Statistical properties of nuclei by the shell model Monte Carlo method

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- Circumventing the odd particle-number sign problem
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Recent review: Y. Alhassid, arXiv:1607.01870 (2016), in a review book, ed. K.D. Launey

Introduction

Statistical properties of nuclei: level density, partition function, entropy,…

Statistical properties, and in particular, 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 statistical properties in the presence of correlations is a challenging many-body problem.

- Often calculated using empirical modifications of the Fermi gas formula

- Mean-field approximations (e.g., Hartree-Fock-Bogoliubov) often miss important correlations and are problematic in the broken symmetry phase.

The configuration-interaction (CI) shell model takes into account 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 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.

Also known in nuclear physics as the shell model Monte Carlo (SMMC) method.

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).

SMMC is the state-of-the-art method for the microscopic calculation of statistical properties of nuclei.

Hubbard-Stratonovich (HS) transformation

Assume an effective Hamiltonian in Fock space with a one-body part and a two-body interaction : $\hat{H} = \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} \sum_\alpha v_\alpha \hat{\rho}_\alpha^2$

ϵ_i are single-particle energies and $\hat{\rho}_\alpha$ are linear combinations of one-body densities $\hat{\rho}_{ij} = a_i^\dagger a_j$.

The HS transformation describes the Gibbs ensemble $e^{-\beta H}$ at inverse temperature $\beta = 1/T$ as a path integral over time-dependent auxiliary fields $\sigma(\tau)$

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

$G_\sigma = e^{-\frac{1}{2} \int_0^\beta |v_\alpha| \sigma_\alpha^2(\tau) d\tau}$ is a Gaussian weight and U_σ is a one-body propagator of non-interacting nucleons in time-dependent auxiliary fields

$$\hat{U}_\sigma = \mathcal{T} e^{-\int_0^\beta \hat{h}_\sigma(\tau) d\tau}$$

with a one-body Hamiltonian $\hat{h}_\sigma(\tau) = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha s_\alpha |v_\alpha| \sigma_\alpha(\tau) \hat{\rho}_\alpha$

$s_\alpha = 1$ for $v_\alpha < 0$, and $s_\alpha = i$ for $v_\alpha > 0$

Thermal expectation values of observables

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

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

Grand canonical quantities in the integrands can be expressed in terms of the single-particle representation matrix $\mathbf{U}_\sigma$ of the propagator :

$$\mathrm{Tr}\,\hat{U}_\sigma = \det(\mathbf{1} + \mathbf{U}_\sigma)$$

$$\langle a_i^\dagger a_j \rangle_\sigma \equiv \frac{\mathrm{Tr}\,(a_i^\dagger a_j \hat{U}_\sigma)}{\mathrm{Tr}\,\hat{U}_\sigma} = \left[\frac{1}{\mathbf{1}+\mathbf{U}_\sigma^{-1}}\right]_{ji}$$

Canonical (i.e., fixed N,Z) quantities are calculated by an exact particle-number projection (using a discrete Fourier transform).

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

Quantum Monte Carlo methods and sign problem

The high-dimensional σ integration is done by Monte Carlo methods, sampling the fields according to a weight $W_\sigma \equiv G_\sigma |\mathrm{Tr}_{\mathcal{A}}\, \hat{U}_\sigma|$

$\Phi_\sigma \equiv \mathrm{Tr}_{\mathcal{A}}\, U_\sigma / |\mathrm{Tr}_{\mathcal{A}}\, U_\sigma|$ is the Monte Carlo sign function.

For a generic interaction, the sign can be negative for some of the field configurations. When the average sign is small, the fluctuations become very large $\Rightarrow$ the Monte Carlo sign problem.

Good-sign interactions

We can rewrite $\hat{H} = \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} \sum_\alpha v_\alpha \left(\rho_\alpha \bar{\rho}_\alpha + \bar{\rho}_\alpha \rho_\alpha \right)$
where $\bar{\rho}_\alpha$ is the time-reversed density.

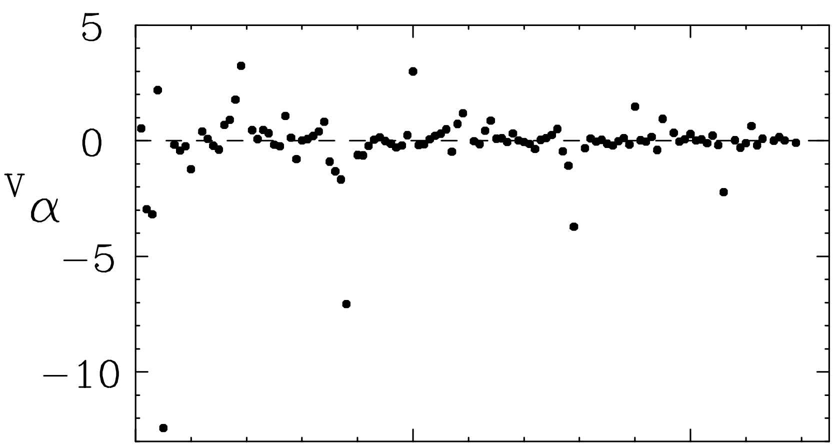
Sign rule: when all $v_\alpha < 0$, $\mathrm{Tr}\, U_\sigma > 0$ for any configuration σ and the interaction is known as a good-sign interaction.

Proof: when all $v_\alpha < 0$, we have $\hat{h}_\sigma = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha \left(v_\alpha \sigma_\alpha^* \rho_\alpha + v_\alpha \sigma_\alpha \bar{\rho}_\alpha \right)$ and $\bar{h}_\sigma = h_\sigma$ $\Rightarrow$ the eigenvalues of U_σ appear in complex conjugate pairs $\{\lambda_i, \lambda_i^*\}$ and $\mathrm{Tr}\, \hat{U}_\sigma = \prod_i |1 + \lambda_i|^2 > 0$.

A practical method for overcoming the sign problem

Alhassid, Dean, Koonin, Lang, Ormand, PRL **72**, 613 (1994).

The dominant collective components of effective nuclear interactions have a good sign.



A family of good-sign interactions is constructed by multiplying the bad-sign components by a negative parameter g

$$H = H_G + gH_B$$

Observables are calculated for $-1 < g < 0$ and extrapolated to $g = 1$.

In the calculation of statistical and collective properties of nuclei, we have used good-sign interactions.

