The deformation dependence of level densities in the configuration-interaction shell model

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- Statistical distributions of deformation in the intrinsic frame
  – without invoking a mean-field approximation!
- Level density vs. intrinsic deformation and excitation energy
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Recent review of AFMC: Y. Alhassid, in *Emergent Phenomena in Atomic Nuclei from Large-Scale Modeling*, ed. K.D. Launey (World Scientific 2017)

Introduction

Modeling of shape dynamics, e.g., fission, requires the knowledge of statistical nuclear properties (level density, …) as a function of deformation.

- Auxiliary-field Monte Carlo (AFMC) is a powerful method for the microscopic calculation of statistical nuclear properties in model spaces that are many orders of magnitude larger than those that can be treated by conventional methods ($\sim 10^{30}$ in heavy nuclei).

- However, statistical properties as a function of intrinsic deformation are not readily available due to the formulation of AFMC in the *spherical* configuration-interaction (CI) shell model approach.

- Theory of deformation up to now has relied on a mean-field approximation which breaks rotational invariance and can miss important correlations.

We have introduced a novel method to calculate exactly the statistical distributions of intrinsic deformation within the rotationally invariant framework of the CI shell model.

The auxiliary-field Monte Carlo (AFMC) method

Start from a CI shell model Hamiltonian H

Gibbs ensemble $e^{-H/T}$ at temperature T can be written as a superposition of ensembles U_σ of *non-interacting* nucleons moving in time-dependent fields $\sigma(\tau)$

$$e^{-H/T} = \int D[\sigma]\, G_\sigma U_\sigma$$

(Hubbard-Stratonovich transformation)

- The integrand reduces to matrix algebra in the single-particle space (of typical dimension ~ 100).
- The high-dimensional σ integration is evaluated by Monte Carlo methods.

Heavy nuclei (lanthanides) in AFMC

CI shell model space:

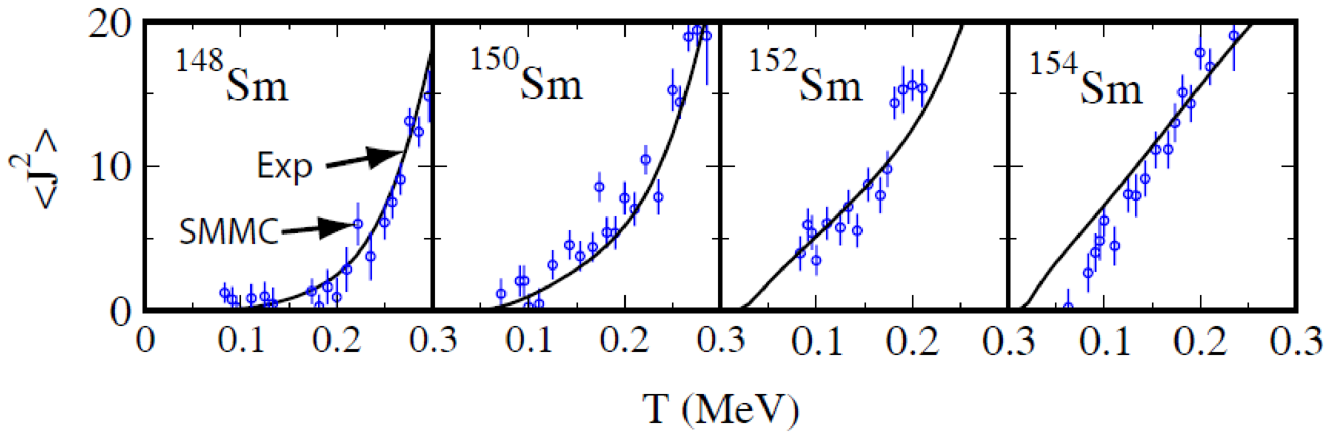
protons: 50-82 shell plus $1f_{7/2}$; neutrons: 82-126 shell plus $0h_{11/2}$ and $1g_{9/2}$

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

Interaction: pairing plus multipole-multipole interaction terms – quadrupole, octupole, and hexadecupole (dominant components of effective interactions)

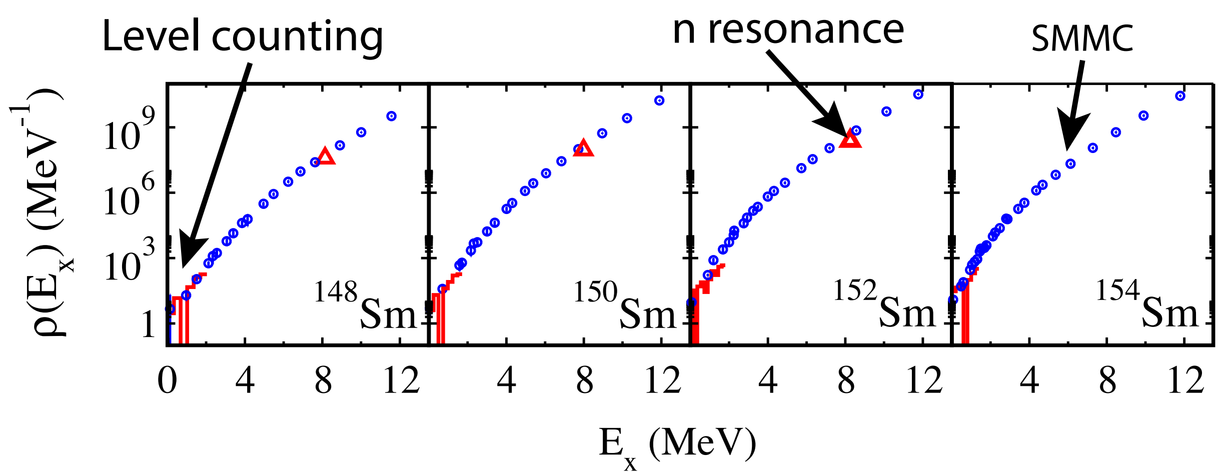
AFMC describes well the crossover from vibrational to rotational collectivity in the framework of the spherical CI shell model.

