Magnetic dipole γ-ray strength functions in heavy odd-mass nuclei from shell-model Monte Carlo

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Outline

1. The shell-model Monte Carlo (SMMC) method and the sign problem in odd-mass nuclei
2. γ-ray strength functions and level densities in heavy nuclei
3. Static-path approximation (SPA) and maximum entropy method (MEM) techniques for computing strength functions
4. Results: M1 γ-ray strength functions in $^{143\text{-}151}$Nd and $^{147\text{-}153}$Sm; Uncertainties are under control and we observe the low-energy enhancement (LEE) in all of these nuclei

Based on a forthcoming article by D.D. and Y. Alhassid

Shell-Model Monte Carlo

- The general goal is to perform nuclear structure calculations starting from a microscopic description of nucleon-nucleon interactions
- Other ab-initio methods have been developed (i.e., no-core shell model, coupled cluster method, lattice field theory), but they are limited to lighter nuclei and/or smaller model spaces due to the computational cost.
- Many calculations of heavy nuclei rely on mean-field approaches which miss important correlations
- The shell-model Monte Carlo (SMMC) enables microscopic calculations of nuclear properties at finite temperature in much larger model spaces than other methods (e.g., 5×10^{26} in ^{153}Sm)

The Hubbard-Stratonovich Transformation

The HS transformation describes the Gibbs ensemble at inverse temperature $\beta = 1/T$ as a path integral over auxiliary fields:

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

This transforms the theory from one of interacting fermions into one of non-interacting fermions in time-dependent fields $\sigma(\tau)$.

The integrand reduces to matrix algebra in the single-particle space in contrast to the combinatorial increase of the many-particle space in direct diagonalization methods.

We use a canonical ensemble by implementing an exact particle-number projection through a discrete Fourier transform.

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

However this projection introduces a sign problem in odd-particle systems at low temperatures.

SMMC in Heavy Nuclei

- The model space for lanthanides:
  protons: the 50-82 shell plus $1f_{7/2}$
  neutrons: the 82-126 shell plus $0h_{11/2}$ and $1g_{9/2}$

- Configuration-interaction Hamiltonian with Wood-Saxon plus spin-orbit s.p. energies and a pairing-plus-multipole interaction (quad., oct., and hexadec.)

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

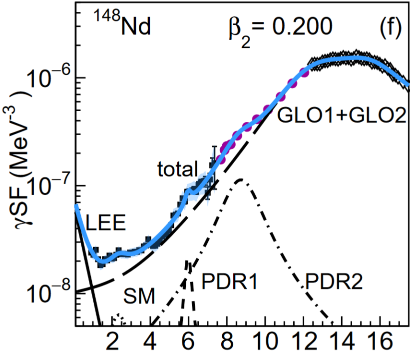
Interaction coefficients in C. Ozen, Y.Alhassid, H. Nakada PRL **110**, 042502 (2013)

γ-ray Strength Functions

The γSF contains important information about collective properties of nuclei and is an input for compound nuclear reaction rates.

In recent years, a low-energy enhancement (LEE) was observed in mid-mass nuclei and a few rare-earth nuclei. If the LEE persists in heavy, neutron-rich nuclei, it can have significant effects on r-process nucleosynthesis A. Larsen, S. Goriely PRC **82**, 014318 (2010).

Shell-model calculations have attributed the LEE to M1 transitions, but are limited to light and mid-mass nuclei. We use the SMMC together with other many-body techniques to calculate the M1 γSF in heavy nuclei.



