Benchmarking mean-field and beyond-the-mean-field methods for calculating level densities

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Introduction

The microscopic calculation of level densities in the presence of correlations is a challenging many-body problem.

The configuration-interaction shell model is a suitable framework to account for correlations but the combinatorial increase of the dimensionality of its model space has hindered its applications in mid-mass and heavy nuclei.

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

SMMC is computationally intensive.

- Mean-field approximations are computationally efficient and have been widely used in the calculation of level densities (S. Goriely, S. Hilaire, et al) but their accuracy has not been well studied.

- We benchmarked mean-field level densities against exact SMMC densities using the same interaction and model space.

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 dimension ~100.
- The high-dimensional σ integration is evaluated by Monte Carlo methods.
- Calculations are done in the *canonical* ensemble of fixed particle number.

Finite-temperature mean-field approximations

The grand potential Ω is minimized at given temperature and chemical potential with respect to the one-body density [Hartree-Fock (HF)] or with respect to the one-body and pairing densities [Hartree-Fock-Bogoliubov (HFB)].

- Formulated in the *grand-canonical* ensemble.

The thermodynamic approach to level densities

The starting point is the partition function $Z(\beta) = Tr\, e^{-\beta H}$ ($\beta = 1/T$)

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

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

where $S(E) = \ln Z + \beta E$ is the entropy and $C = -\beta^2 \partial E / \partial \beta$ is the heat capacity.

β is determined as a function of E using the saddle-point condition

$$-\partial \ln Z / \partial \beta = E$$

Two methods for calculating the partition function

Shell model Monte Carlo (SMMC)

We calculate the thermal energy at fixed particle number N from $E_N(\beta) = < H >_N$ and integrate $-\partial \ln Z_N / \partial\beta = E_N(\beta)$ to find the canonical partition function

. $Z_N(\beta)$

Finite-temperature mean field theory

[Alhassid, Bertsch, Gilbreth, and Nakada, PRC **93**, 044320 (2016)]

- The grand-canonical ensemble of mean-field theory must be reduced to the canonical ensemble: we use exact particle-number projection (after variation)

[Fanto, Alhassid, and Bertsch, PRC **96**, 014305 (2017)].

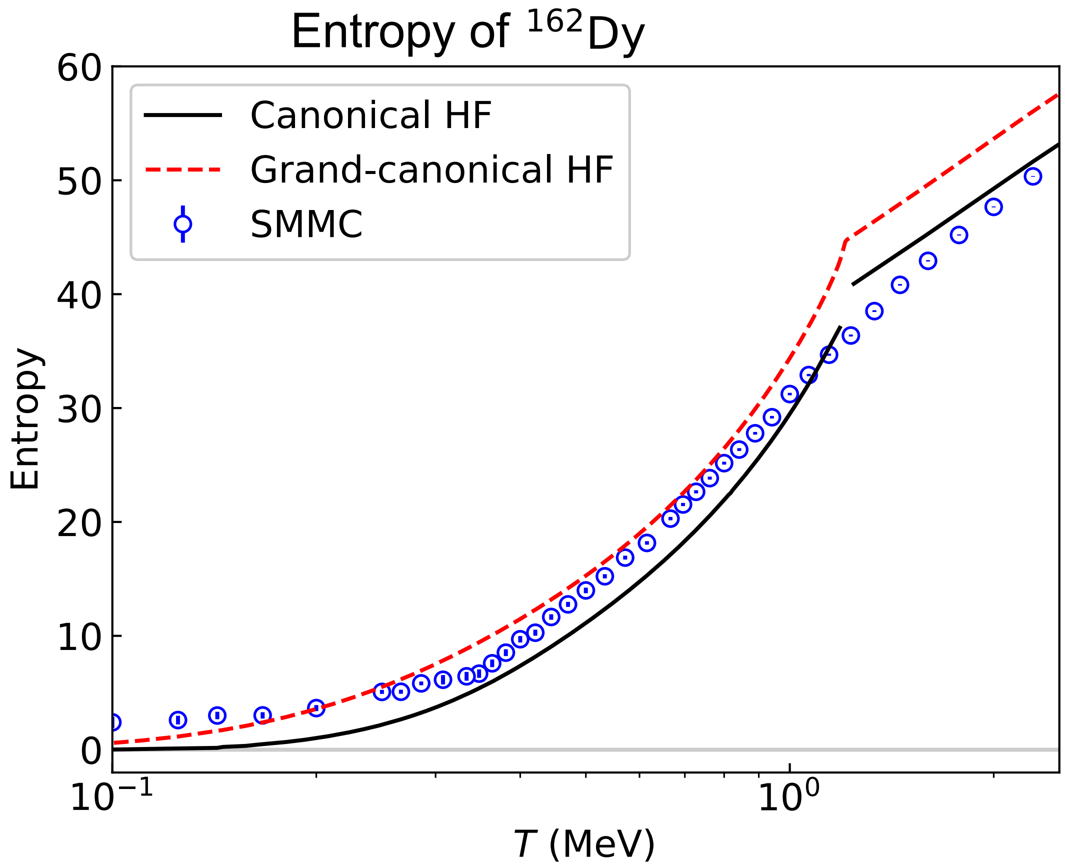
We calculate the canonical partition $Z_N(\beta) = Tr\,[P_N\, e^{-\beta(H_{MF} - \langle V \rangle)}]$
where P_N is the particle-number projection operator and H_{MF} is the (non-interacting) self-consistent mean-field Hamiltonian.

