

# Auxiliary-field quantum Monte Carlo methods for nuclei and cold atoms

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- Auxiliary-field Monte Carlo (AFMC) methods at finite temperature
- Sign problem and good-sign interactions
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- Projection on good quantum numbers (e.g., spin and parity)
- Projection on an order parameter (associated with a broken symmetry)
- Applications to cold atom Fermi gases

Recent review: [Y. Alhassid, arXiv:1607.01870 \(2016\)](#)

# Introduction

The challenge: microscopic calculations of nuclear properties from underlying effective interactions

- Ab initio methods have been developed:

Green function Monte Carlo

No-core shell model

Lattice effective field theory

Coupled cluster (CC) method

...

However, they are mostly limited to light nuclei or to nuclei near shell closure (CC).

- Most microscopic treatments of mid-mass and 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 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.

- The auxiliary-field Monte Carlo (AFMC) method for the shell model enables calculations in model spaces that are many orders of magnitude larger than those that can be treated by conventional diagonalization 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).*

## Hubbard-Stratonovich transformation

Assume an effective Hamiltonian in Fock space with a one-body part and a two-body interaction :

$$\hat{H} = \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} \sum_{\alpha} v_{\alpha} \hat{\rho}_{\alpha}^2$$

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

At inverse temperature  $\beta = 1/T$ , we write  $e^{-\beta \hat{H}} = \left( e^{-\Delta \beta \hat{H}} \right)^{N_t}$  where  $N_t$  is the number of time slices. For each time slice [to order  $(\Delta \beta)^2$  ]

$$e^{-\Delta \beta \hat{H}} \approx \prod_i e^{-\Delta \beta \epsilon_i \hat{n}_i} \prod_{\alpha} e^{-\frac{1}{2} \Delta \beta v_{\alpha} \hat{\rho}_{\alpha}^2}$$

Each interaction factor can be written as an integral over an auxiliary field  $\sigma_{\alpha}$

$$e^{-\frac{1}{2} \Delta \beta v_{\alpha} \hat{\rho}_{\alpha}^2} = \sqrt{\frac{\Delta \beta |v_{\alpha}|}{2\pi}} \int d\sigma_{\alpha} e^{-\frac{1}{2} \Delta \beta |v_{\alpha}| \sigma_{\alpha}^2} e^{-\Delta \beta |v_{\alpha}| s_{\alpha} \sigma_{\alpha} \hat{\rho}_{\alpha}}$$

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

We obtain the HS transformation describing a path integral over time-dependent auxiliary fields  $\sigma(\tau)$

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

Here  $G_\sigma = e^{-\frac{1}{2} \int_0^\beta |v_\alpha| \sigma_\alpha^2(\tau) d\tau}$  is a Gaussian weight,

and  $U_\sigma$  is a one-body propagator of non-interacting nucleons in external time-dependent auxiliary fields

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

$\hat{h}_\sigma(\tau)$  is a one-body Hamiltonian defined for each configuration of the fields

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

## Thermal expectation values of observables

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

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

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

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

The grand canonical expectation value of a one-body observable

$\hat{O} = \sum_{i,j} O_{ij} a_i^\dagger a_j$  is calculated from

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

- The integrand reduces to matrix algebra in the single-particle space (of typical dimension 50 – 100).

## Particle-number projection

In a finite-size system, it is necessary to project on the canonical ensemble of fixed particle number  $\mathcal{A}$ . In the Fock space spanned by  $N_s$  single-particle orbitals, this can be done by an exact discrete Fourier transform.

Canonical partition:

$$\text{Tr}_{\mathcal{A}} U_{\sigma} = \frac{e^{-\beta\mu\mathcal{A}}}{N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m\mathcal{A}} \det \left( \mathbf{1} + e^{i\varphi_m} e^{\beta\mu} \mathbf{U}_{\sigma} \right)$$

where  $\varphi_m = 2\pi m/N_s$  ( $m = 1, \dots, N_s$ ) are quadrature points.

Canonical expectation of an observable  $\mathbf{O}$ :

$$\text{Tr}_{\mathcal{A}} \left( \hat{\mathbf{O}} \hat{U}_{\sigma} \right) = \frac{e^{-\beta\mu\mathcal{A}}}{N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m\mathcal{A}} \det \left( \mathbf{1} + e^{i\varphi_m + \beta\mu} \mathbf{U}_{\sigma} \right) \times \text{tr} \left( \frac{1}{\mathbf{1} + e^{-i\varphi_m - \beta\mu} \mathbf{U}_{\sigma}^{-1}} \mathbf{O} \right)$$

## Quantum Monte Carlo methods and sign problem

The path integrals are done by Monte Carlo methods, sampling the fields according to a weight  $W_\sigma \equiv G_\sigma |\text{Tr}_A \hat{U}_\sigma|$

$\Phi_\sigma \equiv \text{Tr}_A U_\sigma / |\text{Tr}_A U_\sigma|$  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 (compared with 1), the fluctuations become very large  $\Rightarrow$  the Monte Carlo sign problem.

### Good-sign interactions

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

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

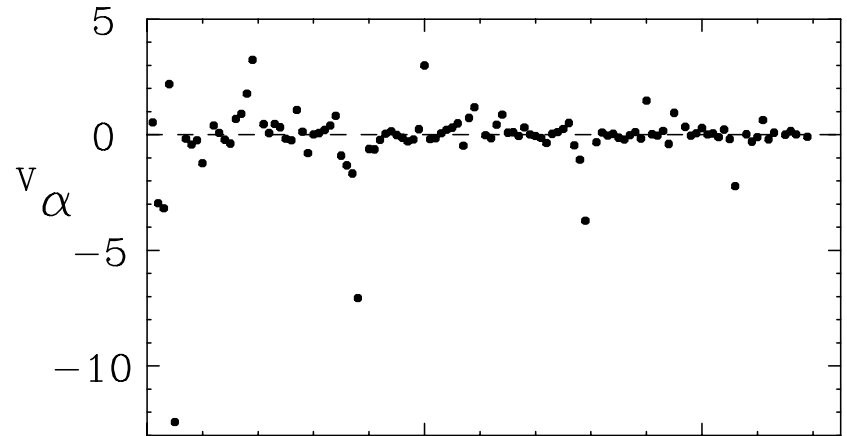
Proof: when all  $v_\alpha < 0$ , we have  $\hat{h}_\sigma = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha (v_\alpha \sigma_\alpha^* \rho_\alpha + v_\alpha \sigma_\alpha \bar{\rho}_\alpha)$   
and  $\bar{h}_\sigma = h_\sigma \Rightarrow$  the eigenvalues of  $U_\sigma$  appear in complex conjugate pairs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



## 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-number sign problem

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

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

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

We calculate the imaginary-time scalar single-particle Green's functions in even-even nuclei for all single-particle orbitals  $\nu = n l j$ :

