The shape distribution of nuclear level densities in the shell model Monte Carlo method

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- Shell model Monte Carlo (SMMC) method and level densities
- Nuclear deformation in the spherical shell model: quadrupole distributions in the laboratory frame
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Recent review of SMMC: Y. Alhassid, arXiv:1607.01870, in a book edited by K.D. Launey (2017)

Introduction

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

- Often calculated using empirical formulas.

- Mean-field approximations can miss important correlations and are problematic in the broken symmetry phase (see talk of Paul Fanto).

The configuration-interaction (CI) shell model is a suitable framework to account for correlations beyond the mean field but the combinatorial increase of the dimensionality of its model space has hindered its applications in mid-mass and 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 ($\sim 10^{30}$) 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 $\sigma(\tau)$

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

Thermal expectation value of an observable O

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\,(\hat{O} e^{-\beta \hat{H}})}{\mathrm{Tr}\,(e^{-\beta \hat{H}})} = \frac{\int \mathcal{D}[\sigma] G_\sigma \langle \hat{O} \rangle_\sigma \mathrm{Tr}\, \hat{U}_\sigma}{\int \mathcal{D}[\sigma] G_\sigma \mathrm{Tr}\, \hat{U}_\sigma}$$

where $\langle \hat{O} \rangle_\sigma \equiv \mathrm{Tr}\,(\hat{O}\hat{U}_\sigma)/\mathrm{Tr}\,\hat{U}_\sigma$

- The calculation of the integrands reduces to matrix algebra in the single-particle space (of typical dimension ~ 100).

- The high-dimensional σ integration is evaluated by Monte Carlo methods.

G.H. Lang, C.W. Johnson, S.E. Koonin, W.E. Ormand, PRC **48**, 1518 (1993);
Y. Alhassid, D.J. Dean, S.E. Koonin, G.H. Lang, W.E. Ormand, PRL **72**, 613 (1994).

Level density in SMMC

Nakada and Alhassid, PRL **79**, 2939 (1997)

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

The level density $\rho(E)$ is related to the partition function by an inverse Laplace transform:

$$\rho(E) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\beta \, e^{\beta E} Z(\beta)$$

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

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

S(E) = canonical entropy

$$S(E) = \ln Z + \beta E$$

C = canonical heat capacity

$$C = -\beta^2 \partial E / \partial\beta$$

Heavy nuclei (lanthanides) in SMMC

CI shell model space:

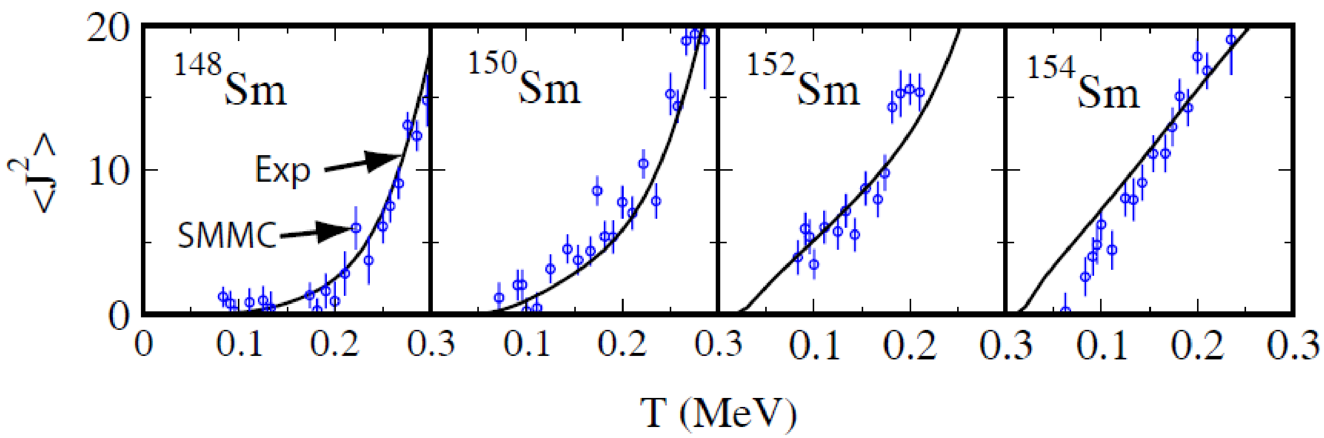
protons: 50-82 shell plus $1f_{7/2}$; neutrons: 82-126 shell plus $0h_{11/2}$ and $1g_{9/2}$

