Nuclear deformation in the laboratory and intrinsic frames

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- Introduction

- Shell model Monte Carlo (SMMC) method: heavy nuclei

- Nuclear deformation in the spherical shell model: quadrupole distributions in the laboratory frame

- Model-independent signatures of quantum and thermal shape transitions

- Quadrupole distributions and level densities vs. intrinsic deformation in the shell model - without using a mean-field approximation!

- Conclusion and outlook

Recent review of SMMC: Y. Alhassid, arXiv:1607.01870, in a book edited by K.D. Launey (2017)

Introduction

Most microscopic treatments of heavy nuclei are based on mean-field methods, e.g., density function theory.

However, important correlations can be missed.

The configuration-interaction (CI) 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 heavy nuclei.

- Conventional diagonalization methods for the shell model are limited to spaces of dimensionality $\sim 10^{11}$.

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

The shell model Monte Carlo (SMMC) 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 $\sigma(\tau)$

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

(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 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 (dominant components of effective interactions)
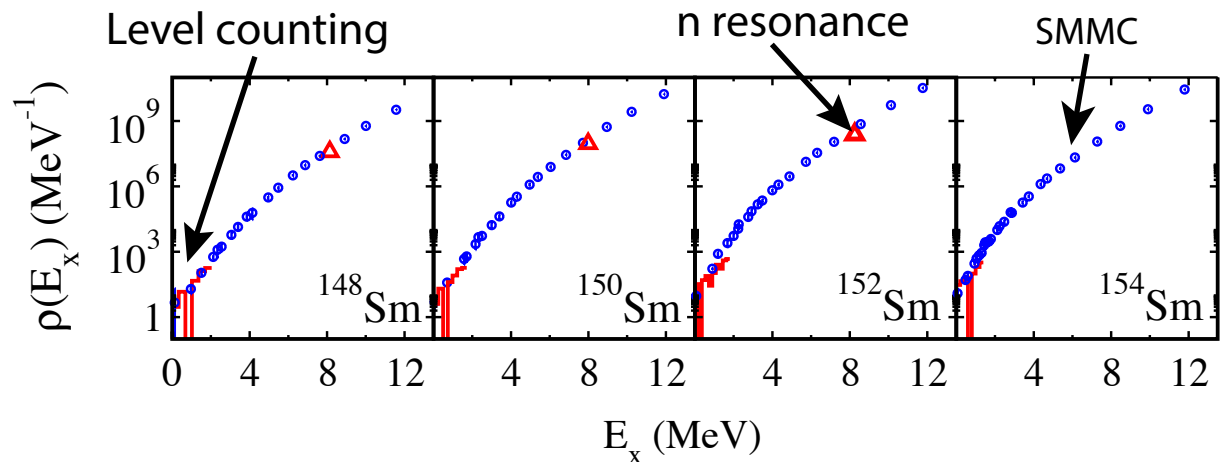
SMMC describes well the crossover from vibrational to rotational collectivity in the framework of the spherical CI shell model.

The dependence of $\langle \vec{J}^2 \rangle$ on temperature T is sensitive to the type of collectivity
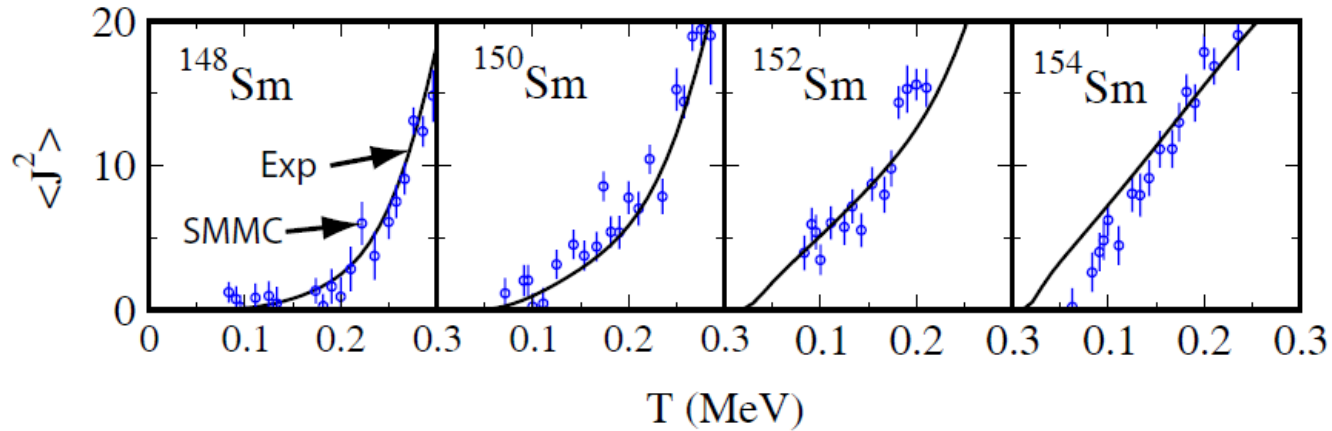
Ozen, Alhassid, Nakada, PRL **110,** 042502 (2013)

