The shell model Monte Carlo approach to level densities: recent developments and perspectives

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- Introduction: the shell model Monte Carlo (SMMC) approach

- Level density in the SMMC approach

- Circumventing the odd-particle sign problem in SMMC
  - Level densities in odd-mass nuclei

- Microscopic emergence of collectivity in heavy nuclei

- Level densities in heavy nuclei and collective enhancement factors

- Spin distributions

- Can we calculate level densities as a function of deformation (useful for fission models) in a spherical shell model approach ?

- Conclusion and prospects.

The shell model Monte Carlo (SMMC) method

- Most microscopic treatments of heavier nuclei are based on mean-field methods but important correlations can be missed.

- The configuration-interaction (CI) shell model accounts for correlations but diagonalization methods are limited to $\sim 10^{11}$ configurations.

The SMMC method enables microscopic calculations in spaces that are many orders of magnitude larger ($\sim 10^{29}$).

Gibbs ensemble $e^{-\beta H}$ $(\beta = 1/T)$ can be written as a superposition of ensembles U_σ of *non-interacting* nucleons 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 integration over σ 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 densities

Level density is the most important statistical nuclear property (Fermi's golden rule, Hauser-Feshbach theory of statistical nuclear reactions, etc.), but its calculation is a difficult many-body problem in the presence of correlations.

- Most approaches are based on empirical modifications of the Fermi gas formula or on mean-field approximations

Level density in the SMMC approach

H. Nakada and Y. Alhassid., PRL **79**, 2939 (1997)

- 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 $Z(\beta)$

- 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; C = canonical heat capacity.

$$S(E) = \ln Z + \beta E \qquad C = -\beta^2 \partial E / \partial \beta$$

Circumventing the odd-particle sign problem in SMMC

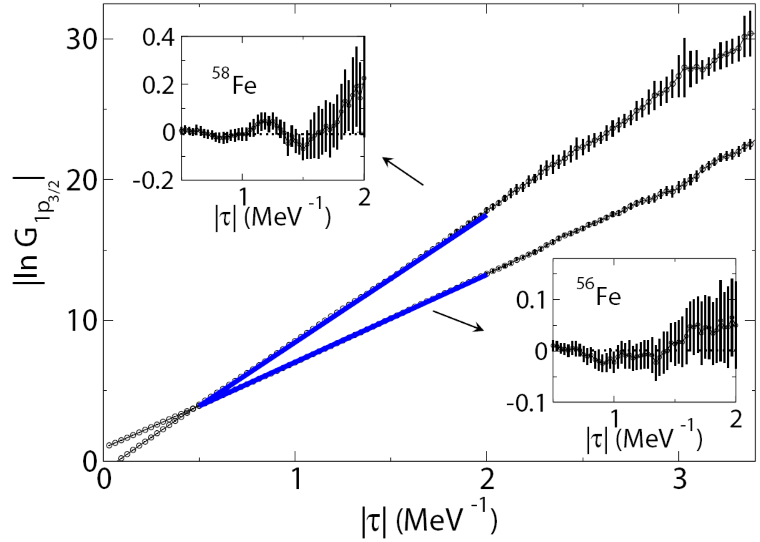
A. Mukherjee and Y. Alhassid, Phys. Rev. Lett. **109**, 032503 (2012)

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.

- A breakthrough was a method we introduced to calculate the ground-state energy of the odd-particle system.

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

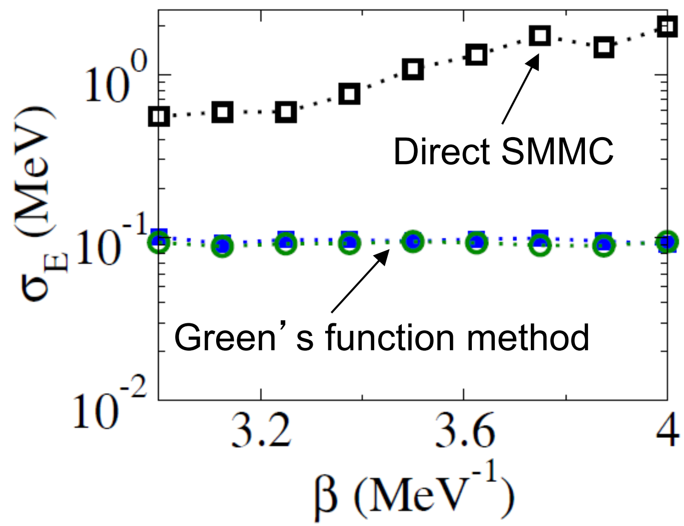
- The energy difference between the lowest energy of the odd-particle system for a given spin j and the ground-state energy of the even-particle system can be extracted from the slope of $\ln G_\nu(\tau)$.

