Level densities by the auxiliary-field Monte Carlo method

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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 auxiliary-field Monte Carlo (AFMC 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 auxiliary-field Monte Carlo (AFMC) method

Start from a configuration-interaction (CI) shell model Hamiltonian H

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.

Level density in AFMC

- 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 $= \partial E / \partial T$

Mid-mass nuclei

CI shell model model space: complete *fpg*9/2-shell.

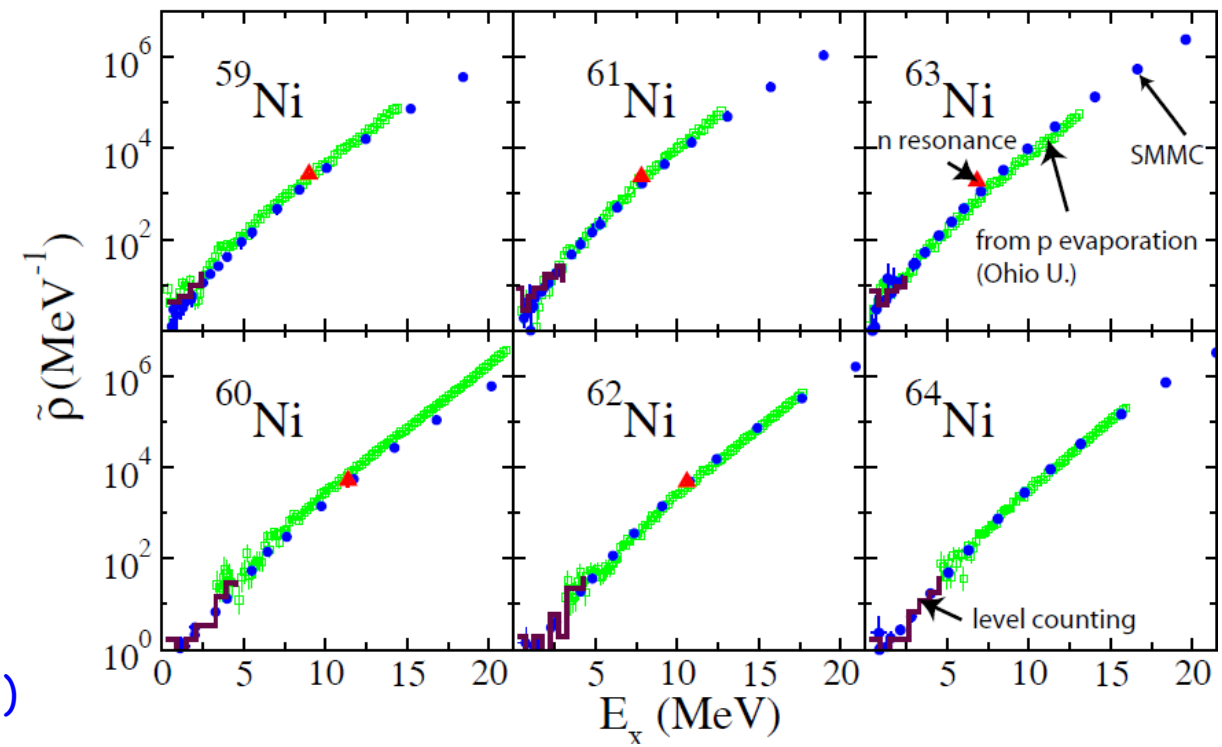
Single-particle Hamiltonian: from Woods-Saxon potential plus spin-orbit

Interaction: includes the *dominant* components of effective interactions

- pairing, g_0=-0.212 MeV determined from odd-even mass differences
- multipole-multipole interaction terms -- quadrupole, octupole, and hexadecupole, determined from a self-consistent condition and renormalized by k_2=2, k_3=1.5, k_4=1.

Level densities in nickel isotopes

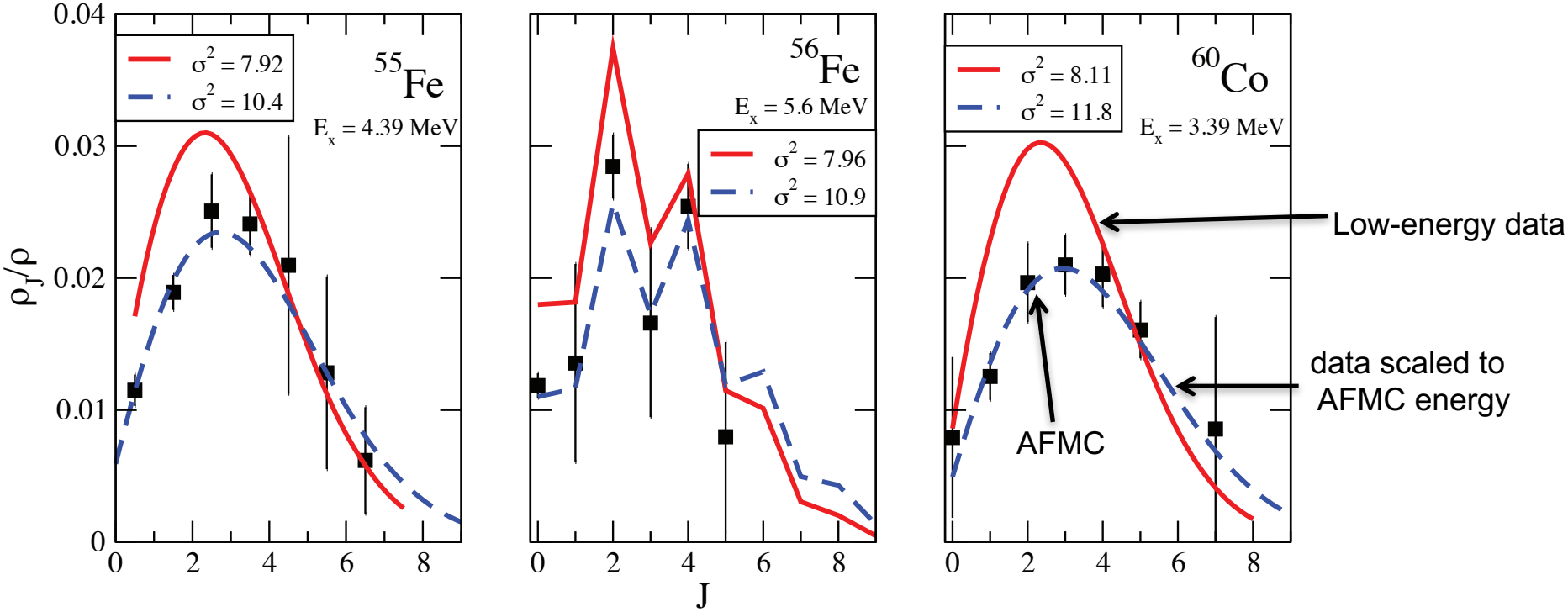
Excellent agreement with experiments:
(i) level counting,
(ii) p evaporation spectra (Ohio U., 2012),
(iii) neutron resonance data.