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)

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



Statistical distributions of deformation in the laboratory frame

Alhassid, Gilbreth, Bertsch, PRL **113**, 262503 (2014)

The challenge is to study nuclear deformation in a framework that preserves rotational invariance (e.g., in the CI shell model) without invoking a mean-field approximation.

The distribution of the axial mass quadrupole Q_{20} in the lab-frame is

$$P(q) = \sum_n \delta(q - q_n) \sum_m \langle q_n | e_m \rangle^2 e^{-e_m/T}$$

where $|q_n\rangle$ are the eigenstates of Q_{20} and $|e_m\rangle$ are the energy eigenstates.

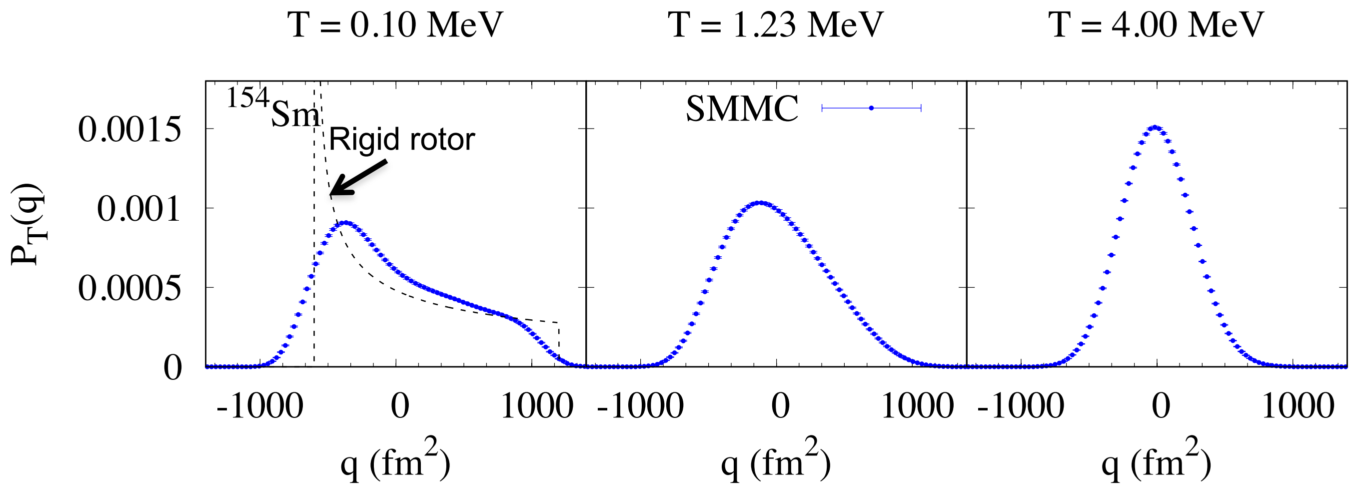
We calculated $P(q)$ using an exact projection on Q_{20}

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

Application to heavy nuclei

^{154}Sm

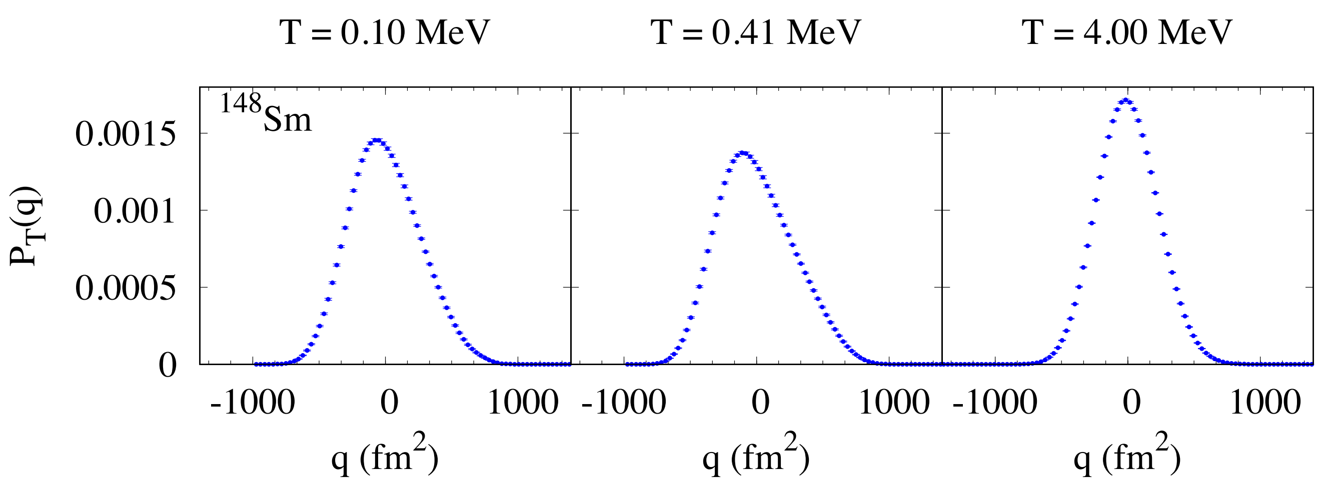
(deformed)



