Level densities of heavy nuclei in the shell model Monte Carlo approach

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- Introduction
- Level densities in the shell model Monte Carlo (SMMC) approach
- Collectivity in heavy nuclei within a shell model approach
- Level densities in heavy nuclei (lanthanides)
- Mean-field approximations
- Nuclear deformation in a spherical shell model approach (important in the modeling of fission)
- Conclusion and prospects.

Level densities

Level densities are important input in the Hauser-Feshbach theory of compound nuclear reactions, but are not always accessible to direct measurement.

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

- Most approaches are based on empirical modifications of the Fermi gas formula or on mean-field approximations that can often miss important correlations.

- The configuration-interaction (CI) shell model accounts for correlations but diagonalization methods are limited to spaces of dimensionality $\sim 10^{11}$.

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

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

Lang, Johnson, Koonin, Ormand, Phys. Rev. C 48, 1518 (1993);
Alhassid, Dean, Koonin, Lang, Ormand, Phys. Rev. Lett. 72, 613 (1994).

Level density in SMMC

[H. Nakada and Y.A., PRL **79**, 2939 (1997)]

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

The *average* level 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 $= \ln Z + \beta E$

C = canonical heat capacity $= \partial E / \partial T$

Collectivity in heavy nuclei in the CI shell model

Heavy nuclei exhibit various types of collectivity (vibrational, rotational, …) that are well described by empirical models.

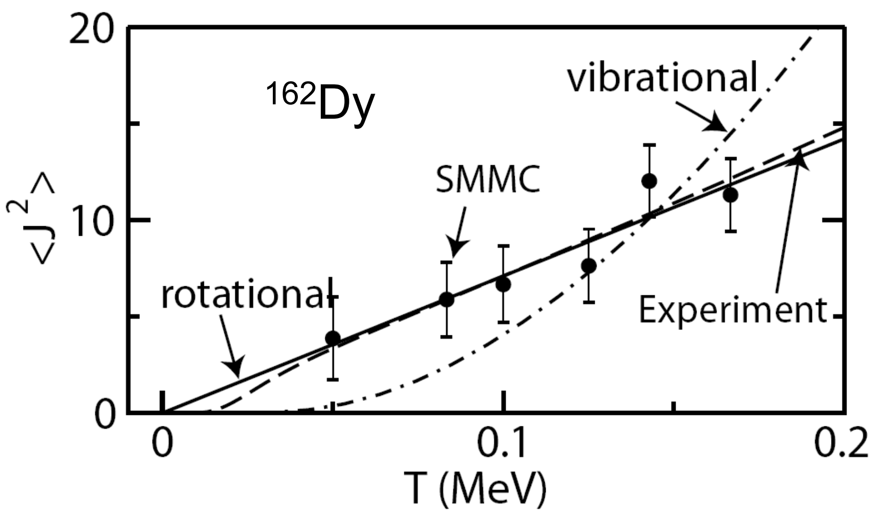
However, a microscopic description in a CI shell model has been mostly lacking.

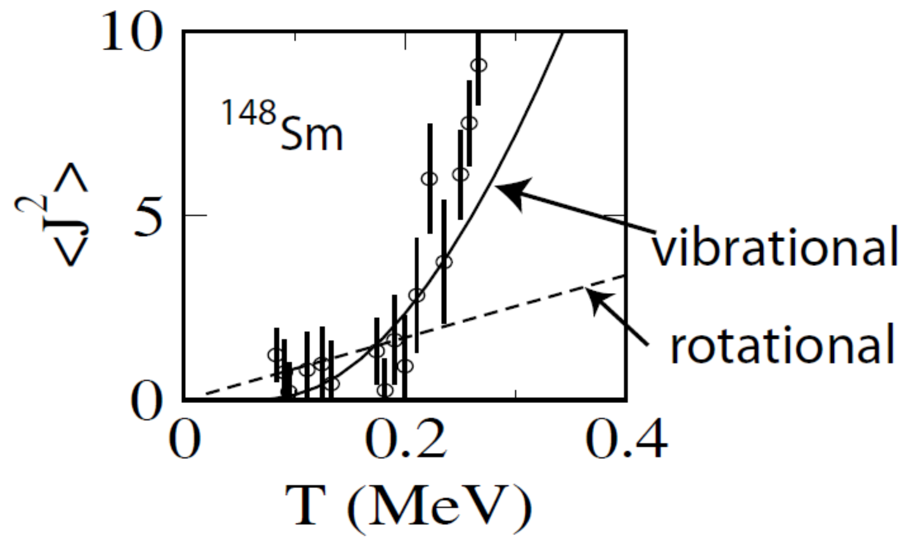
Can we describe vibrational and rotational collectivity in heavy nuclei using a spherical shell model approach in a truncated space ?