Bonett-Matiz, Mukherjee, Alhassid, PRC **88**, 011302 R (2013)

Spin distributions [Alhassid, Liu, Nakada, PRL**99**, 162504 (2007)]

- Use exact spin projection in AFMC



σ^2 = spin cutoff parameter

- Staggering effect (in spin) for even-even nuclei.

- Analysis of experimental data [von Egidy and Bucurescu, PRC **78**, 051301 R (2008)] confirmed our prediction.

Heavy nuclei (lanthanides)

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 (g_p,g_n) plus multipole-multipole interaction terms – quadrupole, octupole, and hexadecupole.

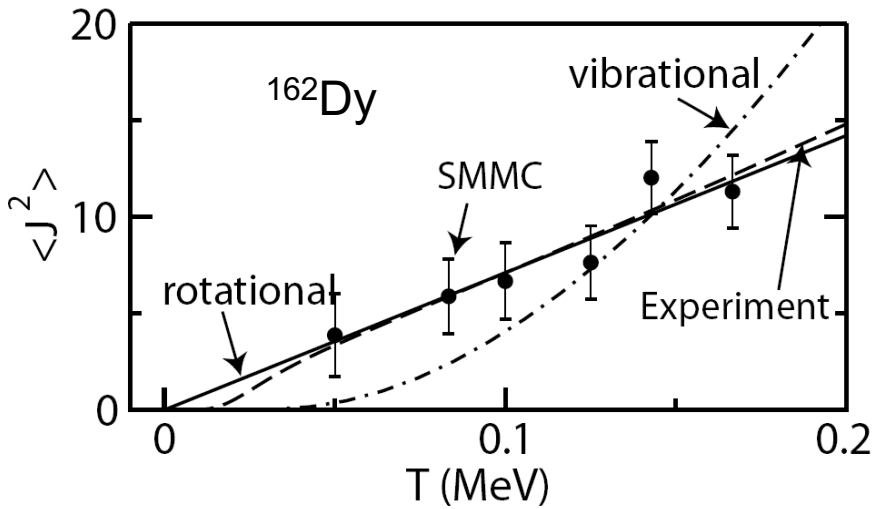
Heavy nuclei exhibit various types of collectivity (vibrational, rotational, …) that are well described by empirical models.

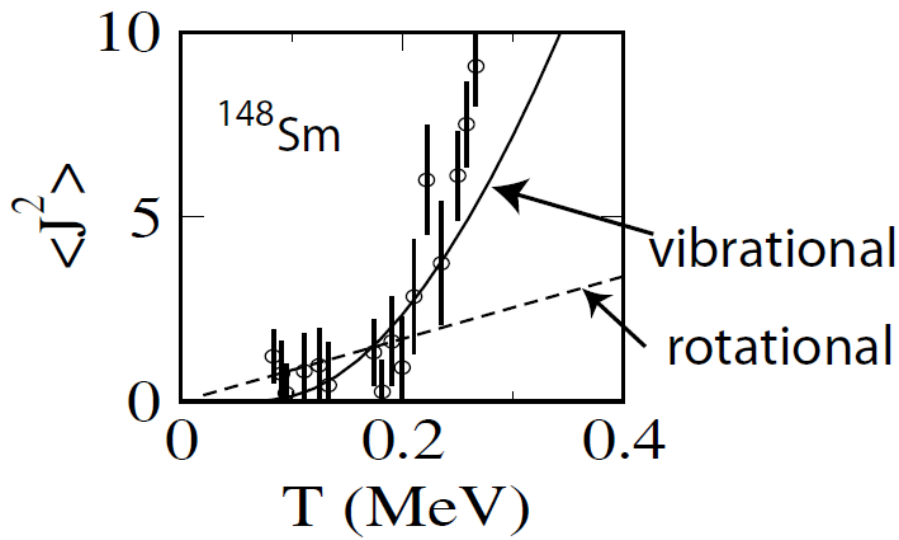
However, a microscopic description in a CI shell model has been lacking.

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

The various types of collectivity are usually identified by their corresponding spectra, but AFMC 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

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

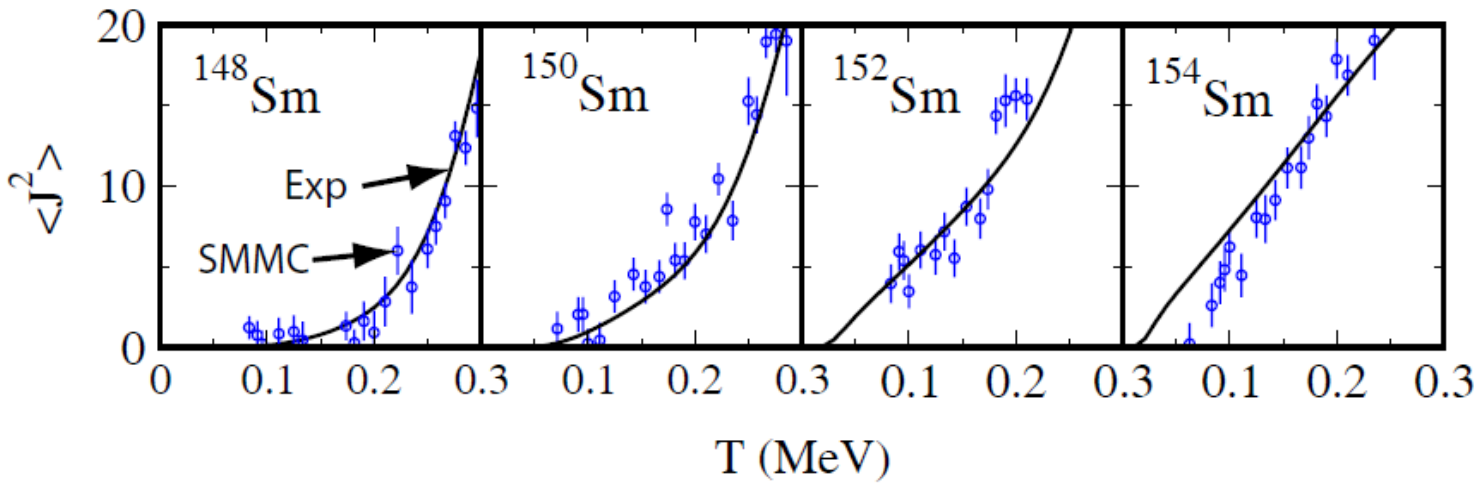
$$\langle \vec{J}^2 \rangle = 30 \frac{e^{-E_{2^+}/T}}{(1-e^{-E_{2^+}/T})^2}$$