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

^{148}Sm

(spherical)



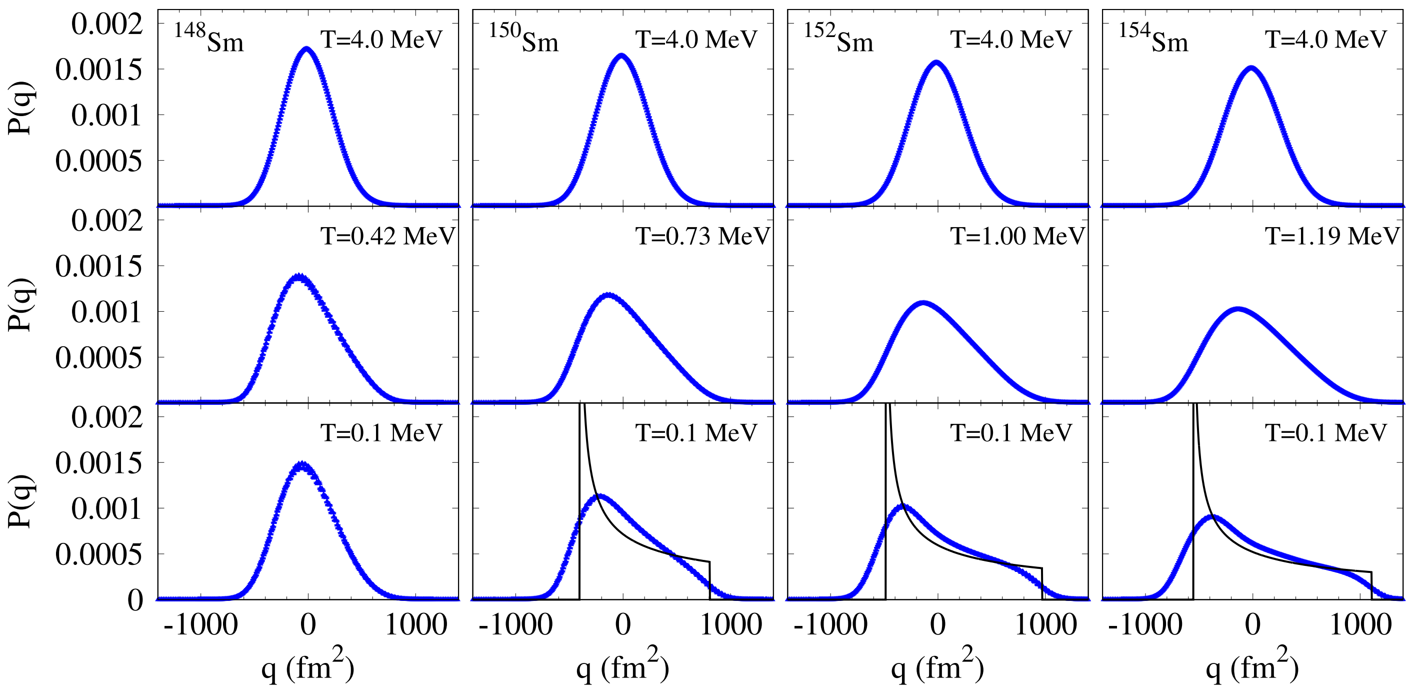
- The distribution is close to a Gaussian even at low temperatures.

Model-independent signatures of quantum and thermal shape transitions

Gilbreth, Alhassid and Bertsch, PRC **97**, 014315 (2018)

Quadrupole shape distributions $P(q_{20})$ in a family of samarium isotopes vs. neutron number N and temperature T

^{148}Sm ^{150}Sm ^{152}Sm ^{154}Sm



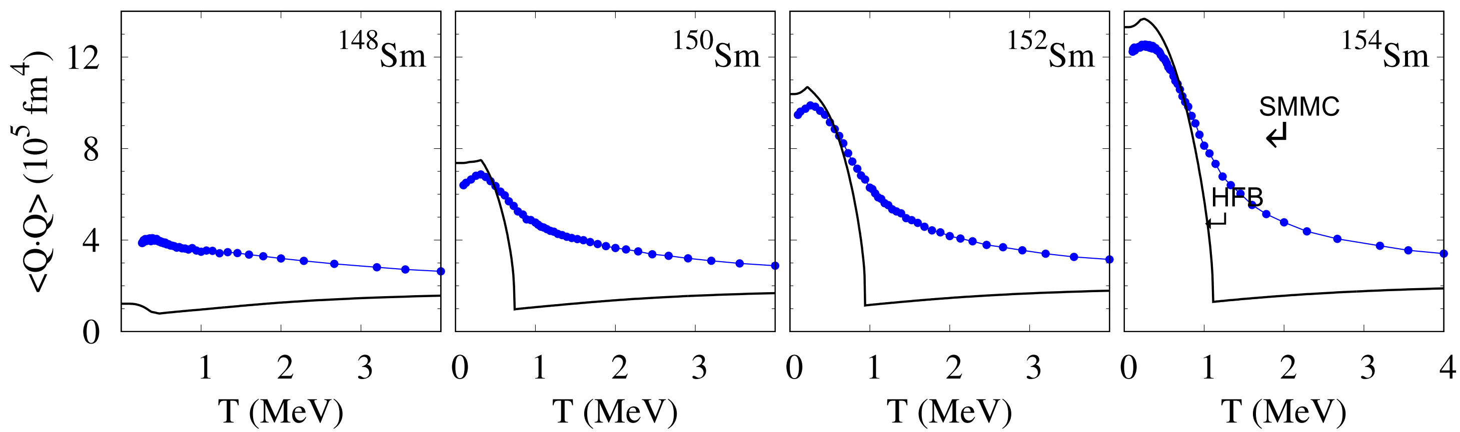
↑ Thermal shape transition vs. temperature (or excitation energy)