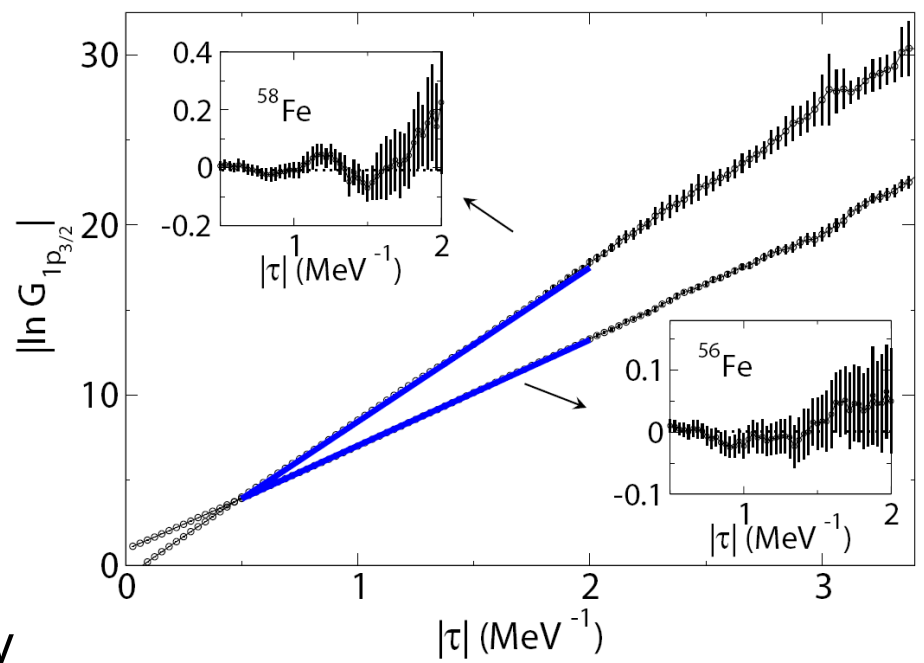
$$G_\nu(\tau) = \sum_m \langle T a_{\nu m}(\tau) a_{\nu m}^\dagger(0) \rangle$$

In the asymptotic regime in  $\tau$  ( $1 < \tau \ll \beta$ )

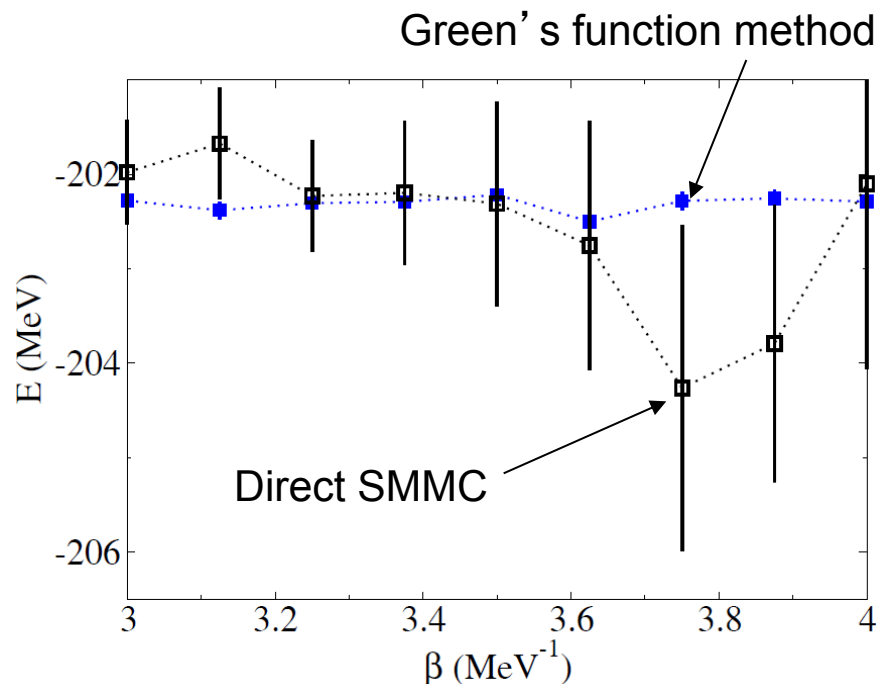
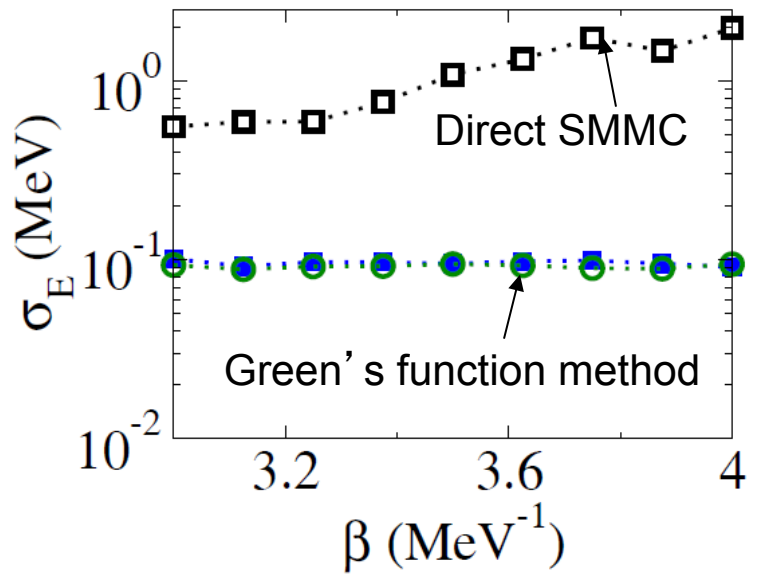
$$G_\nu(\tau) \sim e^{-\beta[E_j(A \pm 1) - E_{gs}(A)] |\tau|}$$

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

- Minimize  $E_j(A\pm 1)$  to find the ground-state energy and its spin  $J=j$



Statistical errors of ground-state energy in direct SMMC vs. Green's function method



## Applications: statistical properties of nuclei

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 measurements.

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

- Most approaches are based on empirical modifications of the Fermi gas formula or on mean-field approximations that can often miss important correlations.
- The configuration-interaction (CI) shell model accounts for correlations but diagonalization methods are limited to spaces of dimensionality  $\sim 10^{11}$ .

The AFMC method enables microscopic calculations in spaces that are many orders of magnitude larger ( $\sim 10^{30}$ ).

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

## Level density in the AFMC

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

- Calculate the thermal energy  $E(\beta) = \langle H \rangle$  versus  $\beta$  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

$C$  = canonical heat capacity

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

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

## Mid-mass nuclei (iron region)

CI shell model model space: complete  $fpg_{9/2}$  shell.

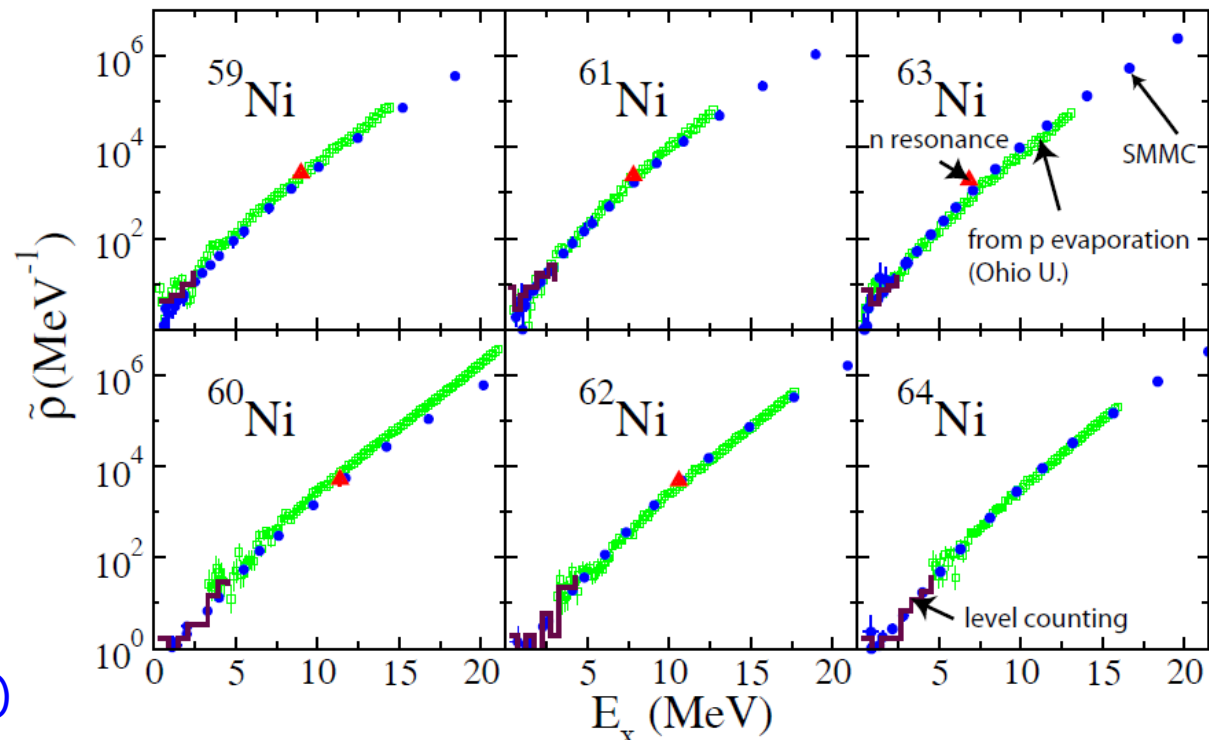
Single-particle Hamiltonian: from Woods-Saxon potential plus spin-orbit

