Auxiliary-field quantum Monte Carlo methods in heavy nuclei

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- Auxiliary-field Monte Carlo (AFMC) methods at finite temperature
- Sign problem and good-sign interactions
- Circumventing the odd particle-number sign problem
- Heavy nuclei
- Nuclear deformation in the spherical shell model: quadrupole distributions in the laboratory frame and in the intrinsic frame
- Possible application of AFMC to neutrinoless double beta decay

Recent review: Y. Alhassid, arXiv:1607.01870, a chapter in a book edited by K.D. Launey (2017)

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 functional 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.

• 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).

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 $\sigma(\tau)$

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

$G_\sigma = e^{-\frac{1}{2} \int_0^\beta |v_\alpha| \sigma_\alpha^2(\tau) d\tau}$ 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.

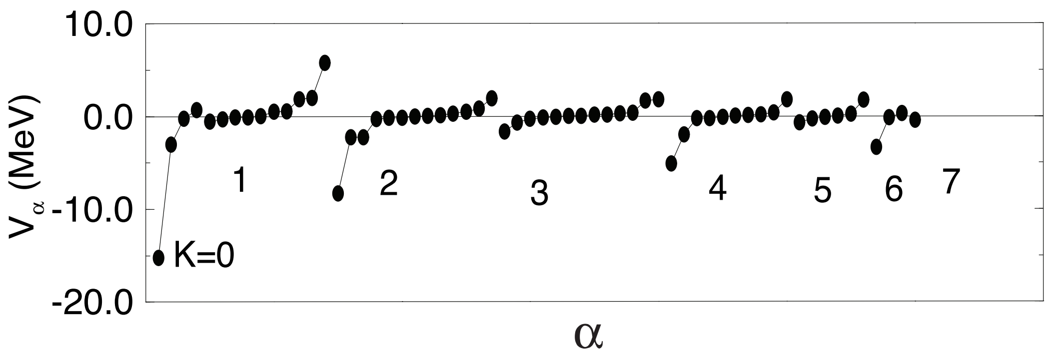
Proof: when all $v_\alpha < 0$, we have $\hat{h}_\sigma = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha \left(v_\alpha \sigma_\alpha^* \rho_\alpha + v_\alpha \sigma_\alpha \bar{\rho}_\alpha\right)$
and $\bar{h}_\sigma = h_\sigma$ $\Rightarrow$ the eigenvalues of U_σ appear in complex conjugate pairs $\{\lambda_i,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

Eigenvalues of effective interaction in fp shell



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 AFMC

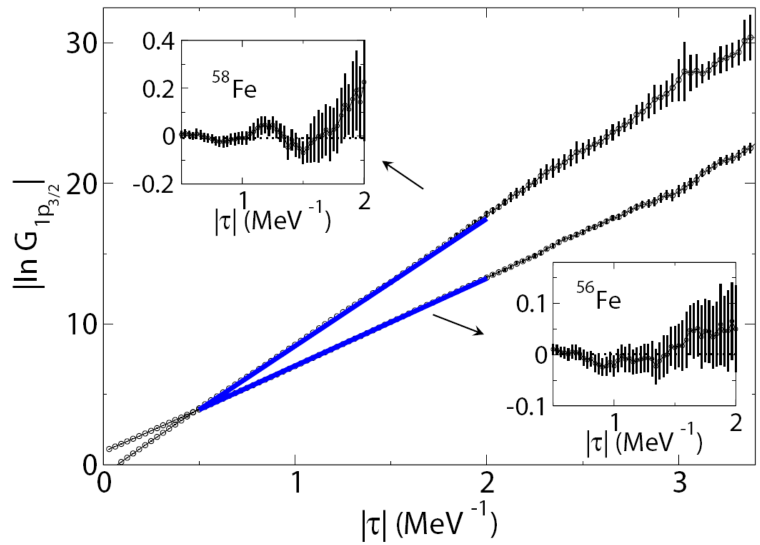
Mukherjee and Alhassid, PRL **109**, 032503 (2012)

Applications of AFMC to odd-even and odd-odd nuclei has been hampered by a sign problem that originates from the projection on 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: $G_\nu(\tau) = \Sigma_m \langle T\, a_{\nu m}(\tau) a^\dagger_{\nu m}(0) \rangle$ for orbitals $\nu = n\, l\, j$