T

N ⟶

Quantum shape transition (at T=0) vs. neutron number

$\langle Q \cdot Q \rangle$ as a function of temperature T for the family of samarium isotopes: AFMC vs. mean-field theory [Hartree-Fock-Bogoliubov (HFB)]



- The sharp kink characterizing the HFB shape transition is washed out as is expected in a finite-size system.
- A signature of this phase transition remains in the rapid decrease of $\langle Q \cdot Q \rangle$ with temperature.
- In AFMC deformation effects survive well above the transition temperature: $\langle Q \cdot Q \rangle$ continues to be enhanced above its mean-field value.

Statistical distributions of deformation in the intrinsic frame

Mustonen, Gilbreth, Alhassid, Bertsch, arXiv:1804.161

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

3 invariants to 4th order: $q\cdot q \propto \beta^2$; $(q\times q)\cdot q \propto \beta^3\cos(3\gamma)$; $(q\cdot q)^2 \propto \beta^4$

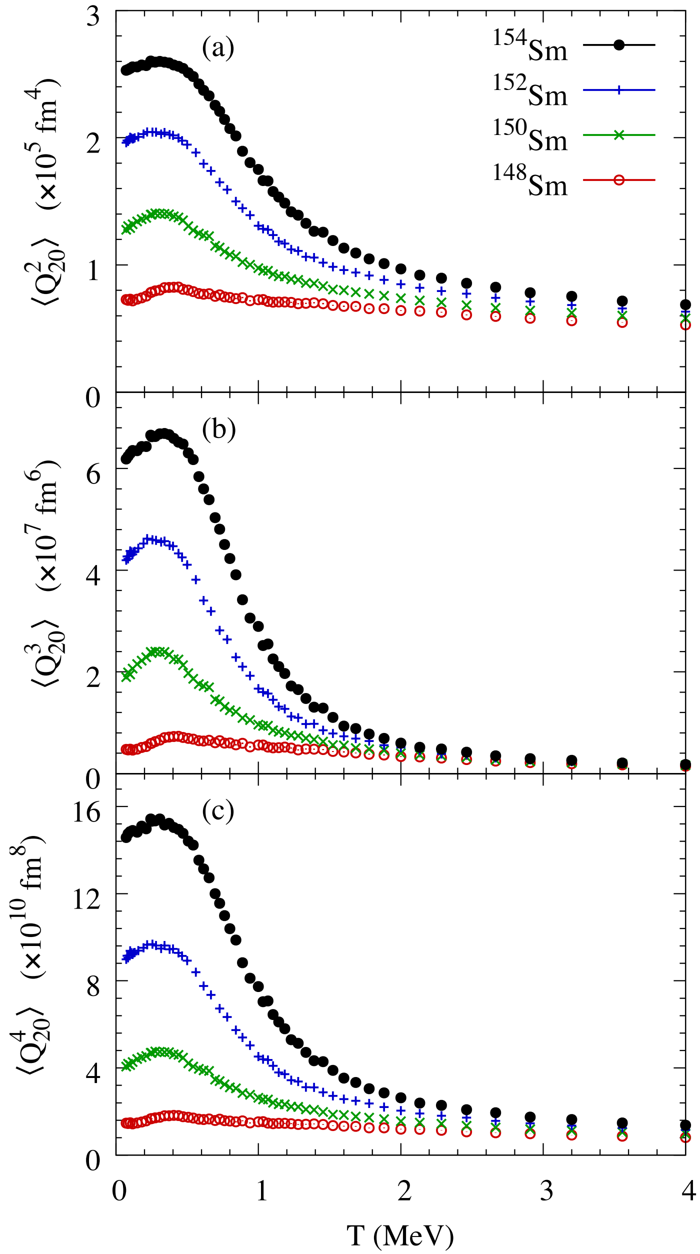
$\ln P(T,\beta,\gamma)$ at a given temperature T is an *invariant* and can be expanded in the quadrupole invariants [a Landau-like expansion: used for the free energy to describe shape transitions in Alhassid, Levit, Zingman, PRL **57**, 539 (1986)]

$$-\ln P(T,\beta,\gamma) = const. + a(T)\beta^2 + b(T)\beta^3\cos 3\gamma + c(T)\beta^4 + \ldots$$