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

Nuclear deformation in the spherical shell model: quadrupole distributions in the laboratory frame

Modeling of shape dynamics, e.g., 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.
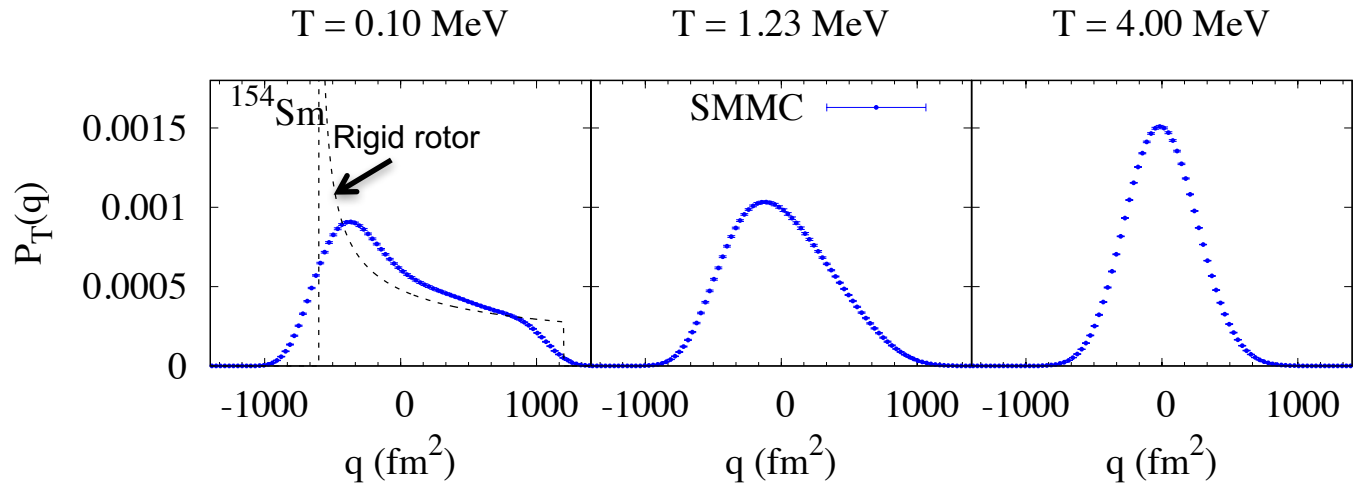
The challenge is to study nuclear deformation in a framework that preserves rotational invariance (e.g., in the CI shell model) without resorting to mean-field approximations.

