Nuclear Level Densities in Actinides by Shell-Model Monte Carlo

Dallas DeMartini

Yale University

9th Workshop on Nuclear Level Densities and Gamma Strength
University of Oslo
May 29, 2024

Outline

1. Applying the shell-model Monte Carlo (SMMC) method to study actinides for the first time
2. Nuclear state and level densities (NLDs)
3. Evidence of the pairing correlations at low excitation energies
4. Results: Our interaction and model space gives level densities that agree with those from Oslo method and predicts NLDs for other actinides

Based on work by D.D. and Y. Alhassid

Possible applications:

- γ-ray strength functions in actinides - two-peak scissor mode; LEE not yet observed in Oslo experiments
- Deformation-dependent NLDs and potential energy surfaces are important inputs to nuclear fission calculations Pei *et. al* PRL (2009)
- Shapes of colliding nuclei, such as in ^{238}U + ^{238}U collisions at RHIC affect elliptic flow and momentum distributions Giacalone *et. al.* PRL (2021)

Challenges (compared to the previously-studied lanthanides):

- Larger single-particle model space greatly increases CPU time and memory costs
- Actinides have lower first excited states ~ 40 keV, compared to lanthanides > 70 keV, requiring larger values of the inverse temperature $\beta = 1/T$ to study ground-state properties

Shell-Model Monte Carlo (SMMC)

- The goal is to calculate nuclear properties starting from a microscopic description of the underlying 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 (e.g, density functional theory) which miss important correlations. In particular, they underestimate the NLDs of deformed nuclei by an order of magnitude or more
- The SMMC enables microscopic calculations of nuclear properties at finite temperature in much larger model spaces than other methods (e.g., $\sim 10^{33}$ in Cf isotopes)

The Hubbard-Stratonovich Transformation

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

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

where $\hat{U}_\sigma$ is the propagator of non-interacting nucleons and G_σ is the Gaussian weight.

This transforms the theory from one of interacting fermions into one of non-interacting fermions in time-dependent fields $\sigma(\tau)$. The integration over the large number of fields requires Monte-Carlo methods

The integrand reduces to matrix algebra in the single-particle space (~ 100 orbitals) in contrast to the combinatorial increase of the many-particle space in direct diagonalization methods.

We use a canonical ensemble of fixed numbers of protons and neutrons by implementing an exact particle-number projection (discrete Fourier transform)

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

Actinide Model Space and Interaction

- The model space for actinides:
  protons: the 82-126 shell plus $1g_{9/2}$
  neutrons: the 126-184 shell plus $1h_{11/2}$

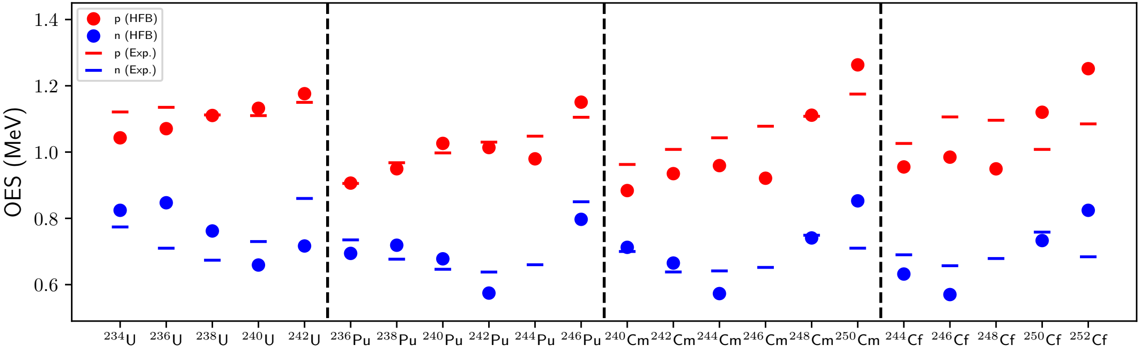
- Configuration-interaction Hamiltonian with Wood-Saxon plus spin-orbit s.p. potential and a pairing-plus-multipole interaction (quadrupole, octupole, and hexadecupole)