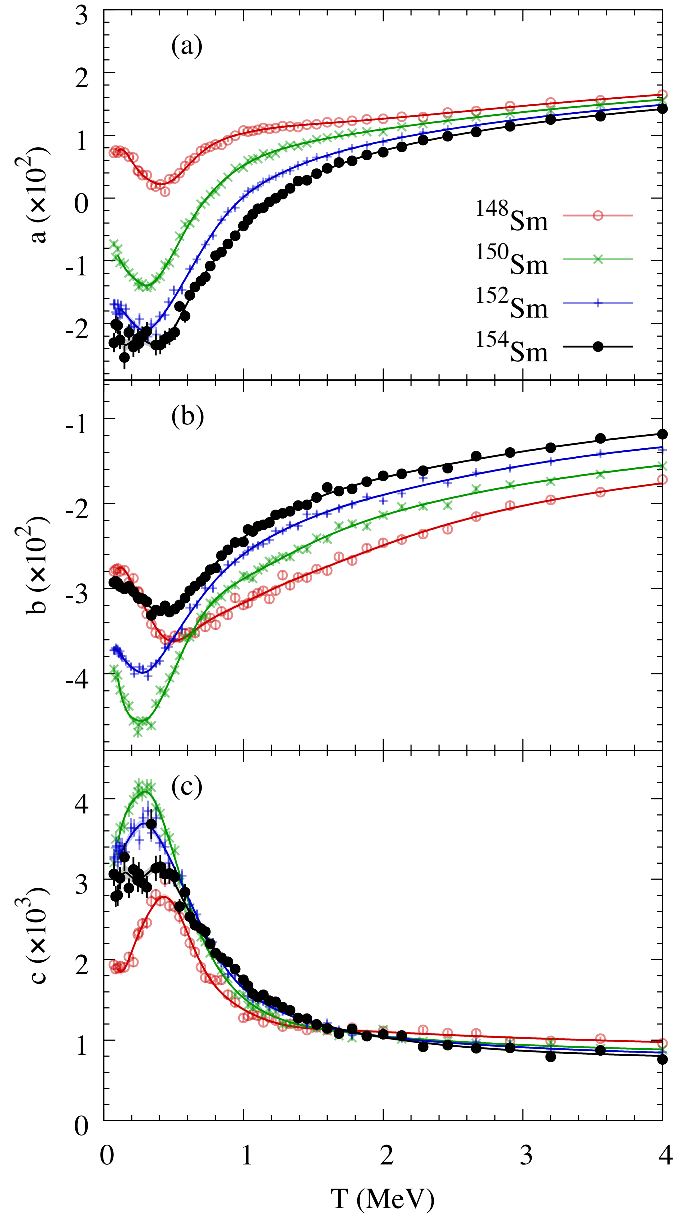
- The expansion coefficients a,b,c… can be determined from the expectation values of the invariants, which in turn can be calculated from the low-order moments of $q_{20}=q$ in the lab frame.

$$< q\cdot q >= 5 < q_{20}^2 >; \quad <(q\times q)\cdot q >= -5\sqrt{\frac{7}{2}} < q_{20}^3 >; \quad <(q\cdot q)^2 >= \frac{35}{3} < q_{20}^4 >$$