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)

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

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

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.

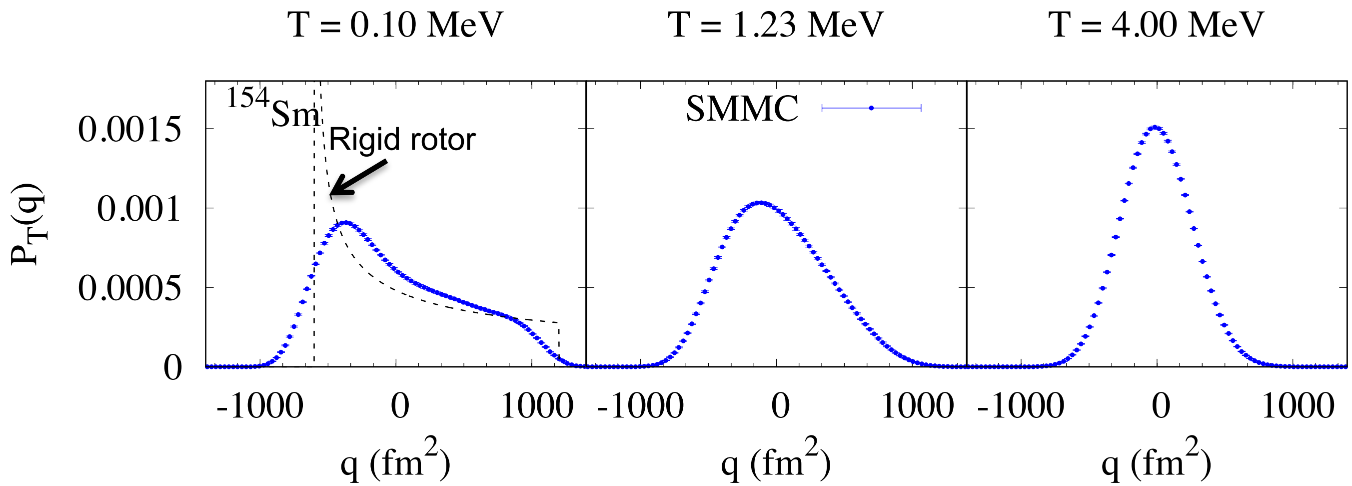
We calculated the distribution of the axial mass quadrupole Q_{20} in the lab frame using an exact projection on Q_{20} (novel in that $[Q_{20}, H] \neq 0$).

