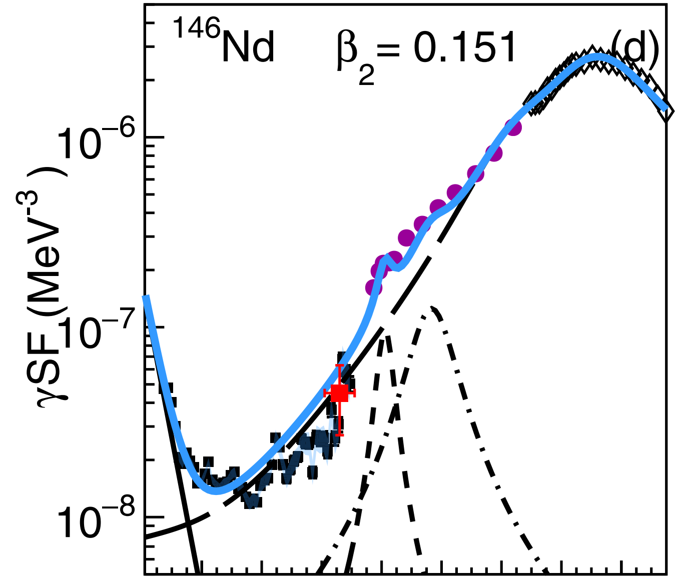
Mustonen, Gilbreth, Alhassid, and Bertsch, PRC **98**, 034317 (2018)

Shape dependence is determined by projecting on the mass quadrupole

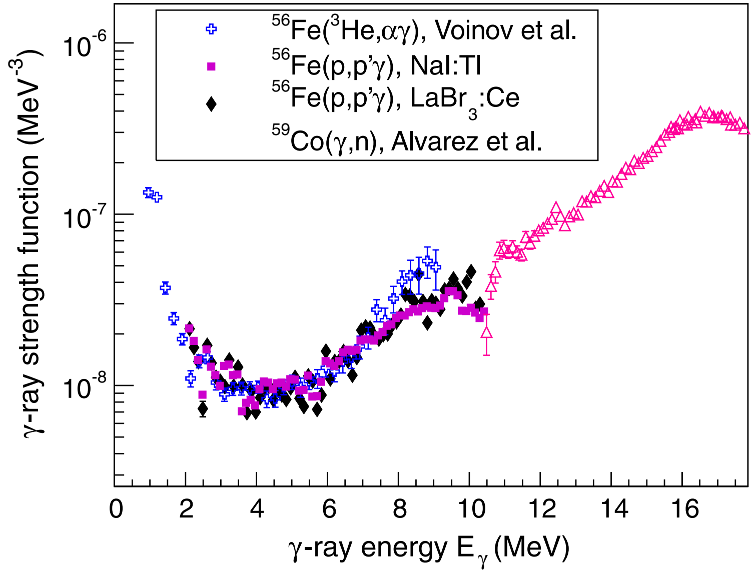
- In strongly deformed nuclei, the contributions from prolate shapes dominate the state density below the shape transition energy.
- In spherical nuclei, both spherical and prolate shapes make significant contributions.

γ-ray Strength Functions (γSF)

In recent years, a low-energy enhancement (LEE) was observed in the γSF 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 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

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

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)