Isoscalar interaction: includes the *dominant* components of effective interactions

- Pairing strength is determined from odd-even mass differences
- Multipole-multipole interaction terms -- quadrupole, octupole, and hexadecupole, determined from a self-consistent condition and renormalized by  $k_2=2$ ,  $k_3=1.5$ ,  $k_4=1$ .

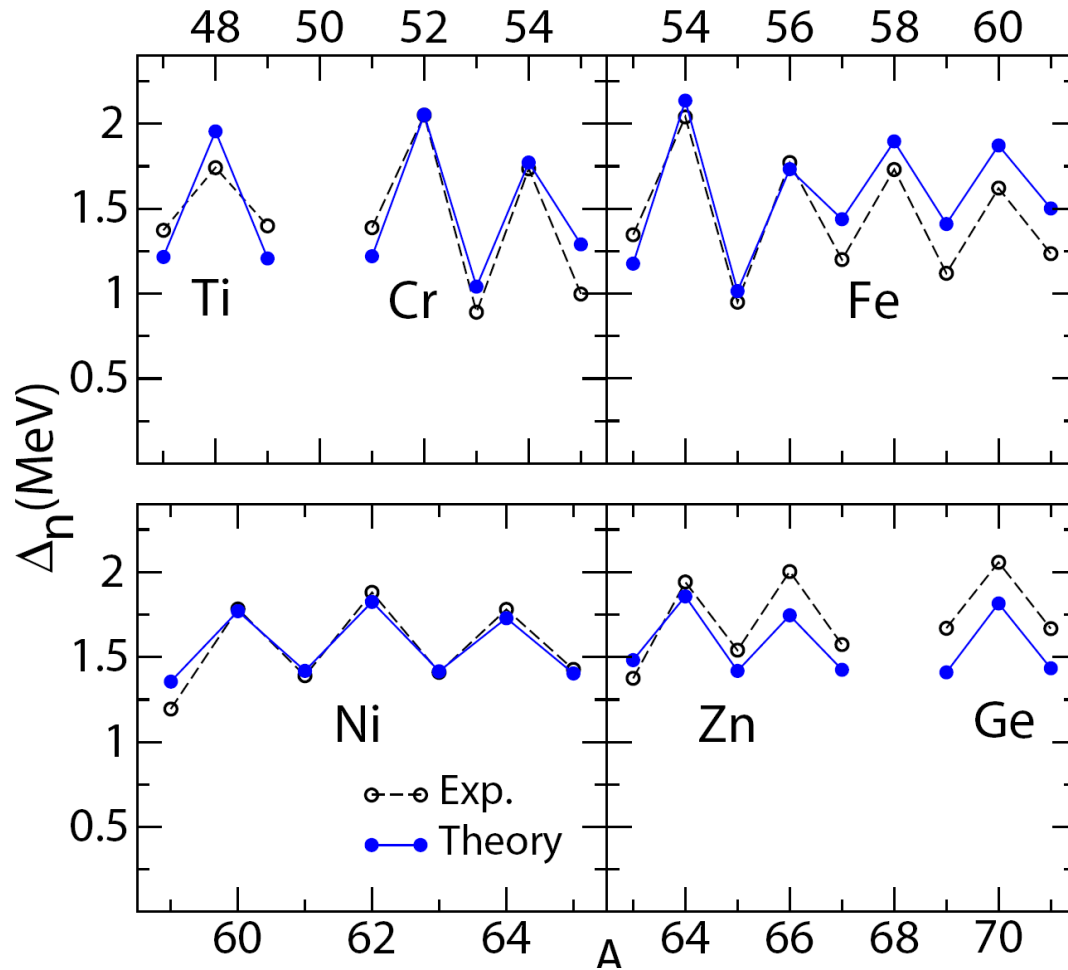
## Level densities in nickel isotopes

Excellent agreement with experiments:  
(i) level counting,  
(ii) proton evaporation Spectra (Ohio U., 2012),  
(iii) neutron resonance data



# Pairing gaps from odd-even mass differences

Mukherjee and Alhassid, PRL 109, 032503 (2012)



- Good agreement with experimental values

## 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 plus multipole-multipole interaction terms  
– quadrupole, octupole, and hexadecupol.

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

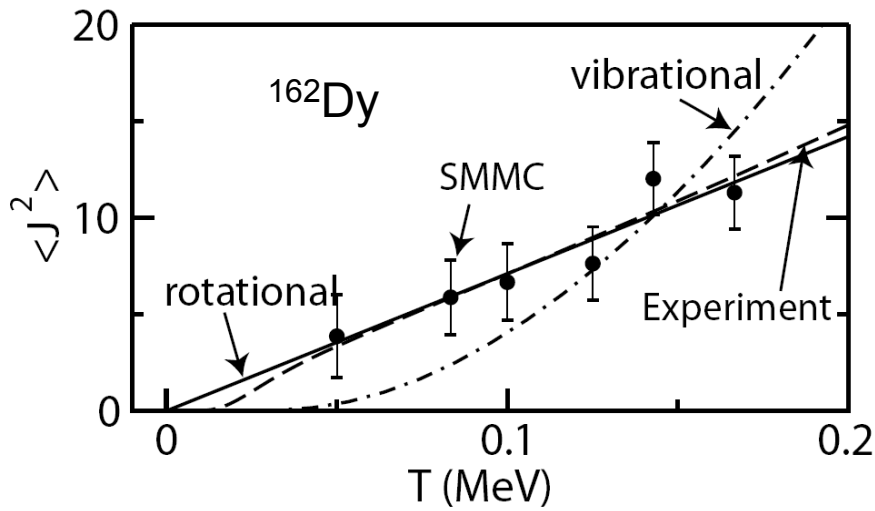
However, a microscopic description in a CI shell model has been lacking.

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.