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

Application to heavy nuclei

^{154}Sm

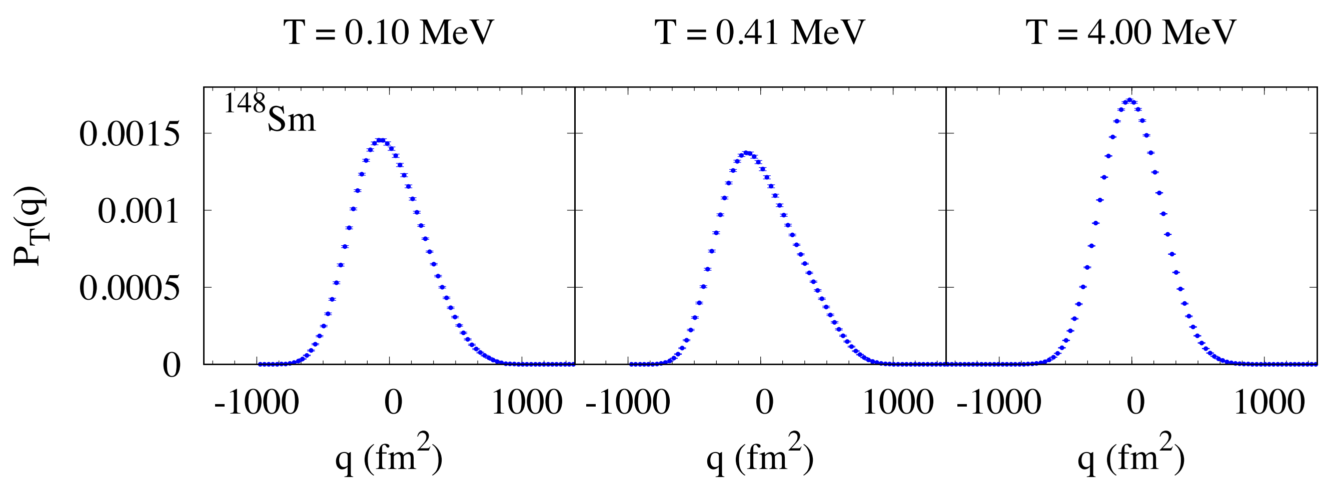
(deformed)



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

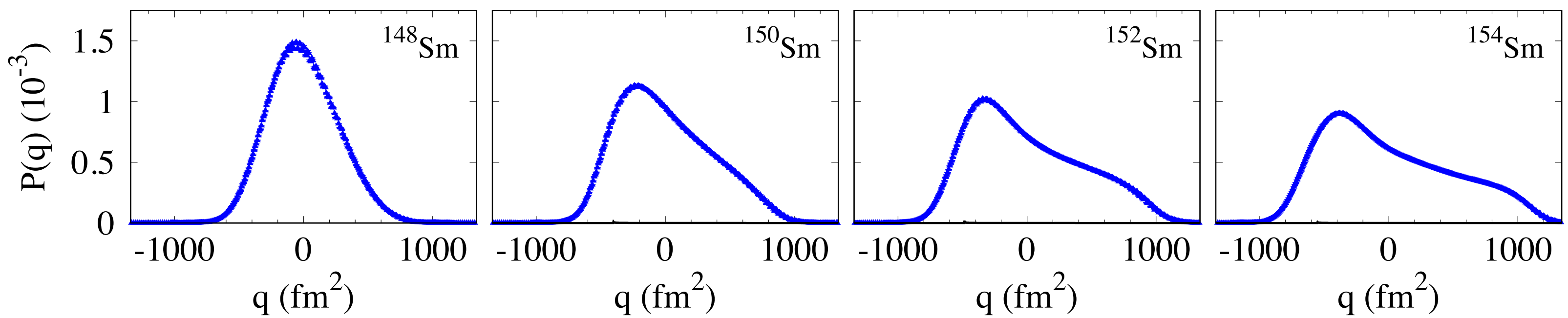
^{148}Sm

(spherical)



