Recent Developments and Applications of the Auxiliary-Field Monte Carlo Method

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Computational Challenges in Nuclear and Many-Body Physics

Nordita, Sept 16, 2014

Outline

- Finite-temperature auxiliary-field quantum Monte Carlo (AFMC) for the canonical ensemble
- Stabilizing canonical-ensemble calculations in AFMC
- Odd particle-number systems in AFMC: Circumventing a sign problem
- Vibrational and rotational collectivity in heavy nuclei
- Nuclear deformation in the spherical shell model approach

Auxiliary-field quantum Monte Carlo (AFMC)

- A method for studying highly-correlated systems which is free of systematic errors
- Advantages:
  - Permits finite-temperature calculations
  - No fixed-node approximations (for good sign interactions)
  - Useful in a variety of systems (electronic structure, nuclear physics, atomic physics, chemistry)
  - Allows calculation of any one- or two-body observable
- Challenges:
  - Sign problem for "repulsive" interactions and certain projections
  - Scaling is $N_s^3 \times N_t$ or $N_s^4 \times N_t$, depending on the application
  - Numerical stability at low temperatures / large model spaces

- Given hamiltonian $\hat{H}$ with one-body and two-body parts, apply the Hubbard-Stratonovich (HS) transformation to obtain

$$e^{-\beta \hat{H}} = \int \underbrace{D[\sigma]}_{\text{Integration measure}} \underbrace{G_\sigma}_{\text{Gaussian weight}} \underbrace{\hat{U}(\sigma)}_{\text{Non-interacting propagator}}$$

Time-dependent auxiliary fields (many)

Integration measure

Non-interacting propagator

Gaussian weight

- A path-integral of a non-interacting propagator with respect to fluctuating time-dependent fields.

- Observables with respect to $\hat{U}(\sigma)$ can be determined using matrix algebra in the single-particle space (typical dimension 50-100's)

- The integral is discretized and observables are sampled stochastically:

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}[e^{-\beta \hat{H}} \hat{O}]}{\mathrm{Tr}\, e^{-\beta \hat{H}}} = \sum_{k=1}^{N_{\mathrm{samp}}} \langle \hat{O} \rangle_{\sigma_k} \qquad \langle \hat{O} \rangle_\sigma = \frac{\mathrm{Tr}[\hat{U}(\sigma)\hat{O}]}{\mathrm{Tr}\, \hat{U}(\sigma)}$$

- $\hat{O} =$ one- or two-body observable; traces can include projections.

Canonical ensemble: exact particle-number projection

- For fixed particle number, we utilize a discrete Fourier Transform

$$\mathrm{Tr}_N[\hat{O}\hat{U}(\sigma)] = \frac{1}{N_s}\sum_{m=1}^{N_s} e^{-i\varphi_m N}\,\mathrm{Tr}_{\mathrm{GC}}[\hat{O}\hat{U}(\sigma)e^{i\varphi_m \hat{N}}]\,.$$

Number of single-particle states (N_s)

Canonical trace, N = number of particles

$\varphi_m \equiv 2\pi m/N_s$

Grand-canonical trace

[W. E. Ormand, et al., Phys. Rev. C **49**, 1422 (1994)]

- Important for finite-size systems such as nuclei, metallic nanoparticles, …

Shell-Model Monte Carlo (SMMC)

- The application of AFMC to atomic nuclei in the configuration-interaction (CI) shell model approach.
- Have studied nuclei in model spaces as large as ~10^{30}
- Successful for calculating statistical and collective properties of nuclei (e.g., level densities, pairing gaps, deformation)

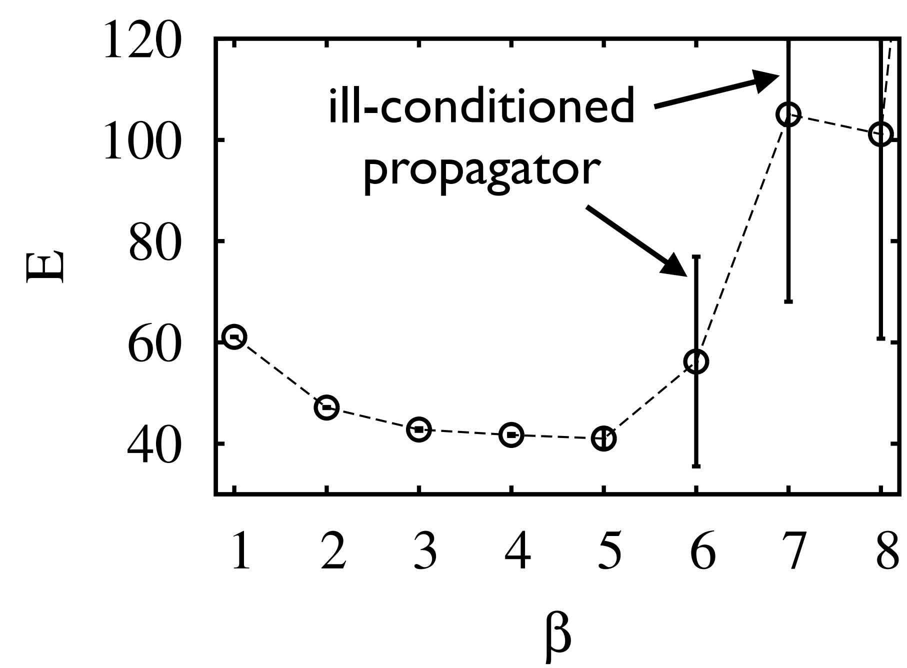
Stabilizing canonical-ensemble calculations in AFMC

C. N. Gilbreth and Y. Alhassid, Computer Physics Communications (2014) (in press)

- Low-temperature AFMC calculations require long chains of matrix products to compute the propagator $\hat{U}$,

$$U(\beta) = U_{N_t} U_{N_t - 1} \cdots U_1, \quad N_t \sim 512$$

- For large N_t, the matrix U becomes ill-conditioned (ratio of largest to smallest eigenvalues is very large). Small and intermediate scales are lost among large numbers, leading to inaccurate results.



Energy vs. inverse temperature for 20 cold atoms in the unitary limit.

- Known solution: Compute a decomposed form of *U*,

[E.Y. Loh Jr and J. E. Gubernatis, 1992]

$$U = ADB = \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} X & & \\ & x & \\ & & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}$$