The large model space required (e.g., ~ 10^{29} in ^{162}Dy) necessitates the use of SMMC.

The various types of collectivity are usually identified by their corresponding spectra, but SMMC does not provide detailed spectroscopy.

The behavior of $\langle \vec{J}^2 \rangle$ versus T is sensitive to the type of collectivity:





$$\langle \vec{J}^2 \rangle = \frac{6}{E_{2^+}} T$$

$\Rightarrow {}^{162}Dy$ is rotational

$$\langle \vec{J}^2 \rangle = 30 \frac{e^{-E_{2^+}/T}}{(1-e^{-E_{2^+}/T})^2}$$

$\Rightarrow {}^{148}Sm$ is vibrational

Alhassid, Fang, Nakada, PRL **101** (2008)

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

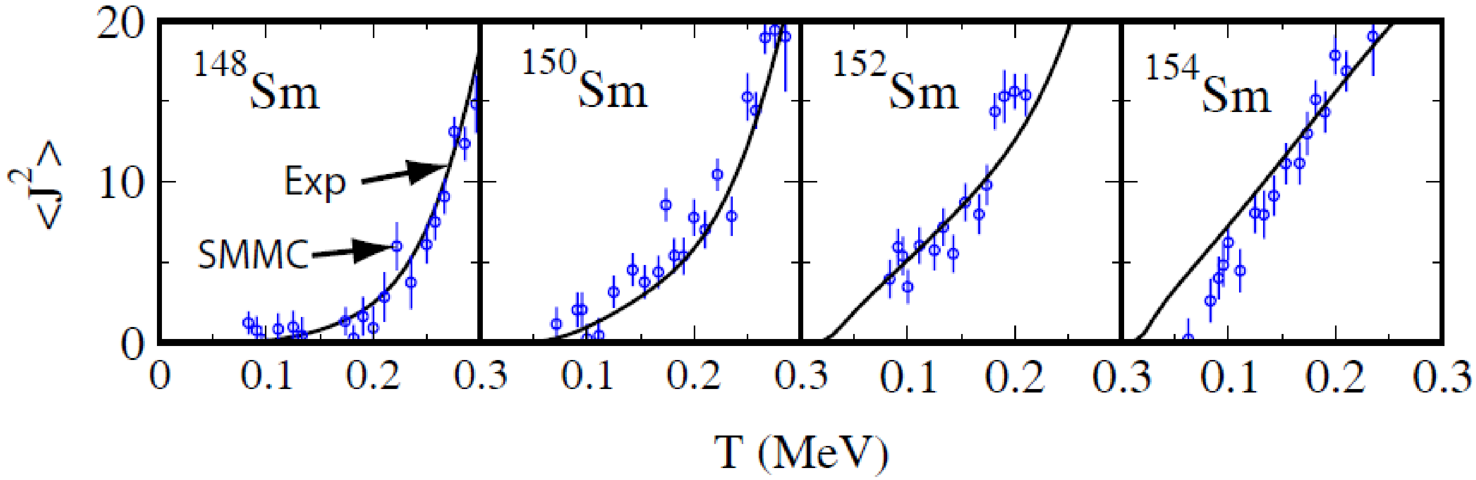
Single-particle model space (using Woods-Saxon plus spin-orbit)