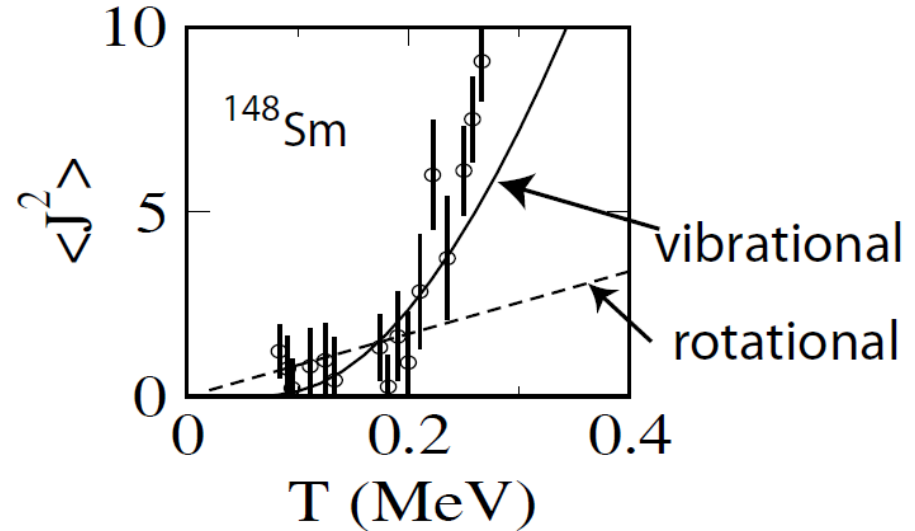
The behavior of  $\langle \vec{J}^2 \rangle$  versus  $T$  is sensitive to the type of collectivity:



$$\langle \vec{J}^2 \rangle = \frac{6}{E_{2^+}} T$$

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

Alhassid, Fang, Nakada, PRL 101 (2008)



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

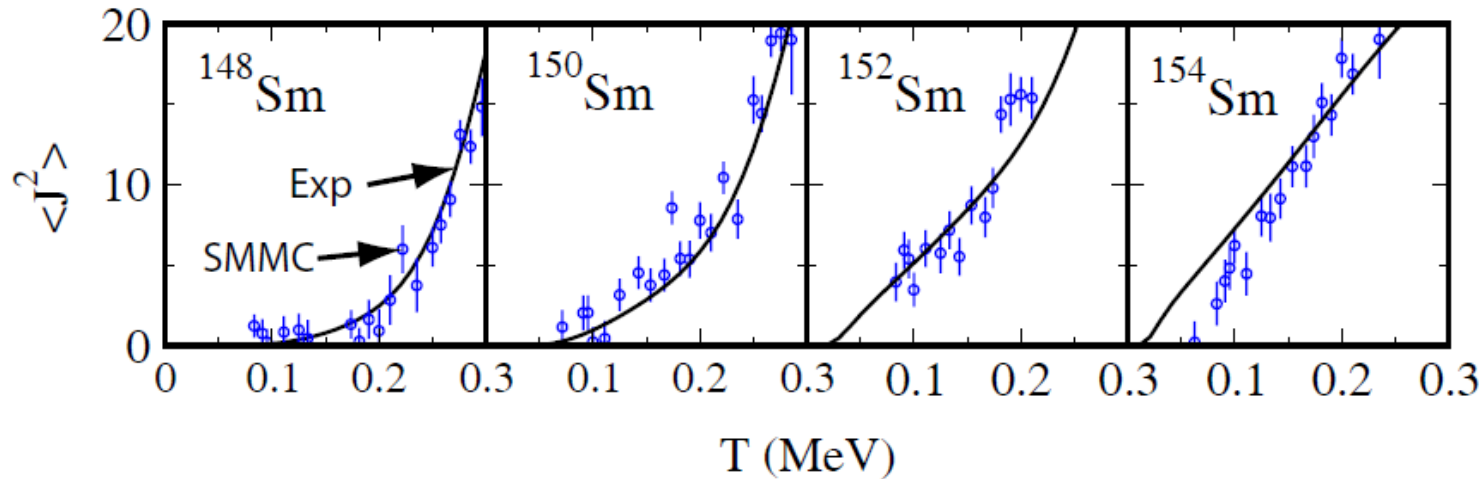
$\Rightarrow$   $^{148}\text{Sm}$  is vibrational

Ozen, Alhassid, Nakada, PRL 110 (2013)

# Crossover from vibrational to rotational collectivity in heavy nuclei

Ozen, Alhassid, Nakada, PRL 110 (2013)

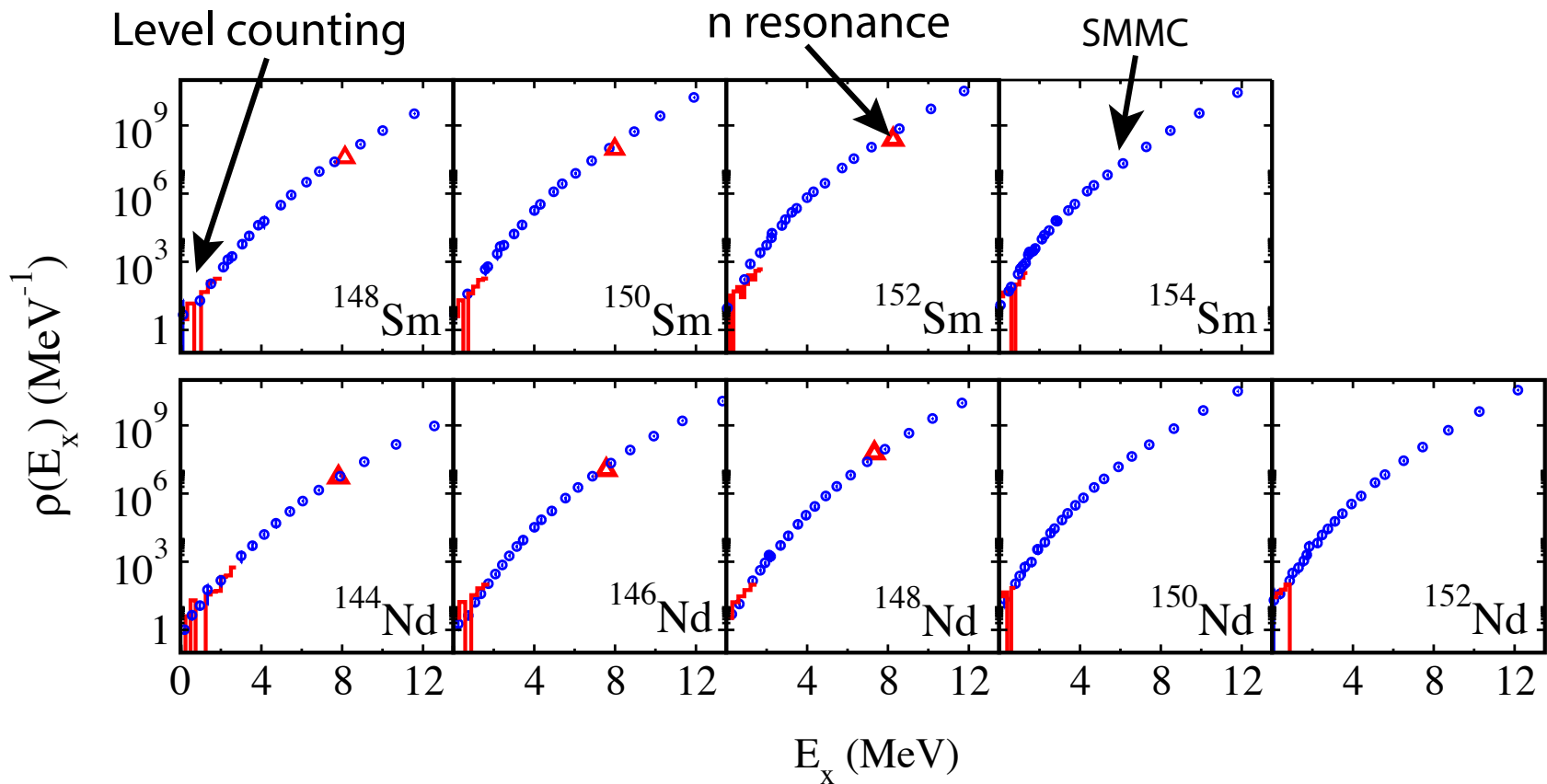
$\langle \bar{J}^2 \rangle$  versus  $T$  in samarium isotopes



- Experimental values are found from  $\langle \bar{J}^2 \rangle = \frac{\sum_{\alpha J} J(J+1)(2J+1)e^{-E_{\alpha J}/T}}{\sum_{\alpha J} (2J+1)e^{-E_{\alpha J}/T}}$  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  $T$ .