Moments $\langle Q_{20}^n \rangle$ $(n=2,3,4)$



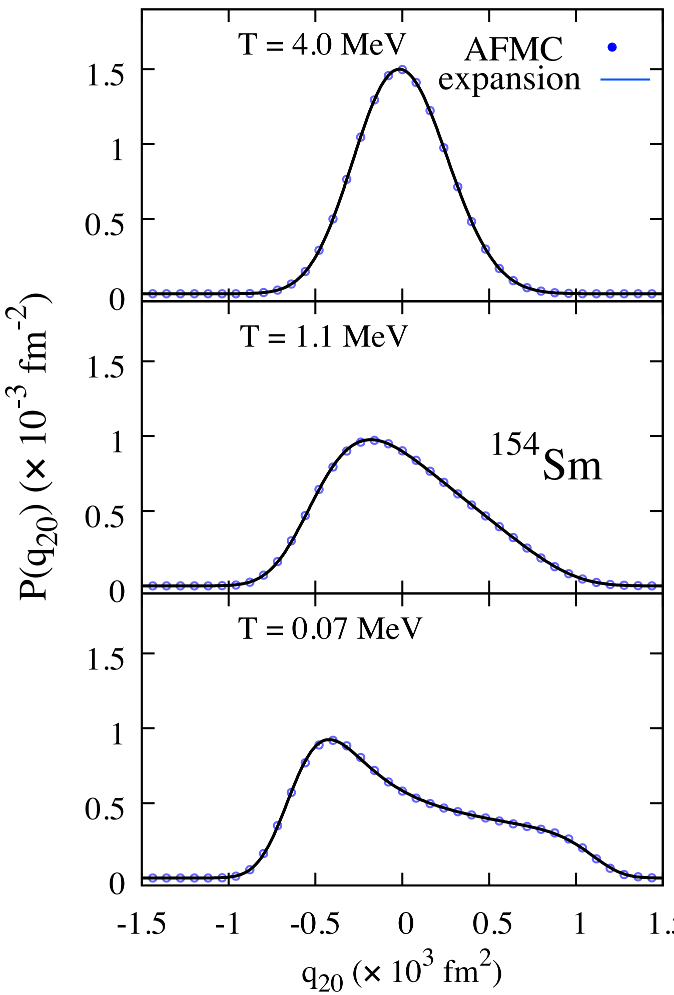
Expansion parametes a, b, c



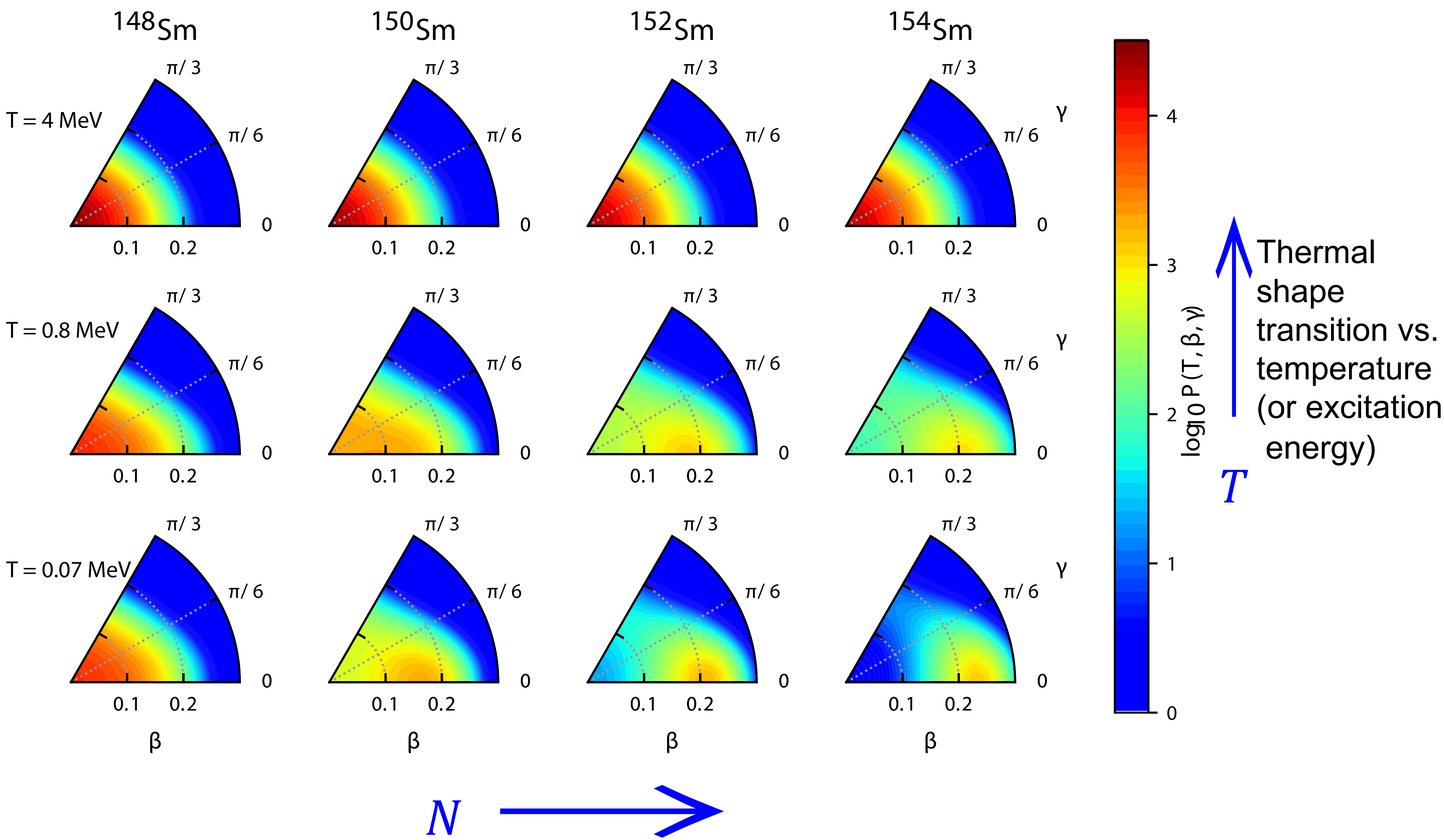
Validation of the Landau-like expansion

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 of this Marginal distribution with $P(q_{20})$ calculated in AFMC !

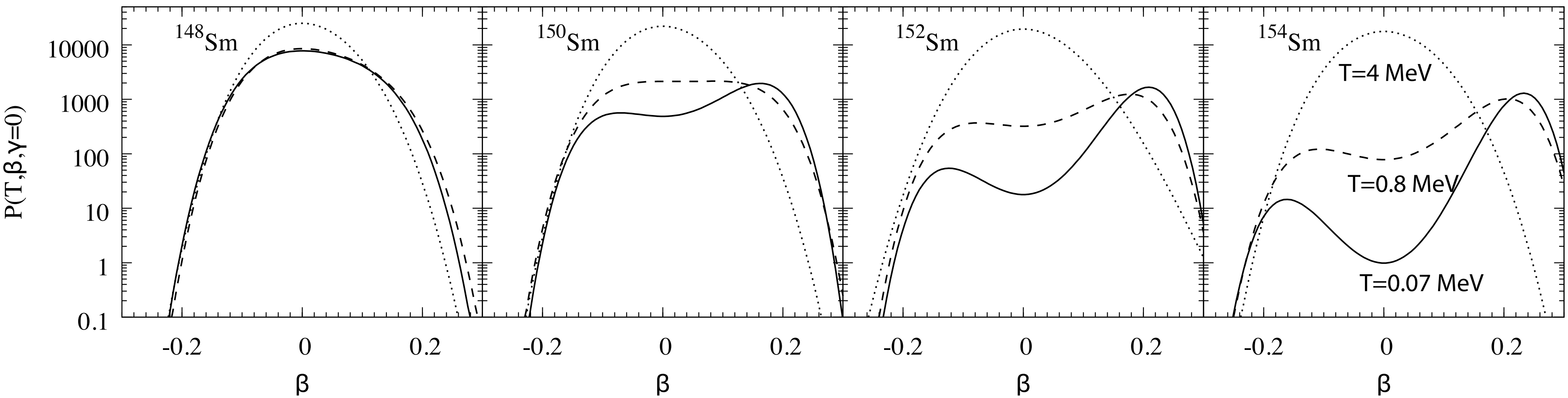


Exact Shape distributions in the intrinsic β,γ variables (no mean field!)