Benchmarking the HF approximation: a deformed nucleus (^{162}Dy)

^{162}Dy is strongly deformed and the proper mean-field theory is the HF

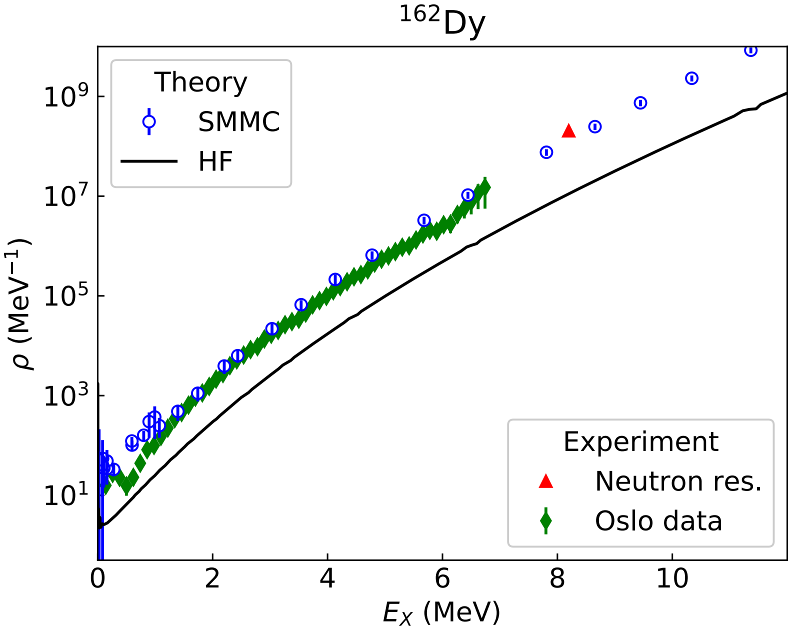
Single particle model space:
protons: 50-82 shell plus $1f_{7/2}$;
neutrons: 82-126 shell plus
$0h_{11/2}$ and $1g_{9/2}$

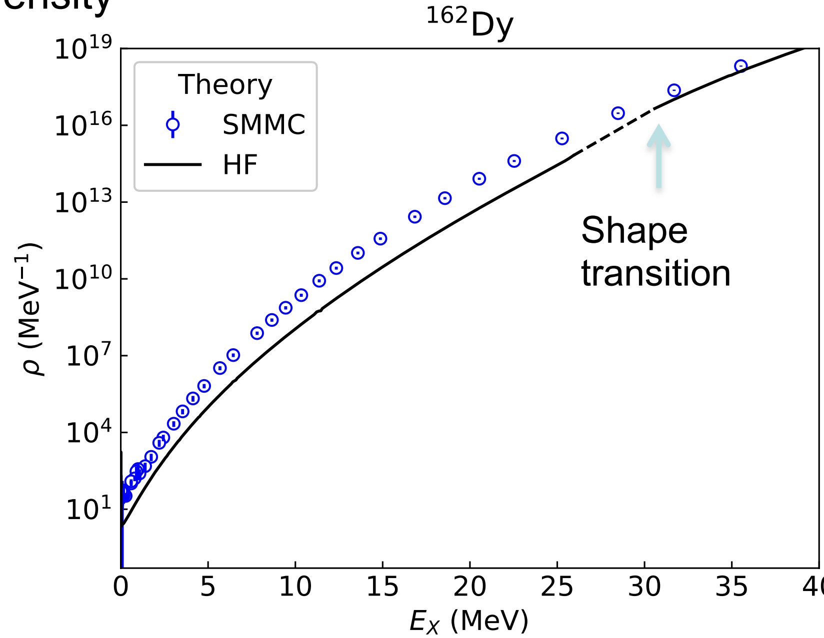
Interaction: pairing + multipole-multipole (quadrupole, octupole, hexadecupole)



- *Grand-canonical* HF entropy overestimates the exact SMMC entropy
- The *canonica*l HF entropy underestimates the SMMC entropy below the shape transition energy.

State density

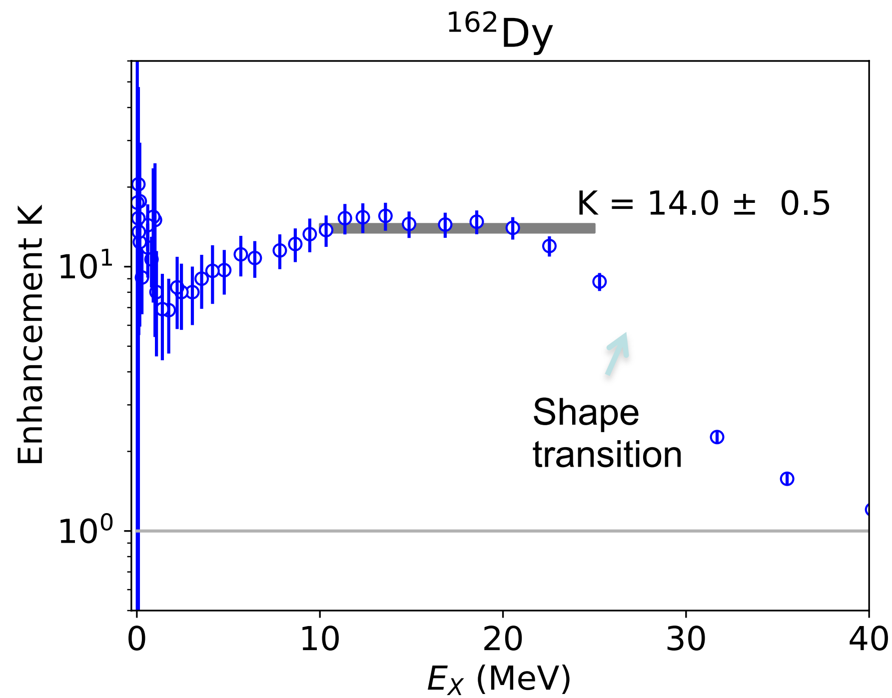




The HF density of a deformed nucleus describes only intrinsic band heads and misses the contribution from rotational states built on top of them: a result of the broken rotational symmetry in the HF.