Circumventing the odd-particle sign problem in SMMC

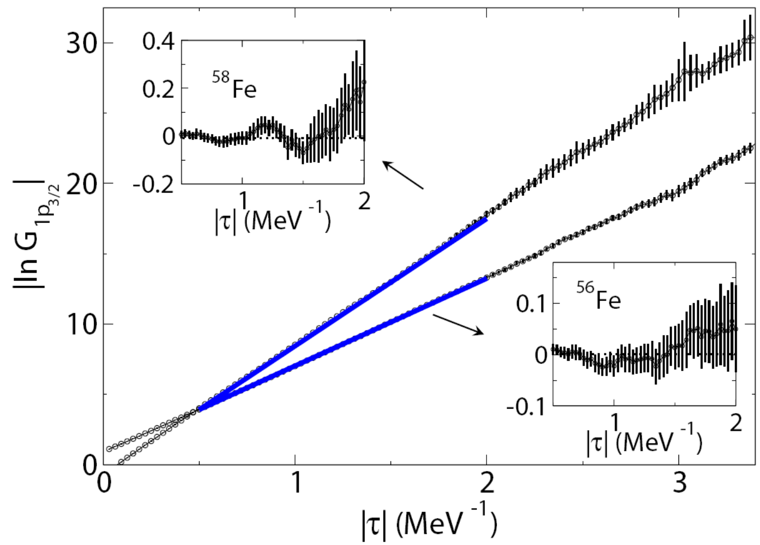
Mukherjee and Alhassid, PRL **109**, 032503 (2012)

Applications of SMMC to odd-even and odd-odd nuclei has been hampered by a sign problem that originates from the projection on odd number of particles.

- We introduced a method to calculate the ground-state energy of the odd-particle system that circumvents this sign problem.

Consider the imaginary-time single-particle Green's functions for even-even nuclei: $G_\nu(\tau) = \Sigma_m \left\langle T\, a_{\nu m}(\tau) a^\dagger_{\nu m}(0) \right\rangle$ for orbitals $\nu = n\, l\, j$

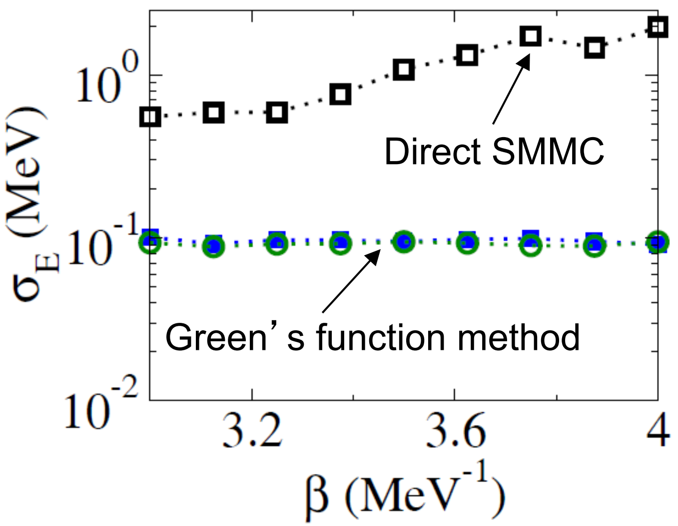
- The energy difference between the lowest energy of the odd-particle system for a given spin j and the ground-state energy of the even-particle system can be extracted from the slope of $\ln G_\nu(\tau)$.

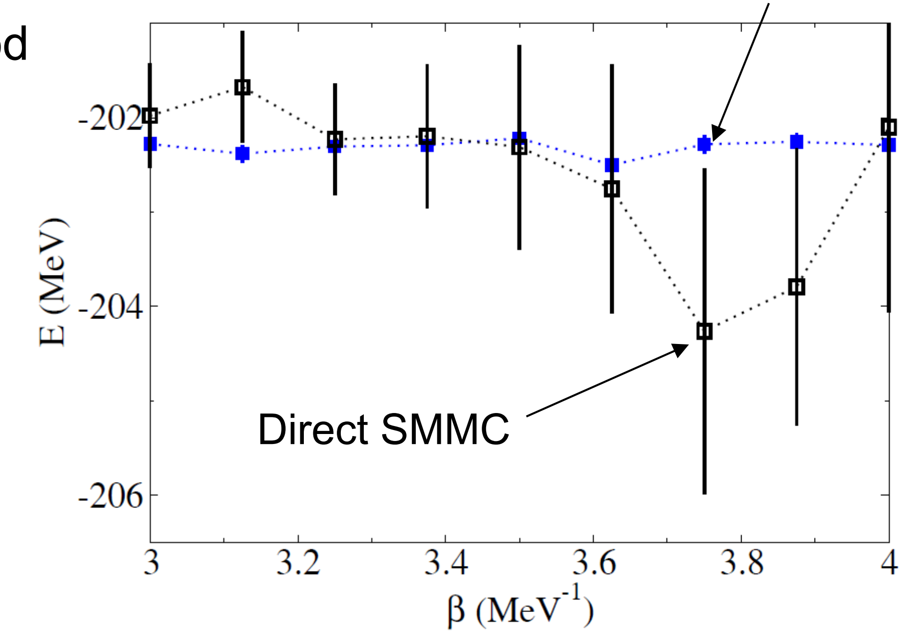


$$G_\nu(\tau) \sim e^{-[E_j(A\pm1) - E_{gs}(A)]\,|\tau|}$$

➡ Minimize $E_j(A\pm1)$ to find the ground-state energy and its spin j.

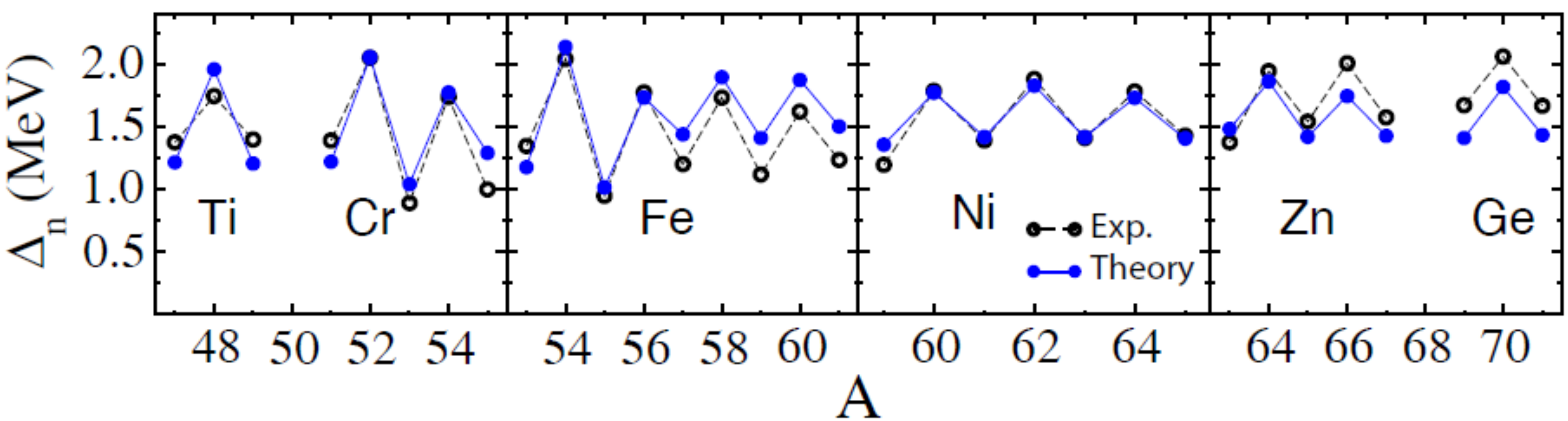
Statistical errors of ground-state energy of direct SMMC versus Green's function method