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

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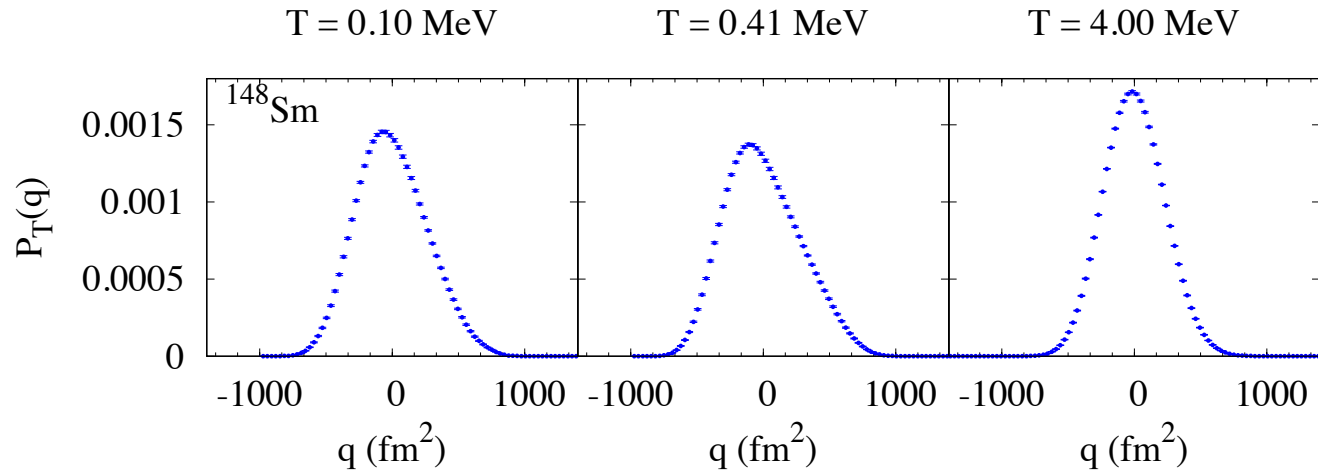
Application to heavy nuclei

T = 0.10 MeV   T = 1.23 MeV   T = 4.00 MeV

^{154}Sm

(deformed)

^{154}Sm   Rigid rotor   SMMC

$P_T(q)$

0.0015

0.001

0.0005

0

-1000   0   1000   -1000   0   1000   -1000   0   1000

$q\ (fm^2)$ $q\ (fm^2)$ $q\ (fm^2)$

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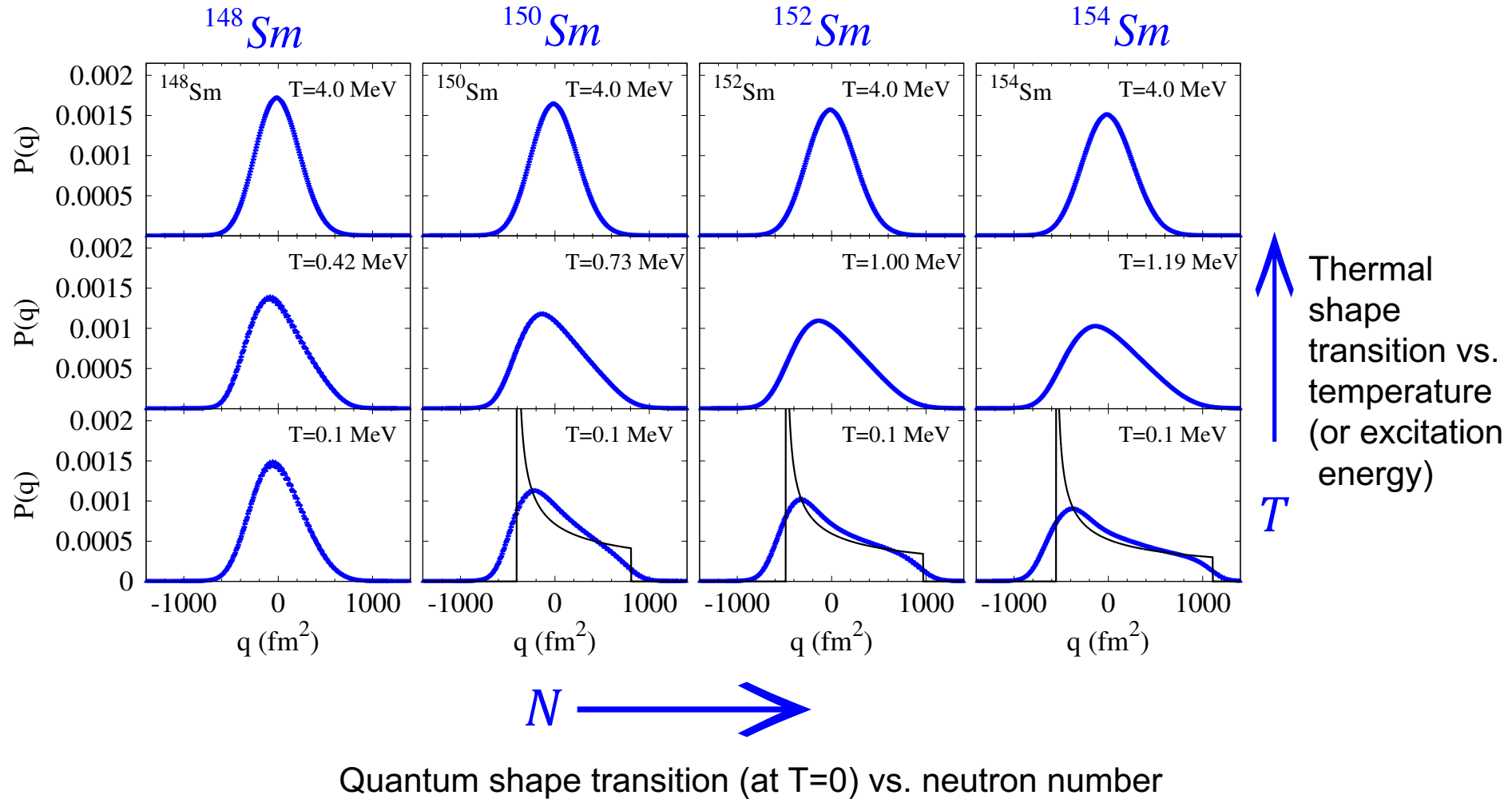 $\Rightarrow$ a model-independent signature of deformation.