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

Crossover from vibrational to rotational collectivity in heavy nuclei

C. Ozen, Y. Alhassid, H. Nakada, Phys. Rev. Lett. 110, 042502 (2013)

$\langle \vec{J}^2 \rangle$ versus T in samarium isotopes

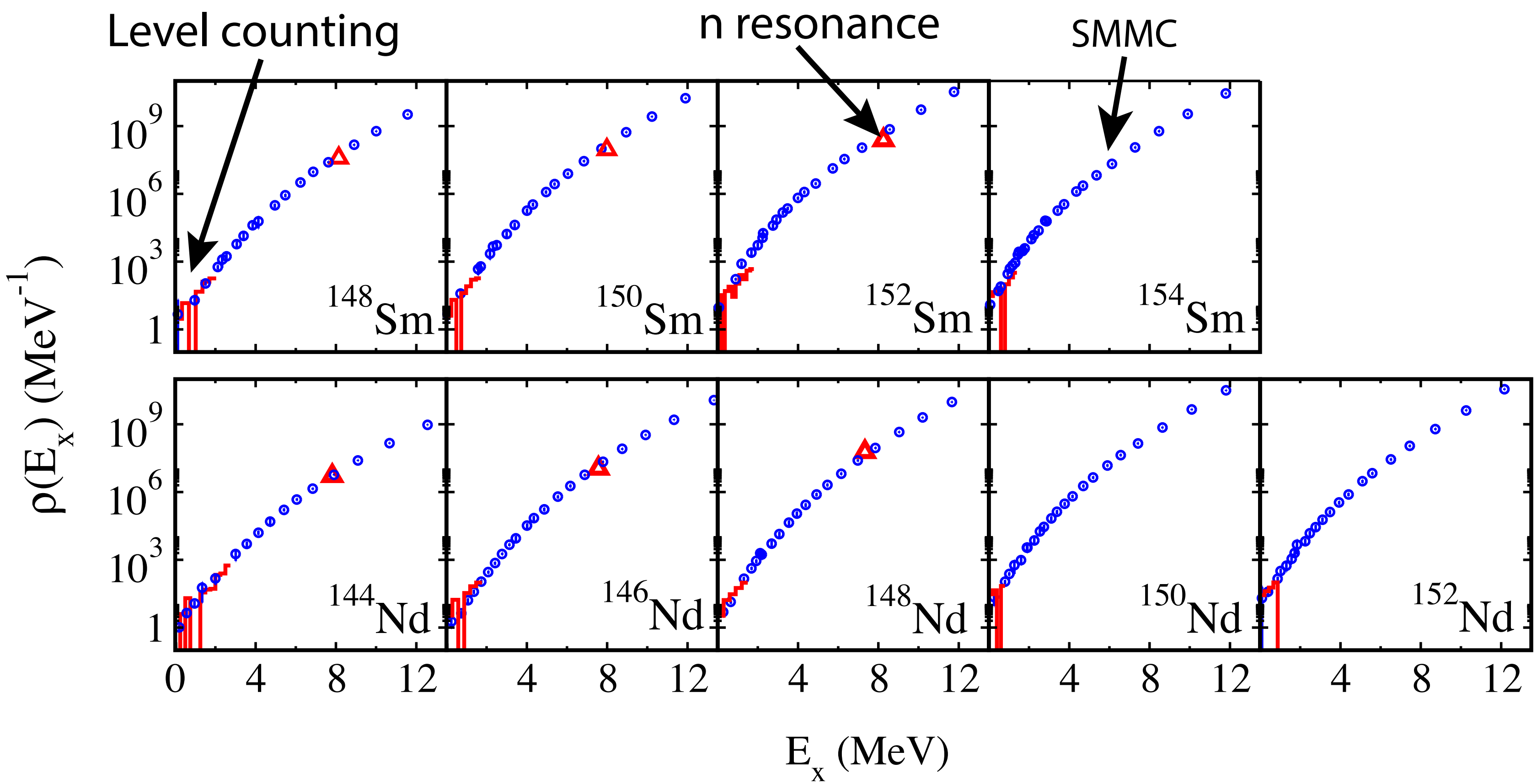


• Experimental values are found from $\langle \vec{J}^2 \rangle = \dfrac{\sum_{\alpha J} J(J+1)(2J+1)e^{-E_{\alpha J}/T}}{\sum_{\alpha J}(2J+1)e^{-E_{\alpha J}/T}}$
where $E_{\alpha J}$ are the experimentally known levels.

• Add the contribution of higher levels using the experimental level density to get an experimental values at higher T.