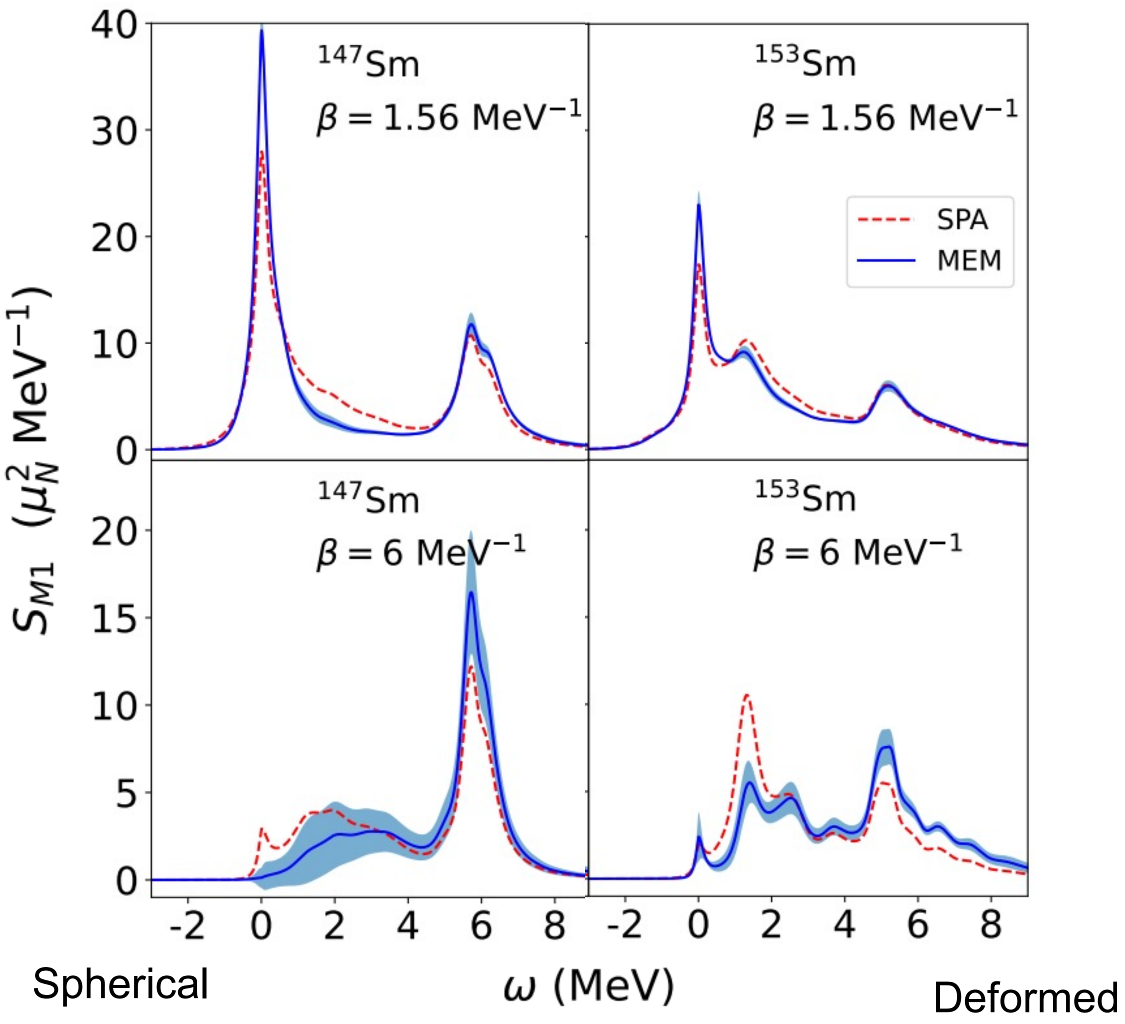
M1 Strength Functions

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)

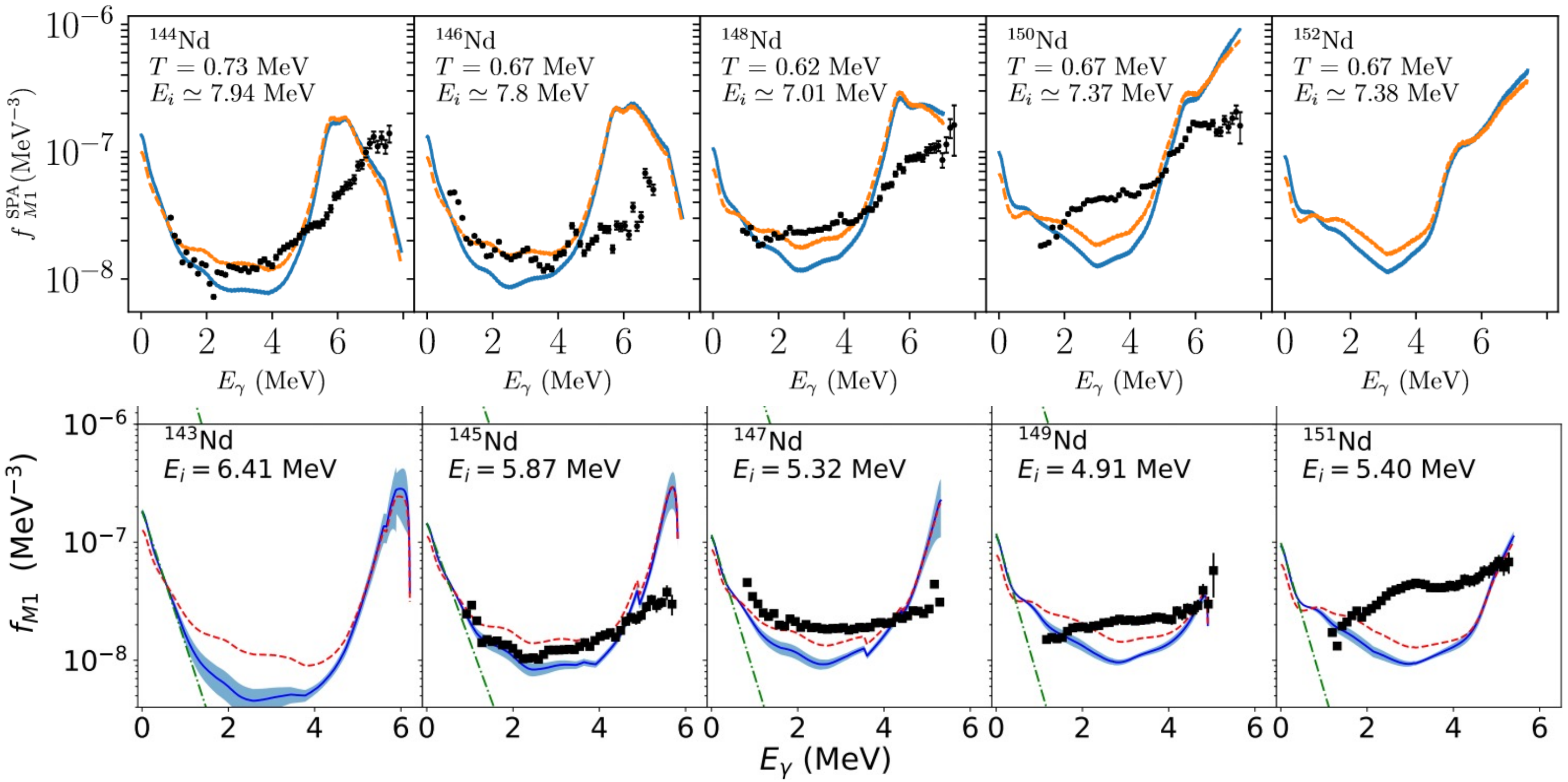
M1 De-excitation Strength Functions

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

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

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
- γSFs 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 γSFs in actinides; Does the LEE persist?
- Shape dependent state densities in actinides - relevant for fission

D.D. is supported by US Department of Energy grant No. DE-SC0019521