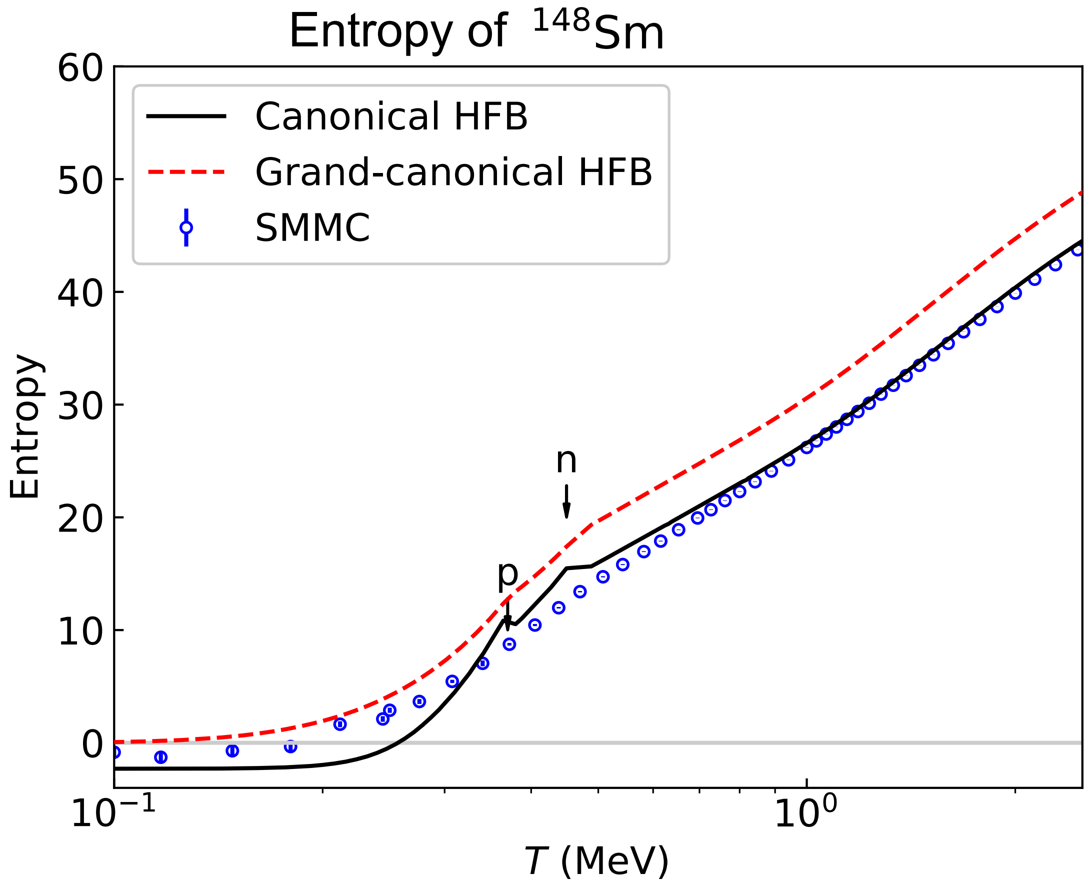
We define the collective enhancement factor K by $K = \rho_{SMMC} / \rho_{HF}$

K decays gradually to ~1 above the shape transition energy



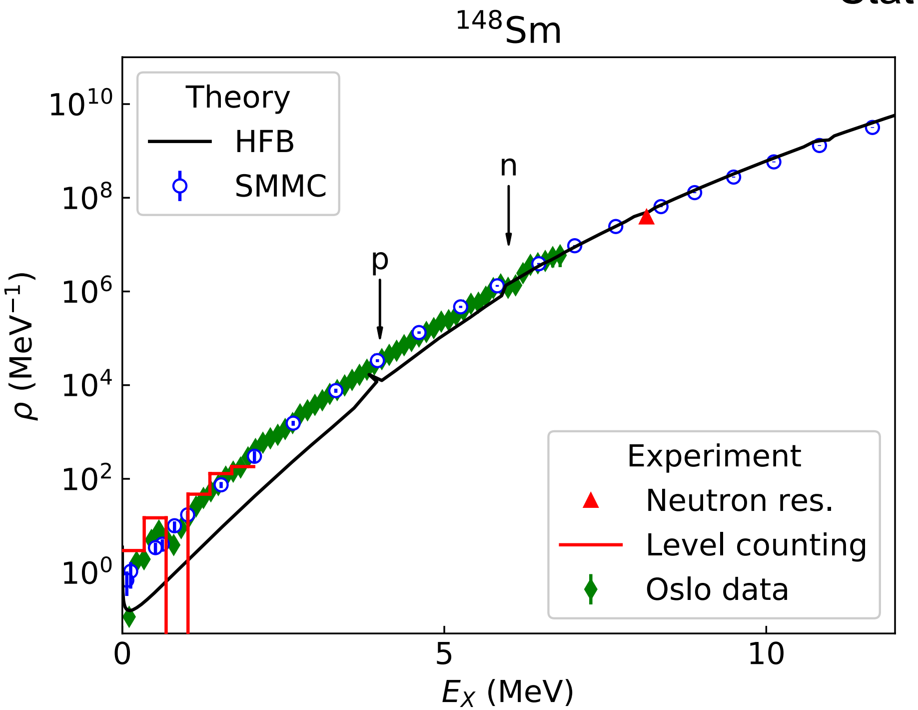
Benchmarking the HFB approximation: a spherical nucleus (^{148}Sm)