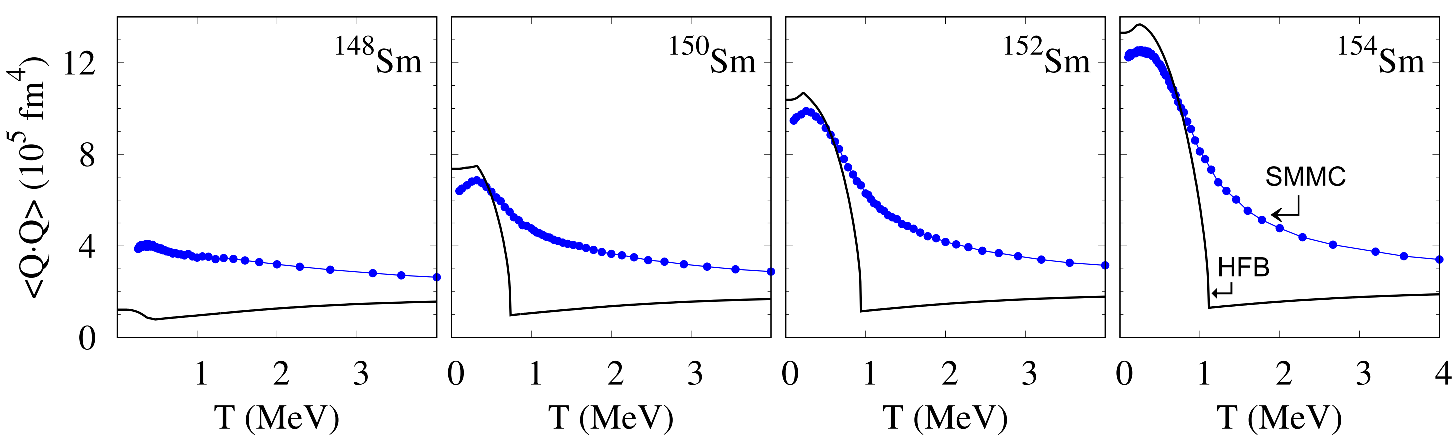
- The distribution is close to a Gaussian even at low temperatures.

Ground-state distributions of $P(q_{20})$ for a family of samarium isotopes



- The distribution $P(q_{20})$ in the lab frame becomes skewed in the crossover from spherical to deformed nuclei

$\langle Q \cdot Q \rangle$ vs. temperature T for a family of samarium isotopes



- The rapid decrease of $\langle Q \cdot Q \rangle$ with temperature is a signature of the sharp shape transition in the mean field results (Hartree-Fock-Bogoliubov)

Quadrupole distributions $P_T(\beta,\gamma)$ in the intrinsic frame

Alhassid, Mustonen, Gilbreth, and 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: $q \cdot q \propto \beta^2$; $(q \times q) \cdot q \propto \beta^3 \cos(3\gamma)$; $(q \cdot q)^2 \propto \beta^4$

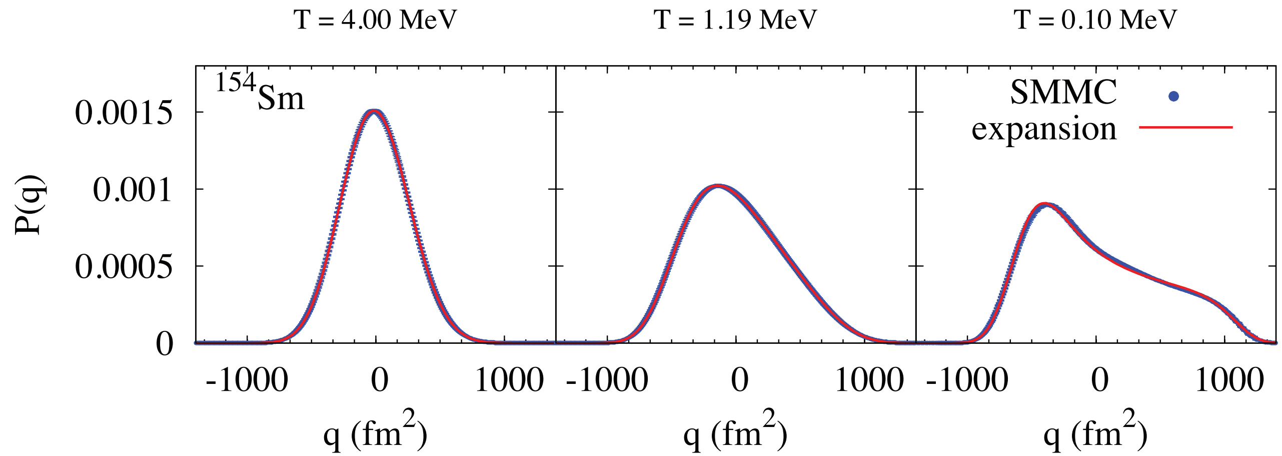
$\ln P_T(\beta,\gamma)$ at a given temperature T is an *invariant* and can be expanded in the quadrupole invariants [a Landau-like expansion, used for the free energy to describe shape transitions in Alhassid, Levit, Zingman, PRL **57**, 539 (1986)]