Pairing gaps in mid-mass nuclei from odd-even mass differences

- SMMC in the complete *$fpg_{9/2}$* shell (in good agreement with experiments)



Statistical properties in the SMMC

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

Partition function

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

Level density

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

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

Mid-mass nuclei

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

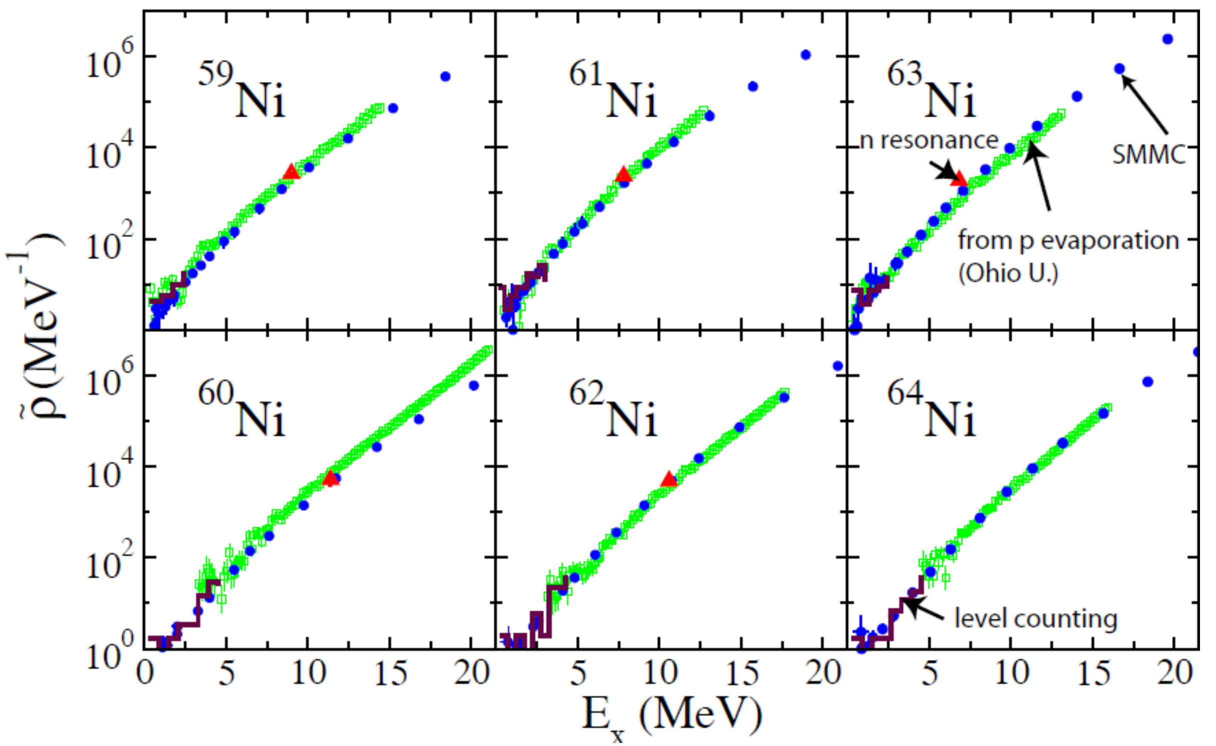
Single-particle Hamiltonian: from Woods-Saxon potential plus spin-orbit

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)

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.

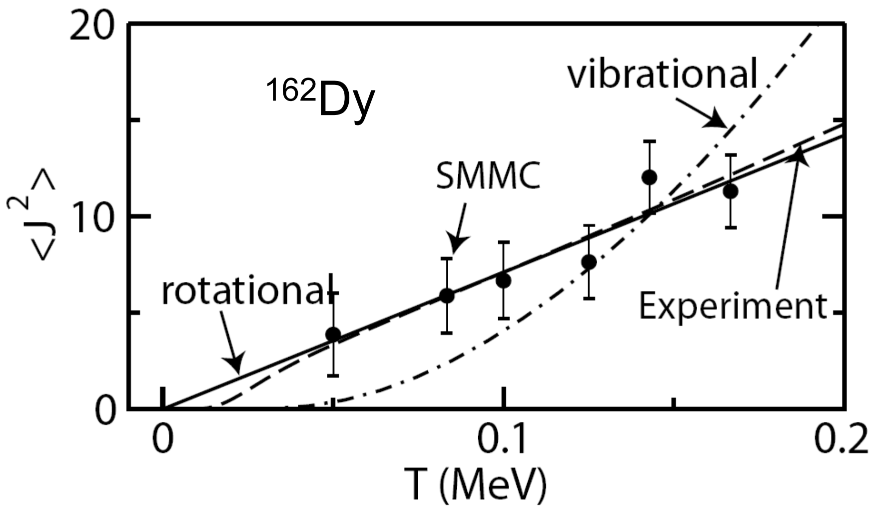
Heavy nuclei exhibit various types of collectivity (vibrational, rotational, …) that are well described by empirical models.

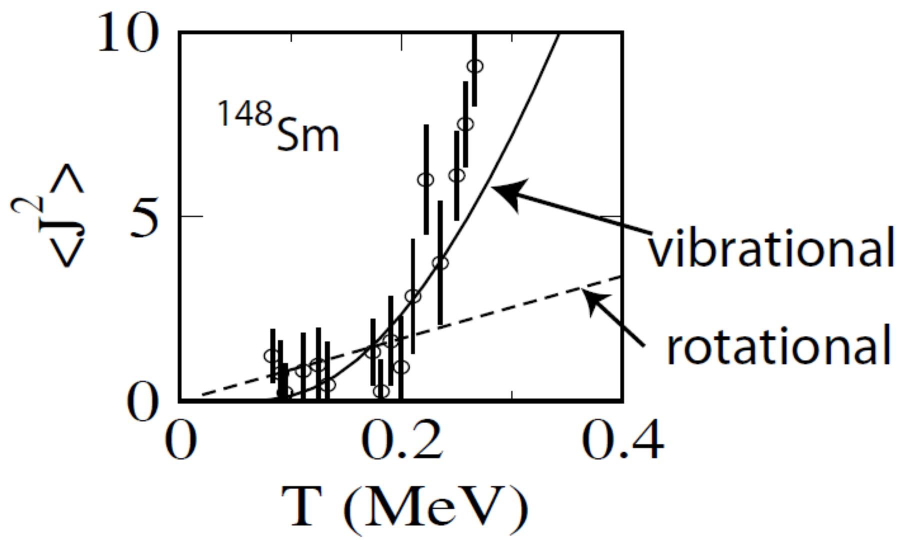
However, a microscopic description in a CI shell model has been lacking.