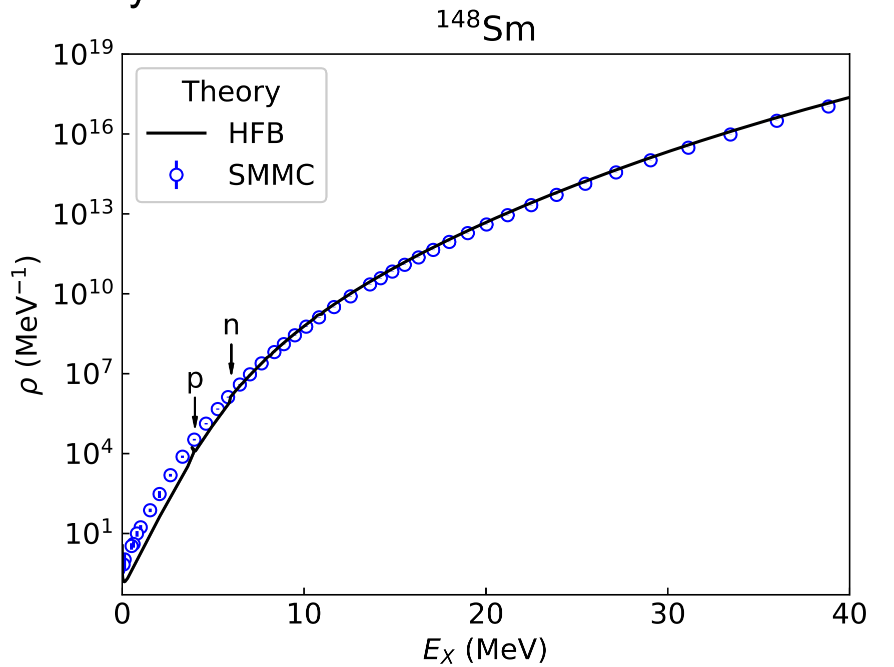
^{148}Sm is nearly spherical with a strong pairing condensate and the proper mean-field theory is the HFB

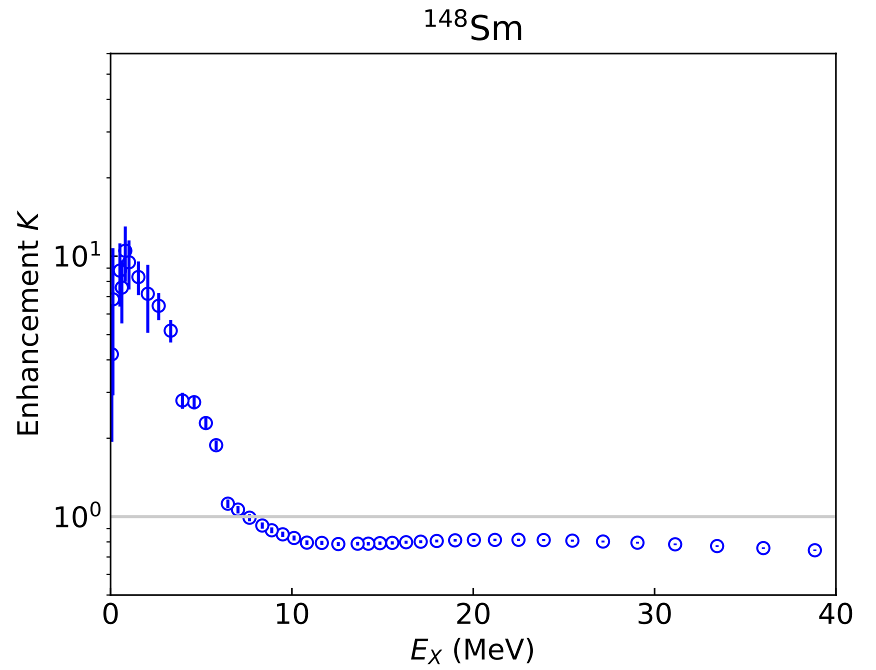


The negative canonical HFB entropy at low temperatures is unphysical and is the result of the inherent violation of particle-number conservation in the HFB.