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

- 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.

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

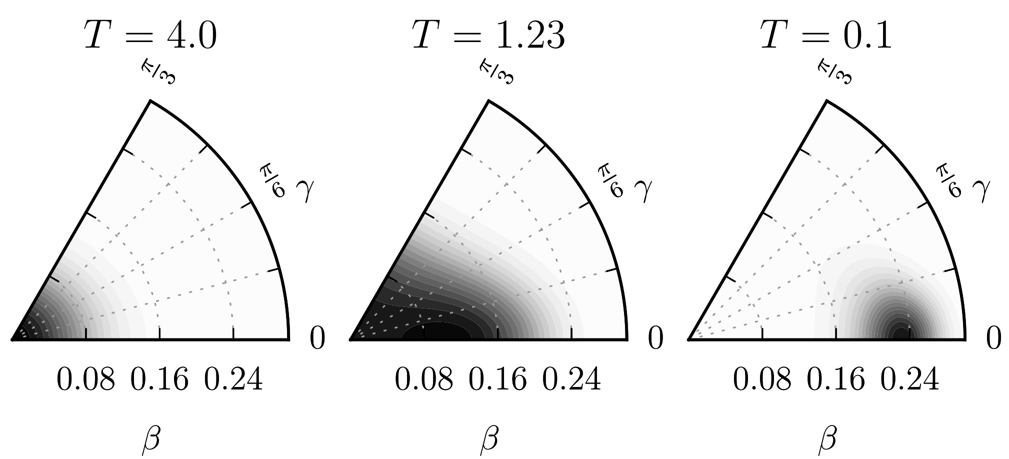
Expressing the invariants in terms of $q_{2\mu}$ in the lab frame and integrating over the $\mu \neq 0$ components, we recover $P(q_{20})$ in the lab frame.