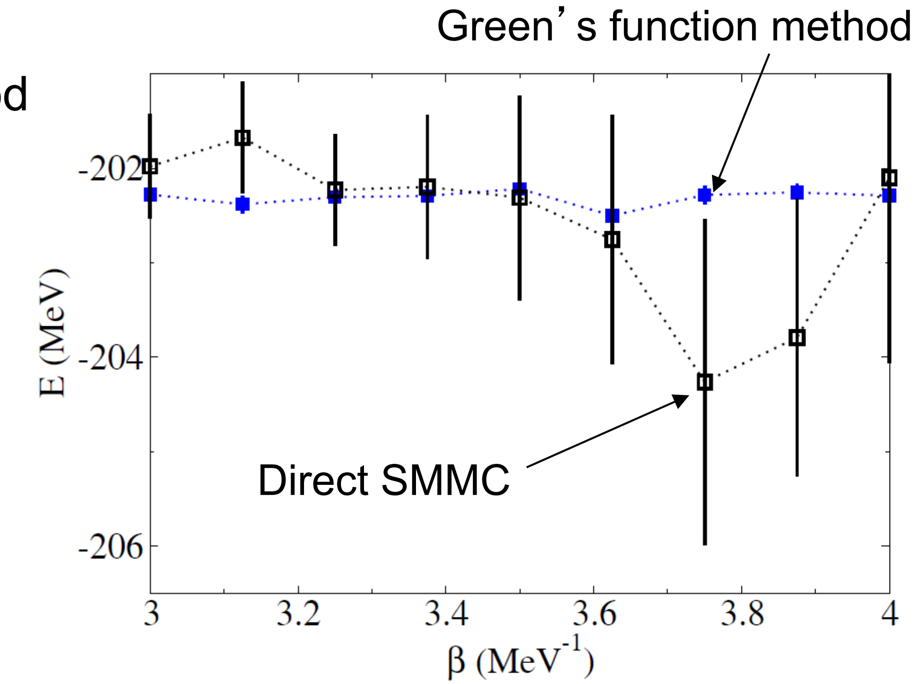


Minimize $E_j(A\pm1)$ to find the ground-state energy and its spin j.

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

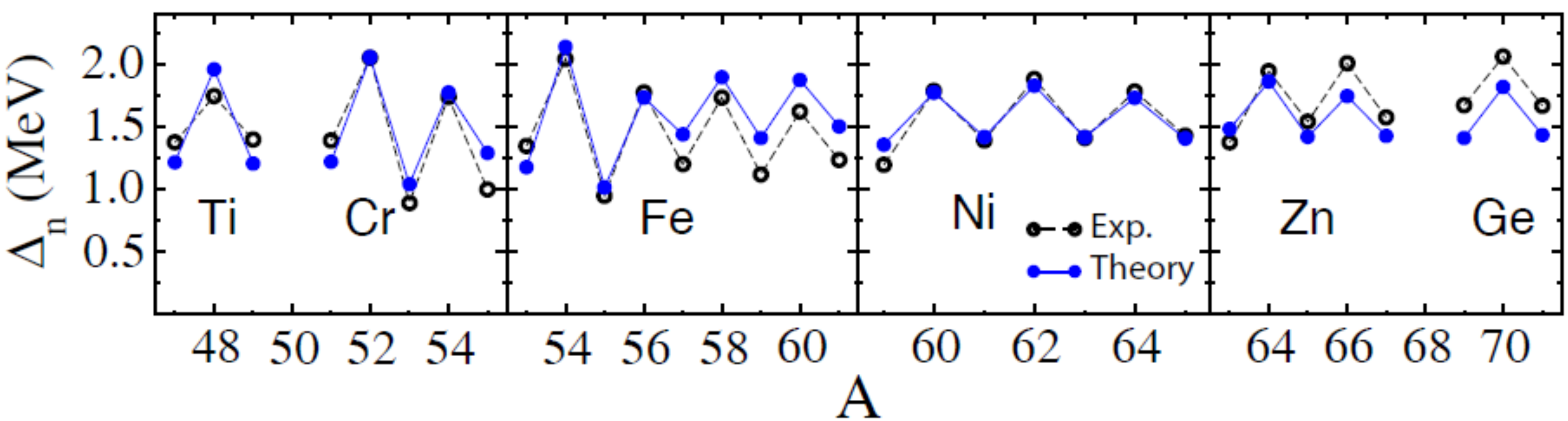
Statistical errors of ground-state energy of direct SMMC versus Green's function method