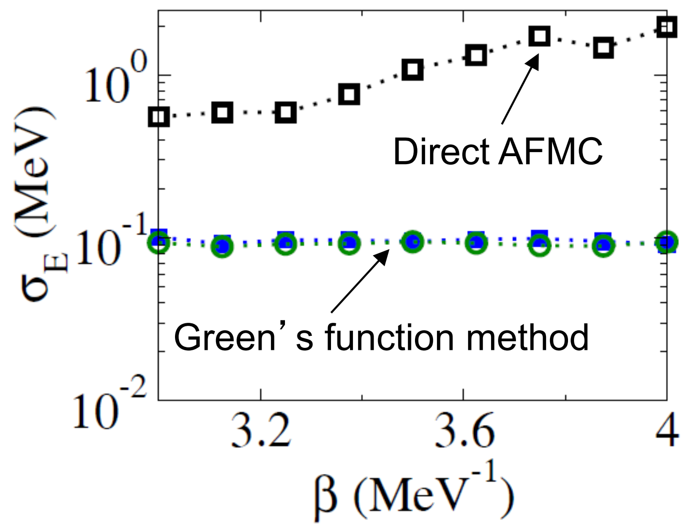
- The energy difference between the lowest energy of the odd-particle system for a given spin j and the ground-state energy of the even-particle system can be extracted from the slope of $\ln G_\nu(\tau)$.