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

- Current empirical N-dependent interaction parameters:
  $\chi_\lambda = \bar{\chi}_\lambda k_\lambda \quad \leftarrow k_\lambda$ are renormalization factors

$$k_2 = 2.29 - \frac{1.124}{(N-148)^2+13.85} - 0.01375(N-148) \qquad k_3 = k_4 = 1$$

$$g_p = 0.10845 + 0.00058(N-148) \qquad g_n = 0.0671 + 0.000517(N-148)^{5/4}$$



Interaction parameters provide good overall agreement of experimental three-point odd even mass staggering (OES), which is estimated with proton and neutron pairing gaps computed in HFB $\Delta_\nu \approx 0.5\,\mathrm{OES}_\nu$

Also tuned parameters to match experimental state densities from level counting at low energies and neutron resonance spacing data

Nuclear State Densities

- Compute the thermal energy $E(\beta) = \langle H \rangle$ over a range of inverse temperatures β from the ground state $\beta \sim 40$ MeV^{-1} up to $\beta = 0$
- The state density $\rho(E_x)$ is the inverse Laplace transformation of the partition function

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

- The average state density is given in the saddle-point approximation

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

where $S(E) = \ln Z + \beta E$ is the entropy and $C = -\beta^2 \frac{\partial E}{\partial \beta}$ is the heat capacity.
Z is calculated by integrating $E(\beta) = -\frac{\partial \ln Z}{\partial \beta}$

- However, most experiments like the Oslo method measure the *level* densities...

Comparing NSD Calculation in ^{236}U

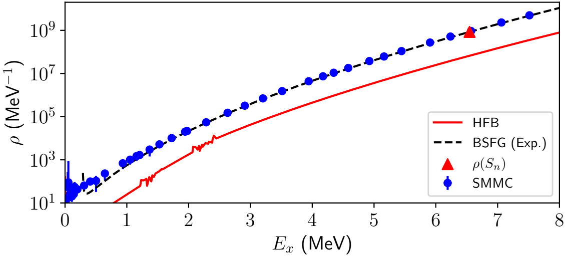
SMMC results agree with back-shifted Fermi gas (BSFG) formula with parameters a and Δ fitted to experimental data

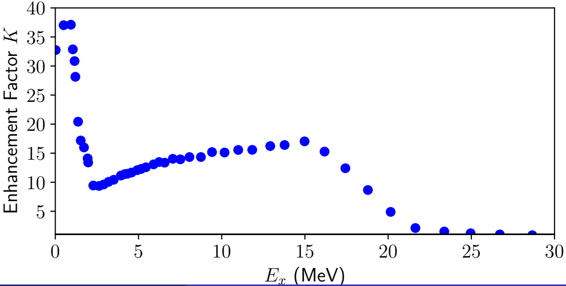
$$\rho_{\mathrm{BSFG}}(E_x) = \frac{\sqrt{\pi} e^{2\sqrt{a(E_x - \Delta)}}}{12 a^{1/4} (E_x - \Delta)^{5/4}}$$

where $a = 26.141$ MeV^{-1} and $\Delta = 0.288$ MeV

Enhancement factor $K = \rho_{SMMC} / \rho_{HFB} > 10$ for energies up to and beyond the neutron separation energy S_n

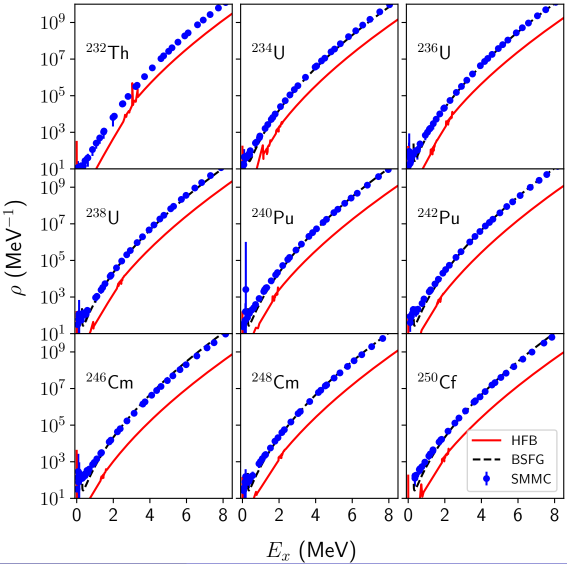
Pairing and shape transitions are clearly visible in K