State density





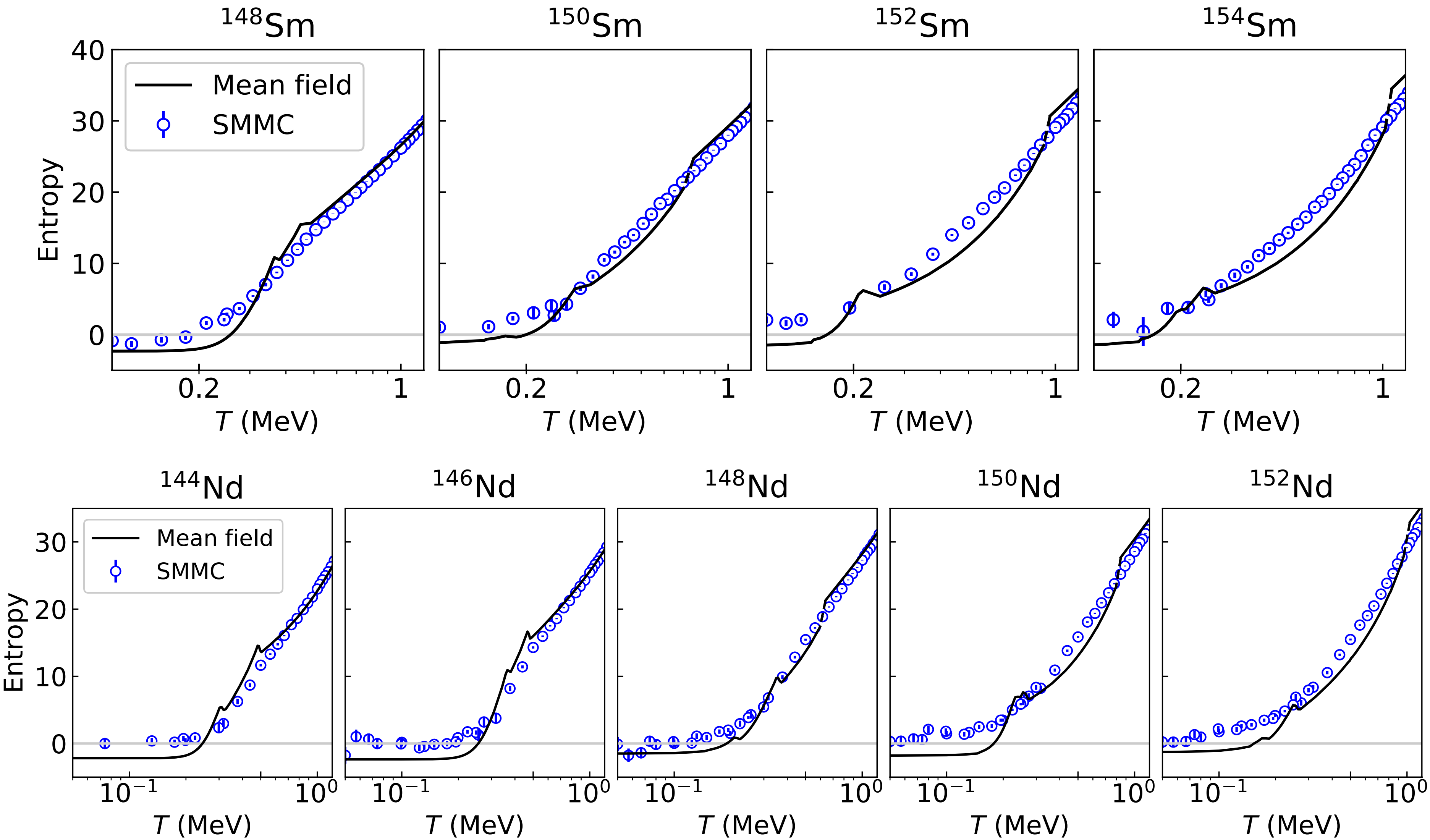


The enhancement of the state density relative to the HFB density below the pairing transition is an artifact of the broken particle-number conservation.

Application to lanthanides: the crossover from spherical to deformed nuclei

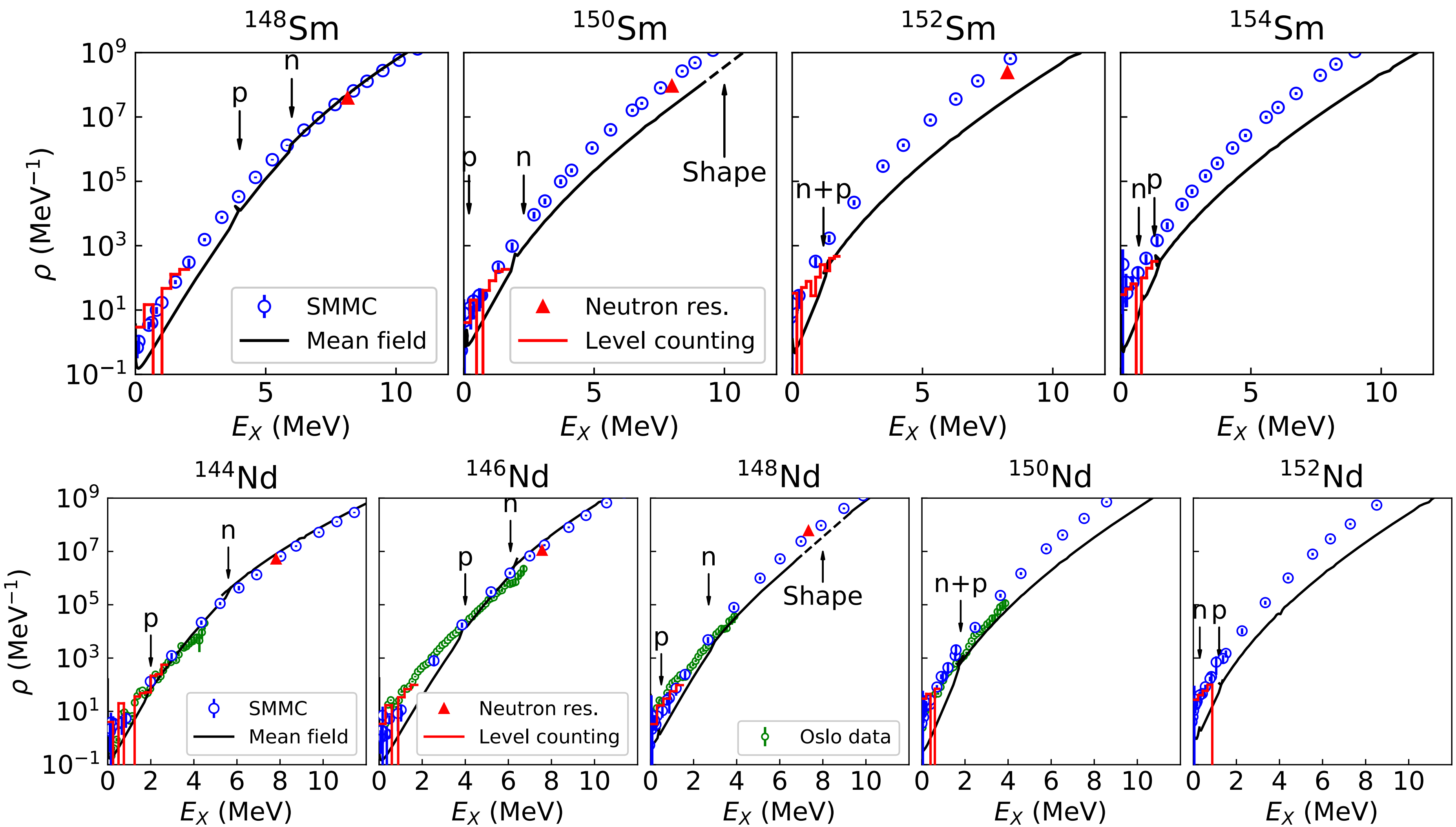
(W. Ryssens and Y. Alhassid)