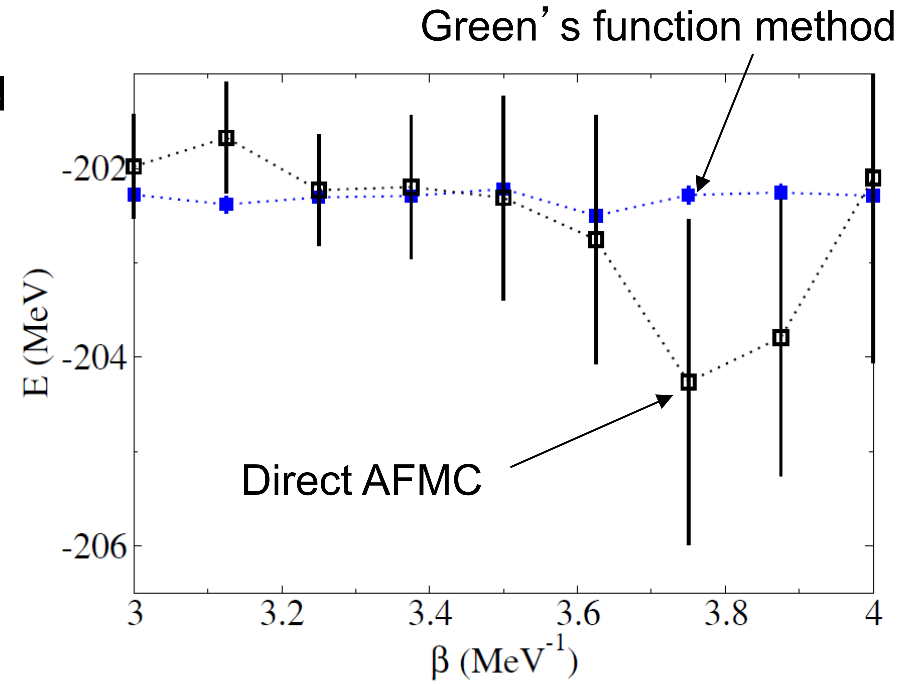


$$G_\nu(\tau) \sim e^{-[E_j(A\pm1) - E_{gs}(A)]\,|\tau|}$$

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

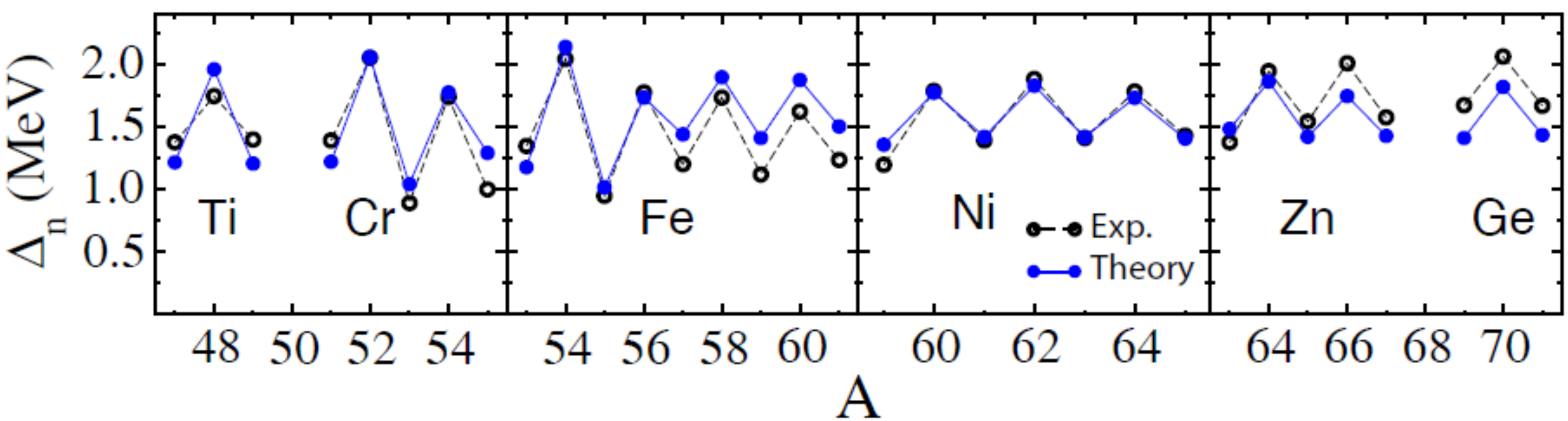
Statistical errors of ground-state energy of Direct AFMC versus Green's function method





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

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



Statistical properties in the AFMC method

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

Partition function

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

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

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

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.

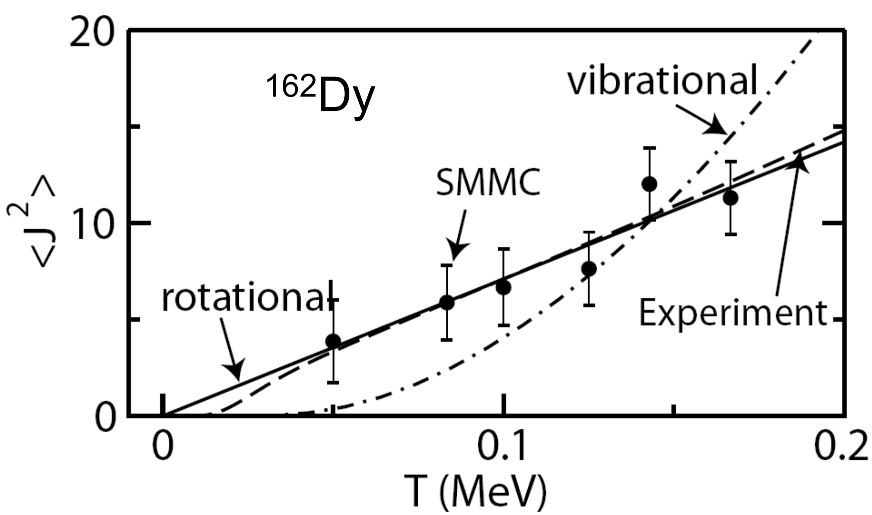
Heavy nuclei exhibit various types of collectivity (vibrational, rotational, …) that are well described by empirical models.

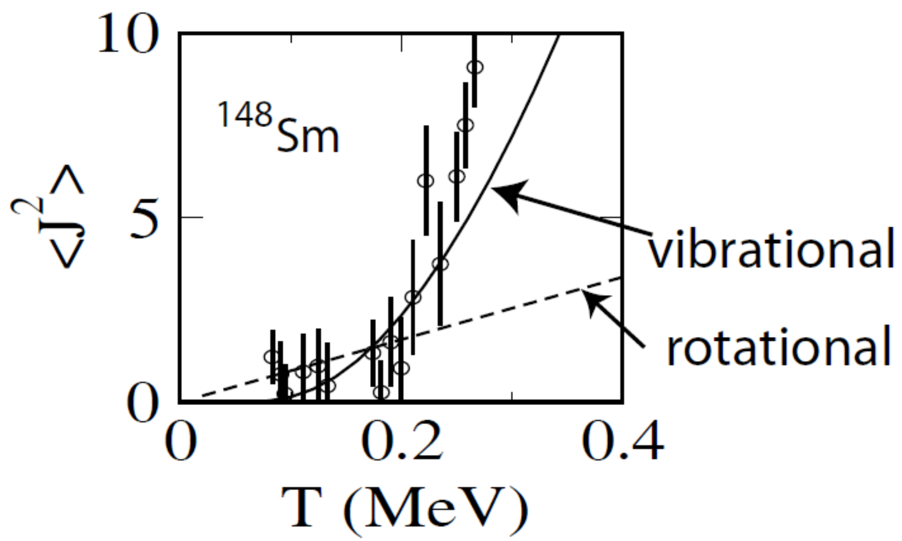
However, a microscopic description in a CI shell model has been lacking.