SMMC describes well the crossover from vibrational to rotational collectivity in good agreement with the experimental data at low T.

Level densities in even samarium and neodymium isotopes



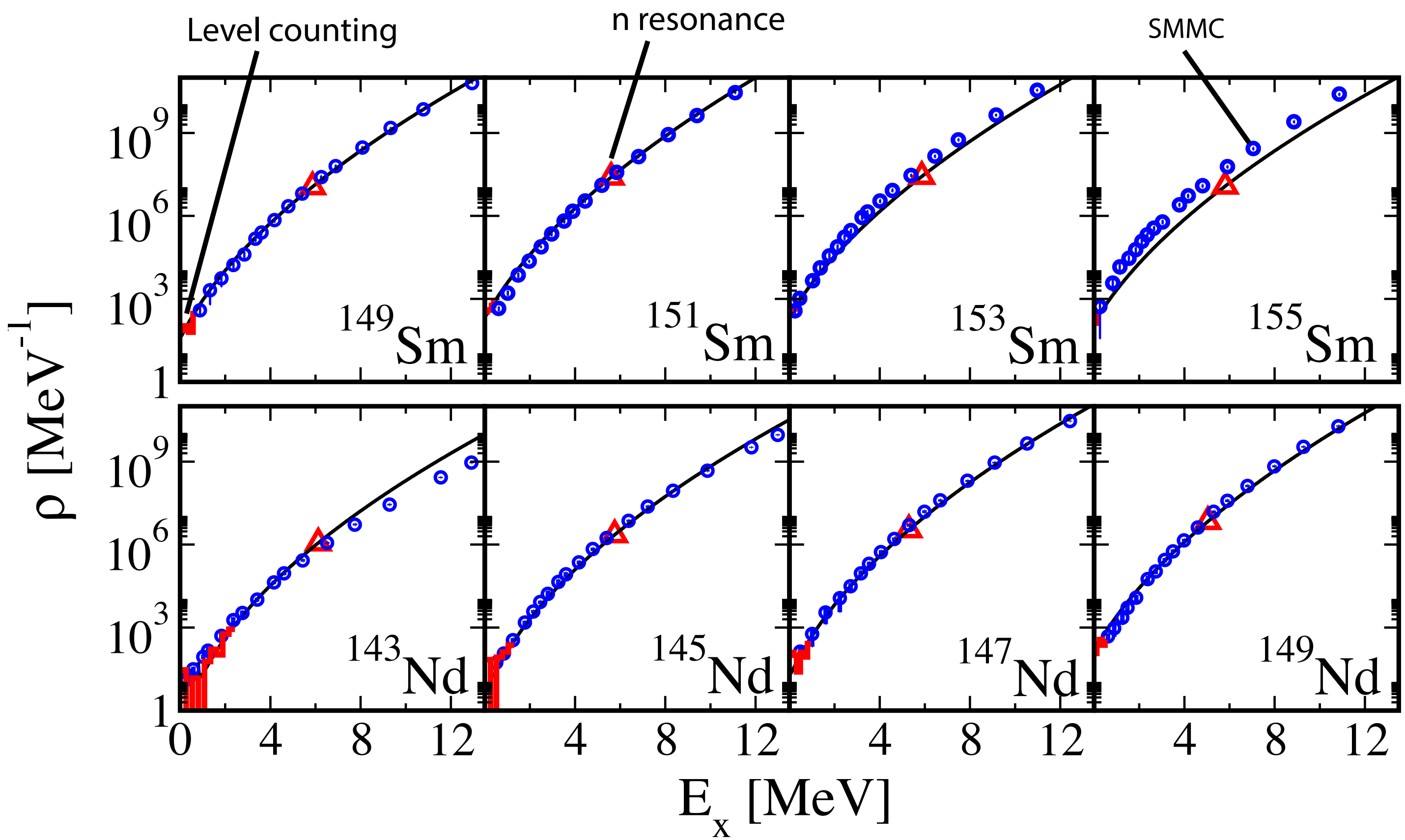
- Good agreement of SMMC densities with various experimental data sets (level counting, neutron resonance data when available).

Level densities in odd samarium and neodymium isotopes

C. Ozen, Y. Alhassid, H. Nakada, PRC **91**, 034329 (2015)

- The projection on odd number of particles introduces a sign problem: it is difficult to determine an accurate ground-state energy E_0.