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

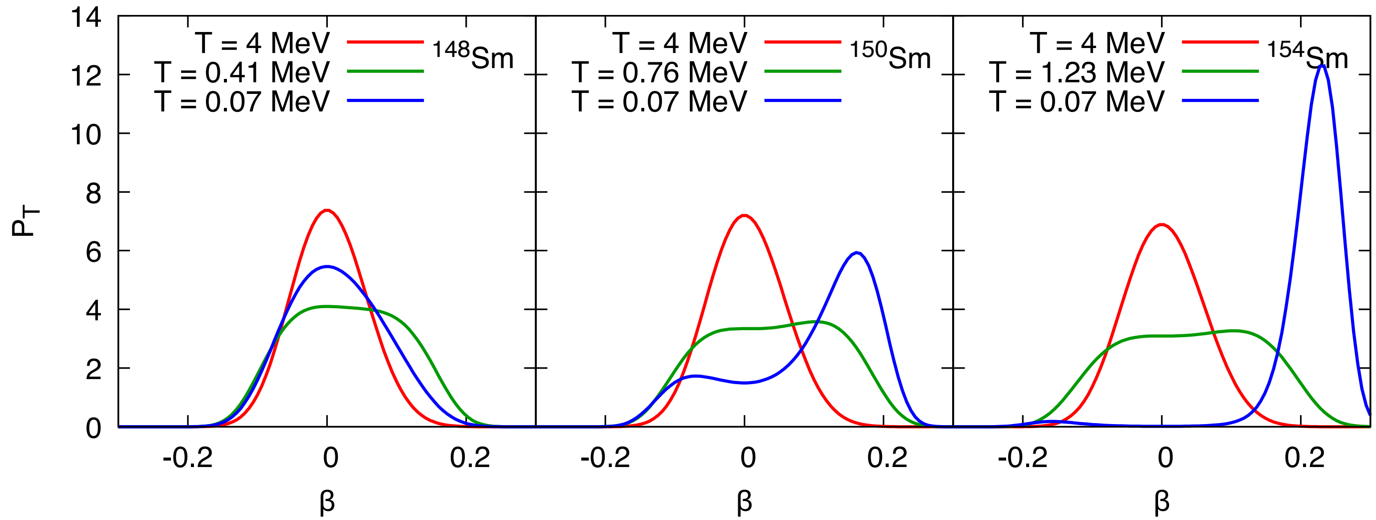
$-\ln P(\beta,\gamma)$

^{154}Sm



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

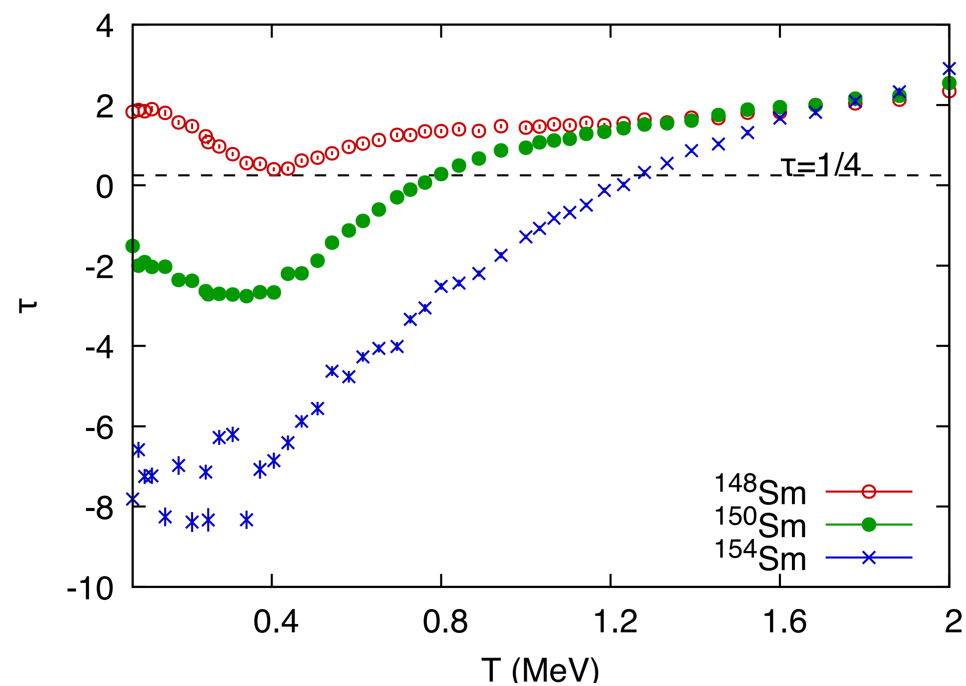
Quadrupole distributions P_T vs. axial deformation β



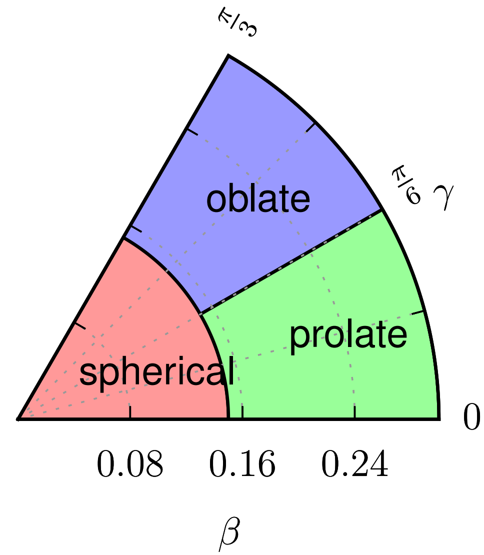
The parameter that controls the equilibrium shape is $\tau = ac / b^2$