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

Alhassid, Fang, Nakada,
PRL **101**, 082501 (2008)

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

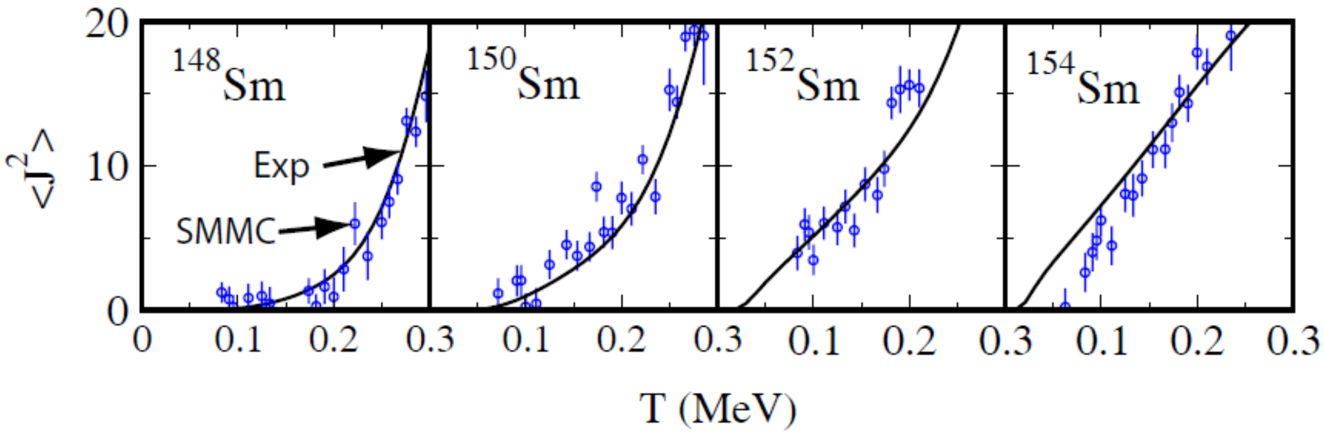
$\Rightarrow {}^{148}Sm$ is vibrational

Ozen, Alhassid, Nakada,
PRL **110**, 042502 (2013)

Crossover from vibrational to rotational collectivity in heavy nuclei

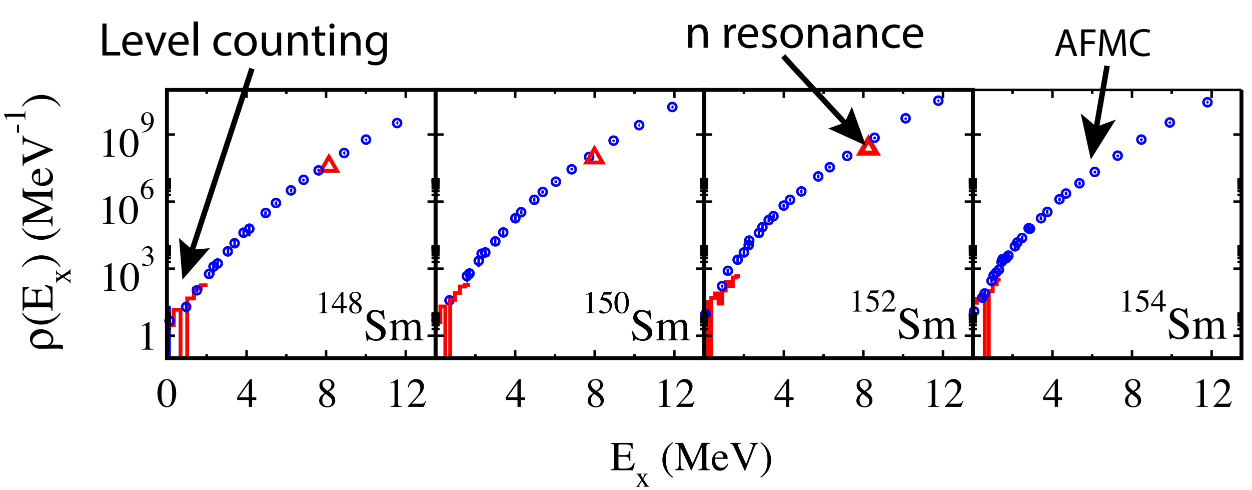
Ozen, Alhassid, Nakada, PRL **110**, 042502 (2013)

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



Level densities in samarium isotopes

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



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.