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

The M1 γSF is the reduced probability for a nucleus with initial energy E_i to emit a photon of energy E_γ via an M1 transition

M1 Strength and Response Functions

$$S_{M1}(E_i;\omega) = \sum_i \sum_f \frac{e^{-\beta E_i}}{Z} |\langle f||\hat{\mathcal{O}}_{M1}||i\rangle|^2 \delta(\omega - E_i + E_f).$$

The imaginary-time response function of the M1 transition operator is defined as

$$R_{M1}(T;\tau) = \langle \hat{\mathcal{O}}_{M1}(\tau)\hat{\mathcal{O}}_{M1}(0)\rangle.$$

The M1 response function is the Laplace transform of the M1 strength.
Using $S_{M1}(T;-\omega) = e^{-\beta\omega} S_{M1}(T;\omega)$, we have

$$R_{M1}(T;\tau) = \int_0^\infty d\omega K(\tau,\omega) S_{M1}(T;\omega), \quad K(\tau,\omega) = e^{-\tau\omega} + e^{(\beta-\tau)\omega}$$

In the SMMC only R_{M1} can be calculated directly. The inversion requires analytic continuation to real time and is numerically ill-defined.
We use the 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 of the prior strength function → we use the SPA

Static-Path Approximation

Consider only static (time-independent) fields: $\sigma_\alpha(\tau) = \sigma_\alpha$ in the HS transformation.

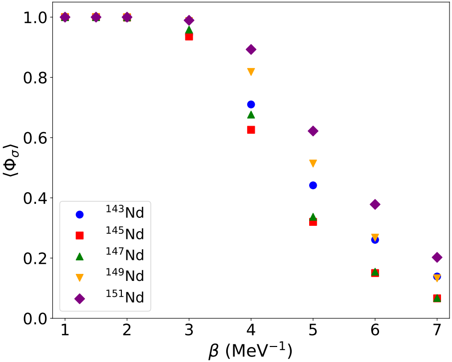
Includes large, static fluctuations around the mean field, but ignores quantum fluctuations - tends toward the SMMC results at large T

The advantages:

- Does not have a sign problem at low temperatures
- S_{M1} can be computed directly as the Fourier transform of the response without the need for analytic continuation
  H. Attias , Y. Alhassid NPA **625** 565 (1997), R. Rossignoli, P. Ring NPA **633**, 613 (1998)

We will combine the SPA strength function with the SMMC response function via the MEM.

Uncertainty Quantification in the MEM

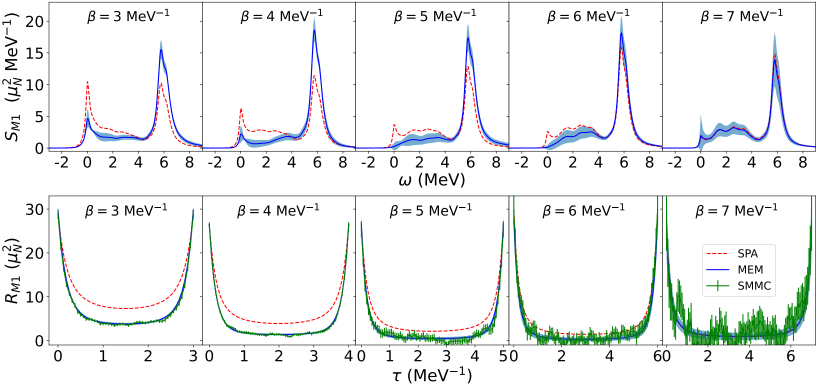


The Monte-Carlo sign begins to fall below 1 at $\beta > 3$ MeV^{-1}

Calculations of the energy typically become too noisy above $\beta \sim 5$ MeV^{-1} to extract g.s. information

How do the MEM strength functions behave as the sign gets worse? We use a jackknife analysis of the MEM strength and response functions.

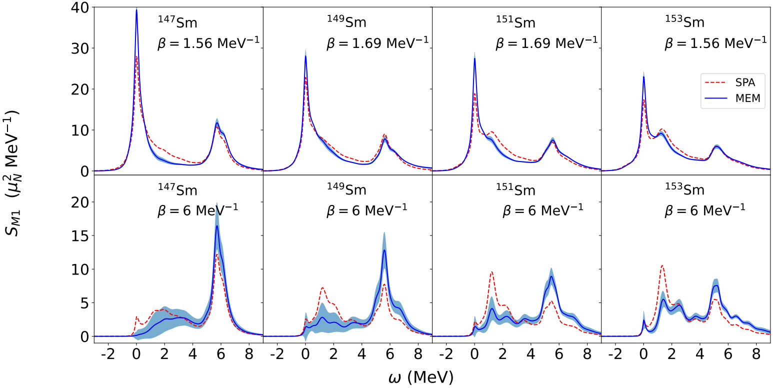
Temperature Evolution of Strength and Response