τ as a function of temperature for the three samarium isotopes

The shape transition occurs at $\tau = 1/4$



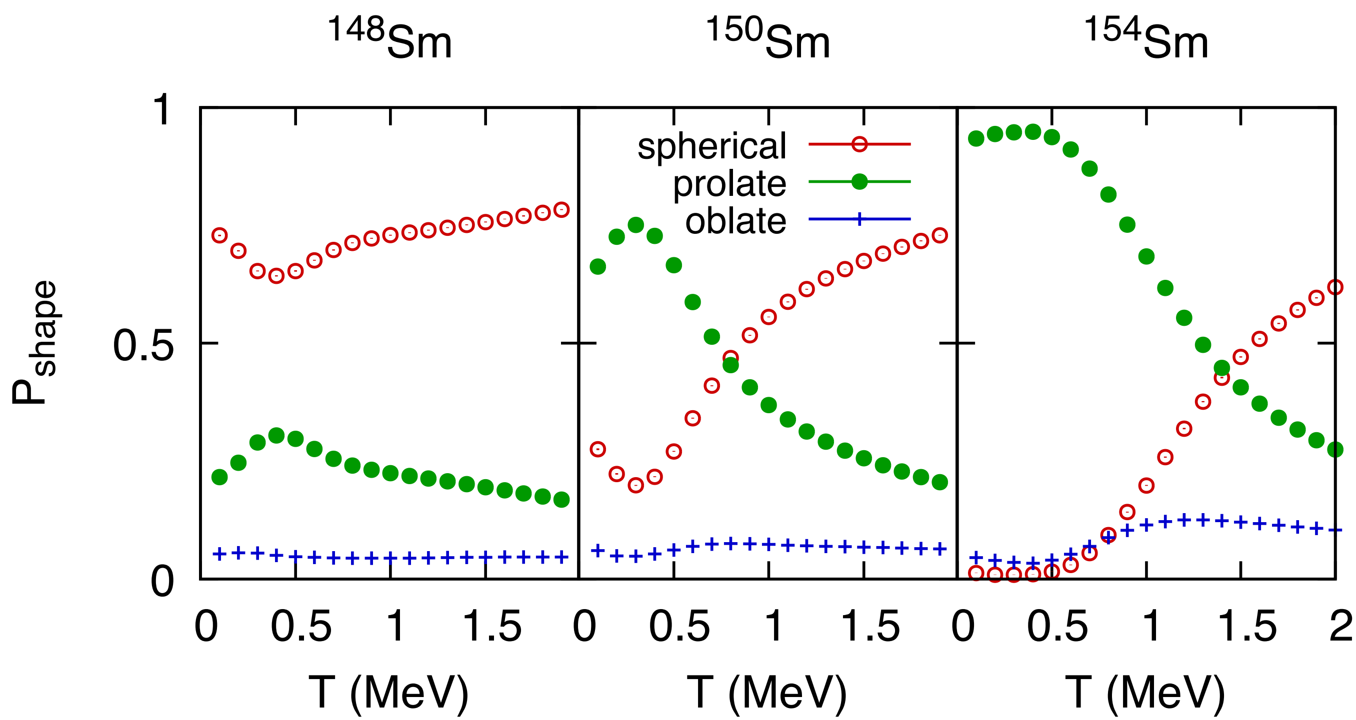
We divide the β,γ plane into three regions: spherical, prolate and oblate.