$\Rightarrow$ ^{148}Sm is vibrational

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

Crossover from vibrational to rotational collectivity in heavy nuclei

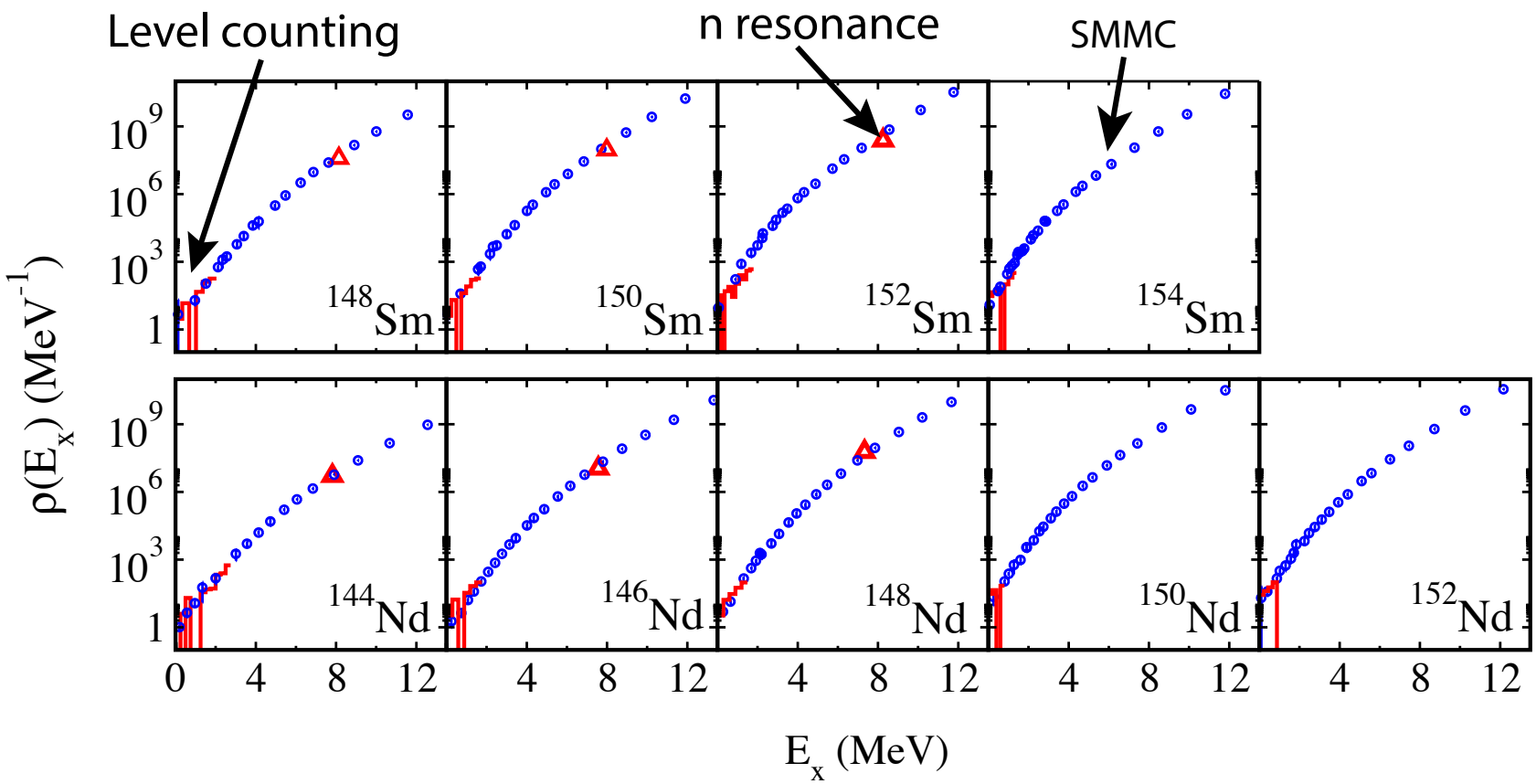
$\langle \vec{J}^2 \rangle$ versus T in samarium isotopes



- 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 samarium and neodymium isotopes