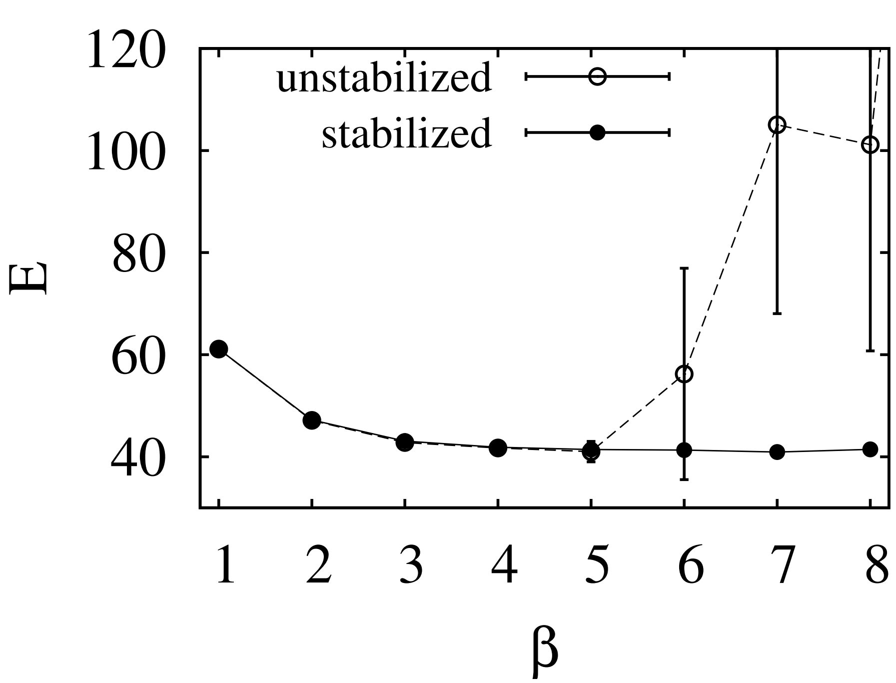
A, B well-conditioned,
$D > 0$ diagonal

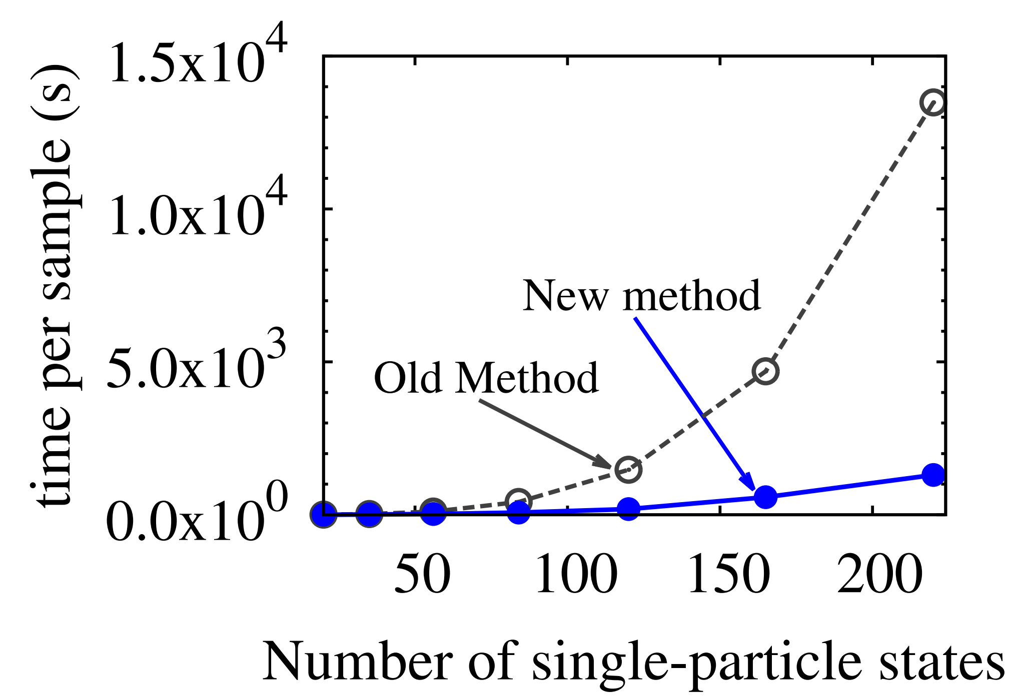
such as singular value decomposition (SVD) or modified Gram-Schmidt (MGS), which explicitly displays scales along the diagonal.

- Canonical trace: $\mathrm{Tr}_N \hat{U} = \frac{1}{N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m N} \det(1 + U e^{i\varphi_m}) \quad (U = ADB)$
- Usual implementation: decompose $1 + U e^{i\varphi_m}$ for every determinant in the Fourier sum. Each decomposition takes $O(N_s^3)$ operations, so the sum requires $O(N_s^4)$ operations.
- Improved method: Consider $A^{-1} U A = DBA$:

$$DBA = \begin{pmatrix} X & & \\ & X & \\ & & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} = \begin{pmatrix} X & X & X \\ X & X & X \\ x & x & x \end{pmatrix}$$

which is "row-stratified" and *similar* to U. Diagonalize once; then each determinant costs $O(N_s)$ operations. The sum now requires only $O(N_s^3)$ operations.



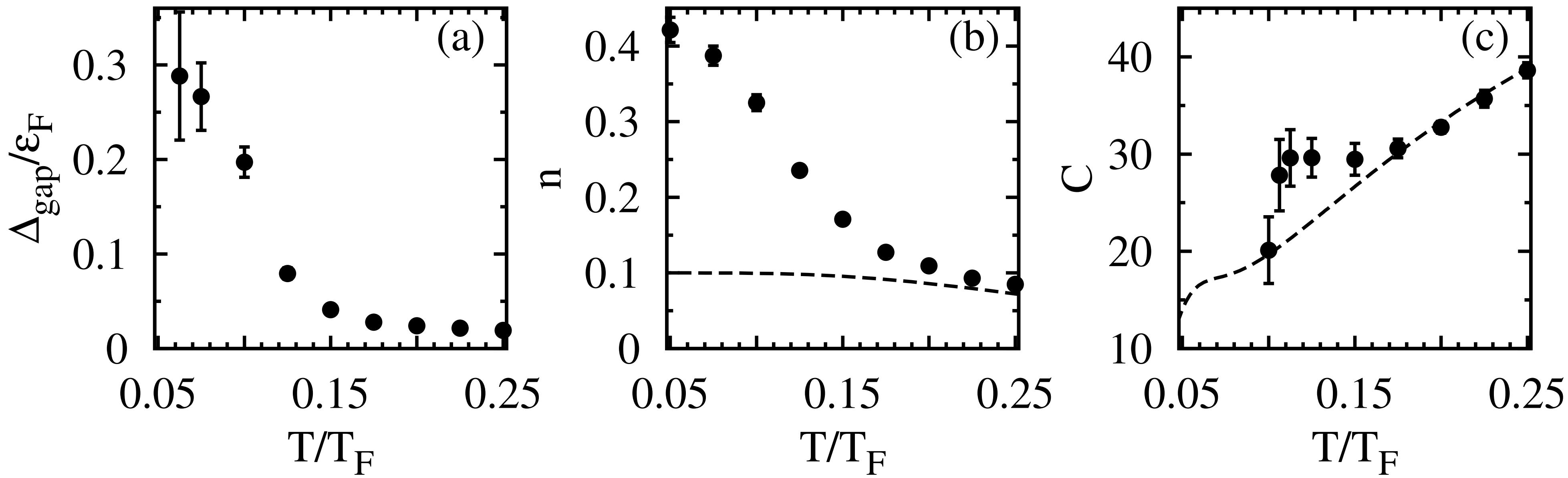


significant speed-up

Application: cold atoms

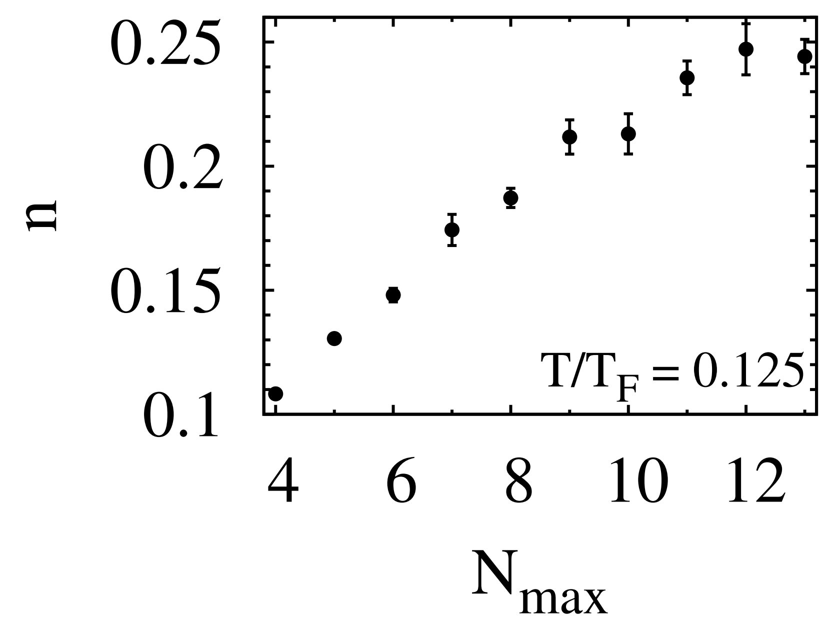
C. N. Gilbreth and Y. Alhassid, Phys. Rev. A **88**, 063643 (2013)

- This new stabilization method allows us to study larger systems that would otherwise not be possible in the canonical ensemble.



pairing gap | condensate fraction | heat capacity

- Cold atoms: 10+10 particles, $N_s = 364$ (10^{38} many-particle states) to reach convergence, in the unitary limit of infinite scattering length.
- First *ab initio* calculation of the heat capacity across the superfluid phase transition.
- Clear signatures of the superfluid phase transition