NSD Results

	a (MeV^{-1})		Δ (MeV)	
Nucleus	Exp.	SMMC	Exp.	SMMC
^{232}Th	-	27.467	-	0.745
^{234}U	25.387	25.779	0.316	0.308
^{236}U	26.141	26.161	0.288	0.260
^{238}U	25.946	26.787	0.273	0.331
^{240}Pu	25.630	25.492	0.282	0.157
^{242}Pu	26.000	25.788	0.259	0.232
^{246}Cm	26.415	25.376	0.543	0.286
^{248}Cm	26.015	25.762	0.500	0.258
^{250}Cf	25.597	24.994	0.527	0.114

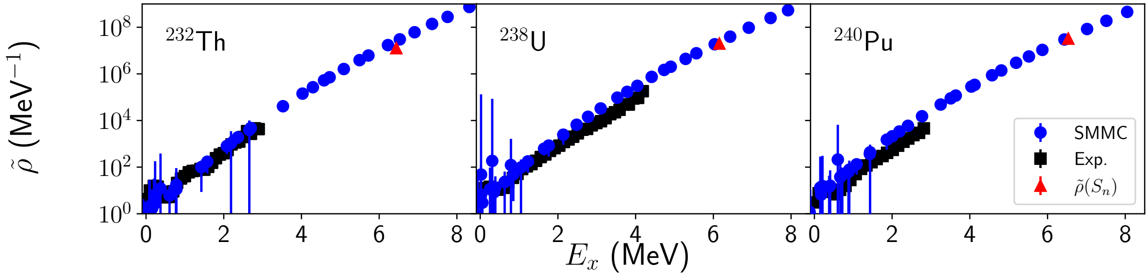


- The state density counts all $2J+1$ degenerate states withing each level. To compute the level density $\tilde{\rho}(E_x)$, we want to count each level only once.
- Perform additional projections onto specific values of spin component M Alhassid, Liu, and Nakada, PRL (2007)

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

- The M-projected state densities can be calculated using a similar saddle-point formula
- By projecting onto $M=0$ ($M=1/2$ for odd-mass nuclei), we count only one state from each level, therefore $\rho_{M=0}(E_x) = \tilde{\rho}(E_x)$
- The spin projection will also enable us to calculate spin distributions at different energies (more on that later)

Comparing NLDs with Oslo Method

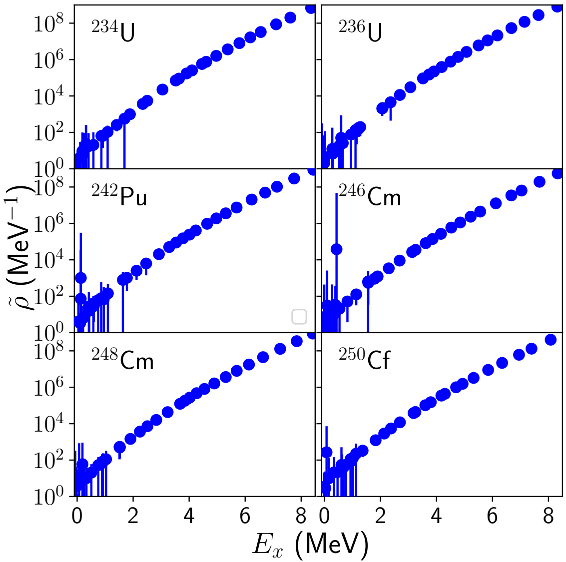


Exp: ^{232}Th, ^{238}U - Guttormsen *et al.* PRC (2013), ^{240}Pu - Zeiser *et al.* PRC (2019)

SMMC NLDs agree well with Oslo data at S_n

Nucleus	S_n (MeV)	$\tilde{\rho}(S_n)$ (10^7 MeV^{-1}) Exp.	SMMC
^{232}Th	6.440	1.27 ± 0.38	2.64 ± 0.43
^{238}U	6.154	2.0 ± 0.8	2.50 ± 0.52
^{240}Pu	6.534	3.27 ± 0.66	3.91 ± 0.73