T = 0.10 MeV   T = 0.41 MeV   T = 4.00 MeV

^{148}Sm

(spherical)

^{148}Sm

$P_T(q)$

0.0015

0.001

0.0005

0

-1000   0   1000   -1000   0   1000   -1000   0   1000

$q\ (fm^2)$ $q\ (fm^2)$ $q\ (fm^2)$

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

Model-independent signatures of quantum and thermal shape transitions

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

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

Thermal shape transition vs. temperature (or excitation energy)

T

$N \longrightarrow$

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

Quadrupole distributions $P_T(\beta,\gamma)$ vs. intrinsic deformation

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 $q_{2\mu}$.

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)]

$$-\ln P_T = a\beta^2 + b\beta^3 \cos 3\gamma + c\beta^4 + ...$$

- 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.

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

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.
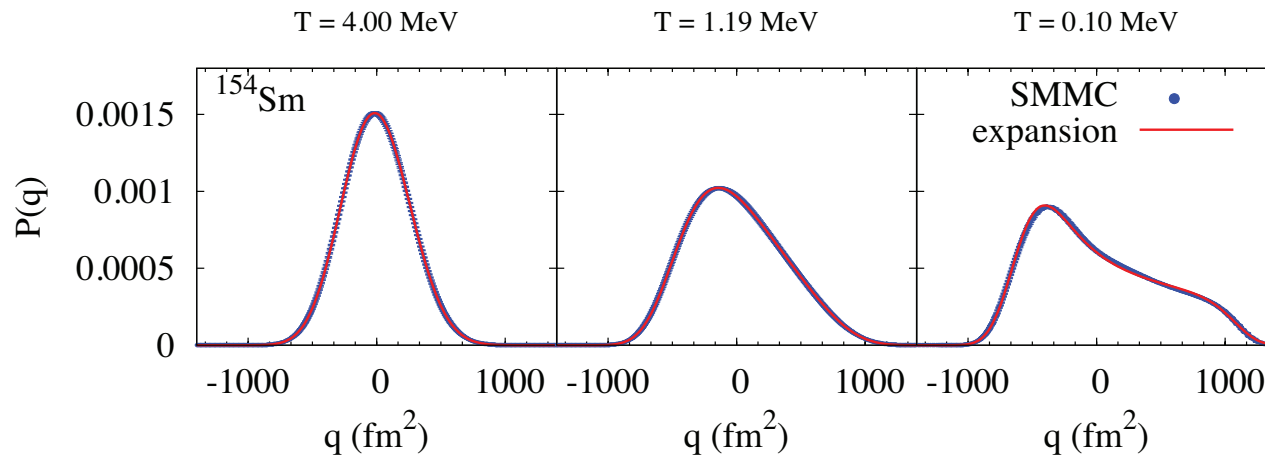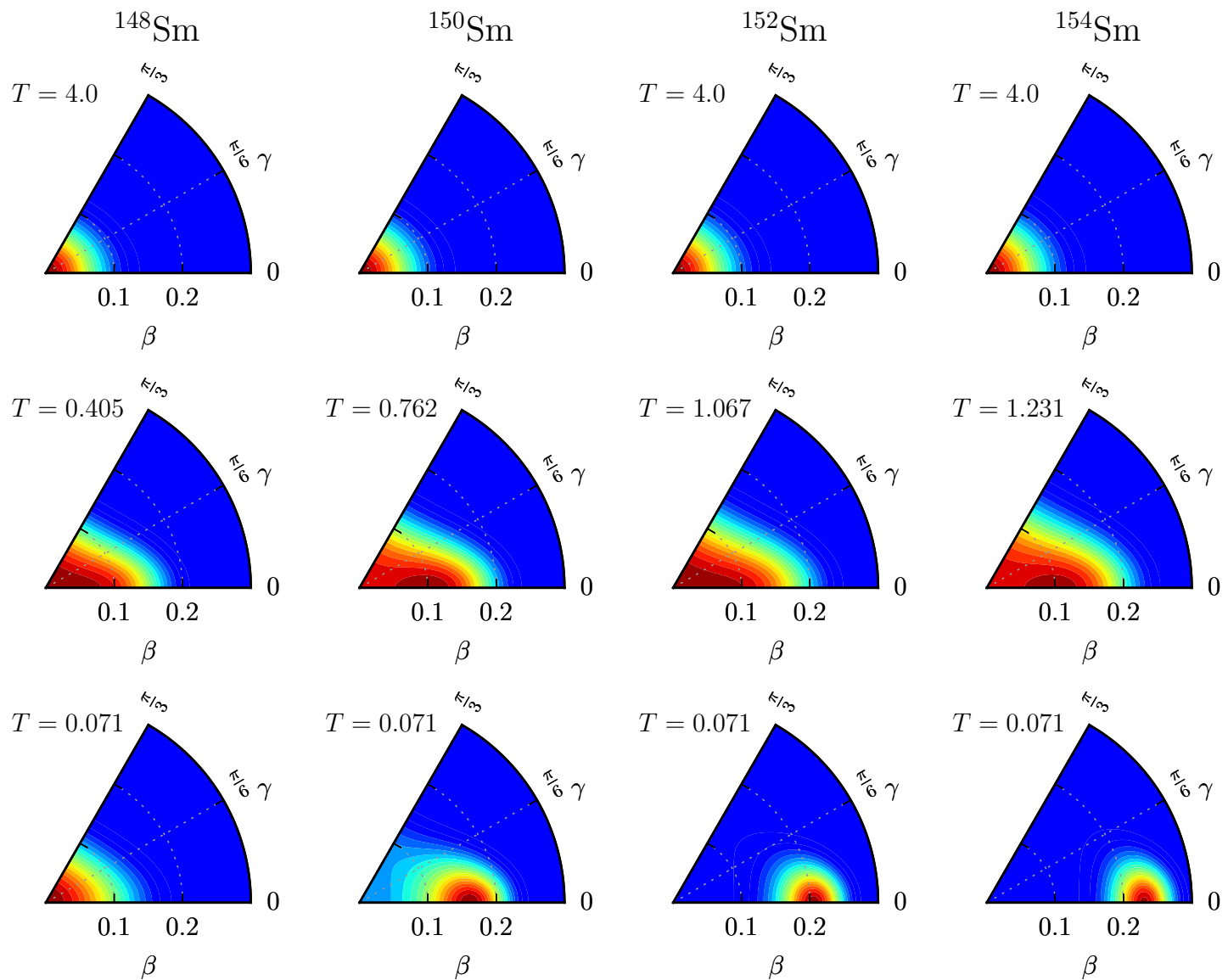

We find excellent agreement with $P(q_{20})$ calculated in SMMC !