Convergence in the number of oscillator shells N_{max}

Odd-particle systems in AFMC: circumventing a sign problem

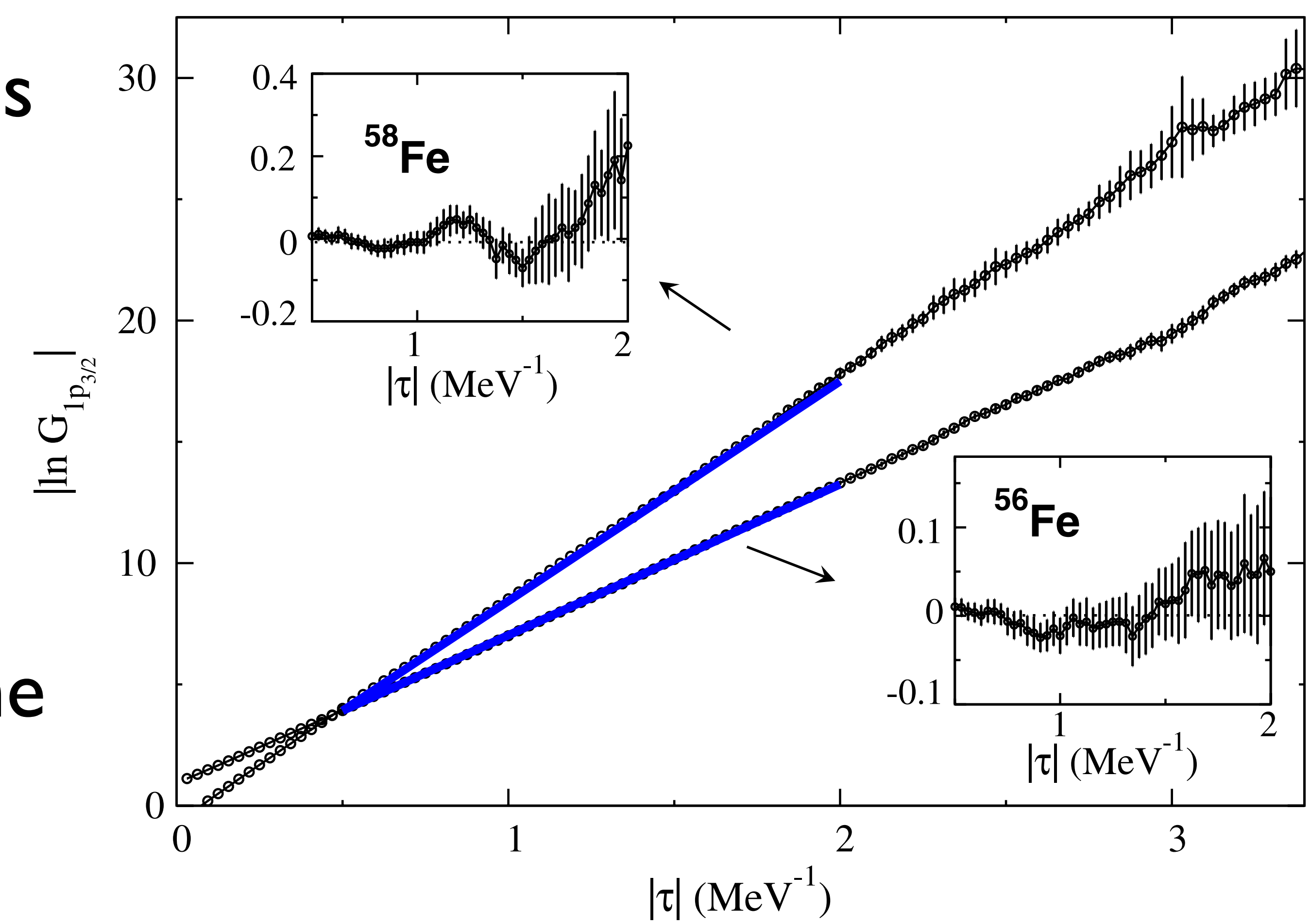
A. Mukherjee and Y. Alhassid, Phys. Rev. Lett. **109**, 032503 (2012)

- Particle-number projection introduces a sign problem which has hampered application of SMMC to odd-even and odd-odd nuclei.
- Breakthrough method: utilize the imaginary-time Green's function,

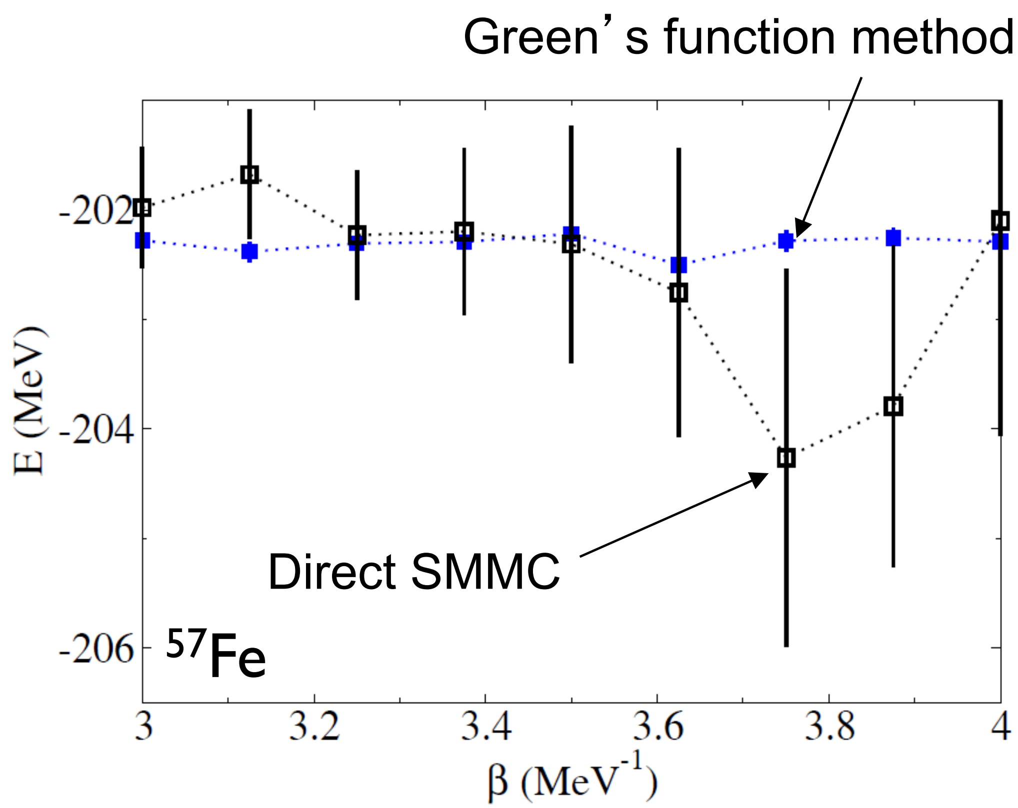
$$G_\nu(\tau) = \sum_m \langle T a_{\nu m}(\tau) a^\dagger_{\nu m}(0)\rangle \qquad \nu = (nlj), \quad m = -j,\ldots,j$$