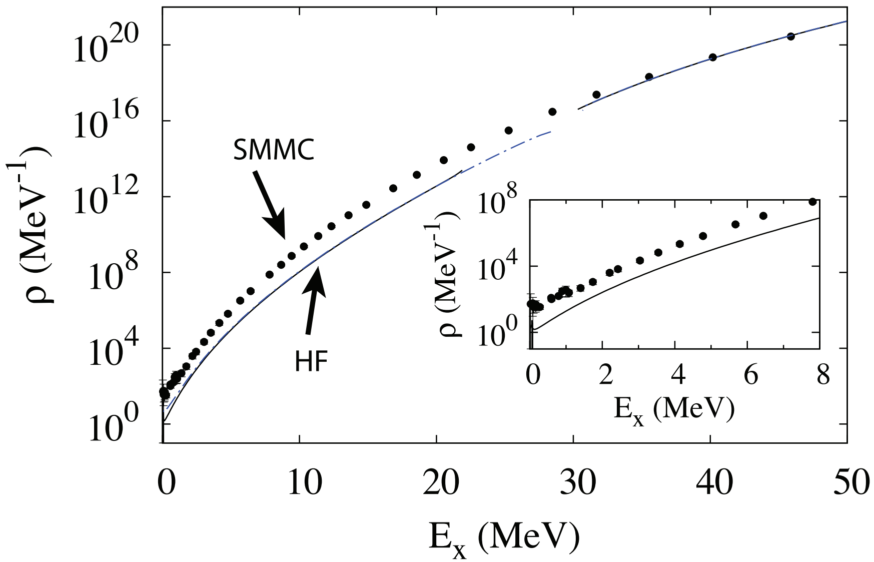
We extracted E_0 by a fit to the experimental thermal energy $E_x(T)$



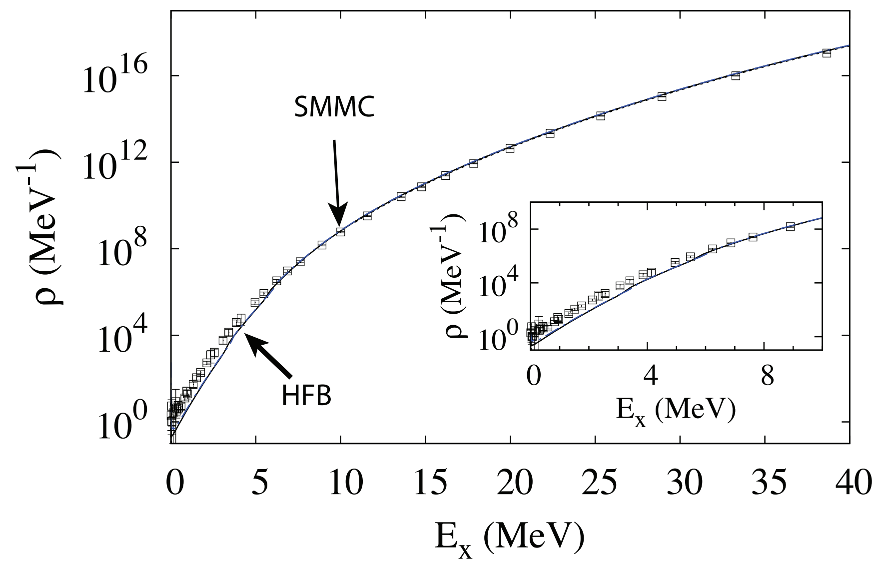
Mean-field approximations

Y. Alhassid, G.F. Bertsch, C.N. Gilbreth and H. Nakada (in preparation)

A deformed nucleus (^{162}Dy): Hartree-Fock (HF) vs. SMMC



A spherical nucleus with strong pairing (^{148}Sm): Hartree-Fock-Bogoliubov (HFB) vs. SMMC



- Particle-number projection is carried out in the saddle-point approximation -- a good approximation in HF but not in HFB (which does not conserve particle number).

- The enhancement of the SMMC density in a deformed nucleus (compared with HF) is due to rotational bands built on top of the intrinsic bandheads.