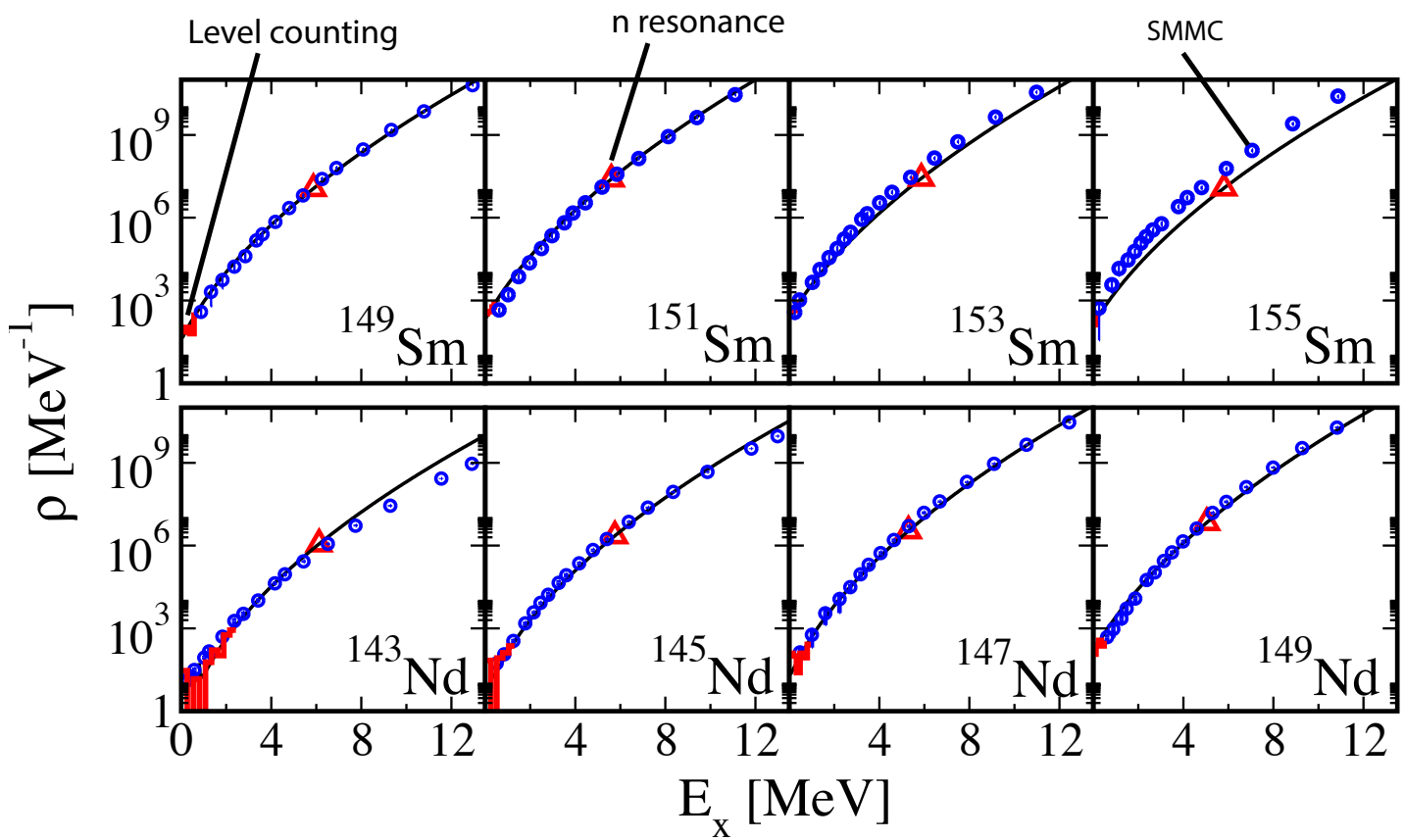
- Good agreement of AFMC densities with various experimental data sets (level counting, neutron resonance data when available).

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 $E_x(T)$



- Work in progress to determine E_0 without using experimental data.

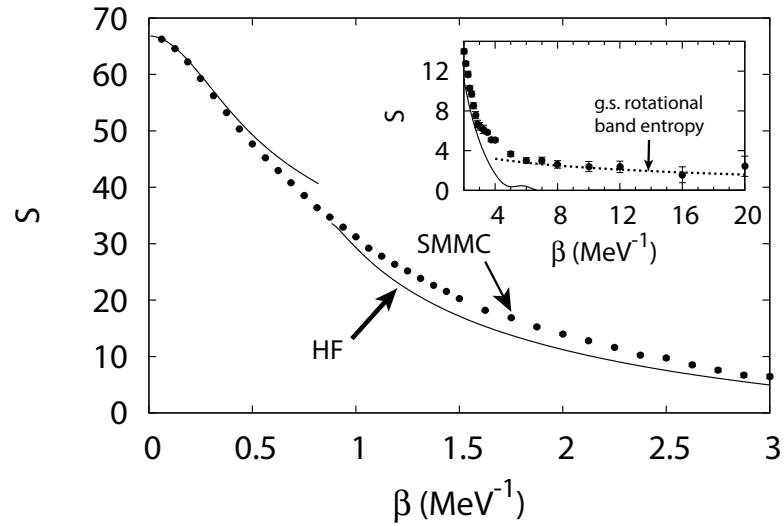
Rotational enhancement in deformed nuclei

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

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

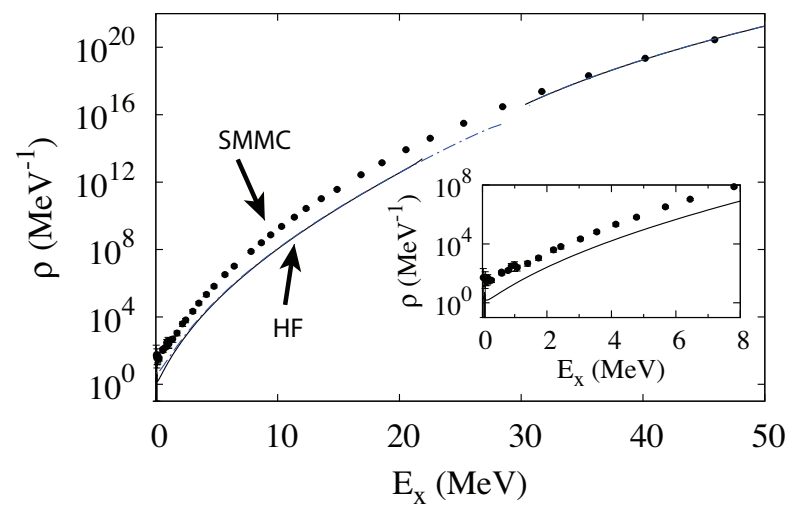
- Particle-number projection in HF is carried out in the saddle-point approximation

The HF entropy of ^{162}Dy goes to zero faster than the AFMC entropy (since it does not contain the contribution from rotational bands).