Uncertainties are small when the sign is close to 1 - good for calculations at S_n ($\beta \sim 1.5$ MeV^{-1})
At $\beta = 7$ MeV^{-1} the SMMC response has little weight in the MEM $\rightarrow$ Since its error bars are too large and the MEM result is biased to the SPA prior

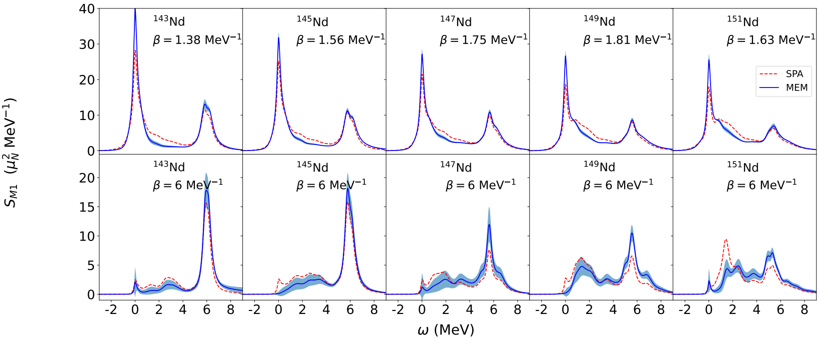
M1 Strengths in Odd-Mass Samarium Isotopes

Top row: M1 strength functions near neutron separation energy



- Bottom row: M1 strength functions near the ground state
- The $\omega = 0$ peak is the LEE!
- Emergence of the scissors mode near ~ 2 MeV as deformation increases.

M1 Strengths in Odd-Mass Neodymium Isotopes



- Similar behavior to samarium
- Apparent 'transfer' of strength from the LEE to the scissors mode in the crossover from spherical to deformed nuclei

Level Densities in Odd-Mass Samarium Isotopes

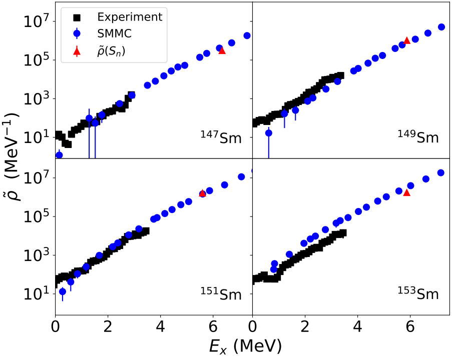
$$f_{M1}(E_i; E_\gamma) = \frac{16\pi\tilde{\rho}(E_i)}{9(\hbar c)^3\tilde{\rho}(E_i - E_\gamma)} S_{M1}(T; -E_\gamma)$$

The state density is computed using the saddle-point approximation from $E(\beta)$ data

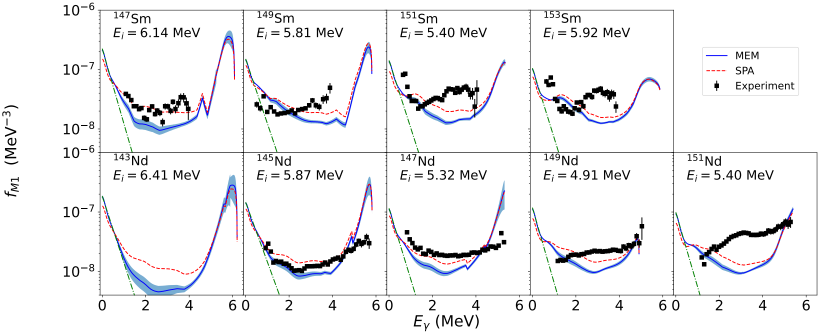
$$\rho(E_x) \approx \sqrt{\frac{\beta^2}{2\pi C}} e^{S(E_x)},$$