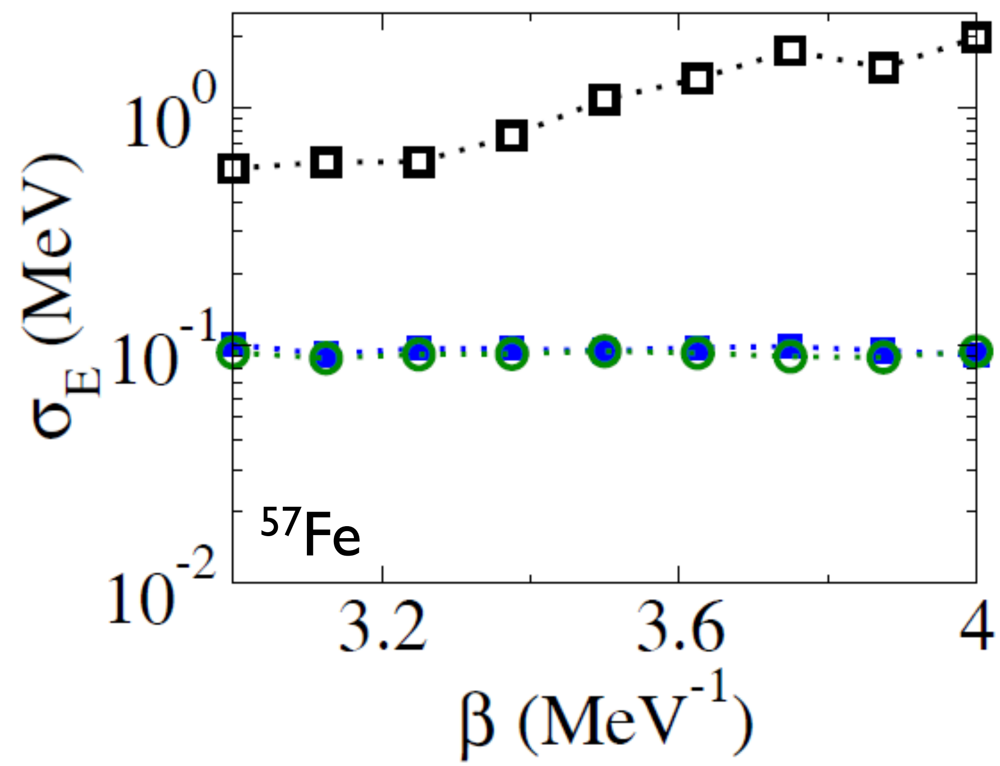
$$G_\nu(\tau) \sim e^{-\beta[E_j(A\pm1) - E_{\rm g.s.}(A)]|\tau|} \qquad (\beta \gg |\tau| \gg 0)$$

- The slope of $\log G_\nu(\tau)$ determines the energy difference between the g.s. of the A-particle system and the lowest energy of the $A \pm 1$ system with angular momentum *j*
- Minimize $E_j(A\pm1)$ to determine the g.s. energy and *j*

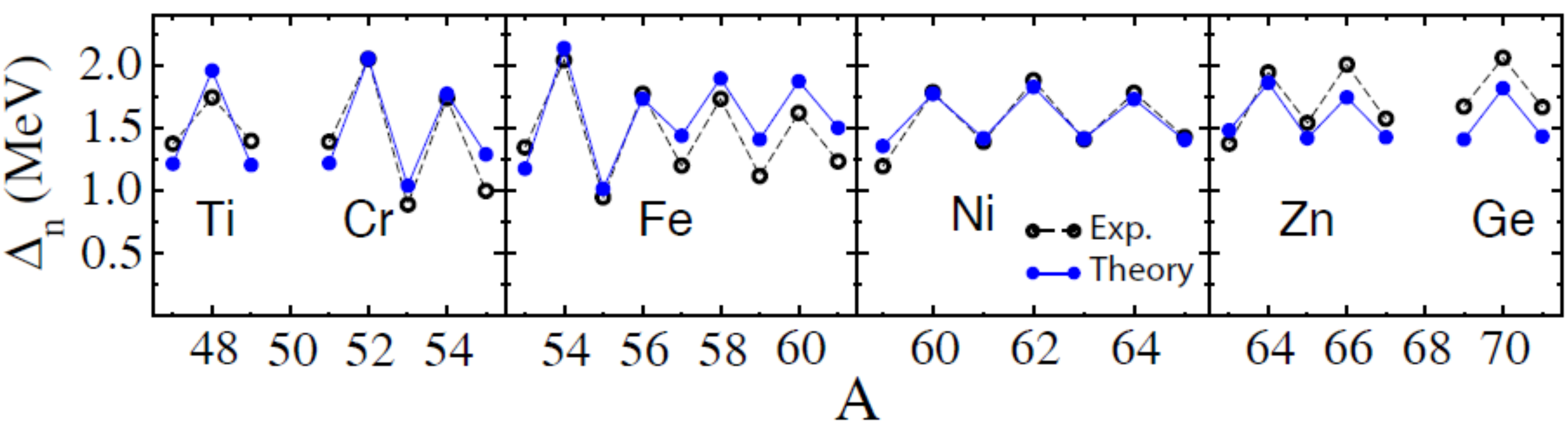


- Statistical errors of ground-state energy





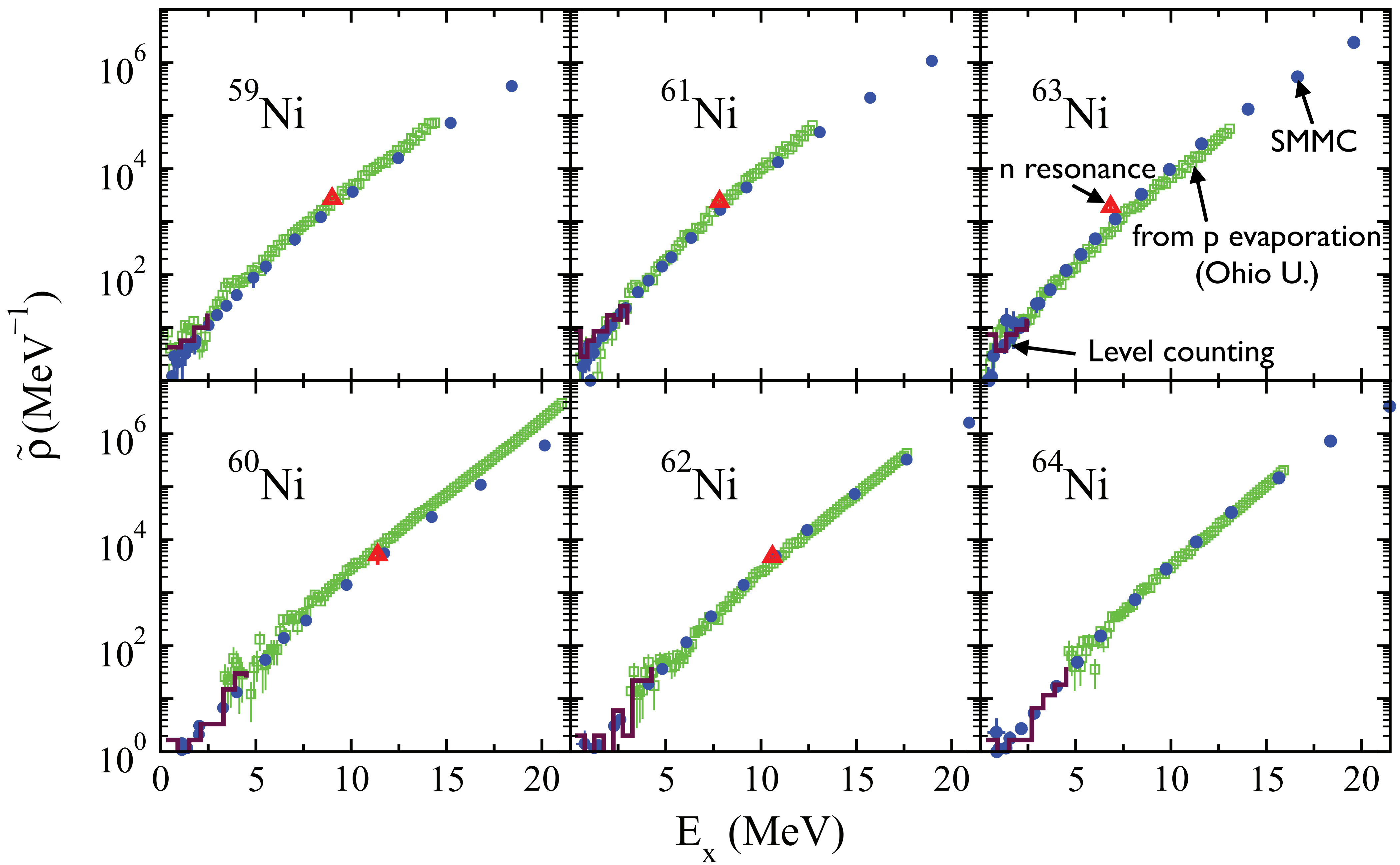
- Pairing gaps in mid-mass nuclei from even-odd mass differences (good agreement with experiments)



Application to nickel isotopes: theory versus experiment

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

- The Green's function method allows calculation of ground-state energies, and hence level densities, of odd-mass isotopes