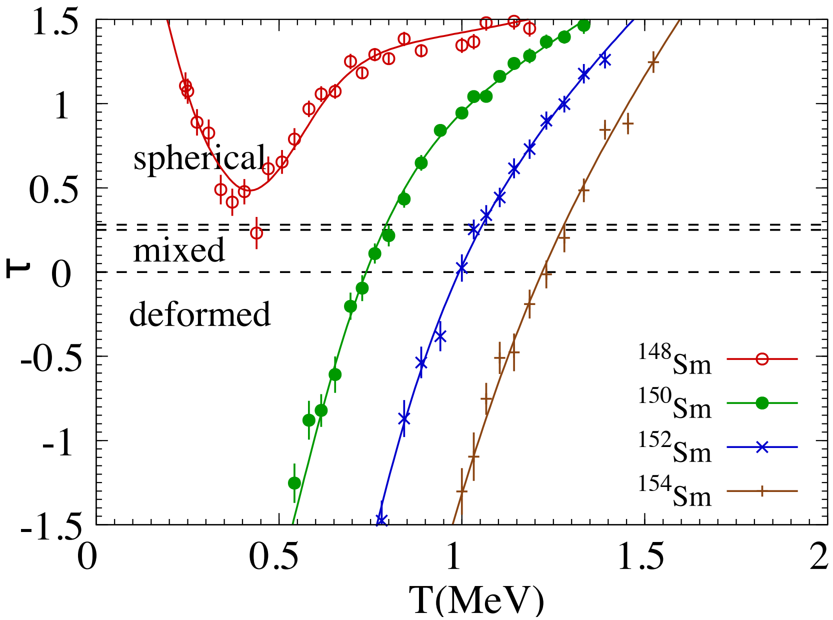


Quantum shape transition (at T=0) vs. neutron number

Axial shape distributions $P(T,\beta,\gamma=0)$

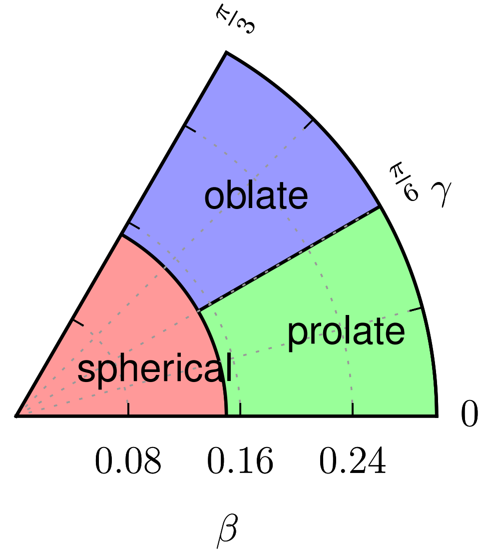


The topography of the Landau expansion distributions is completely determined by the dimensionless parameter $\tau = ac/b^2$



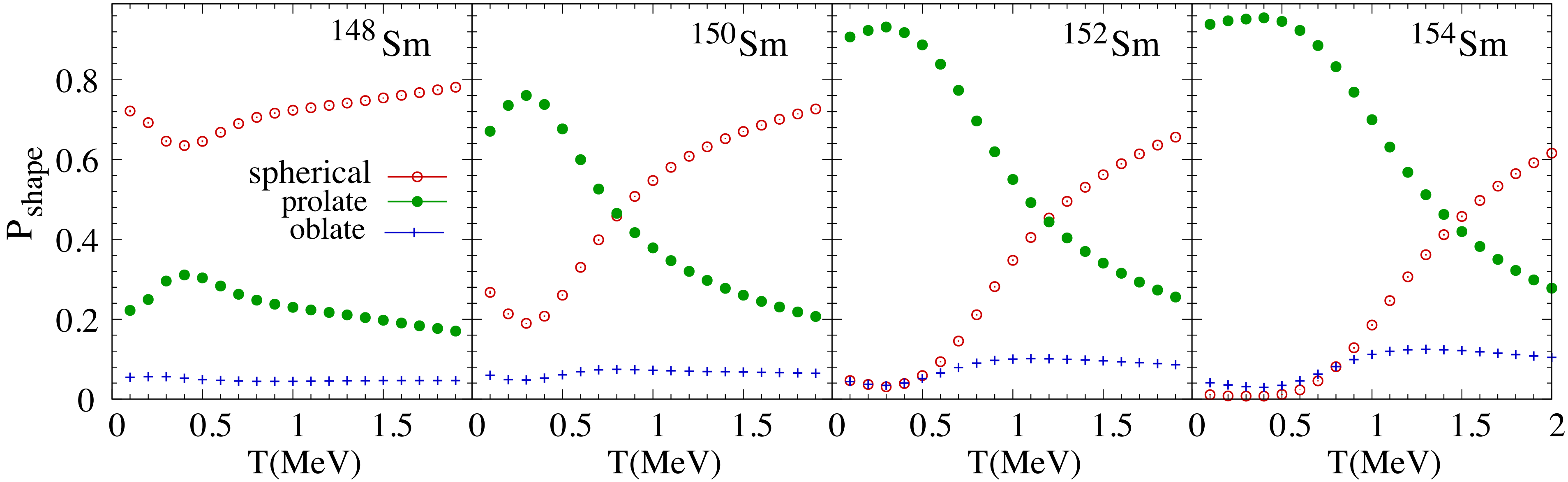
We divide the β,γ plane into three regions: spherical, prolate and oblate.