Nuclear deformation in a spherical shell model approach

Y. Alhassid, C.N. Gilbreth, and G.F. Bertsch, Phys. Rev. Lett. **113**, 262503 (2014)

Modeling of fission requires level density as a function of deformation.

- Deformation is a key concept in understanding heavy nuclei but it is based on a mean-field approximation that breaks rotational invariance.

The challenge is to study nuclear deformation in a framework that preserves rotational invariance.

We calculated the distribution of the axial mass quadrupole in the lab frame using an exact projection on Q_{20} (novel in that $[Q_{20}, H] \neq 0$).

$$P_\beta(q) = \langle \delta(Q_{20} - q) \rangle = \frac{1}{Tr\, e^{-\beta H}} \int_{-\infty}^{\infty} \frac{d\varphi}{2\pi} e^{-i\varphi q} Tr(e^{i\varphi Q_{20}} e^{-\beta H})$$

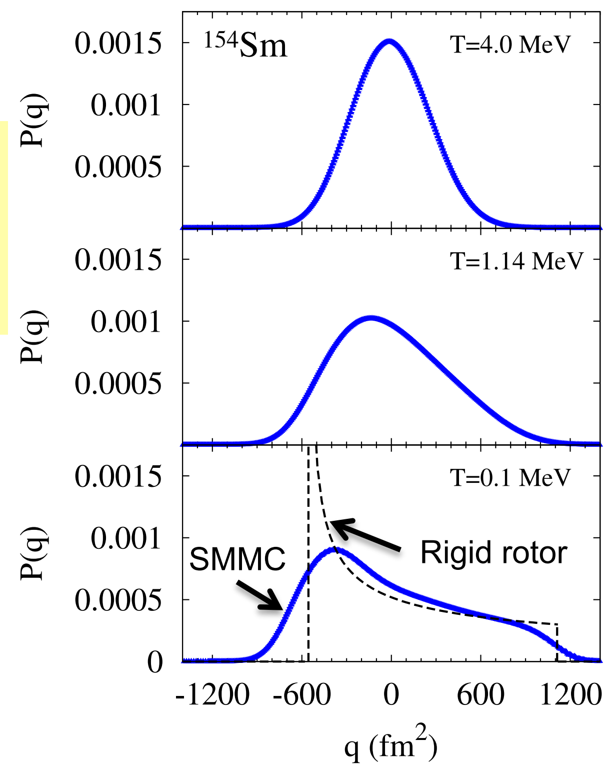
Application to heavy nuclei

^{154}Sm (a deformed nucleus)

- At low temperatures, the distribution is similar to that of a prolate rigid rotor
  ➡ a model-independent signature of deformation.

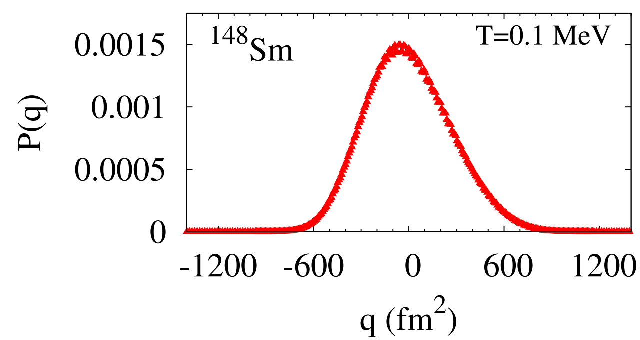
- At the HFB shape transition temperature (T=1.14 MeV), the distribution is still skewed.

- The distribution at high temperatures is close to a Gaussian.



^{148}Sm (a spherical nucleus)

- The distribution is close to a Gaussian even at low temperatures.