Entropy vs. temperature



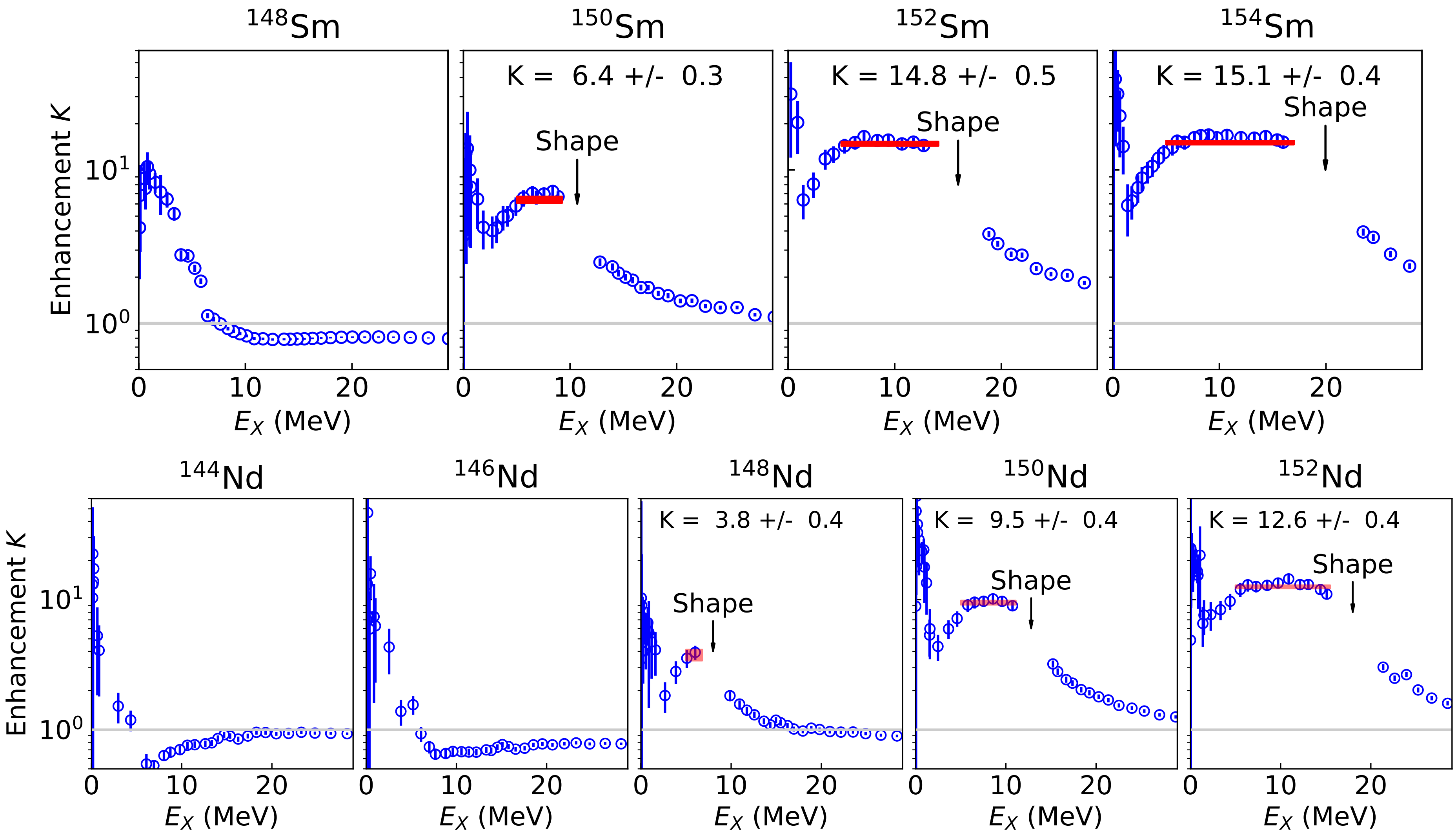
State density

[See also C. Ozen, Y. Alhassid, and H. Nakada, Phys. Rev. Lett. 110, 042502 (2013)]



Oslo data (courtesy of M. Guttormsen) of level densities was converted to state densities using the spin cutoff model with parameter σ determined by SMMC.