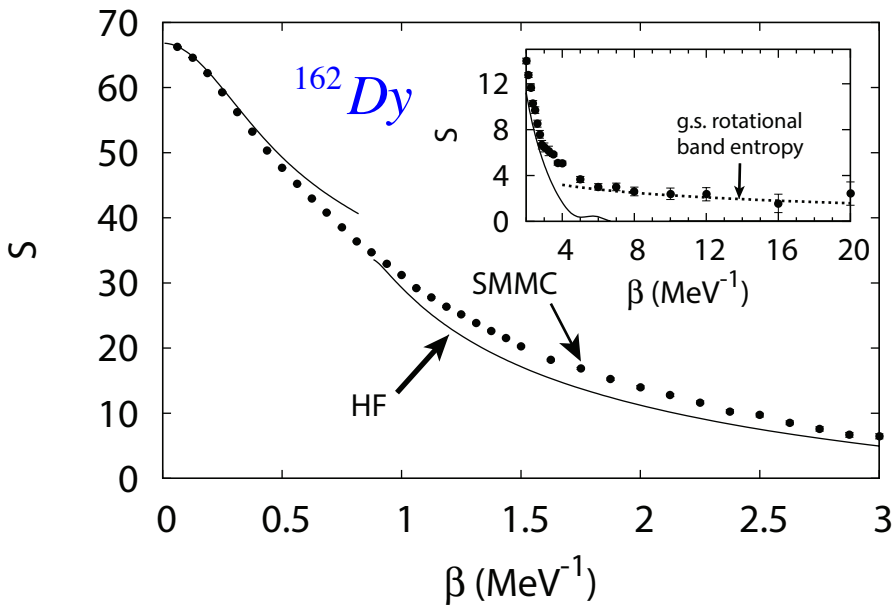


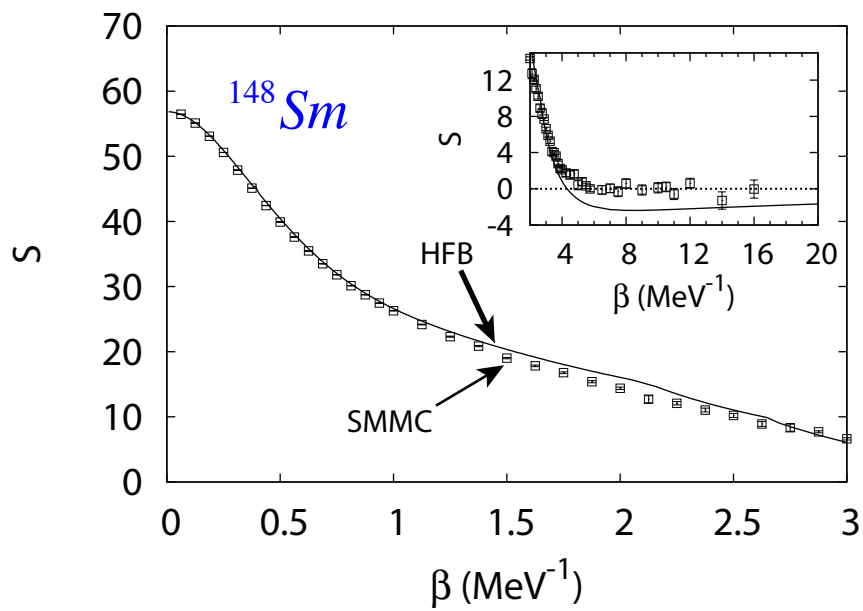
- The enhancement of the AFMC density (compared with HF) is due to rotational bands built on top of the intrinsic bandheads.

- The rotational enhancement gets damped above the shape transition.



Entropy versus β



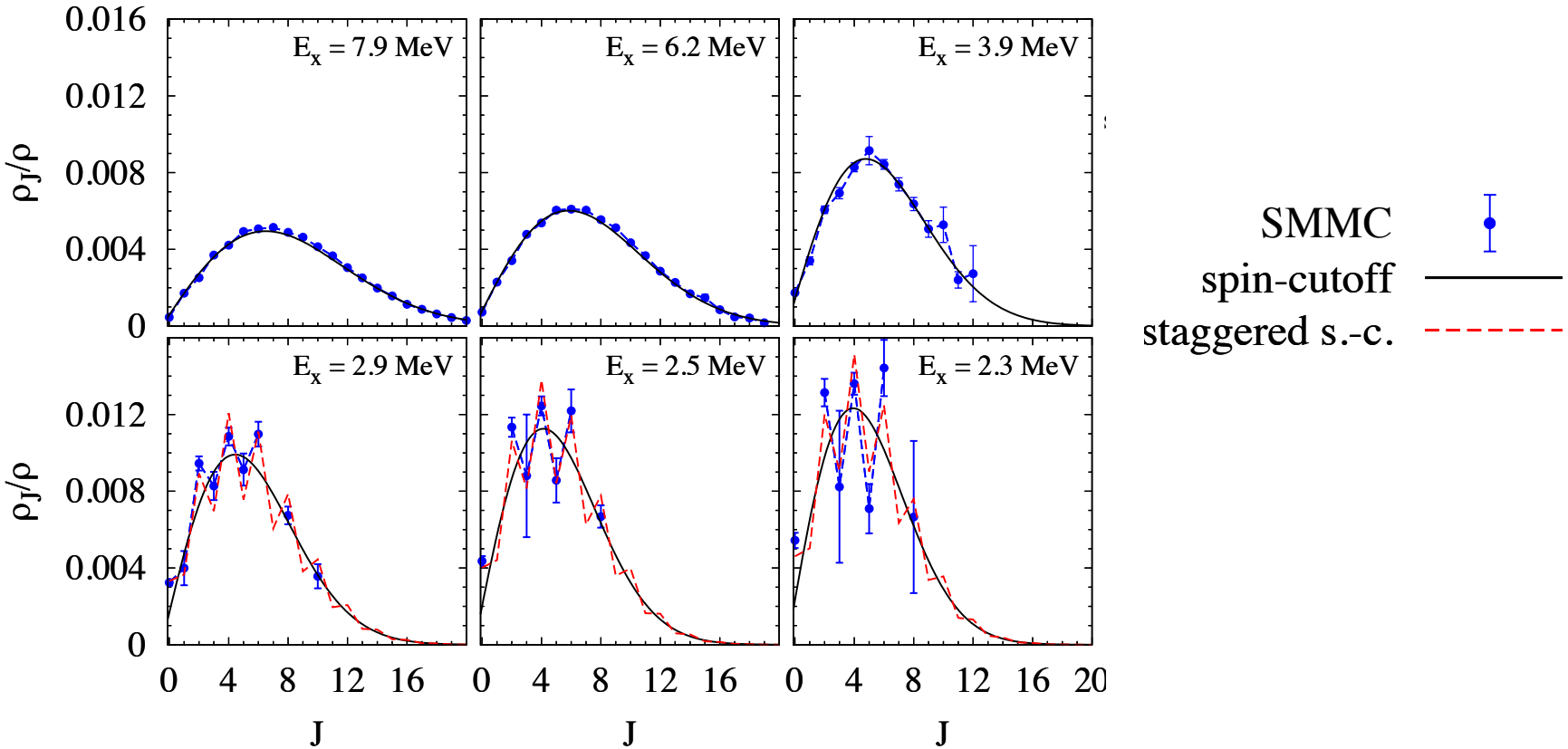


- The HF entropy of ^{162}Dy goes to zero faster than the SMMC entropy (since it does not contain the contribution from rotational bands).