- Excellent agreement with experimental data

Vibrational and rotational collectivity in heavy nuclei

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

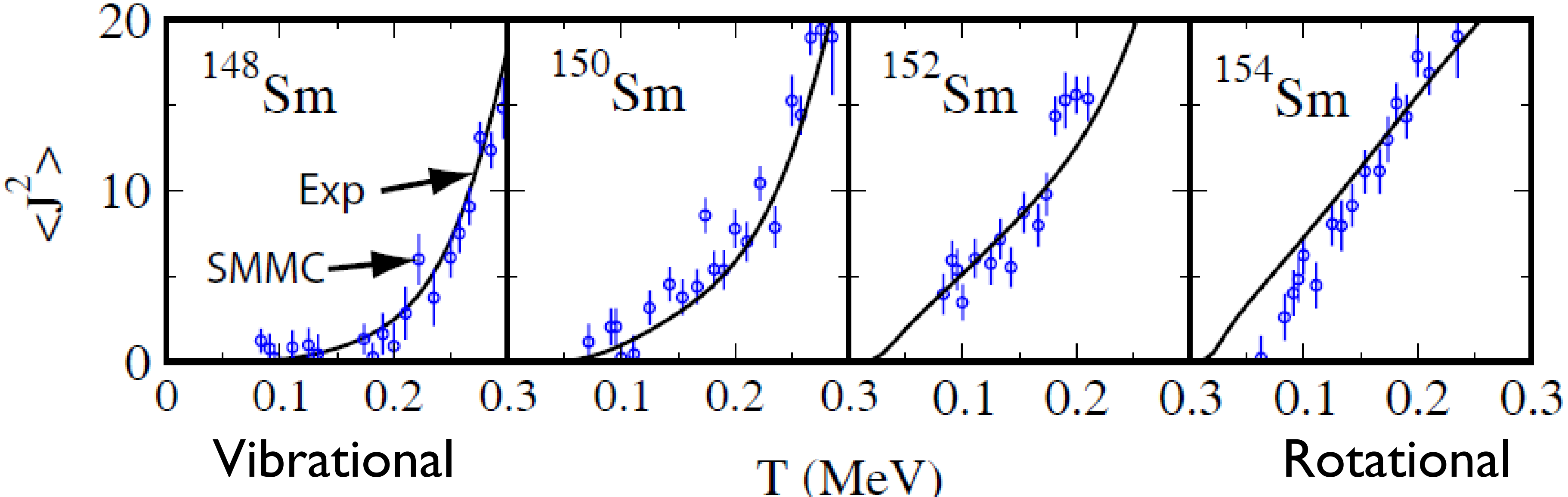
- Heavy nuclei exhibit a crossover from vibrational to rotational collectivity as the number of neutrons increases from shell-closure toward midshell, which is reproduced by empirical models.

- Can the crossover be reproduced microscopically using a truncated spherical shell model approach?

- Technical challenges for microscopic nuclear physics calculations:
  - Large model spaces
  - Small excitation energies (large β required)
  - Numerical stabilization

- Need to identify a signature of collective behavior in nuclei using SMMC, where spectroscopic information is not readily available.

- The low-temperature behavior of $\langle J^2 \rangle$ is sensitive to the type of collectivity.



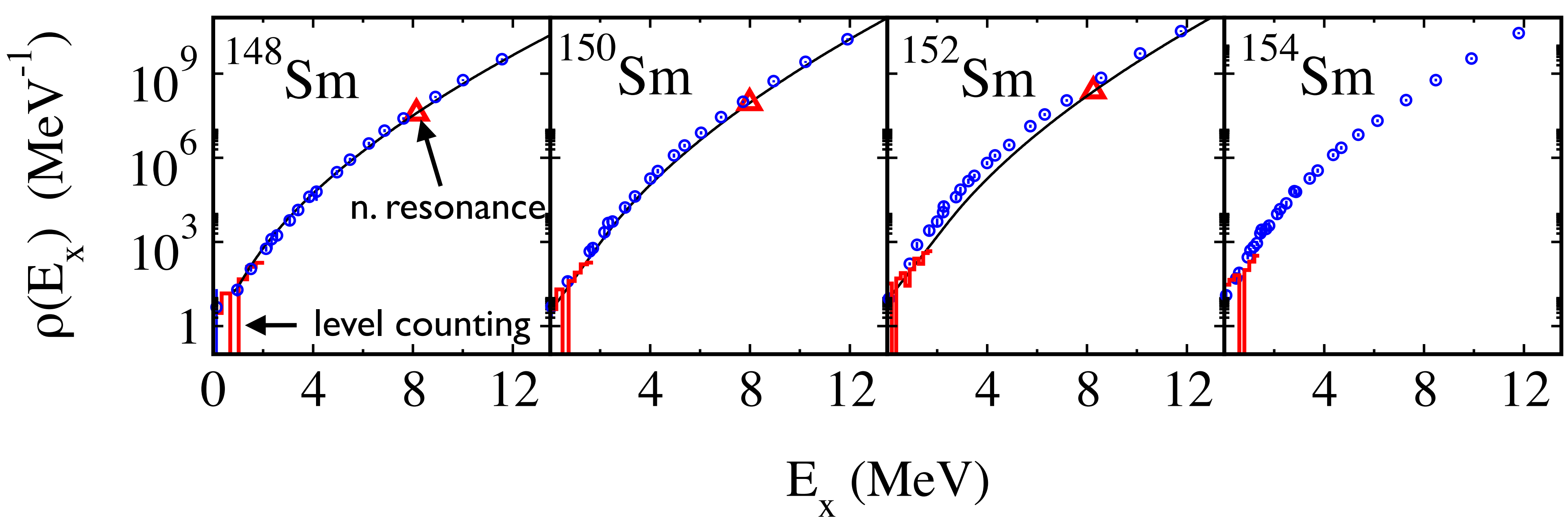
E	Theory (MeV)	Expt (MeV)
148	0.538(31)	0.550
154	0.087(6)	0.082

$$\langle J^2 \rangle_T \approx 30 \frac{e^{-E_{2^+}/T}}{(1-e^{-E_{2^+}/T})^2}$$

$$\langle J^2 \rangle_T \approx \frac{6}{E_{2^+}} T$$

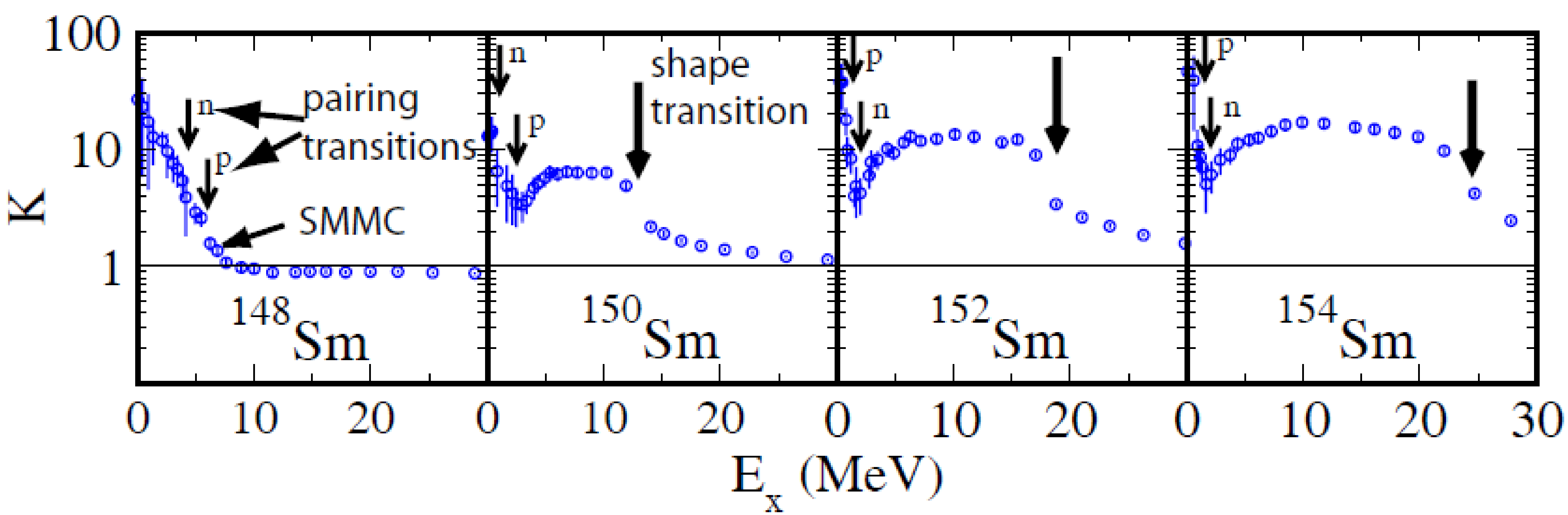
- Clear crossover from vibrational to rotational behavior for samarium isotopes. Values of E_{2^+} agree well with experiment.