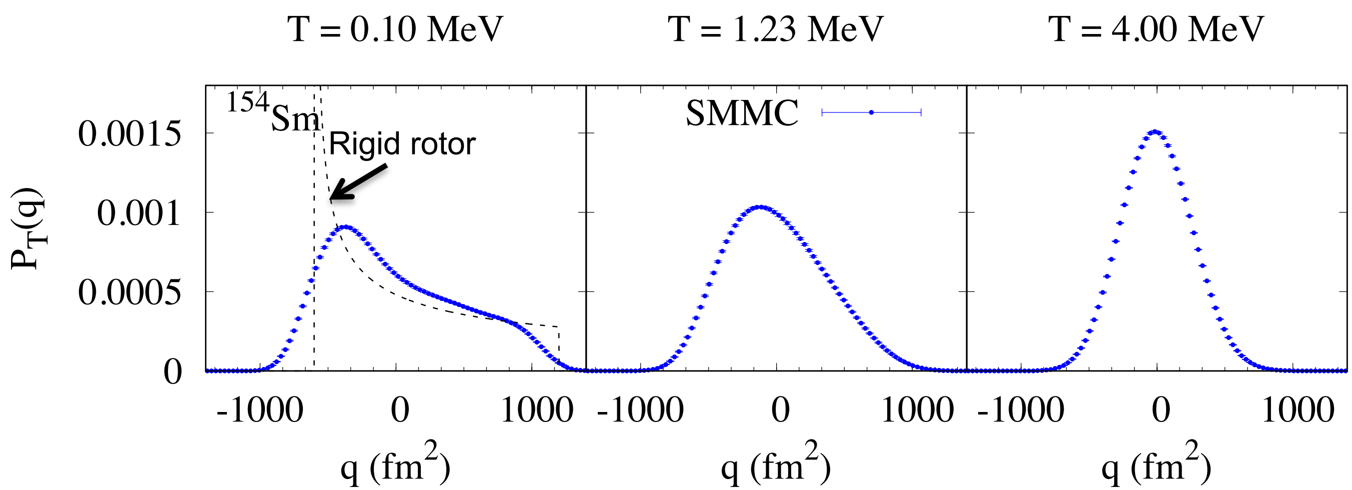
We calculated the distribution of the axial mass quadrupole Q_{20} in the lab frame using an exact projection on Q_{20} (novel in that $[Q_{20}, H] \neq 0$).

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

Application to heavy nuclei

^{154}Sm

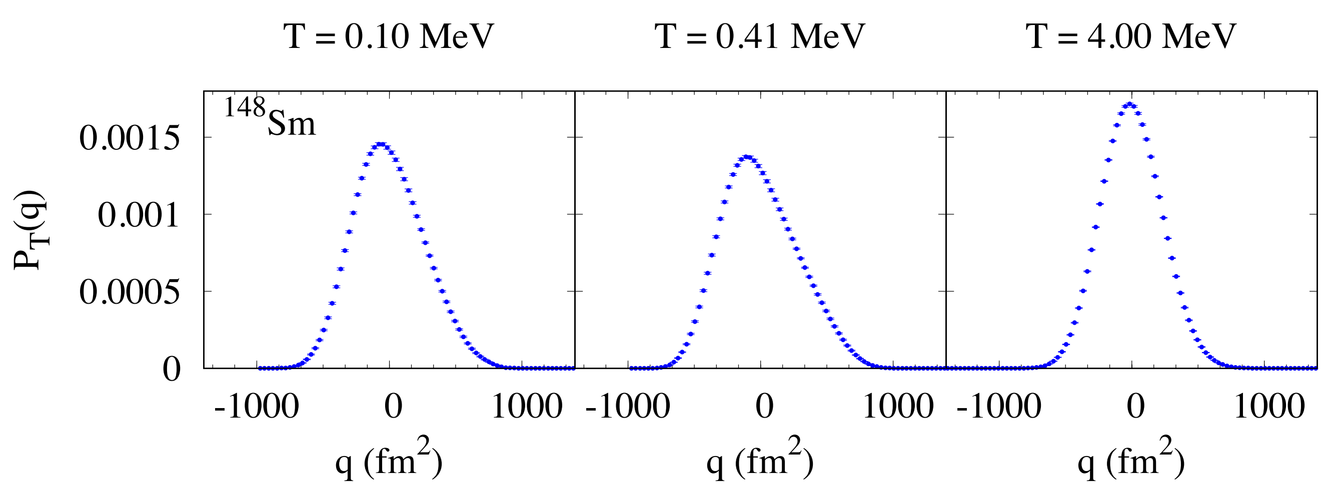
(deformed)