- The HFB entropy of ^{148}Sm becomes negative at large β (saddle-point approximation is not good for particle-number projection).

Spin distributions of level densities in heavy nuclei: ^{162}Dy

Gilbreth, Alhassid, Bonett-Matiz



- Good agreement with spin-cutoff (s.-c.) model at higher excitations.

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

- Odd-even staggering in spin at low excitation energies.

AFMC distributions agree well with an empirical staggered spin cutoff formula based on low-energy counting data

Thermal moment of inertia I vs. excitation energy

I calculated from $\sigma^2 = IT/\hbar^2$

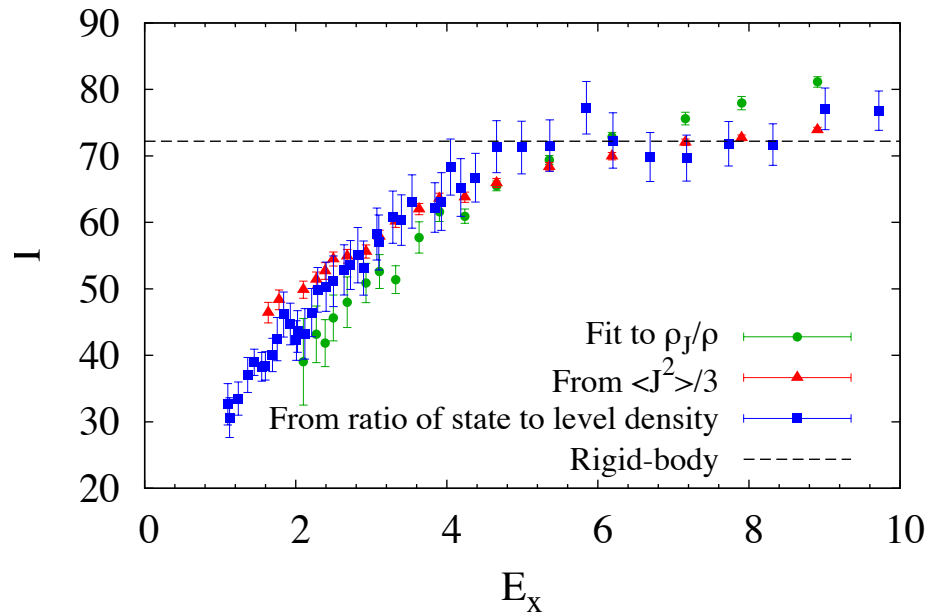
Three methods to determine σ^2

(ii) Fit to spin cutoff model

(ii) From $\sigma^2 = \langle J_z^2 \rangle = \langle \vec{J}^2 \rangle /3$

(iii) From ratio of level to state density

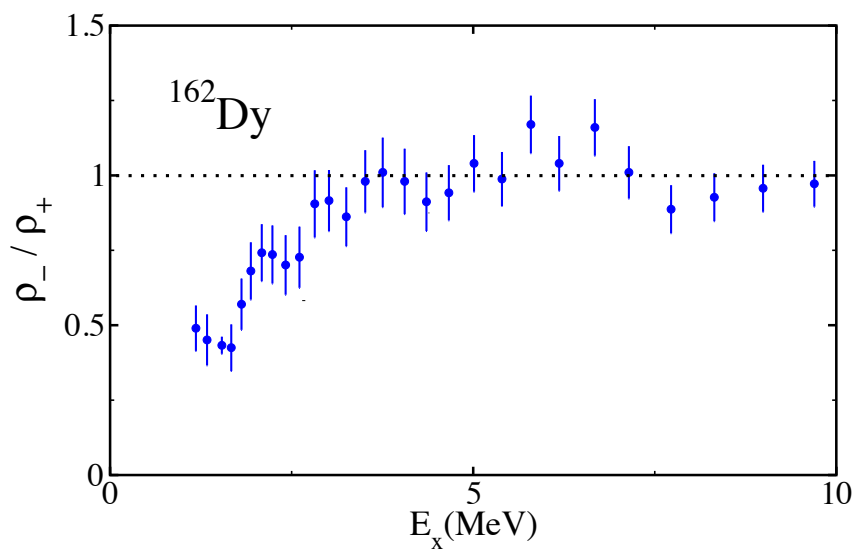
$$\Sigma_J \rho_J(E_x) = \rho_{M=0}(E_x) = \frac{1}{\sqrt{2\pi}\sigma}\rho(E_x)$$



- Moment of inertia I is suppressed by pairing correlations below E_x ~ 5 MeV

Parity ratio vs excitation energy

- Parity ratio is equilibrated at the neutron separation energy



Nuclear deformation in a spherical shell model approach

Alhassid, Gilbreth, Bertsch, PRL **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.