Collective enhancement factor K



- The enhancement below the pairing transition is an artifact of the violation of particle-number conversation in HFB.
- The rotational enhancement is correlated with deformation and decays above the shape transition energy.

Beyond-the-mean-field method: static-path plus random-phase approximation (SPA+RPA)

(P. Fanto and Y. Alhassid)

We integrate over all static (thermal) fluctuations of the mean field plus small time-dependent (quantal) fluctuations around each static fluctuation.

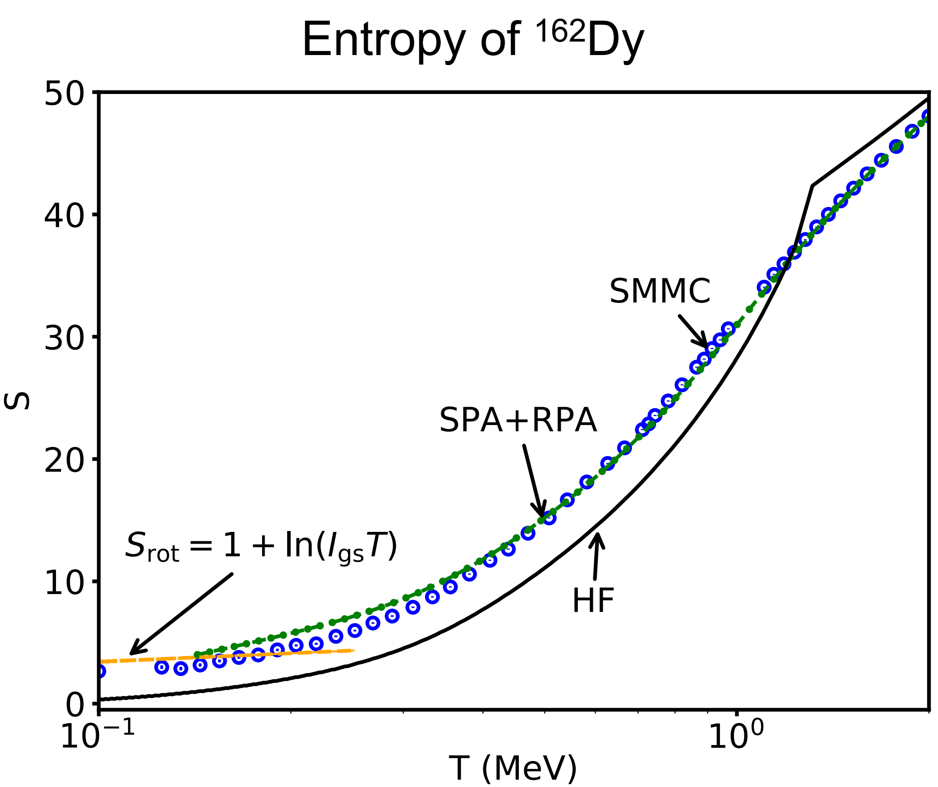
$$Z(\beta) = \int D[\sigma_0]\, e^{-\beta F[\sigma_0,\beta]} C_{RPA}(\sigma_0,\beta)$$