- State densities in samarium isotopes:



Collective enhancement factors

- Mean-field [e.g., Hartree-Fock-Bogoliubov (HFB)] level densities do not include important contributions from collective states.
- Collective enhancement factors are one of the least understood aspects of nuclear level densities.
- We define the collective enhancement factor *K* as the ratio between the SMMC and the HFB level densities.



- The damping of the vibrational and rotational enhancement with excitation energy is correlated with the pairing and shape transitions, respectively.

Nuclear deformations in AFMC

Y. Alhassid, C. N. Gilbreth and G. F. Bertsch, arXiv:1408.0081 [nucl-th]

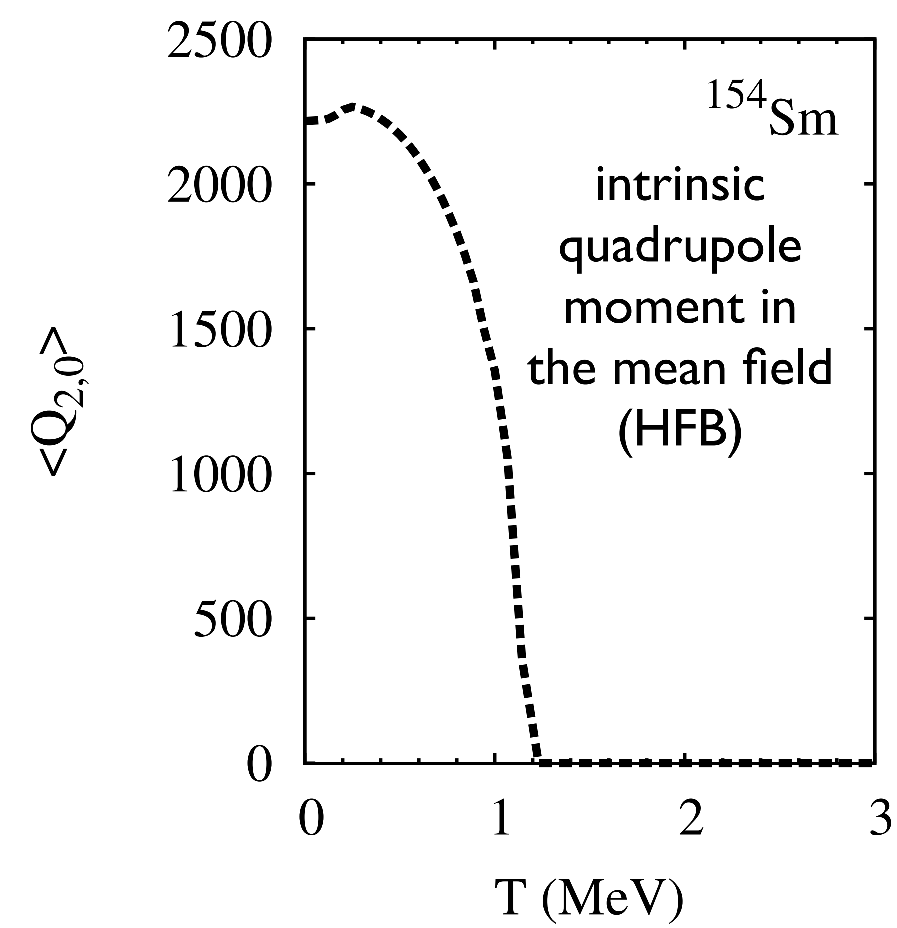
- Mean-field theory is a convenient framework for the study of the intrinsic structure of deformed nuclei, but breaks rotational invariance.
- It also predicts sharp phase transitions, which are washed out in finite systems.
- The challenge is to study nuclear deformation in a framework which *preserves rotational invariance* and captures *finite-size effects*.

Nuclear shapes

$$R = R(\theta,\phi) = R_0\left(1 + \sum_{\lambda,\mu} a^*_{\lambda,\mu} Y_{\lambda,\mu}(\theta,\phi)\right)$$

- The most important nuclear deformation is the quadrupole ($\lambda = 2$), characterized by the mass quadrupole operator

$$Q_{2,\mu} = \sqrt{\frac{16\pi}{5}} \sum_i r_i^2 Y_{2\mu}(\Omega_i)$$ (sum over particles)



- We study the distribution of $\hat{Q}_{2,0}$ by discretizing the Fourier transform

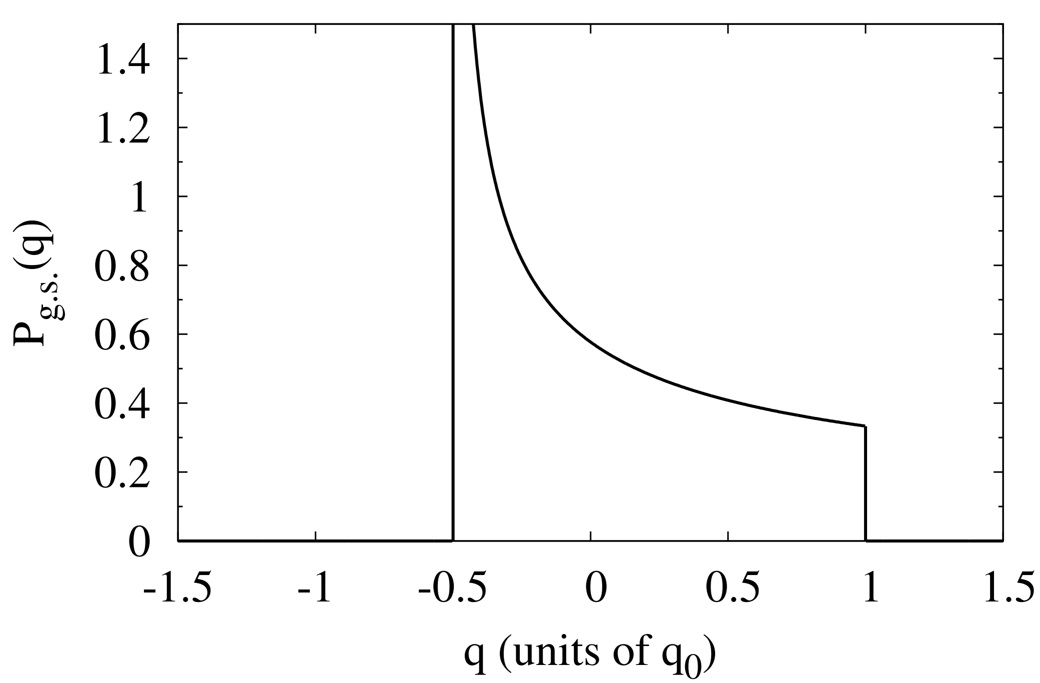
$$P_\beta(q) = \langle \delta(\hat{Q}_{2,0} - q) \rangle = \frac{1}{\mathrm{Tr}\, e^{-\beta \hat{H}}} \int_{-\infty}^{\infty} \frac{d\varphi}{2\pi} e^{-i\varphi q} \mathrm{Tr}\left(e^{i\varphi \hat{Q}_{2,0}} e^{-\beta \hat{H}} \right)$$

- Since $\hat{Q}_{2,0}$ is a one-body operator, we can compute its distribution.
- $[\hat{Q}_{2,0}, \hat{H}] \neq 0$, unlike in other projections (e.g., particle number, spin):