AFMC describes well the crossover from vibrational to rotational collectivity in good agreement with the experimental data at low  $T$ .

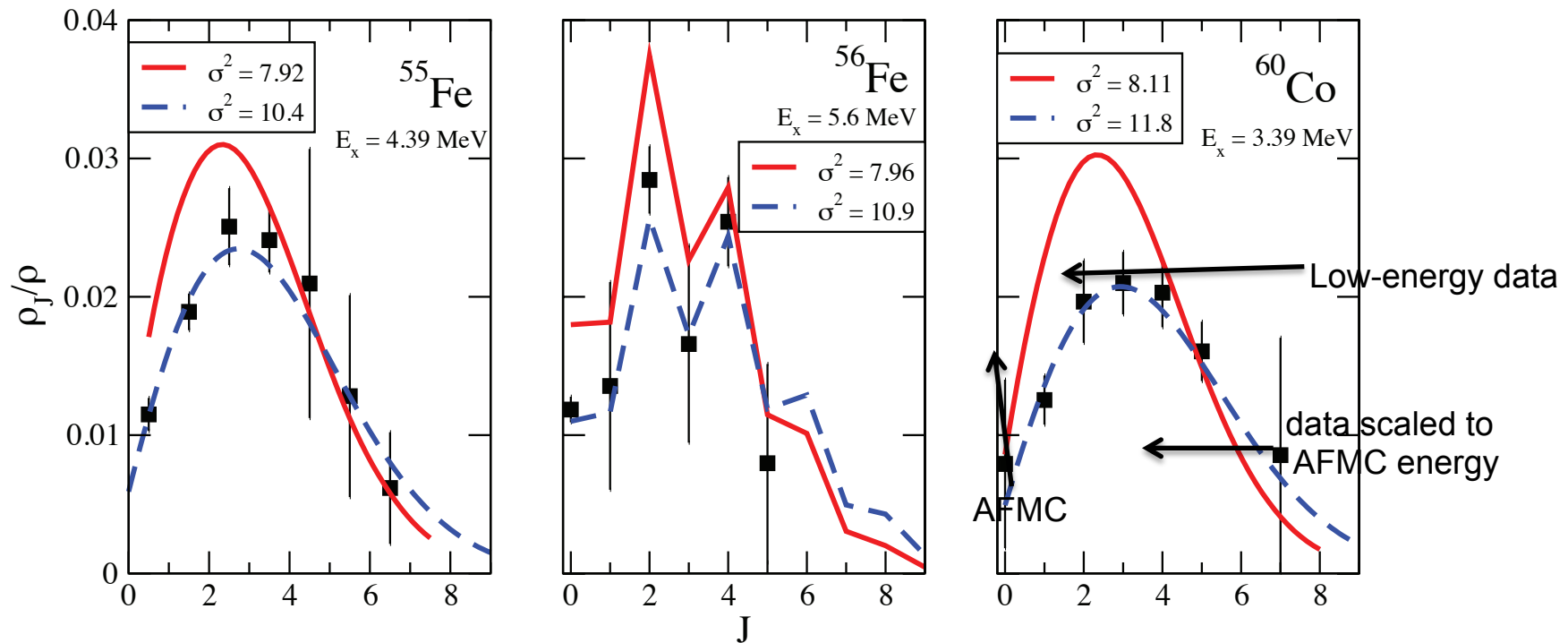
## Level densities in samarium and neodymium isotopes



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

# Projection on good quantum numbers: spin distributions in mid-mass nuclei

[Alhassid, Liu, Nakada, PRL 99, 162504 (2007)]



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

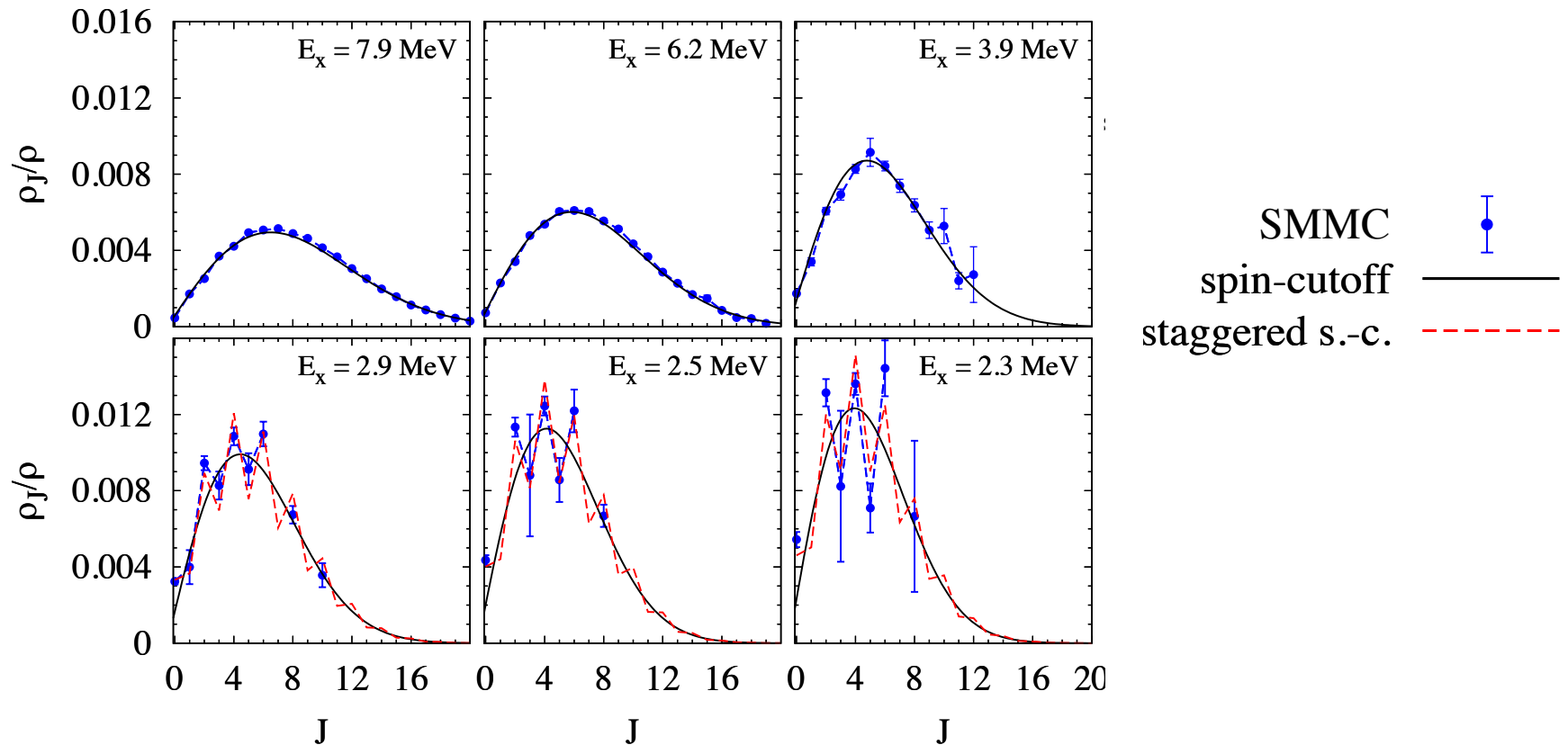
$\sigma^2$  = spin cutoff parameter

- 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: $^{162}\text{Dy}$

Gilbreth, Alhassid, Bonett-Matiz (2016)



- Good agreement with spin-cutoff (s.-c.) model at higher excitations
- 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.