σ_0 = static fields

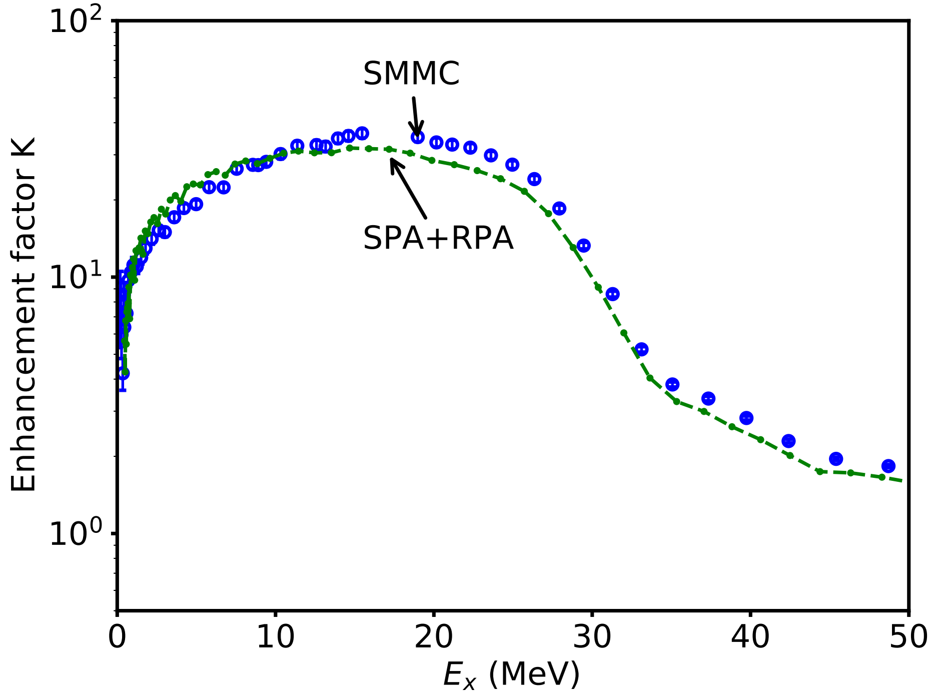
F = free energy

C_{RPA} = RPA correction factor for each σ_0

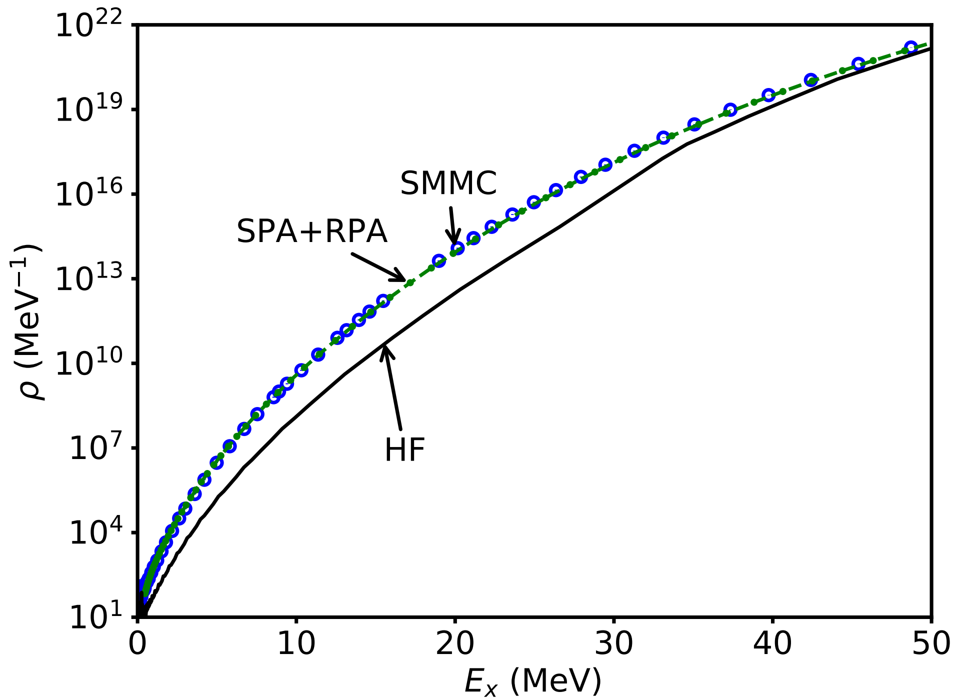
Tested in ^{162}Dy for a quadrupole-quadrupole interaction



Enhancement factor K in ^{162}Dy



State density of ^{162}Dy



- The SPA+RPA reproduces the rotational enhancement in deformed nuclei.

- The rotational symmetry, which is broken in a deformed nucleus in the HF approximation, is restored in the SPA+RPA.

Conclusion

SMMC is a powerful method for calculating level densities in very large model spaces; applications in nuclei as heavy as the lanthanides.

- We benchmarked finite-temperature mean-field approximations to level densities against exact SMMC densities.

- Mean-field theories are formulated in the grand-canonical ensemble and we carry out the reduction to the canonical ensemble by particle-number projection.

- The main deficiencies of a mean-field theory are associated with broken symmetries: (i) broken rotational invariance in deformed nuclei, and (ii) broken particle-number conservation in nuclei with strong pairing correlations.

Outlook

- Thermodynamic approach to level densities in density functional theories (talk by Wouter Ryssens).
- Develop beyond-the-mean-field SPA+RPA methods to overcome the deficiencies associated with the broken symmetries of the mean field (talk by Paul Fanto).

Heavy nuclei (lanthanides) in SMMC

CI shell model space:

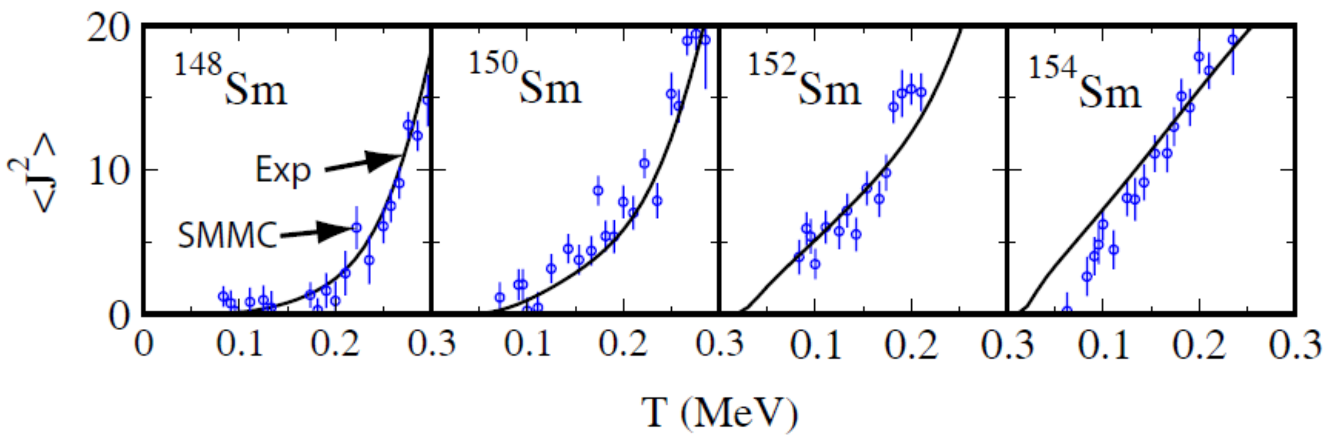
protons: 50-82 shell plus $1f_{7/2}$; neutrons: 82-126 shell plus $0h_{11/2}$ and $1g_{9/2}$

Single-particle Hamiltonian: from Woods-Saxon potential plus spin-orbit

Interaction: pairing plus multipole-multipole interaction terms – quadrupole, octupole, and hexadecupole

We used SMMC to describe the crossover from vibrational to rotational collectivity in the framework of the spherical CI shell model.

The dependence of $\langle \vec{J}^2 \rangle$ on temperature T is sensitive to the type of collectivity



Ozen, Alhassid, Nakada, PRL **110**, 042502 (2013)