Pairing gaps in iron region nuclei from odd-even mass differences

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



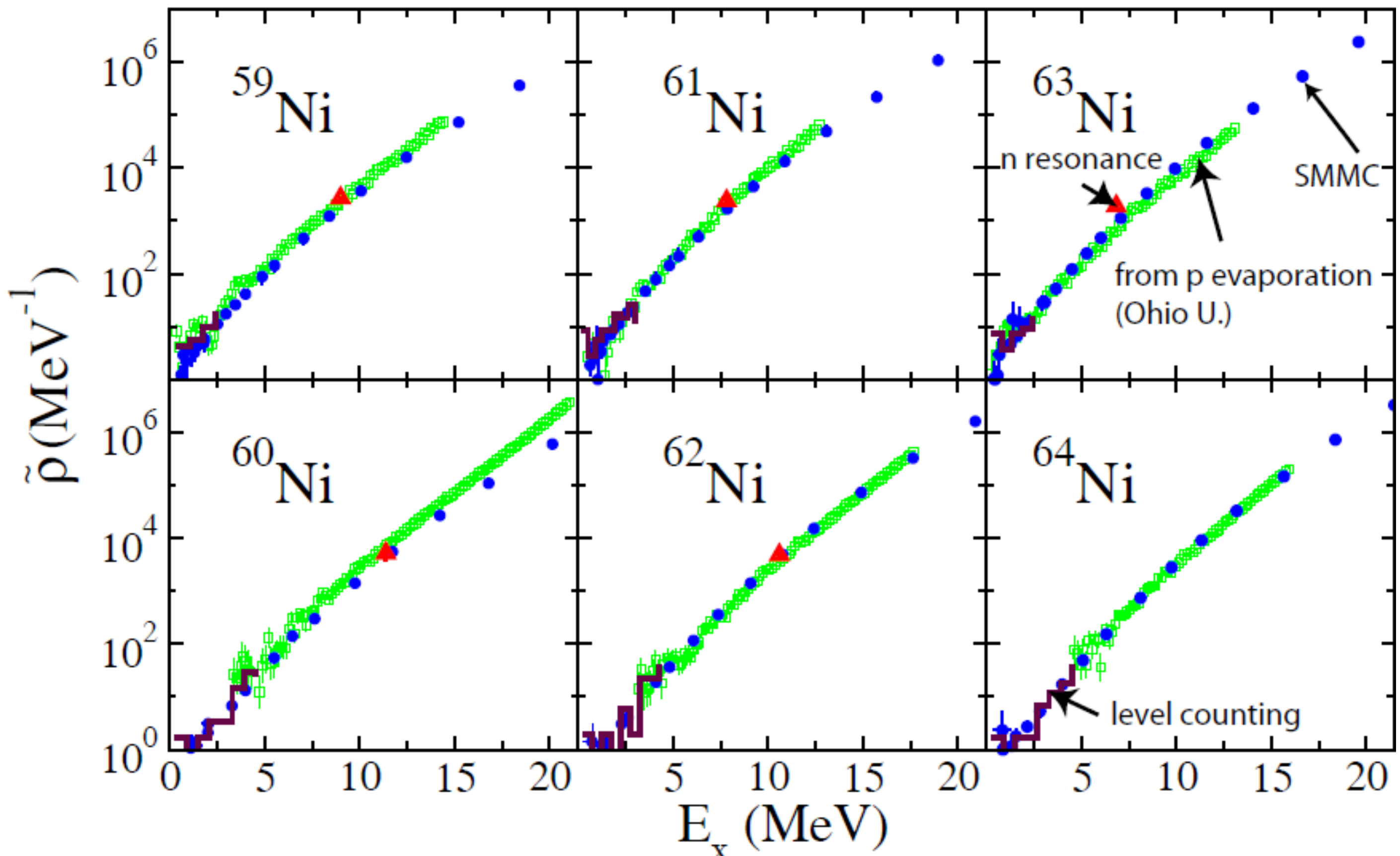
Application to nickel isotopes: theory versus experiment

M. Bonett-Matiz, A. Mukherjee and Y. Alhassid, Phys. Rev. C Rapid Com. **88**, 011302 (2013)

- Recent determination of level densities in nickel isotopes from proton evaporation spectra [A. Voinov et al. (Ohio University group) 2012].

- We can now calculate accurate ground-state energies and thus microscopic level densities for both even-even and even-odd isotopes.