SMMC level densities for Sm isotopes show good agreement from Oslo-method experiments F. Naqvi *et. al.* PRC **99**, 054331 (2019)

Level densities for Nd isotopes first calculated in the same SMMC model in M. Guttormsen *et. al.* PLB **816**, 136206 (2021) and used here for calculating f_{M1}

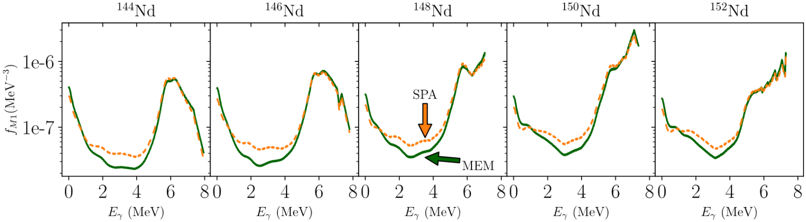


M1 γSF in Odd-Mass Nuclei



- The LEE is seen in all nine odd-mass nuclei
- The scissors mode peak is visible in the deformed nuclei - although at lower energies than in experiment
- Theoretical results were multiplied by a spin-correction factor; experimental results don't distinguish between M1 and E1.
- Experimental data: F. Naqvi *et. al.* PRC **99**, 054331 (2019), M. Guttormsen *et. al.* PRC **106**, 034314 (2022)

M1 γSF in Even-Mass Nuclei



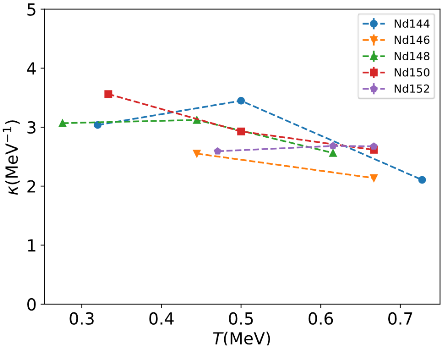
Results for the even-mass Nd isotopes from A. Mercenne, P. Fanto, and Y. Alhassid.

LEE is also seen in all the even-mass nuclei, the spin-flip mode can be more clearly seen due to the higher S_n in even-mass nuclei

The LEE is fit to the form

$$f_{M1}^{\mathrm{LEE}}(E_\gamma) = f_0 e^{-\kappa E_\gamma}$$

The slope parameter depends weakly on temperature except at very low values



Nucleus	κ (MeV^{-1}) [SMMC + MEM]	κ (MeV^{-1}) [exp.]
^{143}Nd	2.59 ± 0.03	–
^{145}Nd	2.31 ± 0.04	1.9 ± 0.2[a]
^{147}Nd	2.75 ± 0.04	1.9 ± 0.2[a]
^{149}Nd	2.92 ± 0.04	–[b]
^{151}Nd	2.88 ± 0.04	–[b]
^{147}Sm	2.92 ± 0.04	3.2 ± 1.0
^{149}Sm	2.50 ± 0.04	5.0 ± 1.0
^{151}Sm	2.62 ± 0.04	5.0 ± 0.5
^{153}Sm	2.70 ± 0.04	5.0 ± 1.0

[a] Experimental value presented is the average value for $^{142,144\text{-}147}$Nd.

[b] No LEE was seen in experiment for ^{149,151}Nd

Conclusions and Outlook

- SMMC enables microscopic computations in very large model spaces such as those required for the lanthanides
- γSFs can be computed in the SMMC using the MEM with the SPA strength as a prior
- The sign problem does not pose an issue for calculations of the γSF near the neutron separation energy
- The LEE is observed theoretically (and experimentally) in heavy, odd-mass nuclei
- We observed a scissors mode built on excited states as the nucleus become more deformed

Outlook:

- Calculation of spin-dependent M1 strength and response functions
- Extend the SMMC to heavier nuclei, e.g., actinides and neutron-rich nuclei