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

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

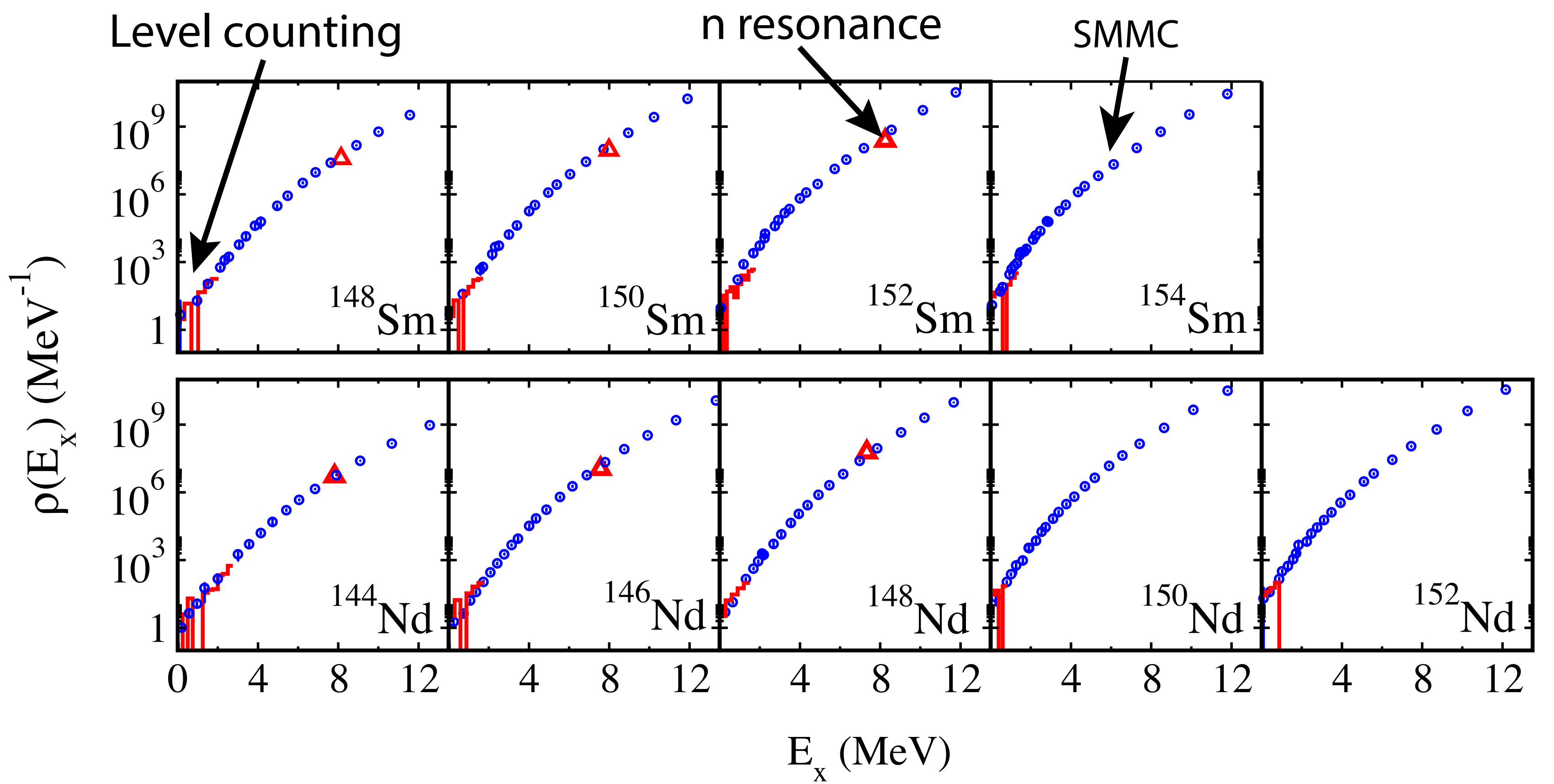
$\Rightarrow {}^{148}Sm$ is vibrational

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

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

Level densities in samarium and neodymium isotopes

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



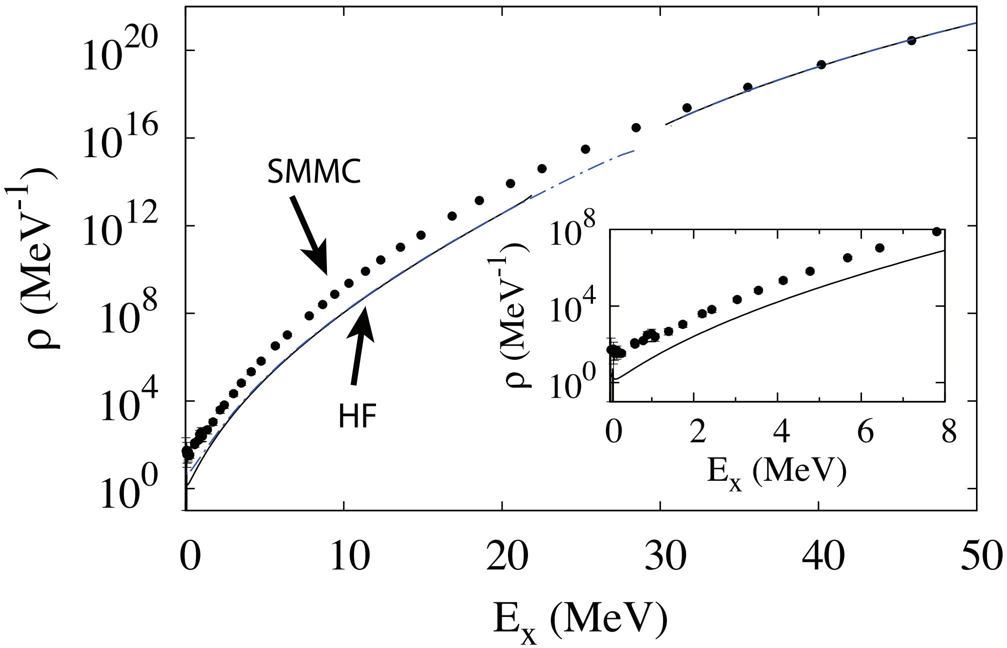
- Good agreement of SMMC densities with various experimental data sets (level counting, neutron resonance data when available).