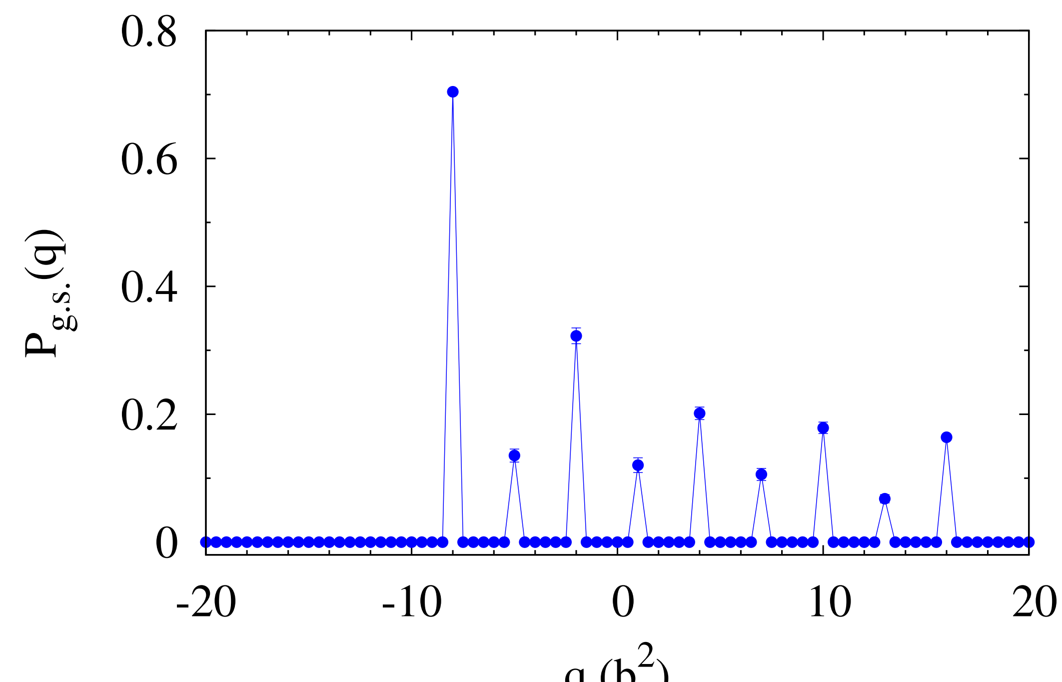
$$P_\beta(q) = \sum_n \delta(q - q_n) \sum_m \langle q, n | e, m \rangle^2 e^{-\beta e_m}$$

- The distribution $P_\beta(q)$ is slow to equilibrate (long decorrelation times). To resolve this problem, we average $P_\beta(q)$ over carefully chosen rotations of $\hat{Q}_{2,0}$ (equivalent to rotating the auxiliary fields).

Prolate rigid rotor with intrinsic quadrupole moment q_0



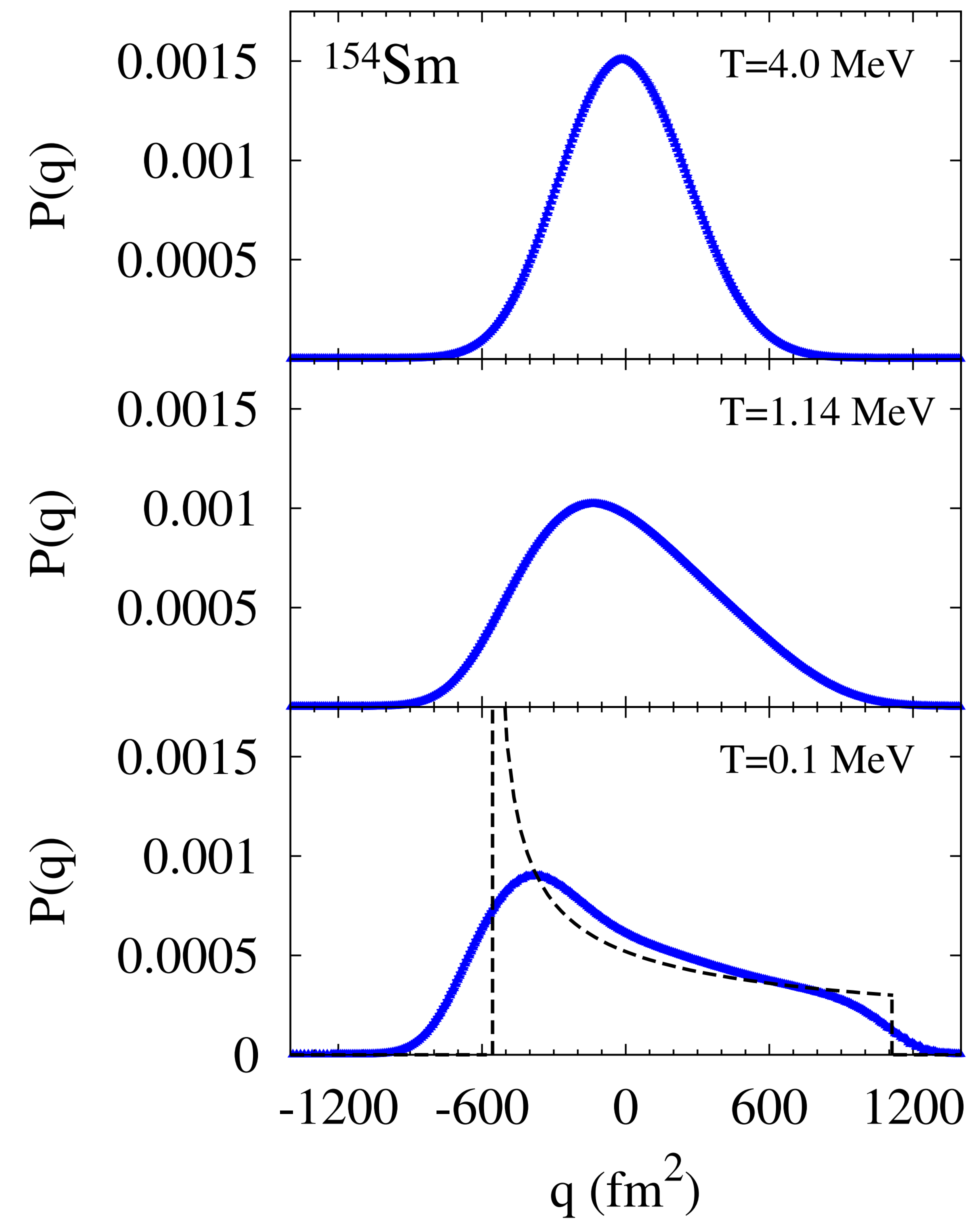
Test case: ^{20}Ne
($Q_{2,0}$ has a discrete spectrum)



Application to ^{154}Sm and ^{148}Sm

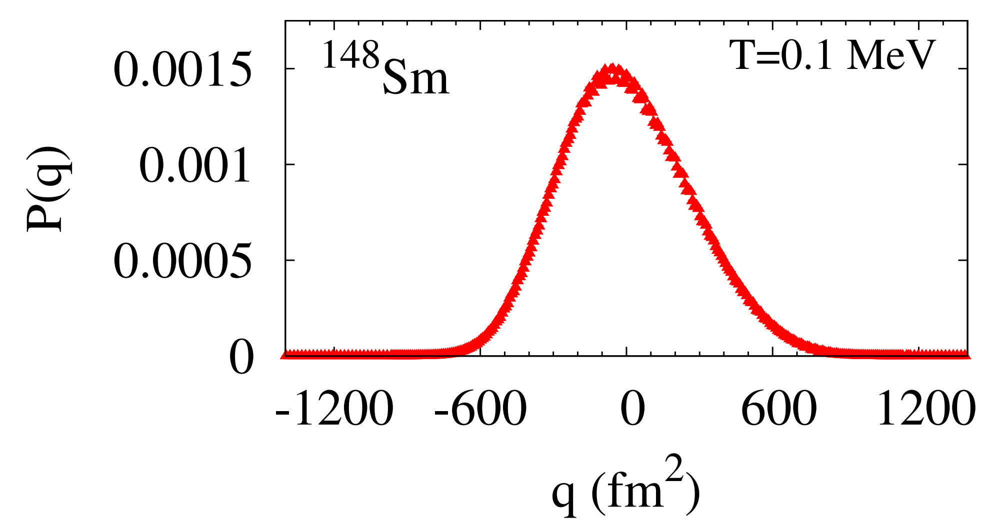
- At $T = \infty$, $P_\beta(q)$ is the many-particle eigenvalue distribution of $\hat{Q}_{2,0}$

^{154}Sm (deformed in HFB)



- The many-particle eigenvalues are closely spaced, giving effectively a continuous distribution.
- At high temperatures, a Gaussian.
- At the mean-field shape transition (T = 1.14 MeV), distribution is skewed.
- At low temperatures, the distribution is similar to that of a prolate rigid rotor, a clear signature of deformation.