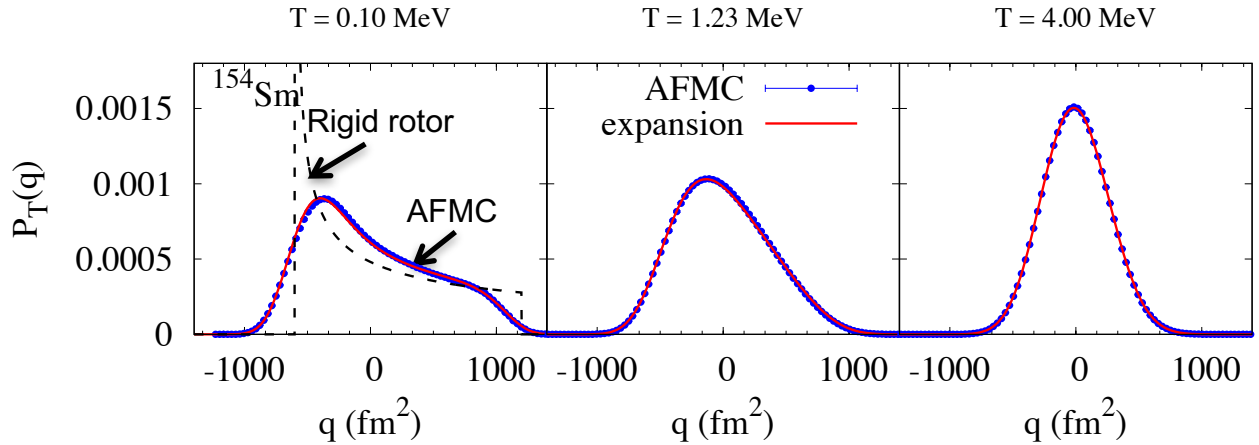
We calculated the distribution of the axial mass quadrupole in the lab frame using an exact projection on Q_{20} (novel in that $[Q_{20}, H] \neq 0$).

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

Application to heavy nuclei

^{154}Sm

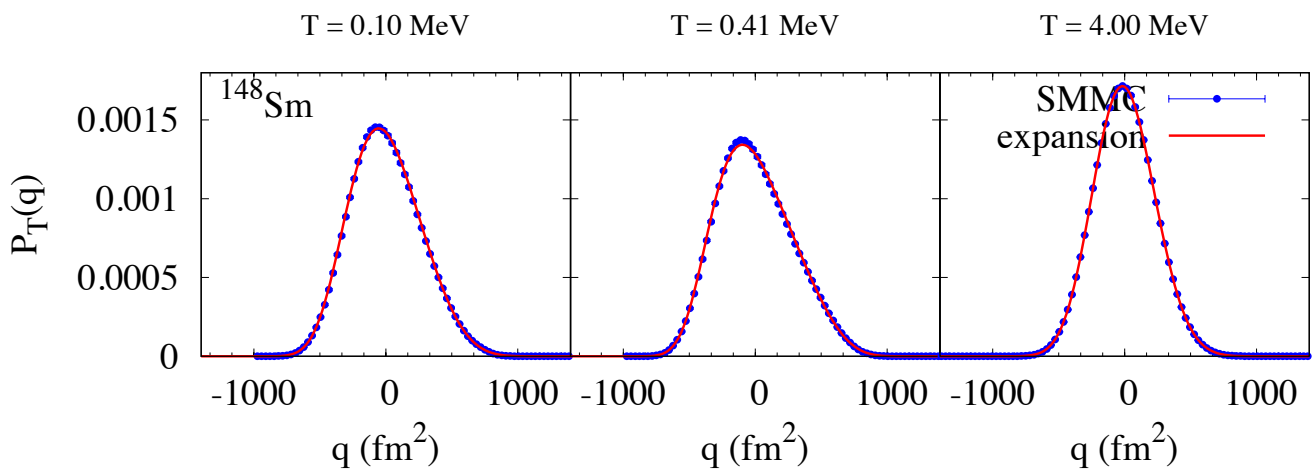
(deformed)



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

^{148}Sm

(spherical)



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

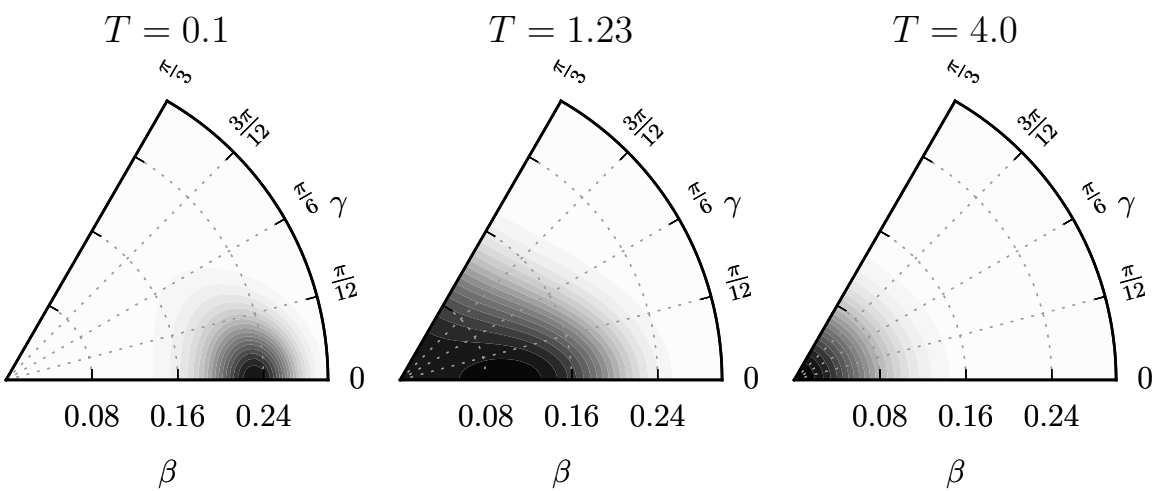
Intrinsic shape distributions $P_T(\beta,\gamma)$

Alhassid, Mustonen, Gilbreth, Bertsch

Information on intrinsic deformation β,γ can be obtained from the expectation values of rotationally invariant combinations of the quadrupole tensor $q_{2\mu}$.