# 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.

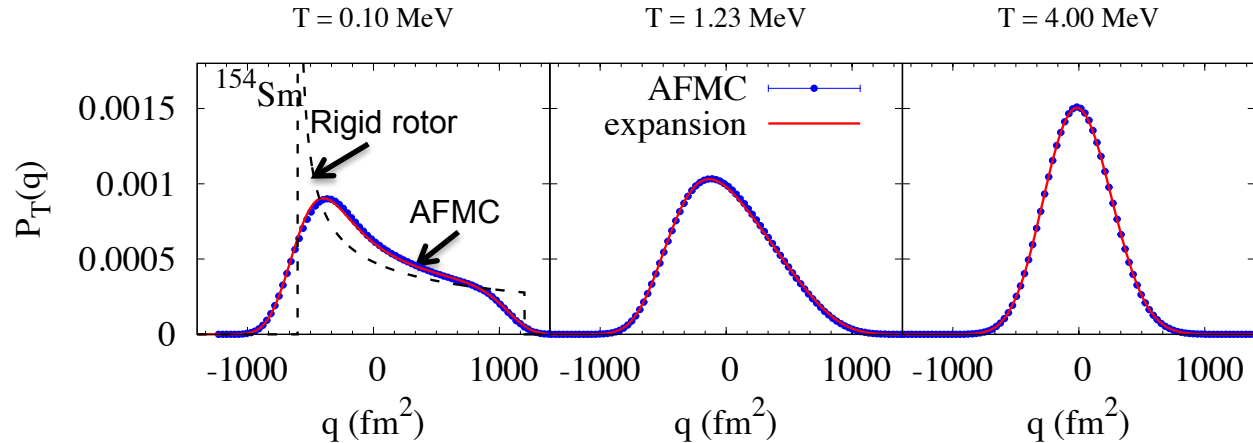
The challenge is to study nuclear deformation in a framework that preserves rotational invariance.

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

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

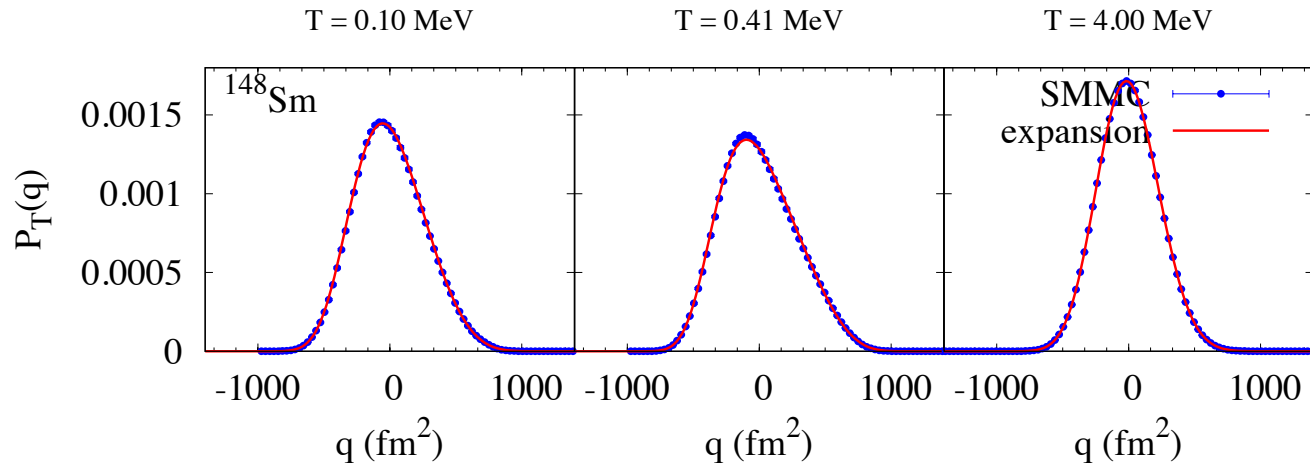
# Application to heavy nuclei

$^{154}\text{Sm}$   
(deformed)



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

$^{148}\text{Sm}$   
(spherical)



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

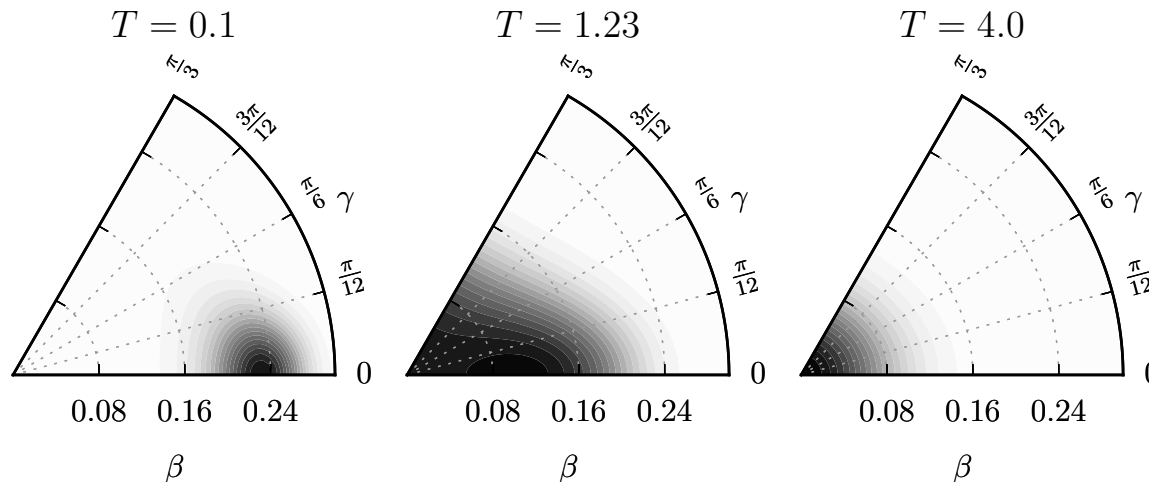
# Intrinsic shape distributions $P_T(\beta, \gamma)$

Alhassid, Mustonen, Gilbreth, Bertsch (2016)

Information on intrinsic deformation  $\beta, \gamma$  can be obtained from the expectation values of rotationally invariant combinations of the quadrupole tensor  $q_{2\mu}$ .

$\ln P_T(\beta, \gamma)$  at a given temperature  $T$  is an invariant and can be expanded in the quadrupole invariants  $-\ln P_T = a\beta^2 - b\beta^3 \cos 3\gamma + c\beta^4 + \dots$ .