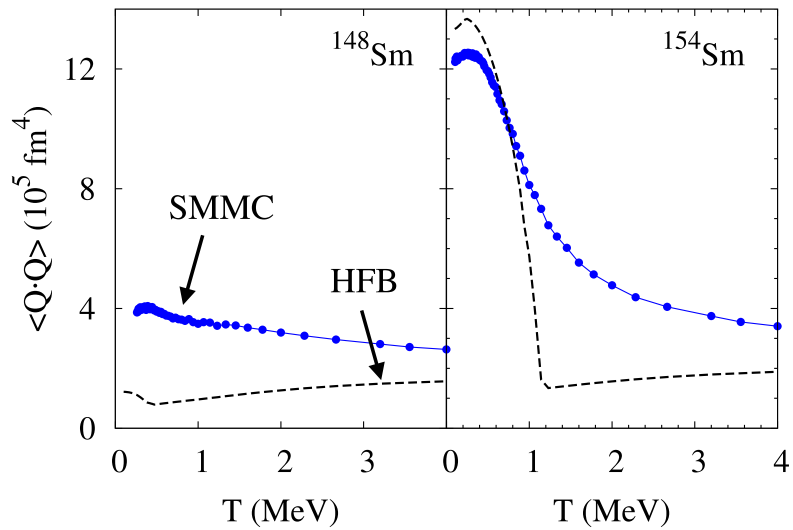
Intrinsic deformation from lab frame distributions

- Information on intrinsic deformation can be obtained from the expectation values of rotationally invariant combinations of the quadrupole tensor $Q_{2\mu}$

  Example: the lowest order invariant is second order $\langle Q \cdot Q \rangle$

Effective value of β :

$$\beta \propto (\langle Q \cdot Q \rangle)^{1/2}$$



The sharp shape transition in HFB is washed out in the finite-size nucleus

An effective value of γ can be determined from the cubic moment of $Q_{2\mu}$

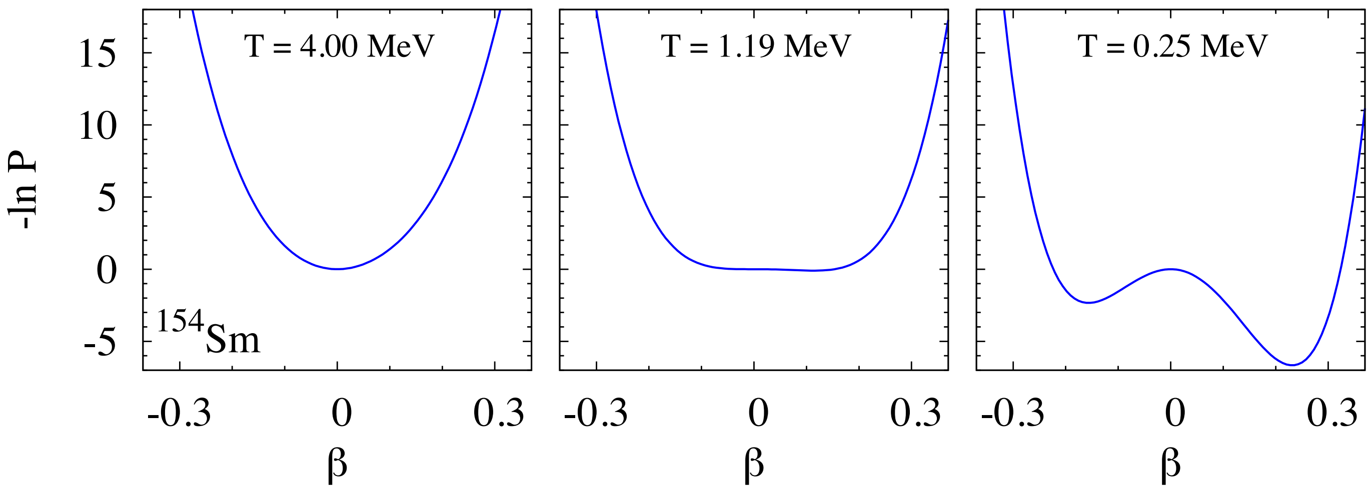
$$\cos 3\gamma = -\sqrt{7/2}\langle (Q \times Q) \cdot Q \rangle / \langle Q \cdot Q \rangle^{3/2}$$