Nucleus	S_n (MeV)	$\tilde{\rho}(S_n)$ (10^7 MeV^{-1})
^{234}U	6.845	6.08 ± 1.07
^{236}U	6.546	4.51 ± 0.83
^{242}Pu	6.310	2.51 ± 0.48
^{246}Cm	6.459	2.60 ± 0.49
^{248}Cm	6.212	2.19 ± 0.45
^{250}Cf	6.624	4.00 ± 0.82



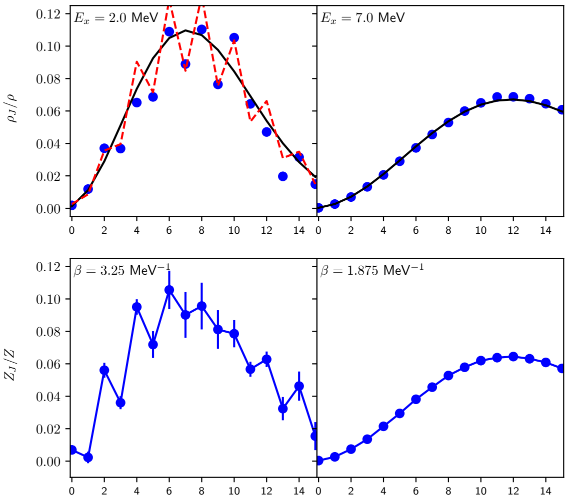
At higher energies, the spin distribution is given by the spin-cutoff model:

$$\frac{\rho_J}{\rho} = \frac{2J+1}{2\sqrt{2\pi}\sigma^3} e^{-J(J+1)/2\sigma^2}$$

Good agreement using the value of σ obtained from the NLD and NSD ratio

Below the pairing transition, the results agree with the empirical staggering formula of von Egidy and Bucurescu, PRC (2008)

Ratio of partition functions displays a similar onset of spin staggering at low temperatures →



Preliminary - uncertainty analysis not complete

Moment of Inertia and Spin Cutoff Parameter σ in ^{240}Pu

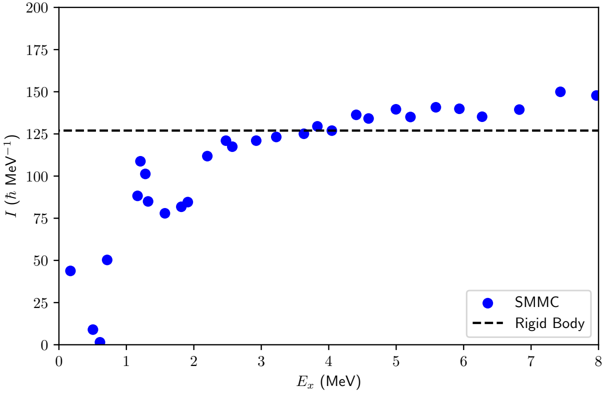
Spin cutoff parameter σ calculated from the ratio of the state and level densities

$$\tilde{\rho}(E_x) = \frac{\rho(E_x)}{\sqrt{2\pi}\sigma}$$

Moment of inertia I computed from

$$I = \frac{\sigma^2 \hbar^2}{T}$$

Moment of inertia decreases at below ~ 4 MeV, indicating the onset of strong pairing correlations



Preliminary - uncertainty analysis not complete

Conclusions and Outlook

Conclusions:

- We successfully extended the SMMC method to actinides, overcoming technical challenges
- SMMC enables microscopic calculations in model spaces that are many orders of magnitude larger than what is possible with direct diagonalization
- Our level densities show good agreement with existing Oslo data and we can make predictions for other nuclei not yet studied experimentally
- Evidence of pairing transitions seen in spin distributions and moment of inertia are in overall agreement with empirical models

Outlook:

- NLD calculations on neighboring actinides, including odd-mass and possibly odd-odd nuclei
- γ-ray strength functions in actinides - Does the LEE persist in these nuclei? Do we see the double-peaked scissor mode?
- Shape-dependent level densities for applications to fission

Work supported by the U.S. DOE grant No. DE-SC0019521. Computational resources provided by the National Energy Research Scientific Computing Center (NERSC).