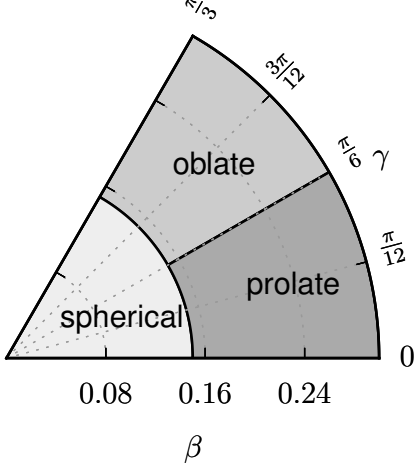
$\ln P_T(\beta,\gamma)$ at a given temperature T is an invariant and can be expanded in the quadrupole invariants $-\ln P_T = A\beta^2 - B\beta^3\cos 3\gamma + C\beta^4 + \ldots$

- 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 $q_{20} = q$



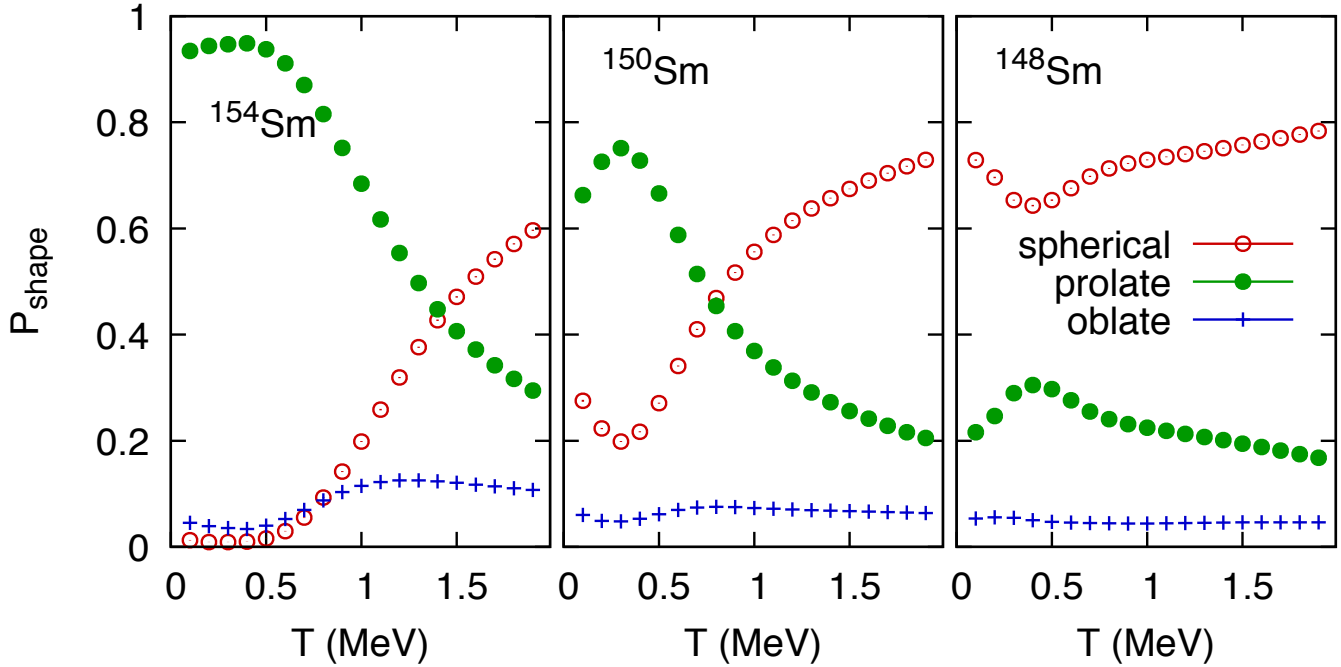
- Mimics a shape transition from a deformed to a spherical shape without using a mean-field approximation !

We divide the β,γ plane into three regions: spherical, prolate and oblate.



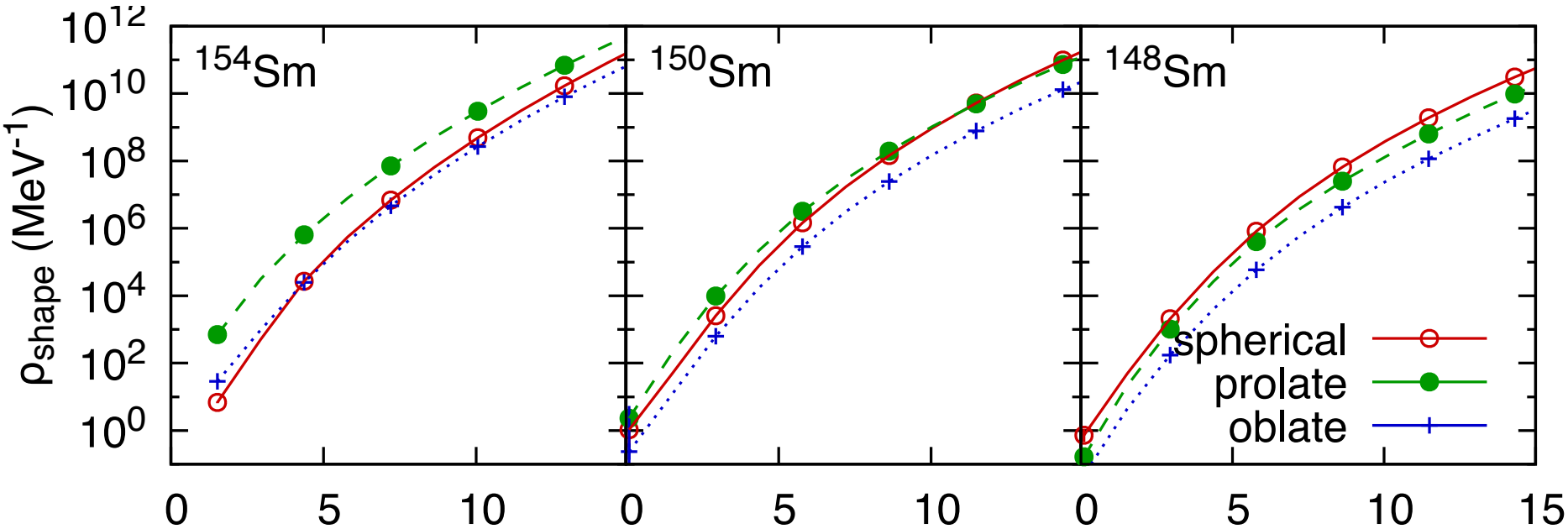
Integrate over each deformation region to determine the probability of shapes versus temperature

- Compare deformed (^{154}Sm), transitional (^{150}Sm) and spherical (^{148}Sm)nuclei



Level density versus intrinsic deformation

- Convert $P_T(\beta,\gamma)$ to level densities vs E_x, β,γ



Conclusion

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

• Microscopic description of rotational enhancement in deformed nuclei.

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

• Level density as a function of deformation in a rotationally invariant framework (CI shell model).

Outlook

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

• Gamma strength functions in AFMC by inversion of imaginary-time response functions.

• Derive *global* effective shell model interactions from density functional theory.