Rotational enhancement in deformed nuclei

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

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

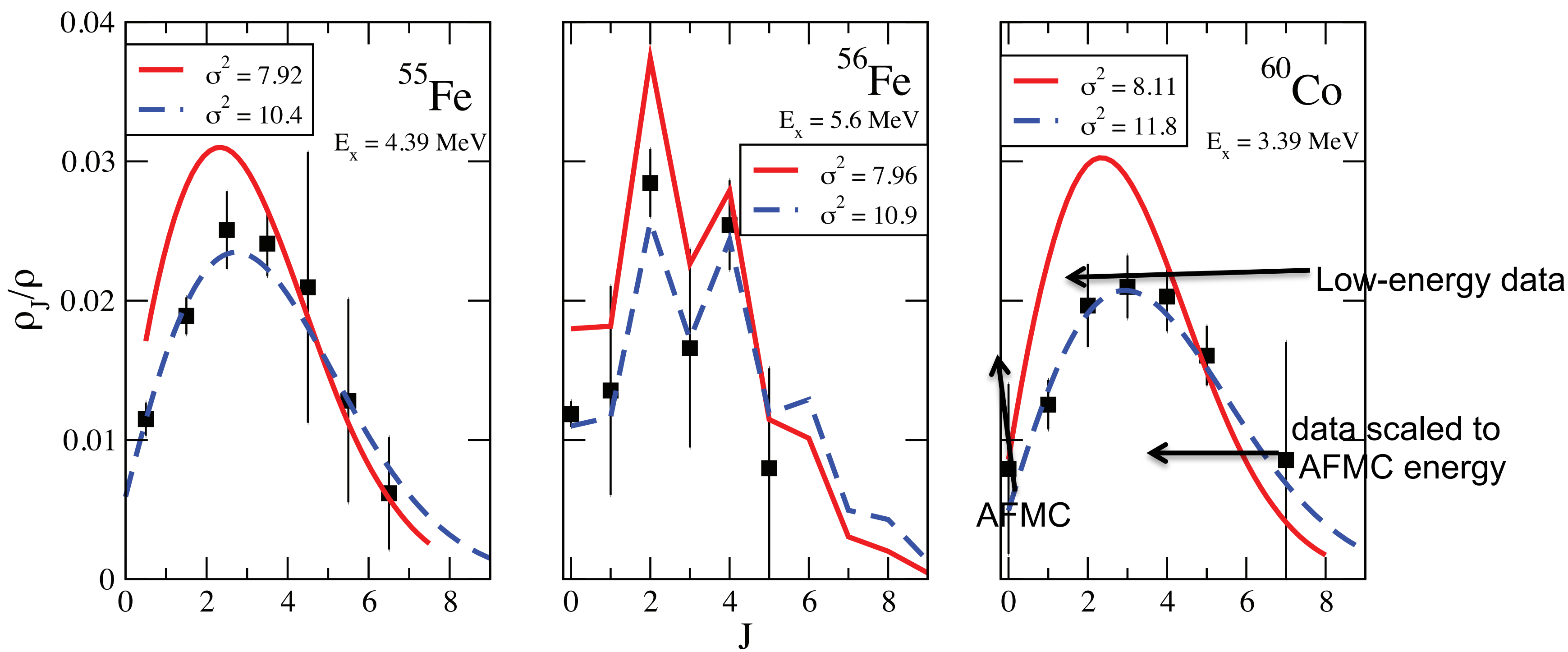
- Particle-number projection is carried out in the saddle-point approximation
- Exact particle-number projection: Fanto, Alhassid, Bertsch, arXiv:1610.08954



- The enhancement of the SMMC 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.

Projection on good quantum numbers: spin distributions in mid-mass nuclei [Alhassid, Liu, Nakada, PRL **99**, 162504 (2007)]



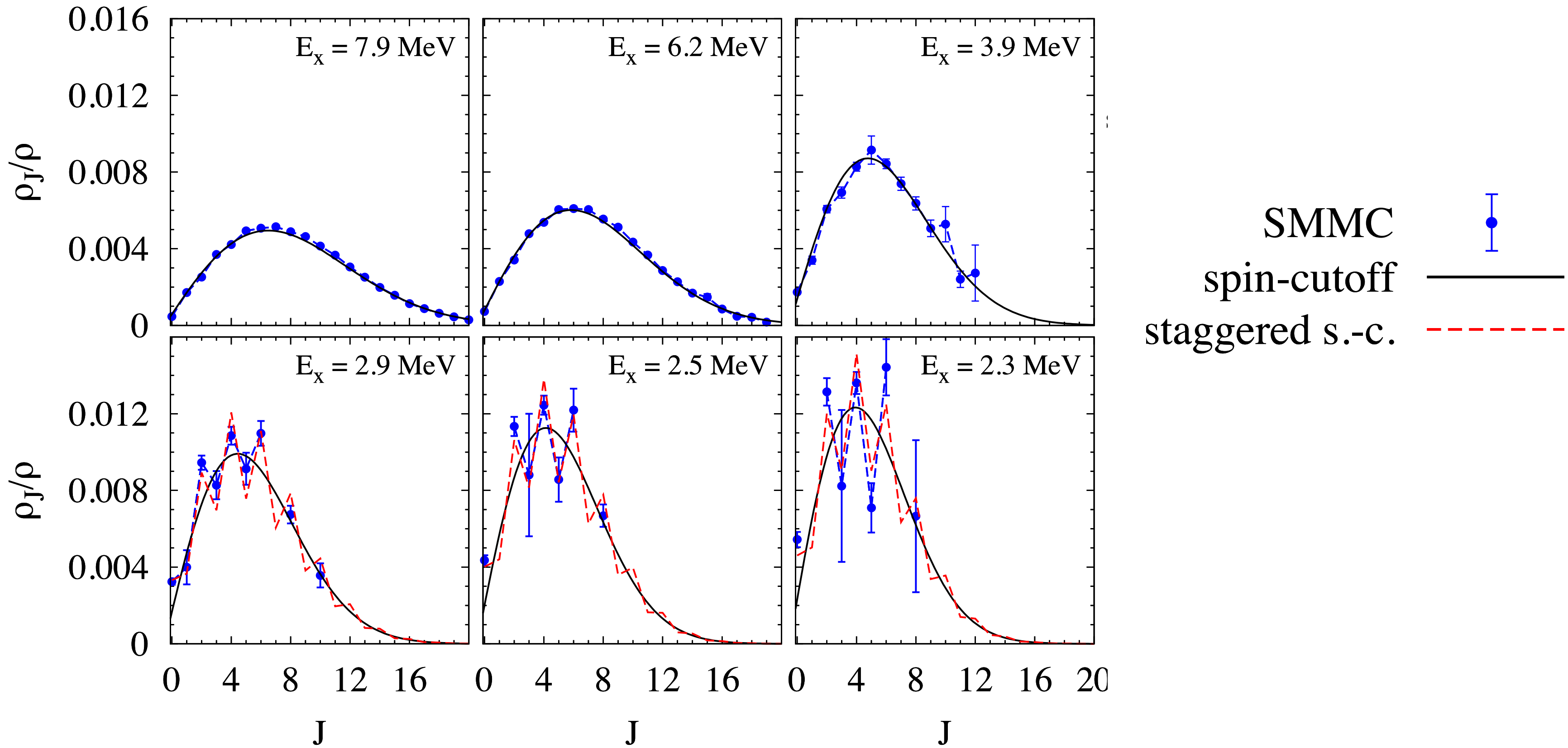
Spin cutoff model: $$\frac{\rho_J}{\rho} = \frac{2J+1}{2\sqrt{2\pi}\sigma^3} e^{-J(J+1)/2\sigma^2}$$ σ^2 = spin cutoff parameter

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

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

Spin distributions 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 (von Egidy and Bucurescu).