- 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.

Quadrupole distributions $P_T(\beta,\gamma)$ vs. intrinsic deformation

Mustonen, Alhassid, Gilbreth, Bertsch

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

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

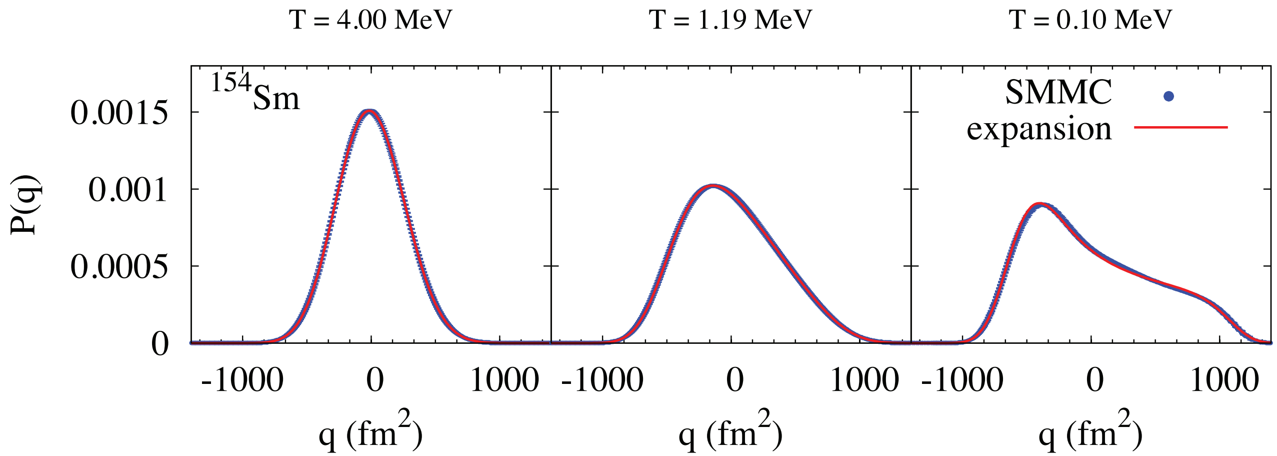
$\ln P_T(\beta,\gamma)$ at a given temperature T is an *invariant* and can be expanded in the quadrupole invariants [a Landau-like expansion, used for the free energy to describe shape transitions in Alhassid, Levit, Zingman, PRL **57**, 539 (1986)]

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

- 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.

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

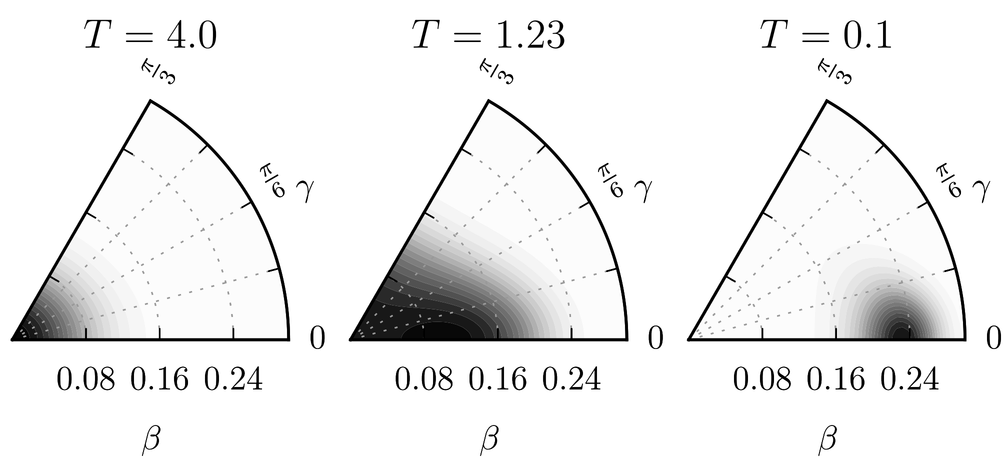
Expressing the invariants in terms of $q_{2\mu}$ in the lab frame and integrating over the $\mu \neq 0$ components, we recover $P(q_{20})$ in the lab frame.