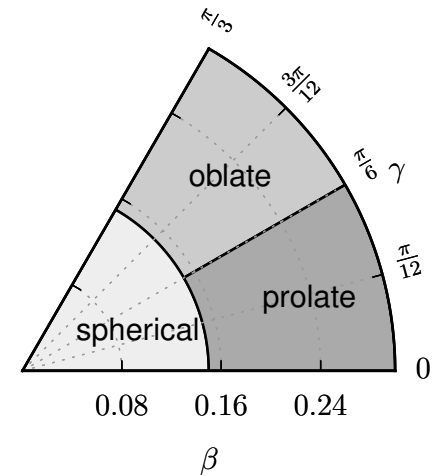
- The expansion coefficients  $a, b, c, \dots$  can be determined from the expectation values of the invariants, which in turn can be calculated from the low-order moments of  $q_{20} = q$ .



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

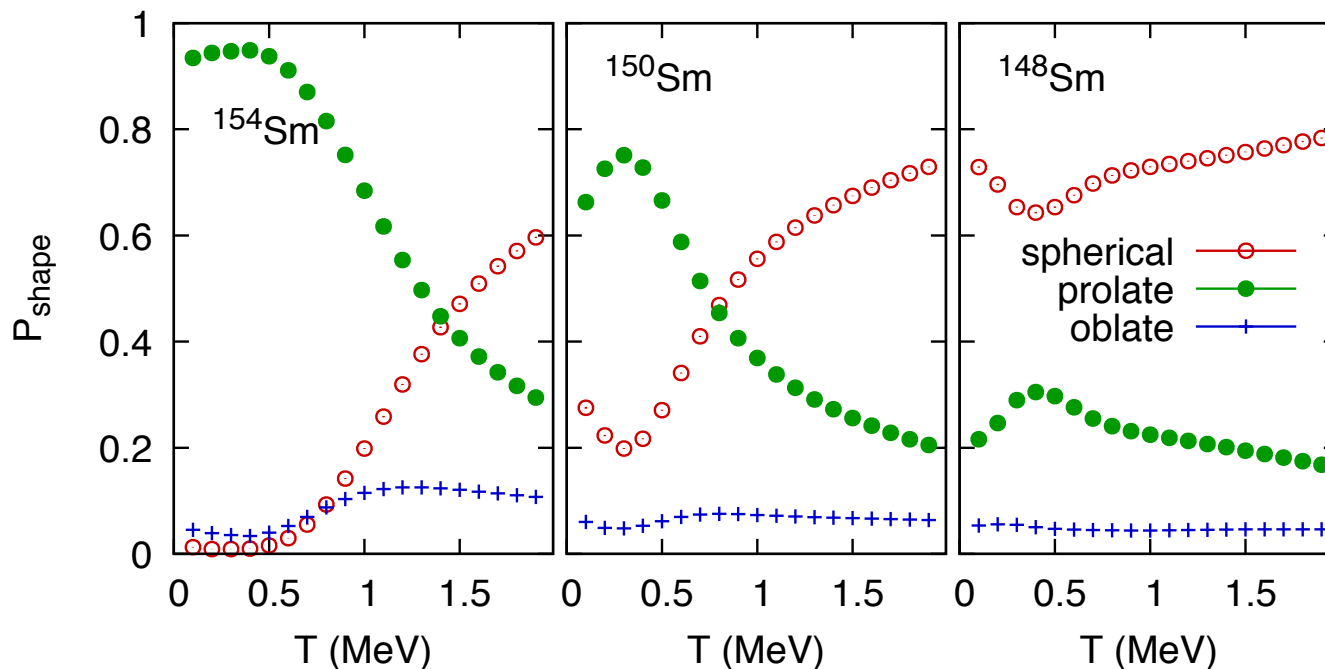


We divide the  $\beta, \gamma$  plane into three regions: spherical, prolate and oblate.



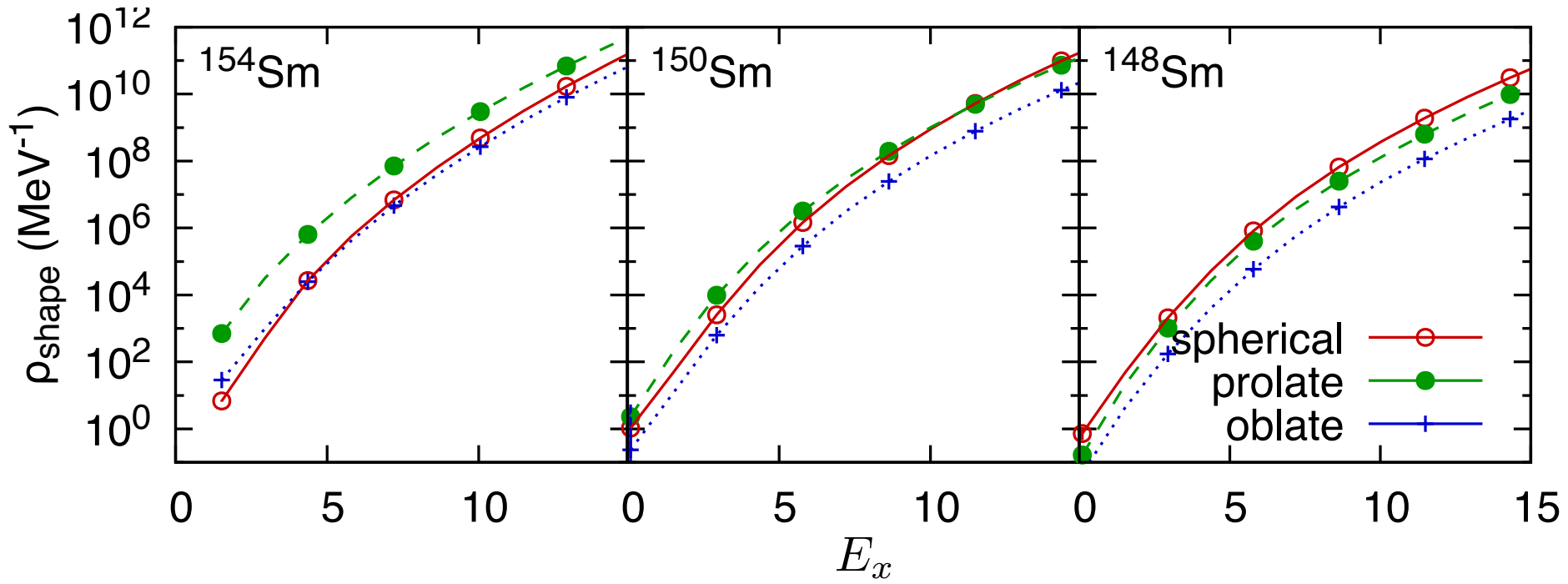
Integrate over each deformation region to determine the probability of shapes versus temperature.