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



Microscopic emergence of collectivity in heavy nuclei

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

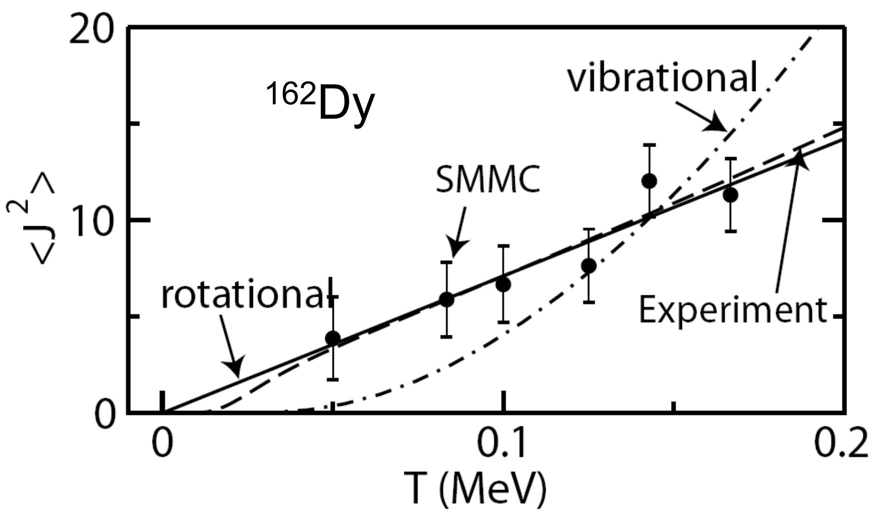
However, a microscopic description (e.g., CI shell model) has been lacking.

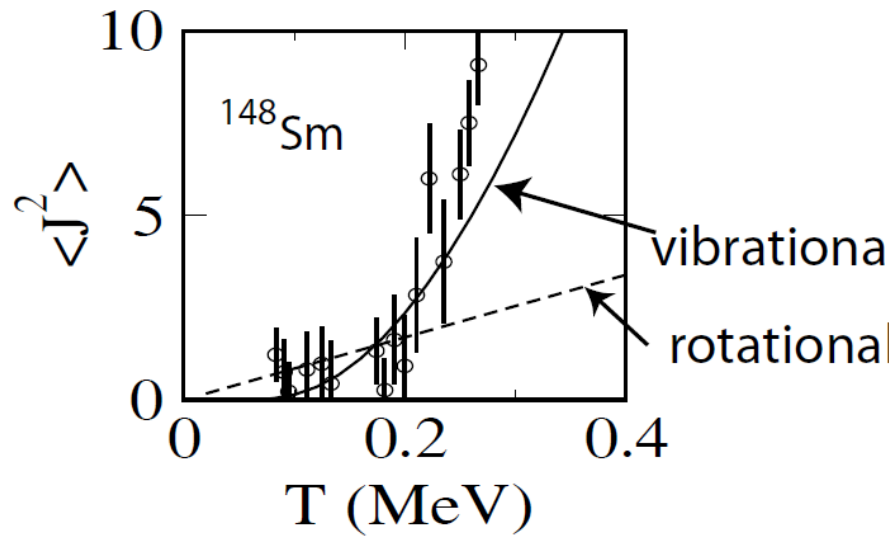
Can we describe vibrational and rotational collectivity in heavy nuclei using the framework of the CI shell model ?

The large model space required (e.g., ~ 10^{29} in rare-earth nuclei) necessitates the use of SMMC.

The various types of collectivity are usually identified by the corresponding spectra, but SMMC does not provide detailed spectroscopy.

The behavior of $<\vec{J}^{\,2}>$ versus T is sensitive to the type of collectivity:





$$<\vec{J}^{\,2}> = \frac{6}{E_{2^+}} T$$

$\Rightarrow {}^{162}Dy$ is rotational

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

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

Y. Alhassid, L. Fang, H. Nakada, PRL (2008)

C. Ozen, Y. Alhassid, H. Nakada, PRL (2013)

Single-particle model space:

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

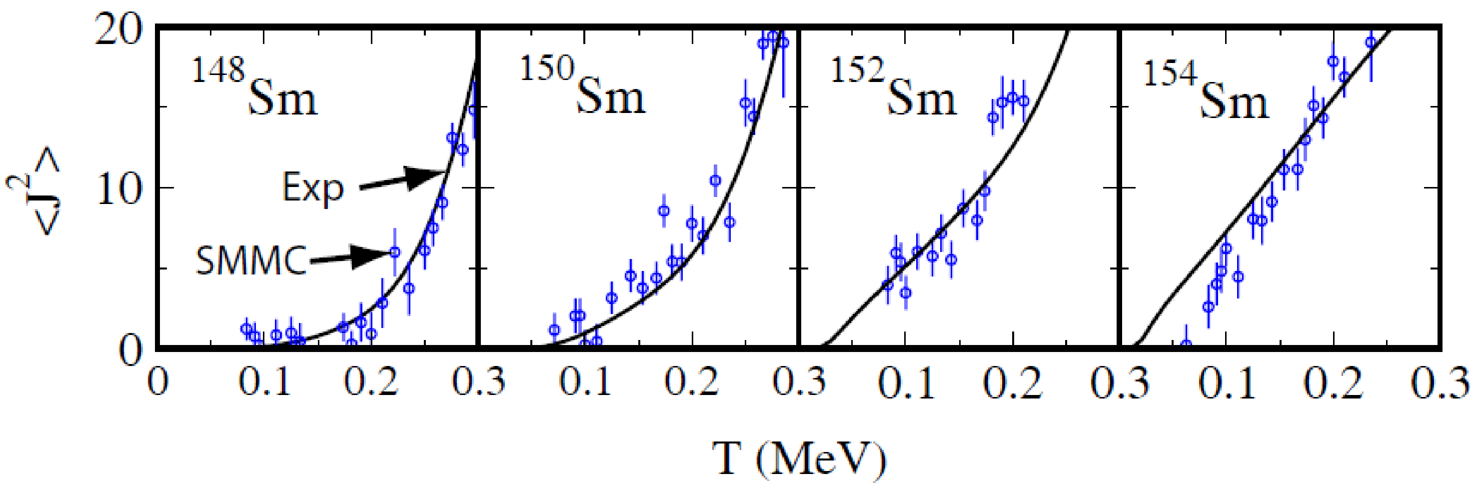
Crossover from vibrational to rotational collectivity in heavy nuclei

C. Ozen, Y. Alhassid, H. Nakada, Phys. Rev. Lett. **110**, 042502 (2013)

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

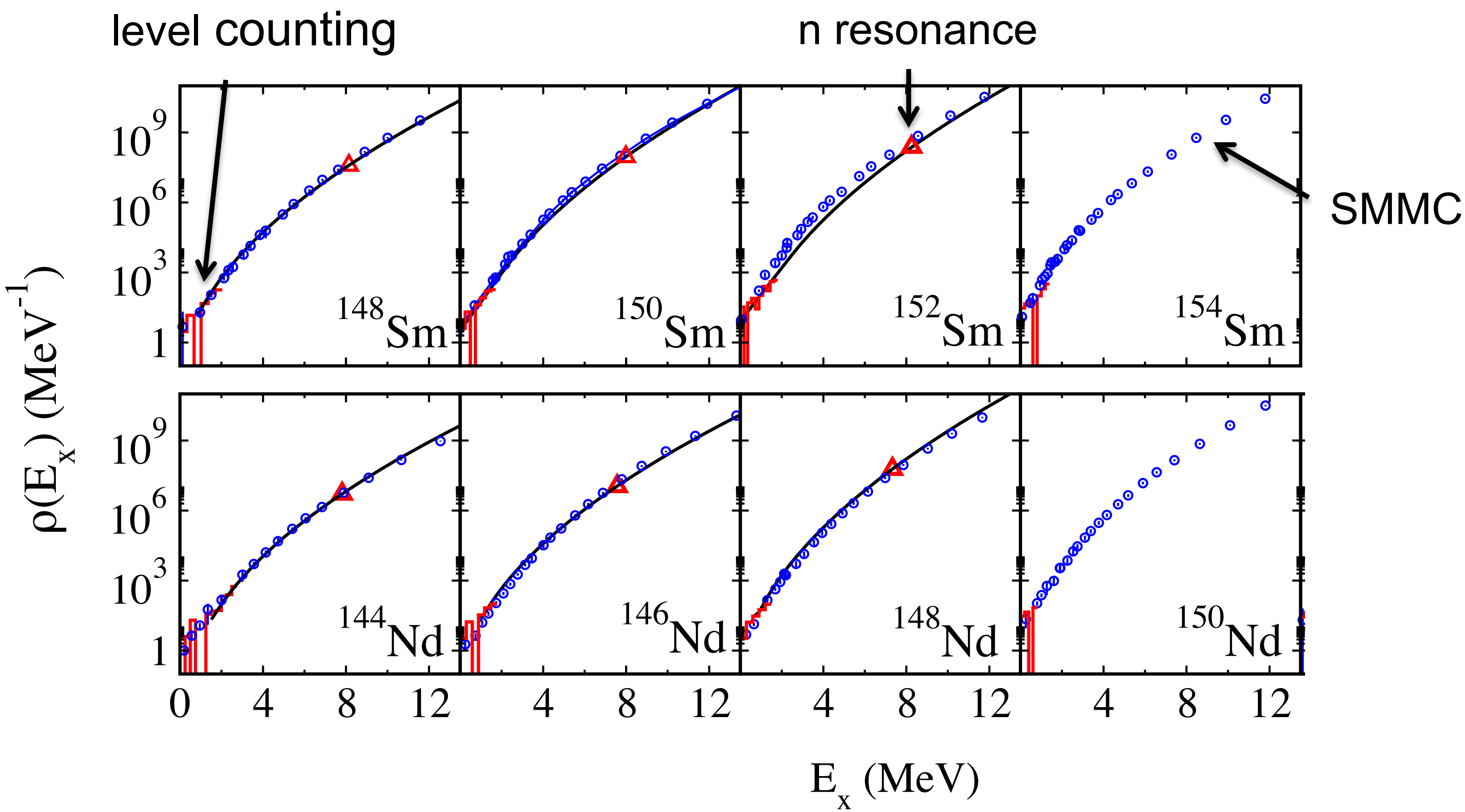
- Experimental values are found from $\langle \vec{J}^2 \rangle = \dfrac{\sum_{\alpha J} J(J+1)(2J+1)e^{-E_{\alpha J}/T}}{\sum_{\alpha J}(2J+1)e^{-E_{\alpha J}/T}}$
where $E_{\alpha J}$ are the experimentally known levels.