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

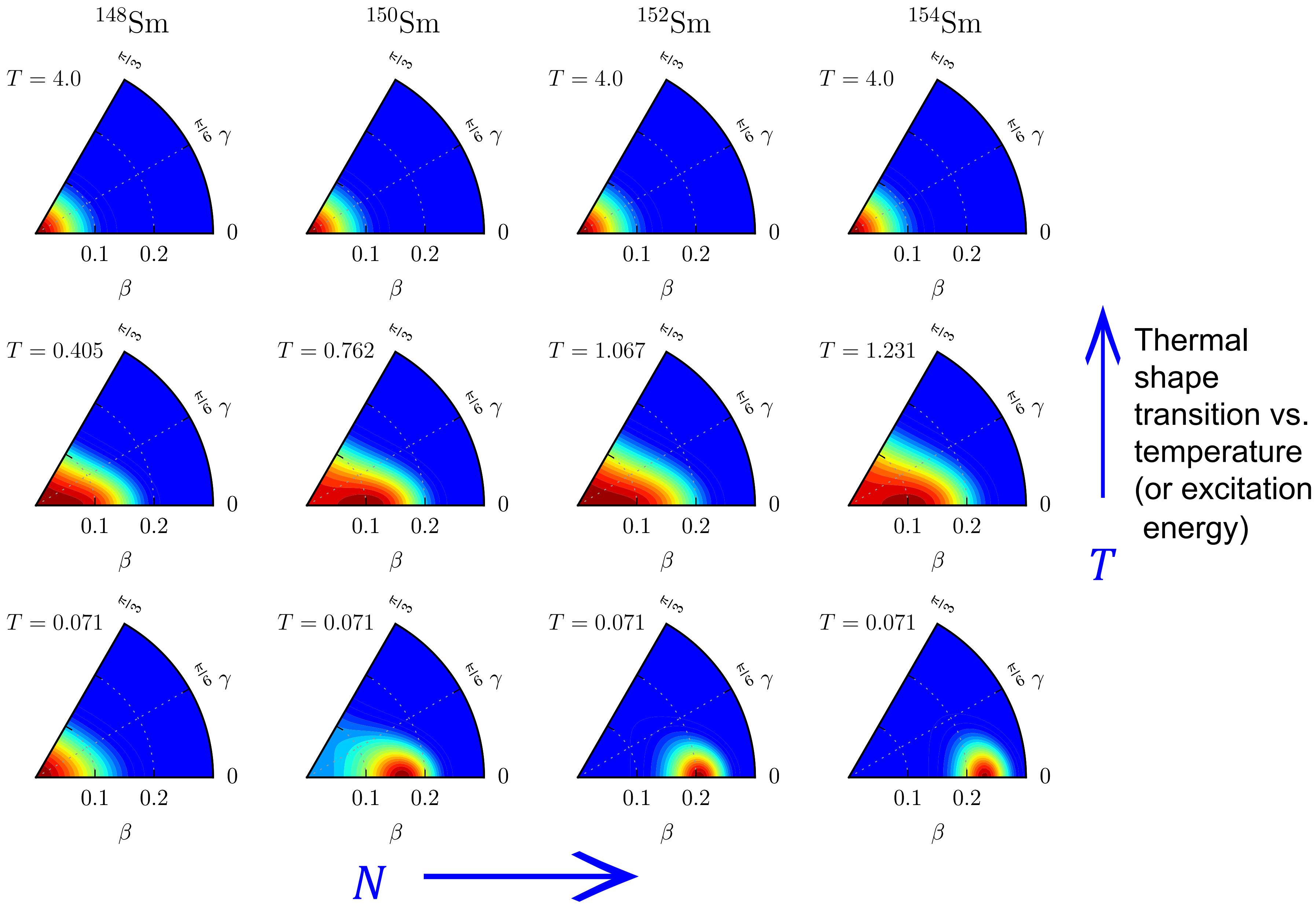
$-\ln P(\beta,\gamma)$

^{154}Sm



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

Shape distributions in the intrinsic β,γ variables

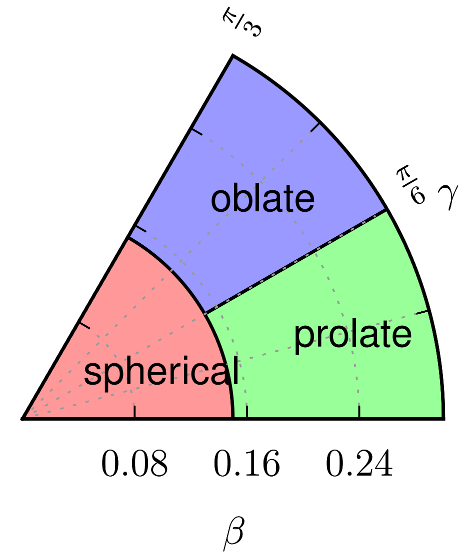