$-\ln P(\beta,\gamma)$

^{154}Sm
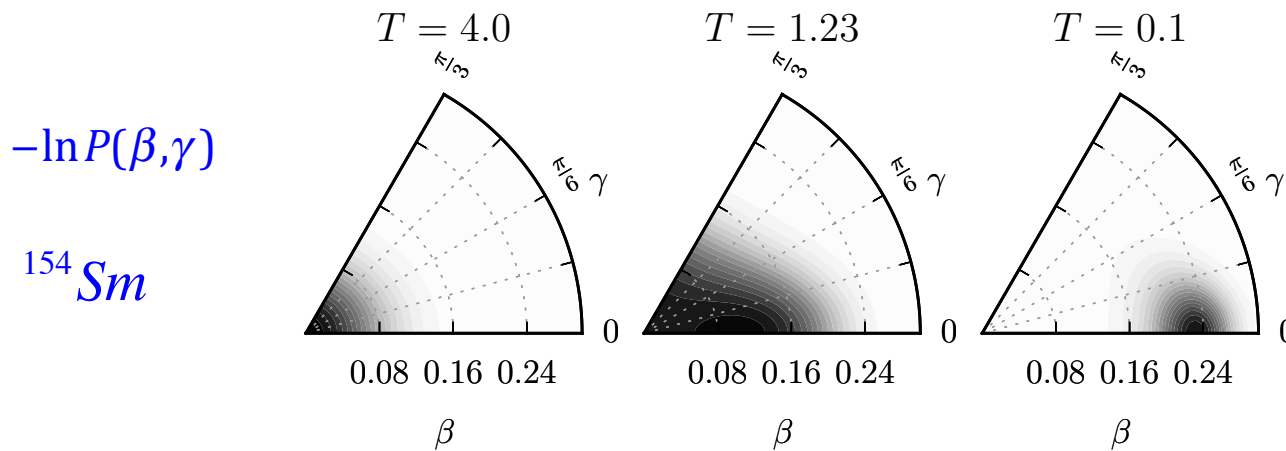
- Mimics a shape transition from a deformed to a spherical shape without using a mean-field approximation !

Shape distributions P_T in the intrinsic β, γ variables

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

$T = 4.0$

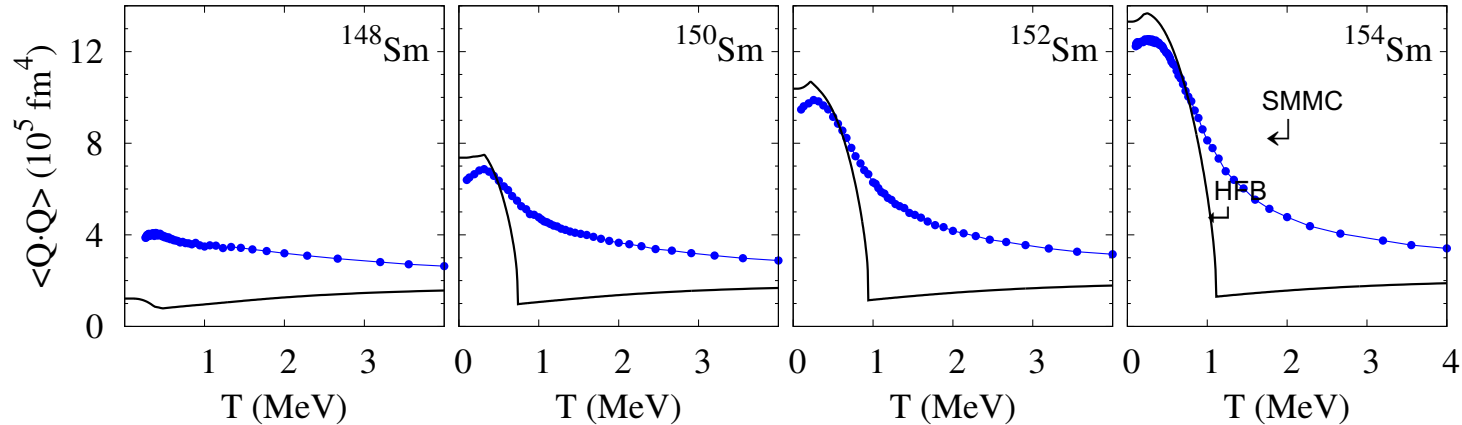$T = 0.405$ $T = 0.762$ $T = 1.067$ $T = 1.231$