Integrate over each deformation region to determine the probability of shapes using the appropriate metric



$$\prod_\mu dq_{2\mu} \propto \beta^4 |\sin(3\gamma)| d\beta d\gamma$$

- Compare deformed (^{154}Sm, ^{152}Sm), transitional (^{150}Sm) and spherical (^{148}Sm) nuclei



Level density versus intrinsic deformation

The shape-dependent partition $Z(T,\beta,\gamma)$ is calculated from

$$P(T,\beta,\gamma) = Z(T,\beta,\gamma) / Z(T)$$

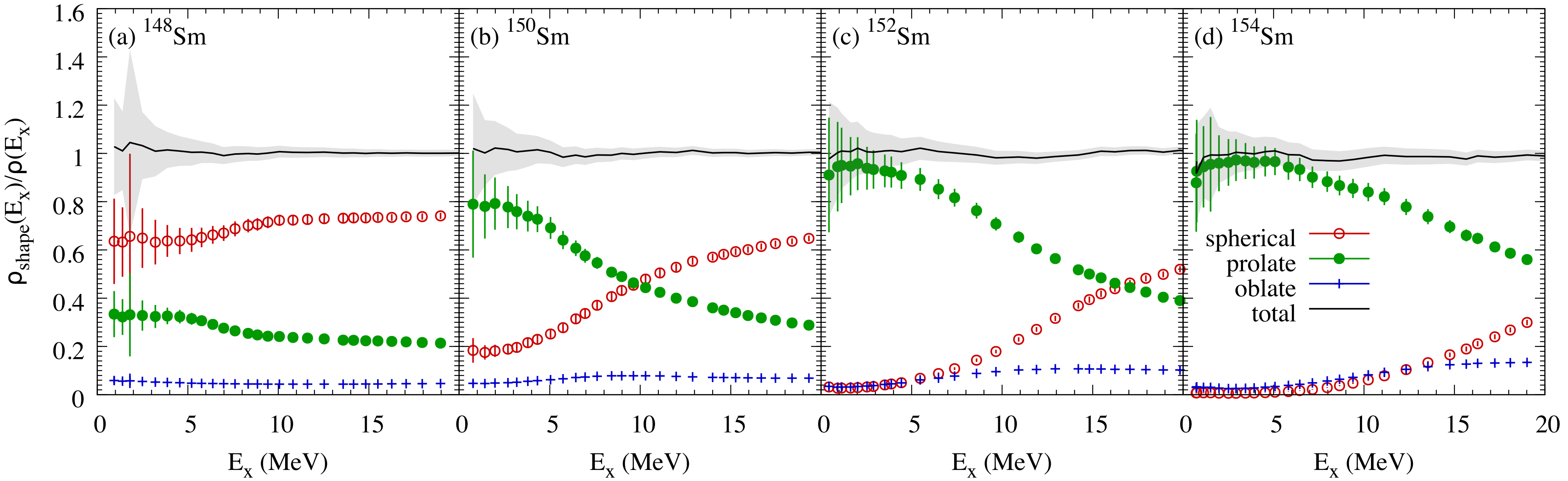
The average level density $\rho(E,\beta,\gamma)$ at energy E and intrinsic deformation β,γ is determined from $Z(T,\beta,\gamma)$ in the saddle-point approximation

$$\rho\left(E,\beta,\gamma\right) \approx \frac{1}{\sqrt{2\pi T^2 C(T,\beta,\gamma)}} e^{S\left(T\beta,\gamma\right)}$$

$S(T,\beta,\gamma) = \ln Z(T,\beta,\gamma) + E / T$ is the canonical entropy

$C(T,\beta,\gamma) = T \partial S(T,\beta,\gamma) / \partial T$ is the canonical heat capacity

Fraction of the level density in each shape region $\rho_{shape}(E_x)/\rho(E_x)$ versus excitation energy



In well-deformed nuclei, the contributions from prolate shapes dominate the level density below the shape transition energy.

In spherical nuclei, both spherical and prolate shapes make significant contributions.

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.

- The mass quadrupole distribution in the laboratory frame is a *model - independent* signature of deformation.

- Quadrupole distributions in the intrinsic frame can be determined in a rotationally invariant framework (the CI shell model) using a Landau-like expansion *without* invoking a mean-field approximation.

- Deformation-dependent level densities can now be calculated in AFMC.

Outlook

- Applications to shape dynamics within a spherical shell model approach

- Extend AFMC to actinides (applications to fission)

- Method can be applied within any nuclear model that preserves rotational symmetry (e.g., the conventional CI shell model)

Outlook (continued)

In broader terms, we have introduced a method to calculate statistical properties of a finite-size many-body system that undergoes a symmetry-breaking phase transition in the thermodynamic limit.

The challenge is to calculate the distribution of the order parameters of the transition in a framework that preserves the exact symmetry and without invoking a mean-field approximation.

Key ingredients:

- Construction of the marginal distribution of one or more components of the order parameters by using a projection.
- Determination of the expectation values of low-order polynomial combinations of the order parameters that preserve the symmetry.
- Expansion of the logarithm of the distribution of the order parameters in the above invariants.