Thermal moment of inertia I vs. excitation energy

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

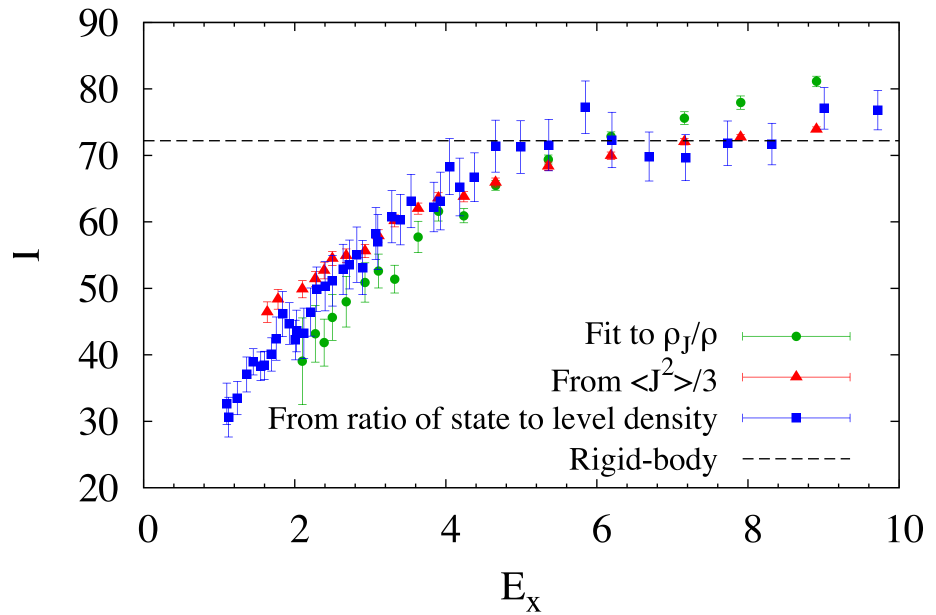
Three methods to determine σ^2

(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

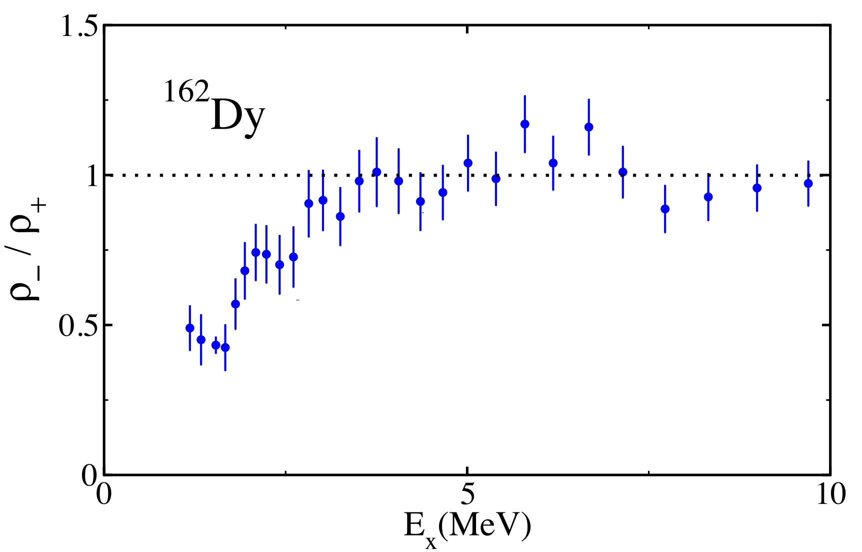
$$\Sigma_J \rho_J(E_x) = \rho_{M=0}(E_x) = \frac{1}{\sqrt{2\pi}\sigma}\rho(E_x)$$



- 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



Projection on an order parameter (associated with a broken symmetry)

Example: 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.

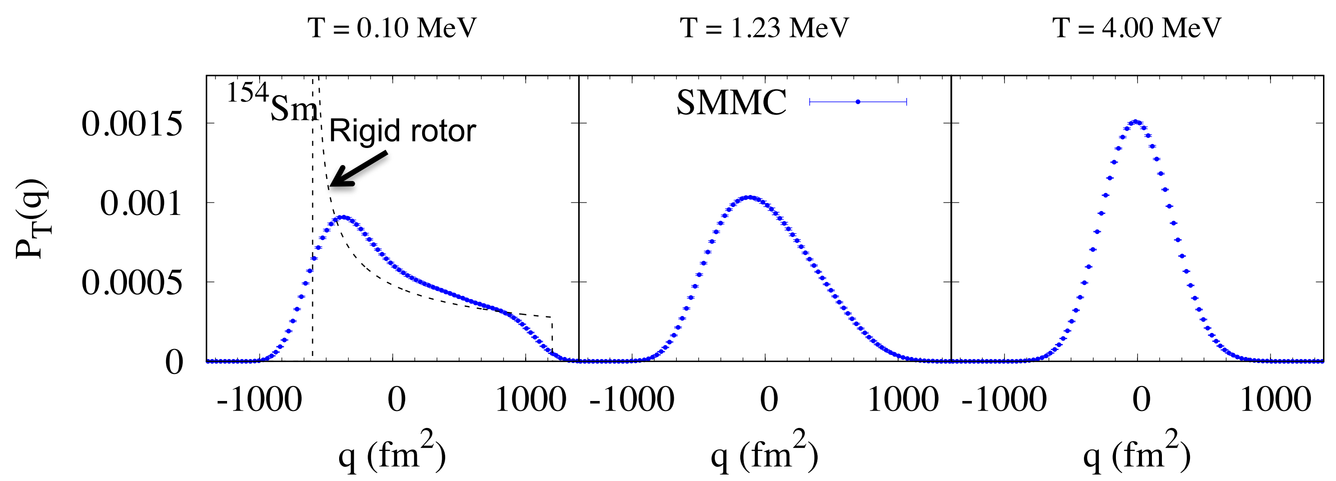
We calculated the distribution of the axial mass quadrupole in the lab frame using an exact projection on Q_{20} (novel in that $[Q_{20}, H] \neq 0$).