$T = 0.071$

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: SMMC 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 SMMC deformation effects survive well above the transition temperature: $\langle Q \cdot Q \rangle$ continues to be enhanced above its mean-field value.
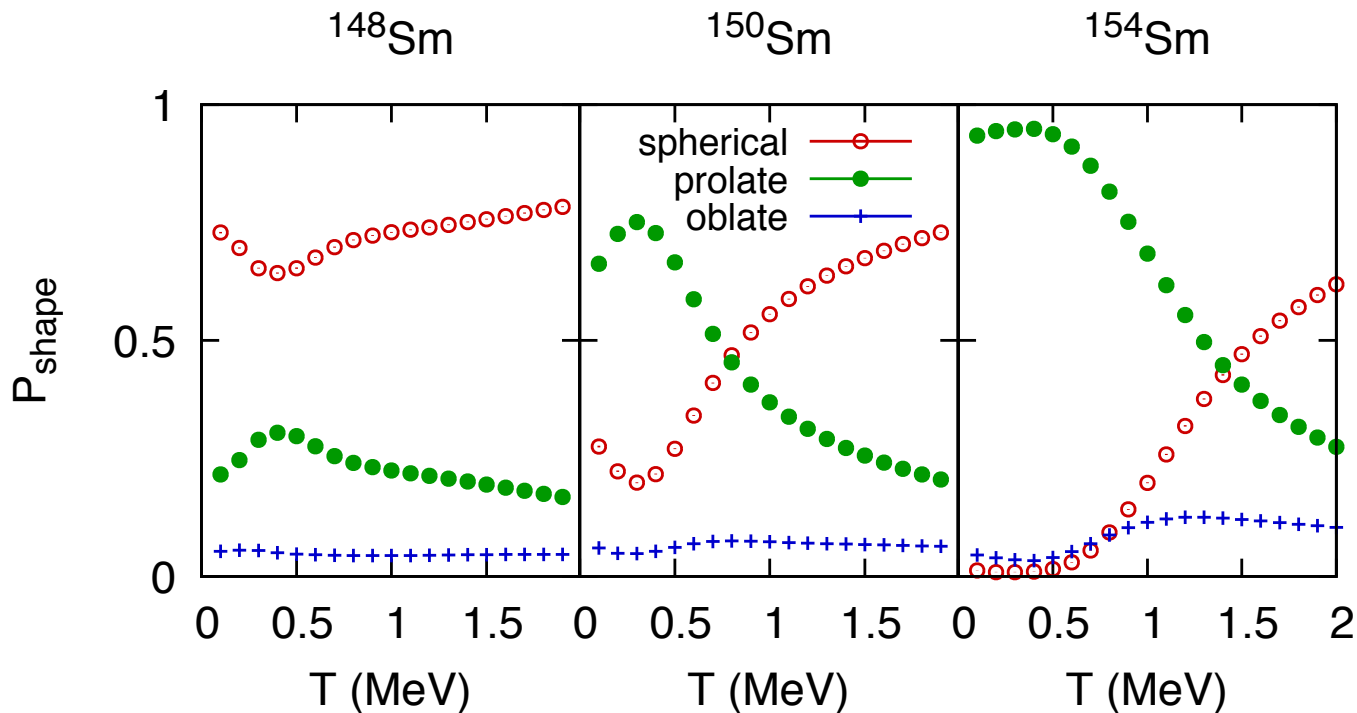
We divide the β, γ plane into three regions: spherical, prolate and oblate.