- The quadrupole invariants can be calculated from lab frame moments of Q_{20}

Intrinsic shape distributions $P_T(\beta,\gamma)$

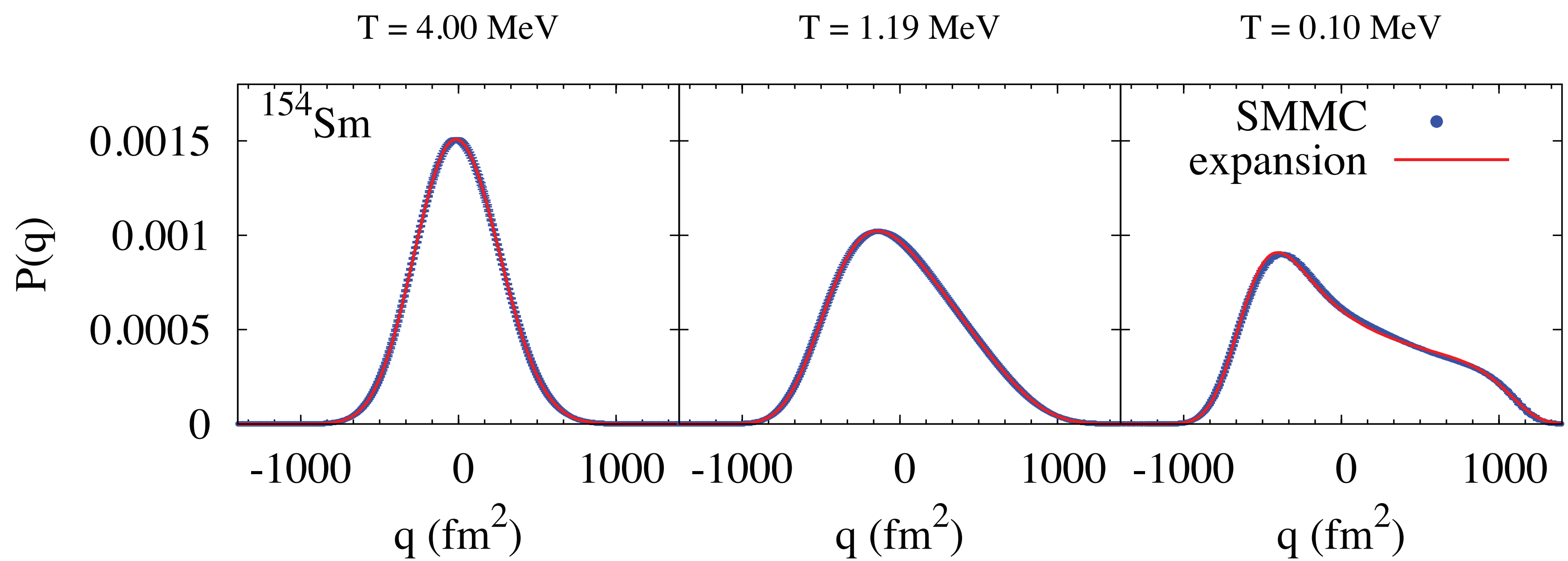
$\ln P_T(\beta,\gamma)$ at a given temperature T is an invariant and can be expanded in the quadrupole invariants $-\ln P_T = A\beta^2 - B\beta^3\cos 3\gamma + C\beta^4 + \ldots$

- The expansion coefficients A,B,C,… can be determined from the expectation values of the invariants, which in turn can be calculated from the low-order moments of $q_{20} = q$



- Mimics a shape transition from a deformed to a spherical shape without using a mean-field approximation !

Expressing the invariants in terms of $q_{2\mu}$ in the lab frame and integrating over the $\mu \neq 0$ components, we recover $P[q_{20}]$ in the lab frame.



We find excellent agreement with $P[q_{20}]$ calculated in SMMC !

A promising method for calculating level densities vs. deformation:

Construct the joint level density distribution $\rho(\beta,\gamma,E_x) = \rho(E_x) P_{E_x}(\beta,\gamma)$

where $P_{E_x}(\beta,\gamma)$ is the intrinsic shape distribution at given excitation energy E_x

Conclusion

• SMMC is a powerful method for the microscopic calculation of level densities in very large model spaces; recent applications in nuclei as heavy as the lanthanides.

• Microscopic description of collectivity in heavy nuclei.

• Spin distributions in even-even heavy nuclei: odd-even staggering at low excitation energies; spin cutoff model at higher excitations.

• Description of nuclear deformation in a rotationally invariant framework (CI shell model).

Prospects

• Other mass regions (actinides, unstable nuclei,…).

• Level densities as a function of deformation (useful for modeling of fission).

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