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

Application to heavy nuclei

^{154}Sm

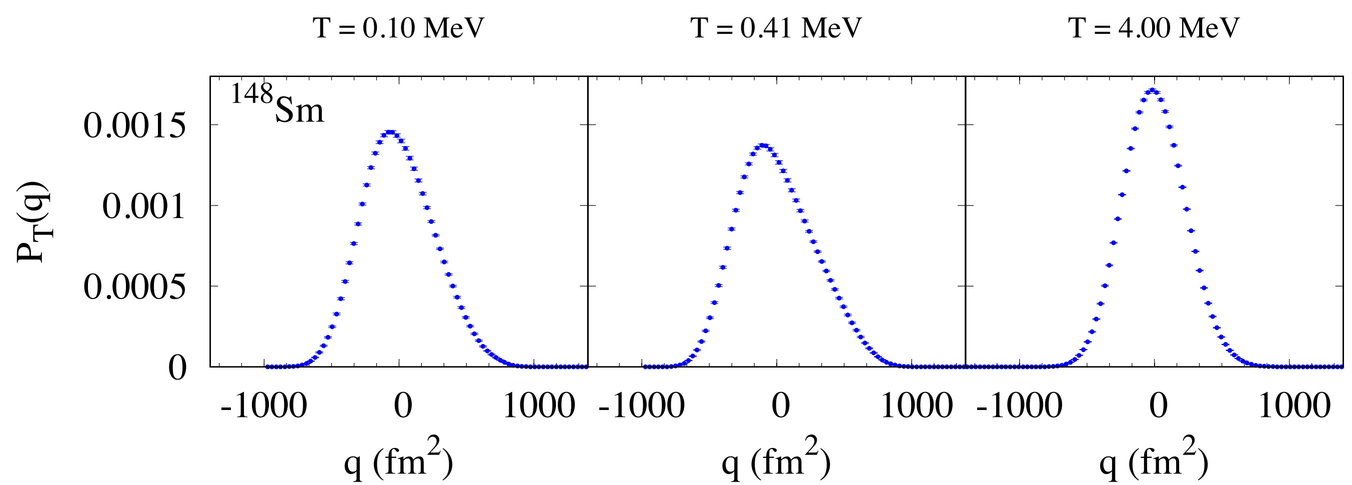
(deformed)



- 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 $q_{2\mu}$.

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

(β,γ are the intrinsic deformation parameters)

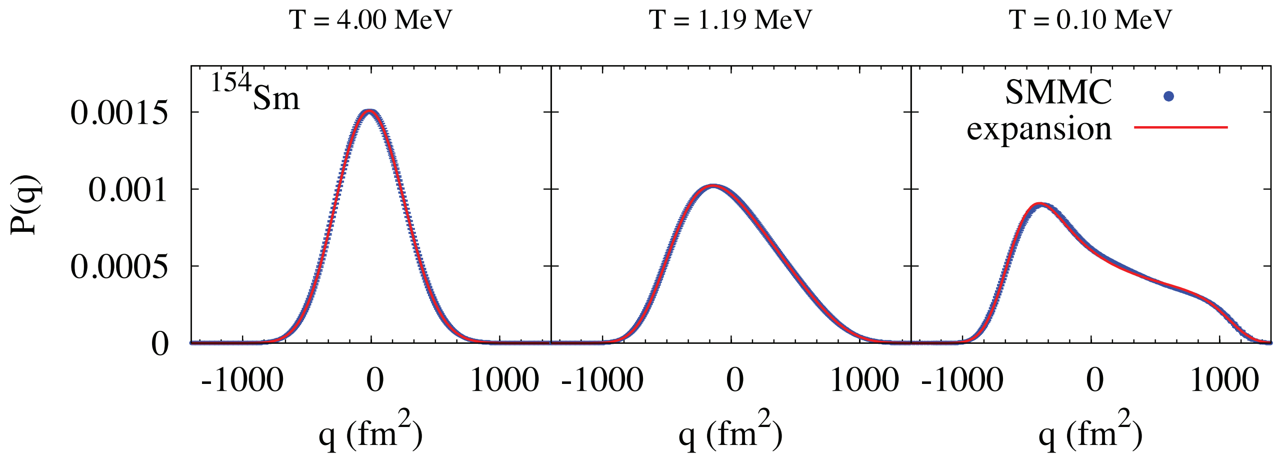
$\ln P_T(\beta,\gamma)$ at a given temperature T is an invariant and can be expanded in the quadrupole invariants (Landau-like expansion)

$$-\ln P_T = A\beta^2 - B\beta^3 \cos 3\gamma + C\beta^4 + \ldots$$

- 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.

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

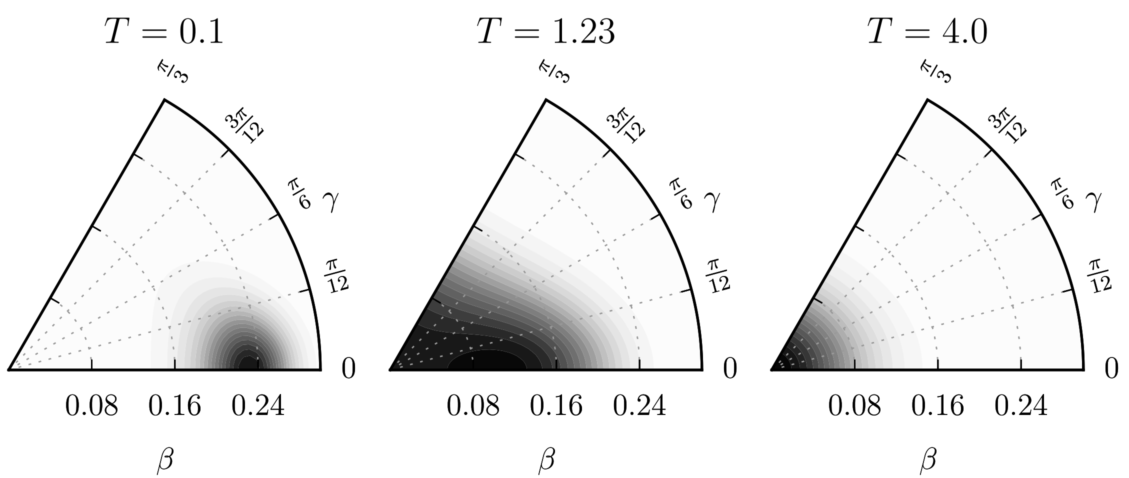
Expressing the invariants in terms of $q_{2\mu}$ in the lab frame and integrating over the $\mu \neq 0$ components, we recover $P[q_{20}]$ in the lab frame.