- Compare deformed ( $^{154}\text{Sm}$ ), transitional ( $^{150}\text{Sm}$ ) and spherical ( $^{148}\text{Sm}$ ) nuclei:



# Level density versus intrinsic deformation

- Convert  $P_T(\beta, \gamma)$  to level densities vs  $E_x, \beta, \gamma$

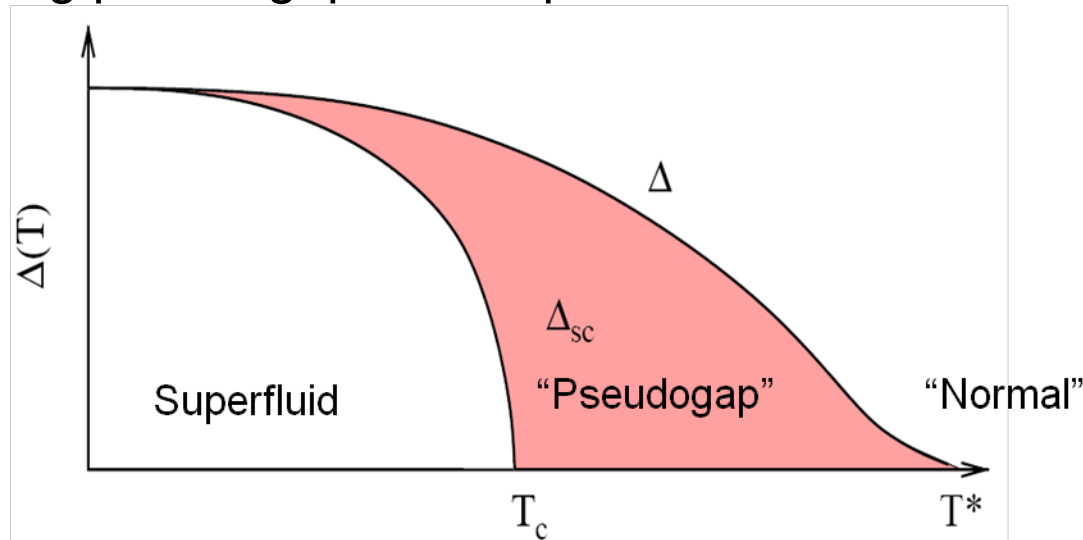


# Application to the trapped cold atom Fermi gas condensate

Gilbreth and Alhassid, PRA **88**, 063643 (2013)

Study the nature of the superfluid phase transition in the finite trapped Fermi gas condensate.

- Are there pairing pseudogap effects prior to condensation in the unitary gas ?



[Q. Chen et al., Physics Reports **412** (2005) 1-88]

Monte Carlo calculations of the homogenous gas suggested a pseudogap.

Magieriski, Wlazlowski, Bulgac and Drut, PRL **103**, 210403 (2009)

Signatures of pairing correlations:

(i) Model-independent gap (requires the canonical ensemble)

$$\Delta_{gap} \equiv [2E(N_{\uparrow}, N_{\downarrow} - 1) - E(N_{\uparrow}, N_{\downarrow}) - E(N_{\uparrow} - 1, N_{\downarrow} - 1)]/2$$

(ii) Heat capacity

Numerical differentiation *inside* the path integral, taking into account *correlated* errors that reduce the statistical errors by an order of magnitude.

[Liu and Alhassid, PRL **87**, 022501 (2001)]

(iii) Condensate fraction

Define a pair correlation matrix for good angular momentum L :

$$C_L(ab, cd) = \langle A_{LM\uparrow\downarrow}^{\dagger}(ab) A_{LM\uparrow\downarrow}(cd) \rangle$$

where  $A_{LM\uparrow\downarrow}^{\dagger}(ab)$  is a pair creation operators of particles in orbitals a and b.

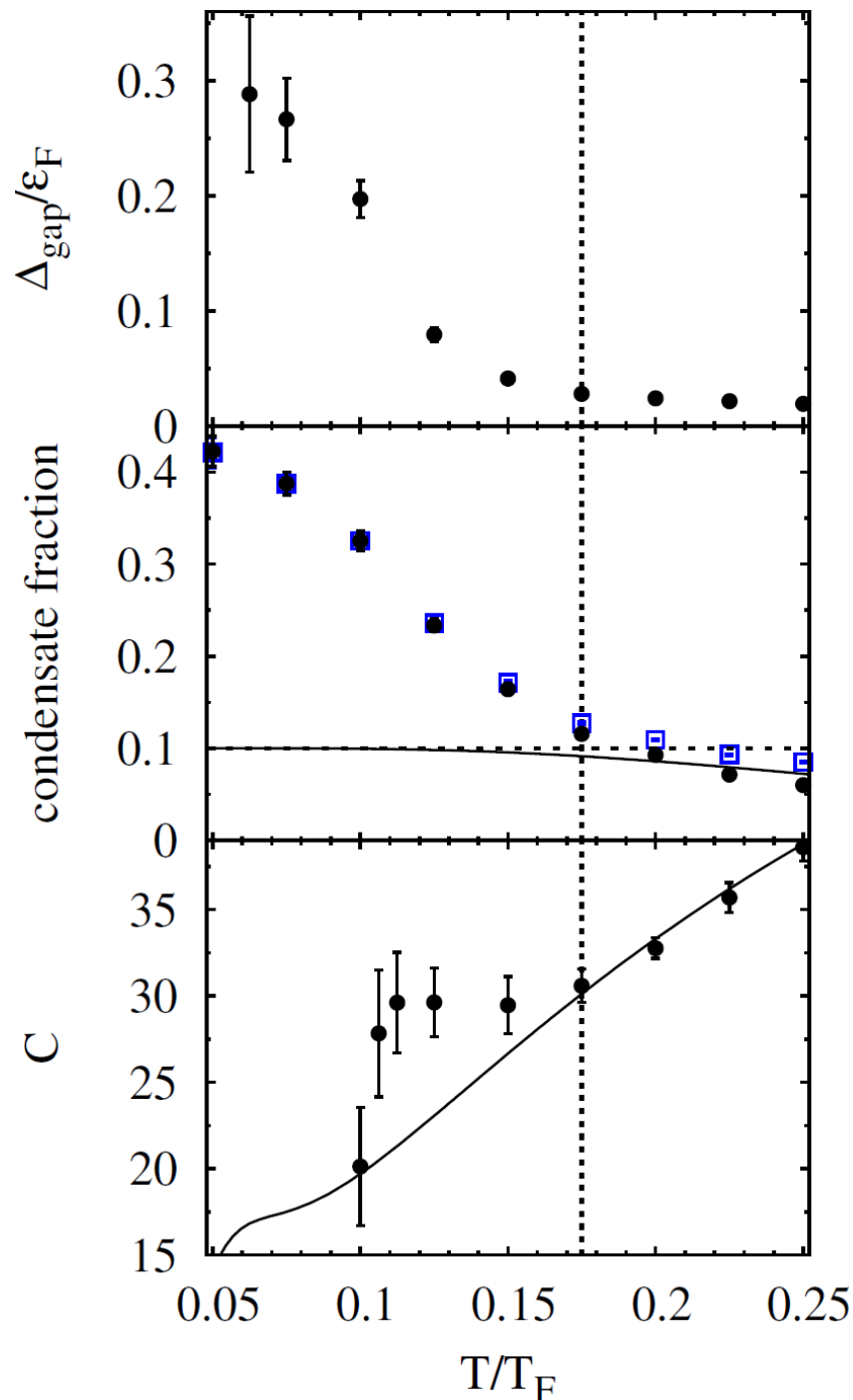
Maximal eigenvalue occurs for L=0 and defines the condensate.

## AFMC results for 20 atoms (10+10) in the unitary gas

- Clear signatures of the superfluid phase transition below  $T/T_F \approx 0.175$

- In the finite-size trapped system, the gap does not appear to lead the condensate fraction as temperature decreases.

⇒ No clear signature of a pseudogap phase in the energy-staggering pairing gap for the finite condensate



## Conclusion

- Finite-temperature AFMC is a powerful method for the microscopic calculation of statistical properties (e.g., level densities) of nuclei in very large model spaces; applications in nuclei as heavy as the lanthanides.
- Microscopic description of collectivity in heavy nuclei.
- Spin distributions: odd-even staggering in even-even nuclei at low excitation energies; spin cutoff model at higher excitations.
- Statistical properties as a function of intrinsic deformation in a rotationally invariant framework (CI shell model).

## Outlook

- Other mass regions (actinides, unstable nuclei,...).
- Gamma strength functions in AFMC by inversion of imaginary-time response functions.
- Derive *global* effective shell model interactions from density functional theory.