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

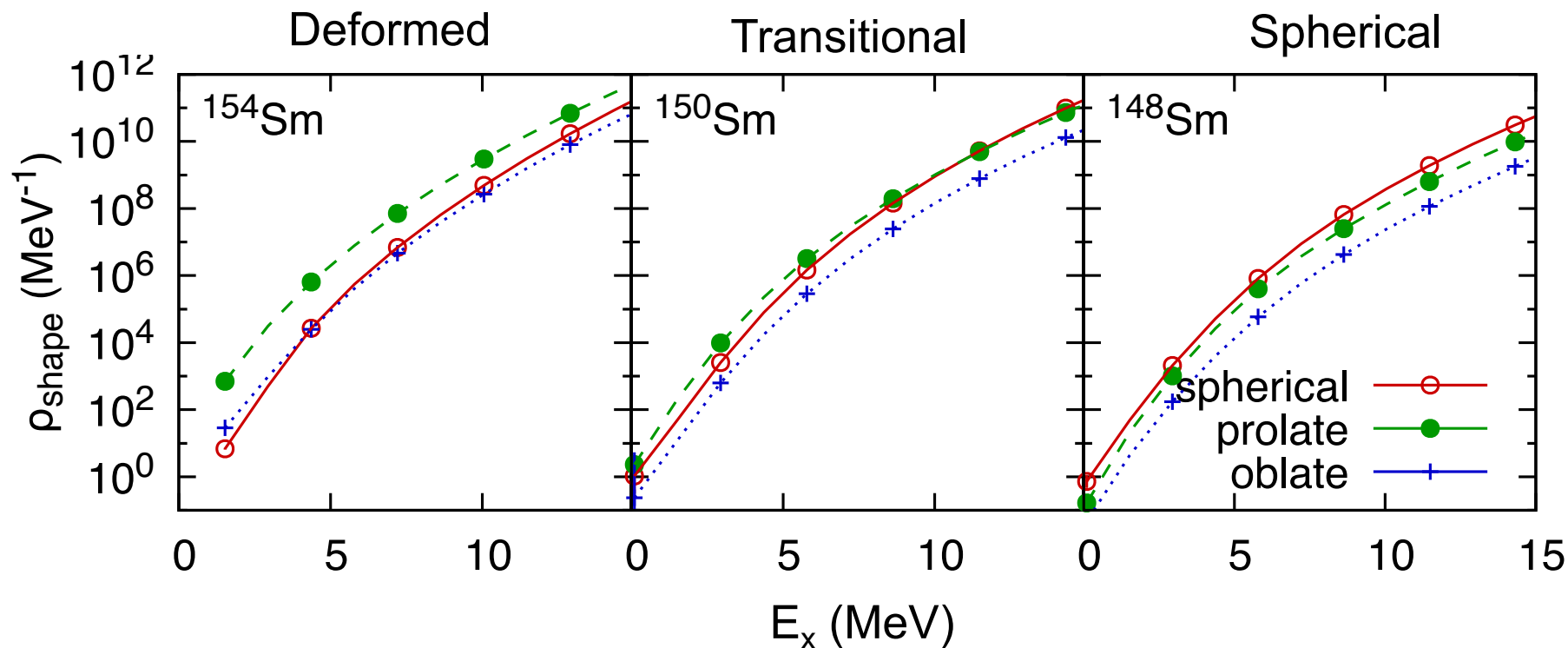$$\prod_\mu dq_{2\mu} \propto \beta^4 |\sin(3\gamma)| d\beta d\gamma$$
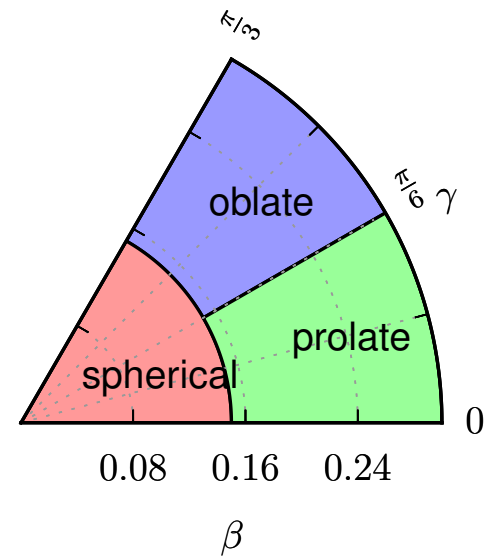
- Compare deformed (^{154}Sm), transitional (^{150}Sm) and spherical (^{148}Sm) nuclei

Level density versus intrinsic deformation

- Use the saddle-point approximation to convert $P_T(\beta, \gamma)$ to level densities vs. E_x, β, γ (canonical $\Rightarrow$ micro canonical)

In strongly 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

- SMMC is a powerful method for the microscopic calculation of collective and statistical nuclear properties 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) - describe quantum and thermal shape transitions *without* using a mean-field approximation.

- Deformation-dependent level densities can now be calculated in SMMC

Outlook

- Generalize to other shapes (e.g., octupole)

- Method can be applied to calculate *exact* shape distributions in other nuclear models.

- Applications to shape dynamics