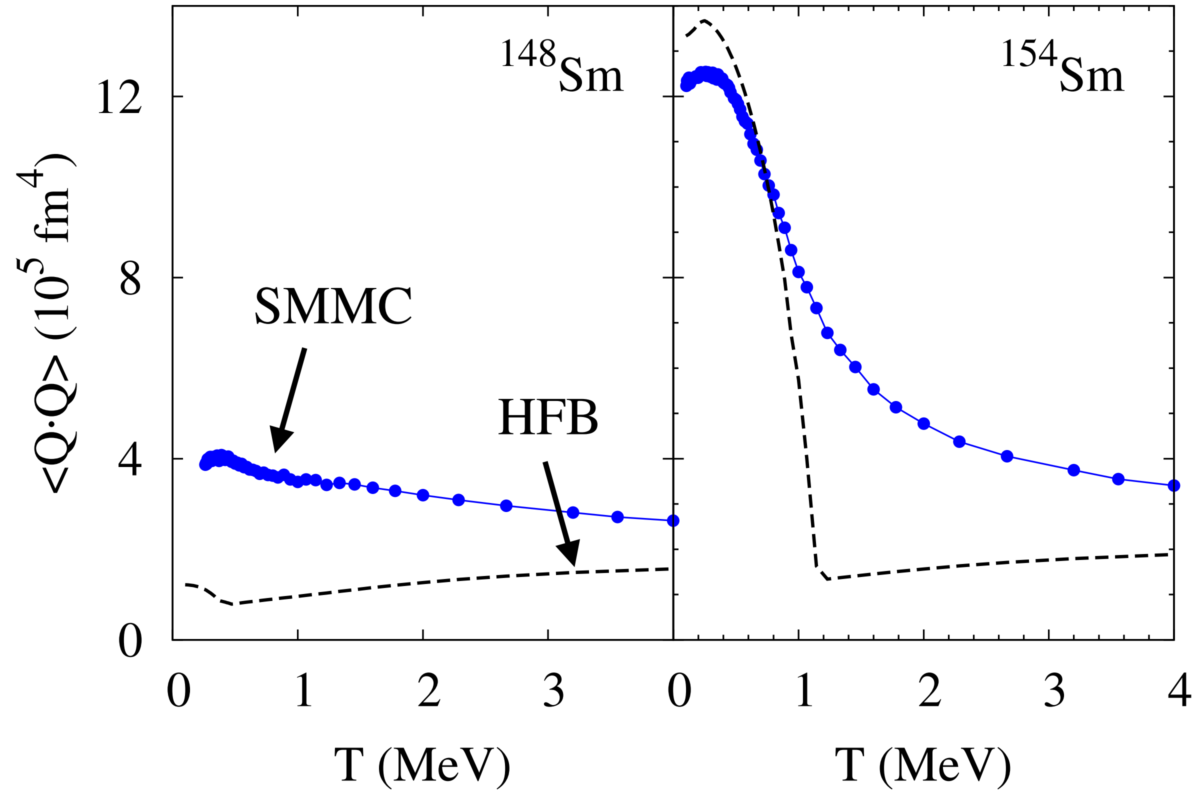
^{148}Sm (spherical in HFB)



- $P_\beta(q)$ is close to a Gaussian even at low temperatures.

Intrinsic deformation

- Information on the intrinsic deformation can be obtained from rotationally invariant combinations of $\hat{Q}_{2,\mu}$, which are related to the moments of $\hat{Q}_{2,0}$.



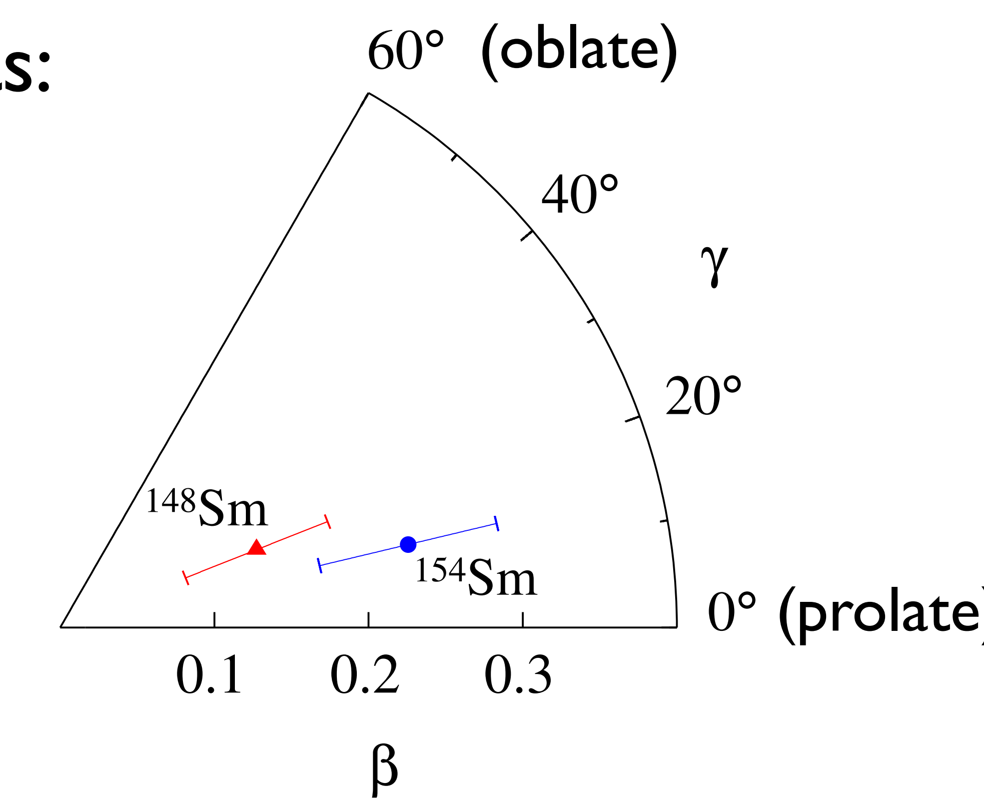
- In the intrinsic frame $a_{2,1} = a_{2,-1} = 0$ and

$$a_{2,0} = \beta \cos\gamma, \quad a_{2,2} = a_{2,-2} = \frac{1}{\sqrt{2}} \beta \sin\gamma$$

- The intrinsic deformation parameters β, γ can be determined from the quadrupole invariants:

$$\beta = \frac{\sqrt{5\pi}}{3r_0^2 A^{5/3}} \langle \hat{Q} \cdot \hat{Q} \rangle^{1/2} \; ; \quad \cos 3\gamma = -\sqrt{\frac{7}{2}} \frac{\langle (\hat{Q} \times \hat{Q}) \cdot \hat{Q} \rangle}{\langle \hat{Q} \cdot \hat{Q} \rangle^{3/2}}$$

$$(\Delta\beta/\beta)^2 = \left[\langle (\hat{Q} \cdot \hat{Q})^2 \rangle - \langle \hat{Q} \cdot \hat{Q} \rangle^2 \right]^{1/2} / \langle \hat{Q} \cdot \hat{Q} \rangle$$



- Allows us to extract information about intrinsic deformation in the rotationally invariant framework of SMMC.

Conclusion

- We have circumvented the long-standing odd-particle sign problem for the calculation of ground-state energies in shell model calculations.
- $\langle J^2 \rangle_T$ provides a signature of collective behavior in nuclei, allowing a description of the transition from vibrational to rotational collectivity.
- We have introduced a new method for stabilizing canonical-ensemble AFMC calculations which scales as $O(N_s^3)$ instead of $O(N_s^4)$.
- Nuclear deformation can be studied in a framework which preserves rotational invariance and finite-size effects, and allows model-independent extraction of intrinsic deformation parameters.

Prospects

- Level densities at fixed intrinsic deformation (input to fission models)
- Application to other mass regions