- 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

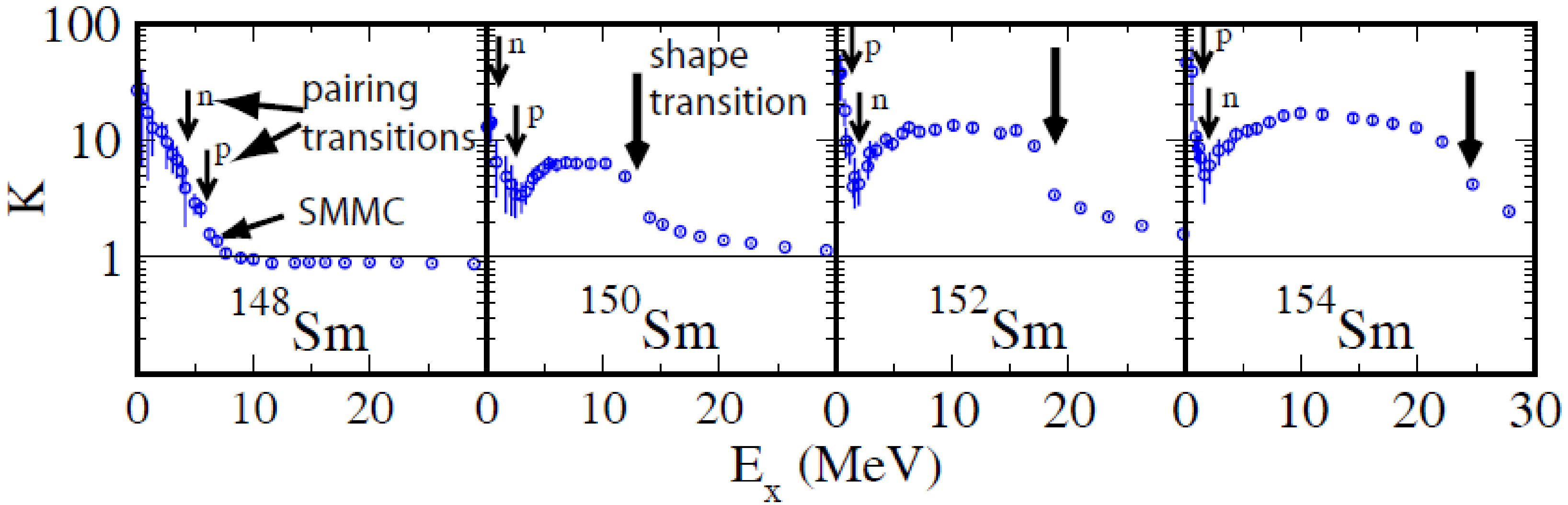


- Excellent agreement of SMMC densities with various experimental data sets.

Collective enhancement factor

Collective enhancement factors K are one of the least understood topics in level densities and are usually treated empirically.

We define K as the ratio of the SMMC state density to the Hartree-Fock-Bogoliubov (HFB) intrinsic density.