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

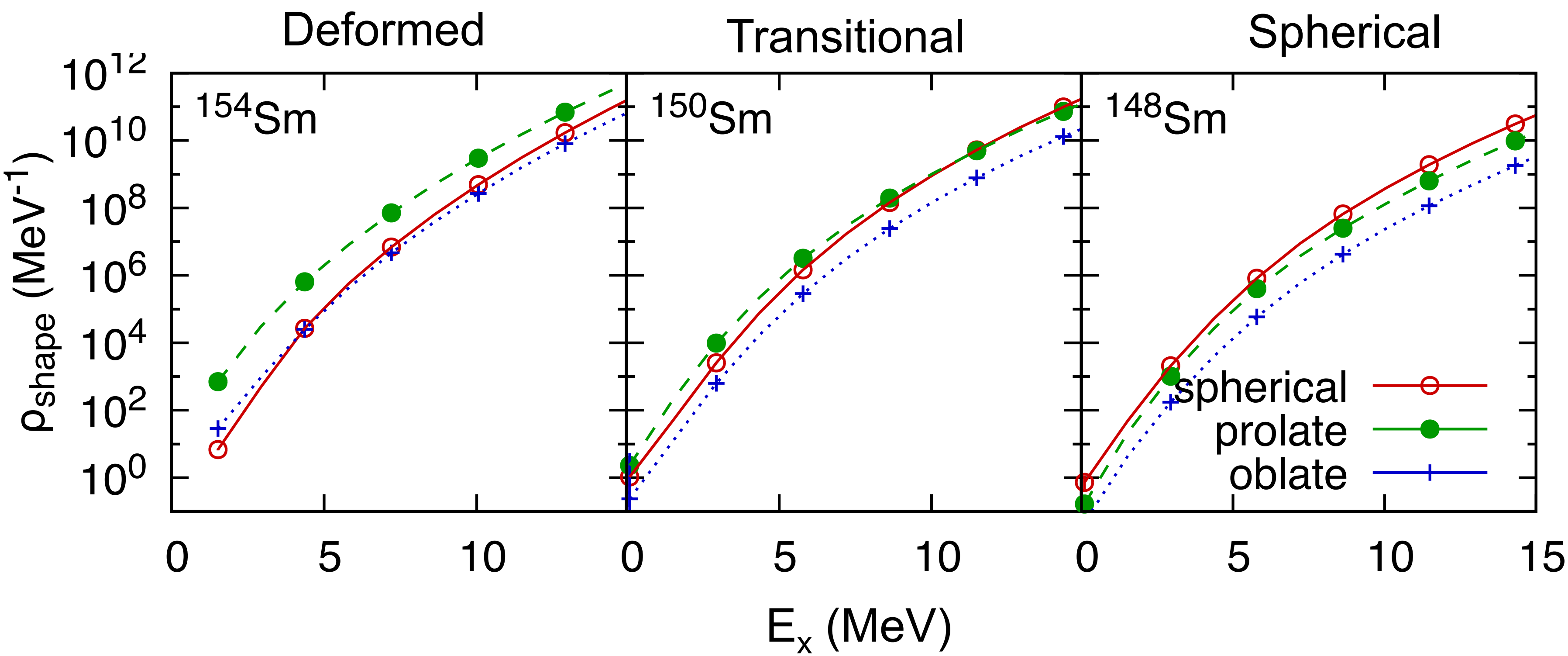
$$\prod_{\mu} dq_{2\mu} \propto \beta^4 |\sin(3\gamma)| d\beta d\gamma$$

- 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 ⇒ micro canonical)



In strongly deformed nucleus, the contributions from prolate shapes dominate the level density below the shape transition energy.

In a spherical nucleus, both spherical and prolate shapes make significant contributions.

Conclusion

- SMMC 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 axial 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 (e.g., the CI shell model) using a Landau-like expansion.

- Mimics shape transitions without using a mean-field approximation.

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

Outlook

- Applications to shape dynamics within a spherical shell model approach.

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