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

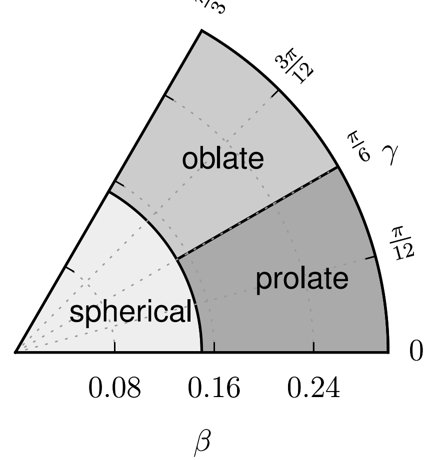
$-\ln P(\beta,\gamma)$

^{154}Sm



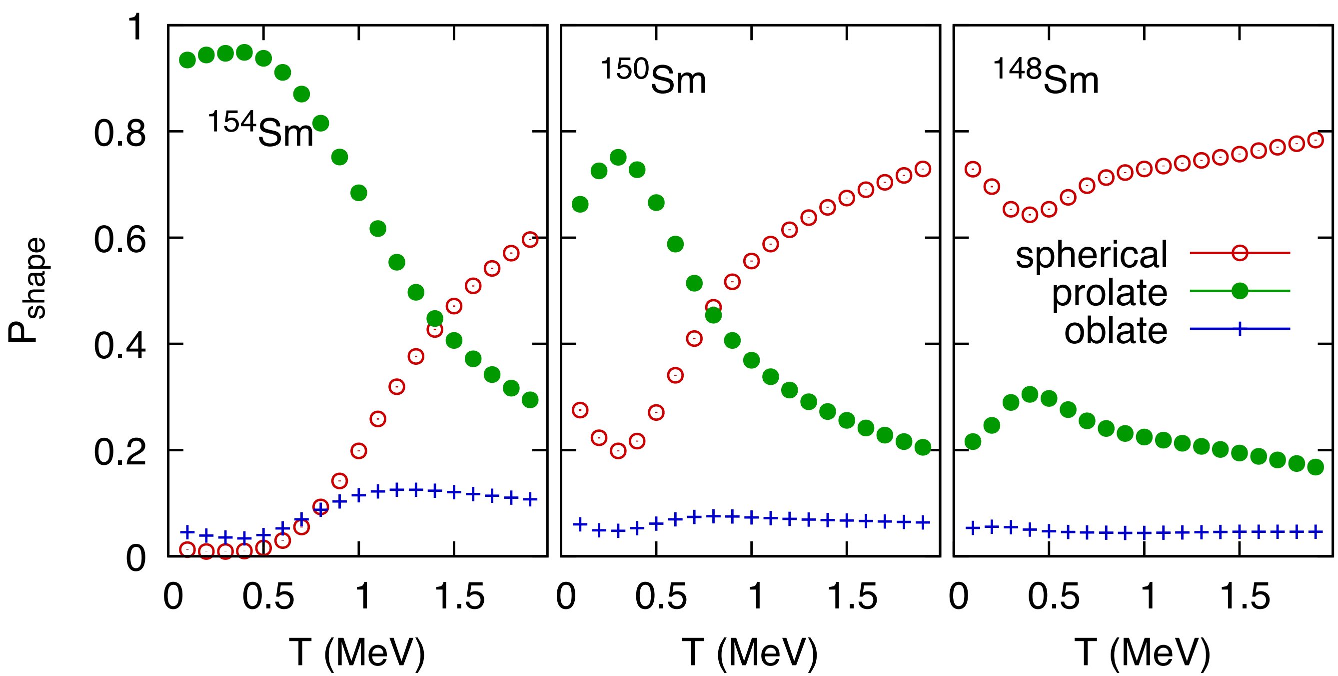
- Mimics a shape transition from a deformed to a spherical shape without using a mean-field approximation !

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



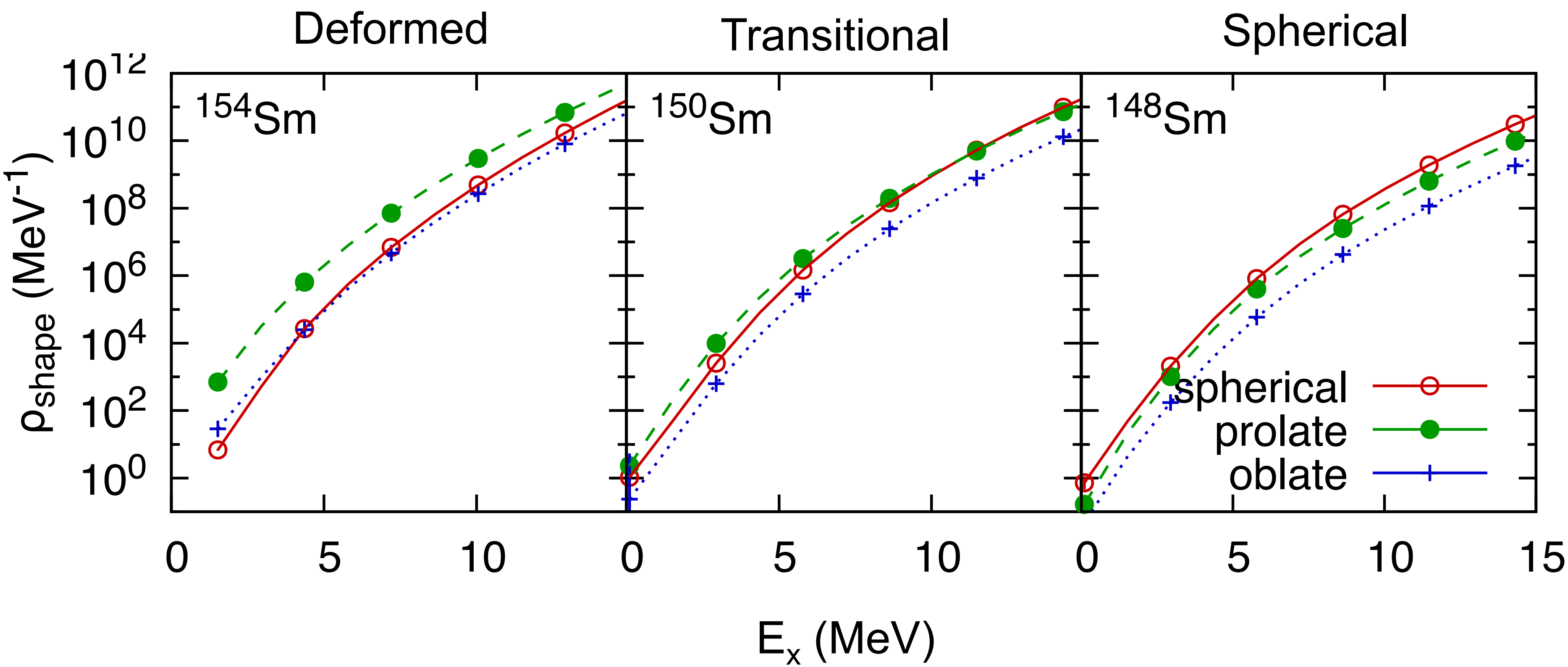
Integrate over each deformation region to determine the probability of shapes versus temperature

- 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

- 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.

- 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.

- Deformation-dependent level density in a rotationally invariant framework (CI shell model).

Outlook

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

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