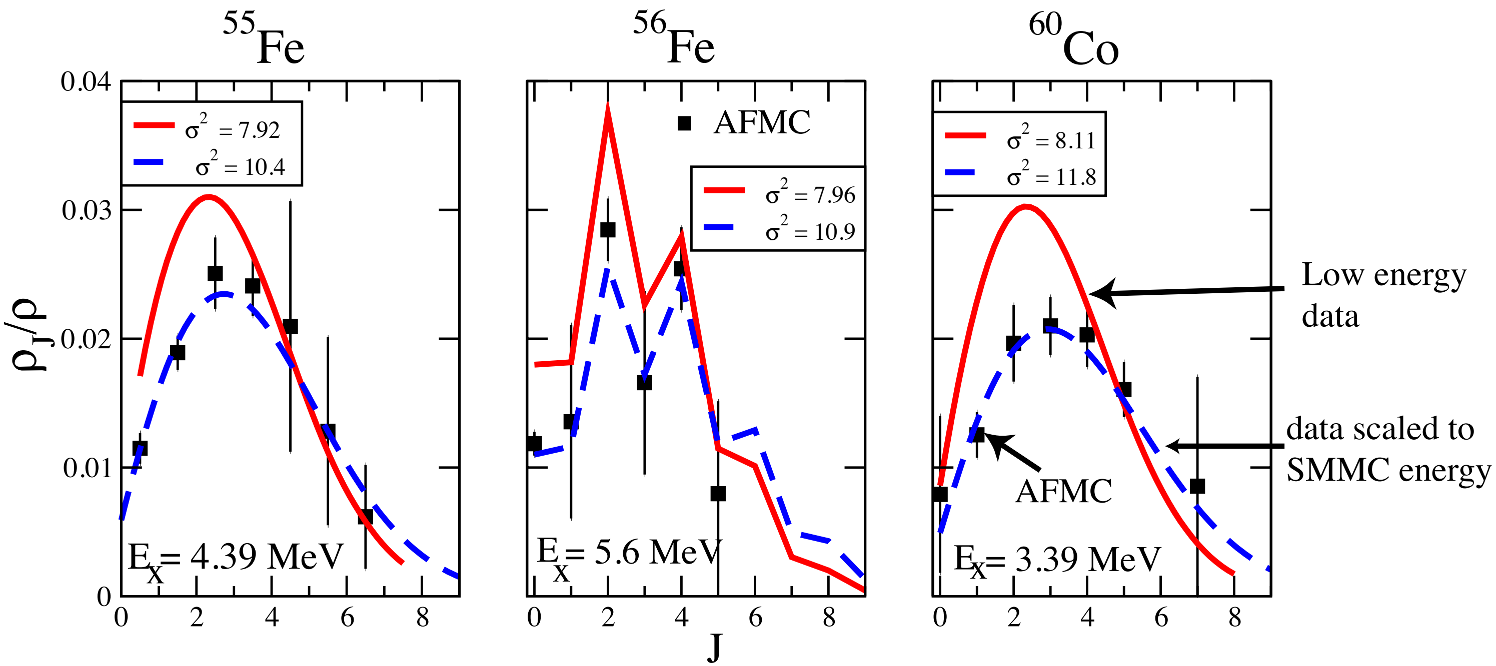
• The damping of vibrational enhancement is correlated with the pairing transition

• A regime of rotational enhancement up to the shape transition.

• The damping of rotational enhancement is correlated with the shape transition.

Spin distributions in SMMC

Y. Alhassid, S. Liu and H. Nakada, Phys. Rev. Lett. **99**, 162504 (2007)



σ^2 = spin cutoff parameter (increases with excitation energy).

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

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

Nuclear deformation in a spherical shell model approach

Y. Alhassid, C.N. Gilbreth, and G.F. Bertsch, arXiv:1408:0081 (2014)

Fission dynamics requires level densities 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 $[Q_{20}, H] \neq 0$).

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

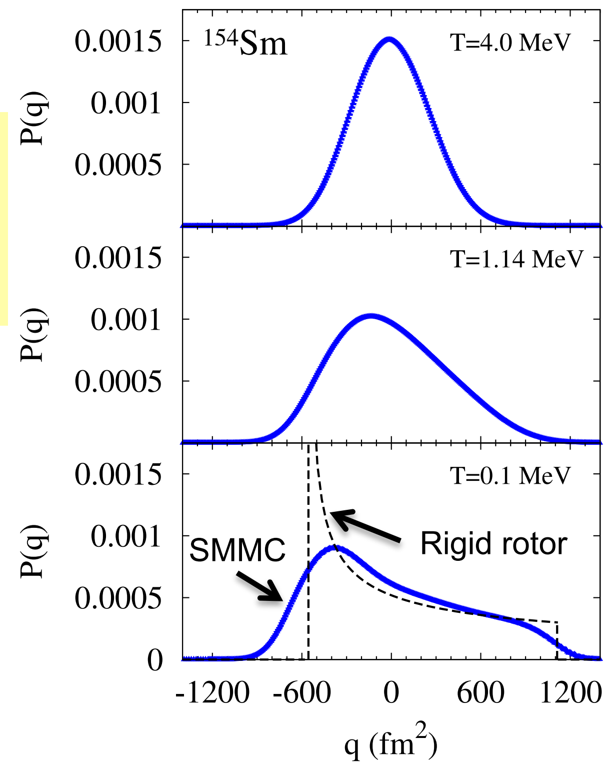
Application to rare-earth nuclei

^{154}Sm (a deformed nucleus)

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

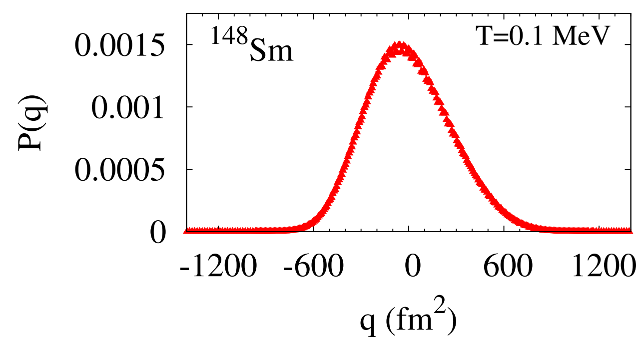
- At the HFB shape transition temperature (T=1.14 MeV), the distribution is still skewed.

- The distribution at high temperatures is close to a Gaussian



^{148}Sm (a spherical nucleus)

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



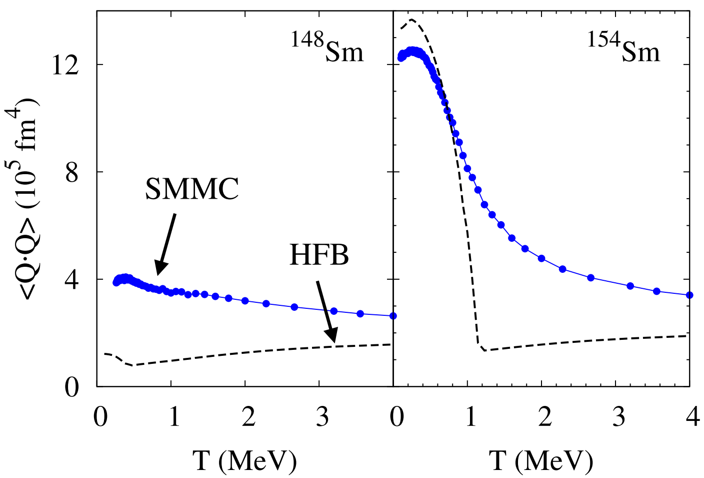
Intrinsic deformation from lab frame distributions

- Information on intrinsic deformation can be obtained from the expectation values of rotationally invariant combinations of $Q_{2\mu}$

Example: the lowest order invariant is second order $\langle Q \cdot Q \rangle$

$$\beta \propto (\langle Q \cdot Q \rangle)^{1/2}$$

The sharp shape transition in HFB is washed out in the finite-size nucleus



$$\cos 3\gamma = -\sqrt{\frac{7}{2}} \frac{\langle (Q \times Q) \cdot Q \rangle}{\langle Q \cdot Q \rangle^{3/2}}$$

- The quadrupole invariants can be calculated from lab frame moments of Q_{20}

➡ Construct the joint level density distribution $\rho(\beta, E_x) = \rho(E_x) P_{E_x}(\beta)$

where $P_{E_x}(\beta)$ is the intrinsic shape distribution at given excitation energy E_x

Conclusion

- SMMC is a powerful method for the microscopic calculation of level densities in very large model spaces.
- We have circumvented the odd-particle sign problem in SMMC, enabling the calculation of level densities of odd-mass nuclei.
- Microscopic description of collectivity in heavy nuclei.
- Damping of the collective vibrational and rotational enhancement factors of level densities correlates with the pairing and shape phase transitions.
- Description of nuclear deformation in a rotationally invariant framework.

Prospects

- Other mass regions (actinides, unstable nuclei,…).
- Level densities as a function of deformation (useful for fission).
- Derive *global* effective shell model interactions from density functional theory.