Quantum shape transition (at T=0) vs. neutron number

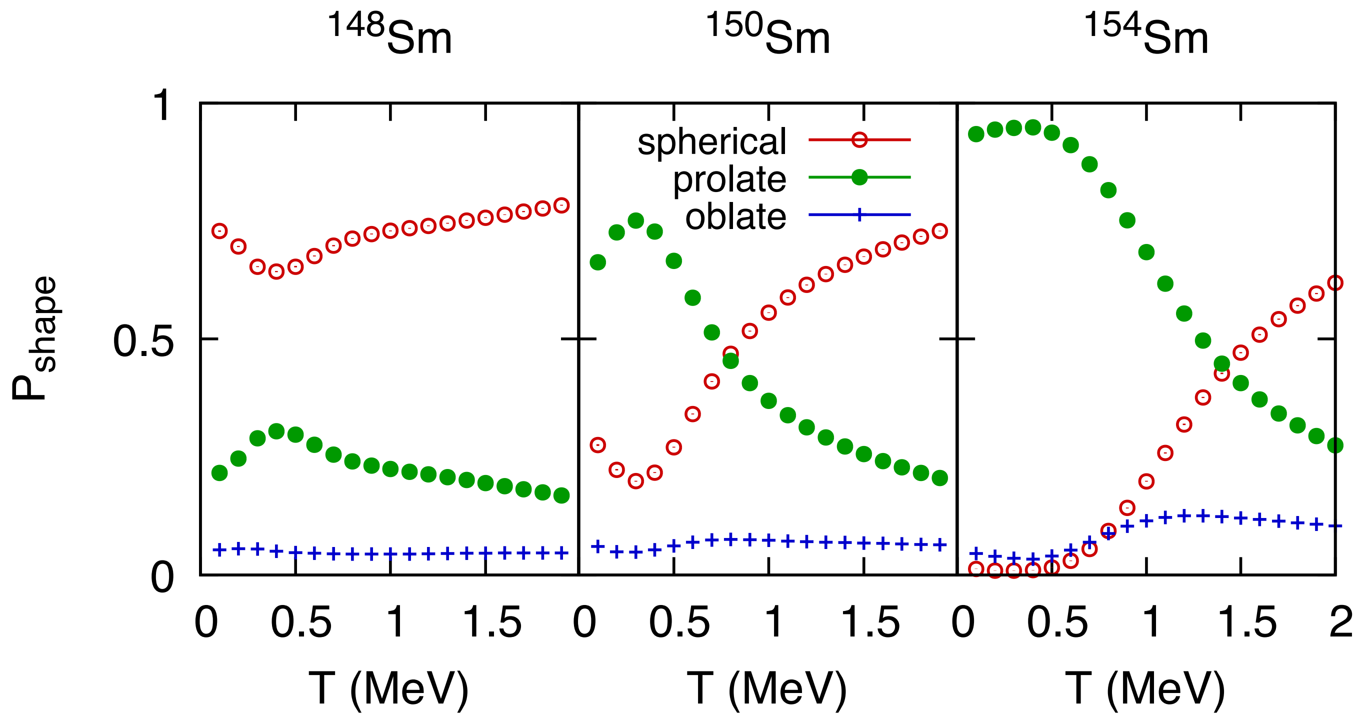
We divide the β,γ plane into three regions: spherical, prolate and oblate.

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

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

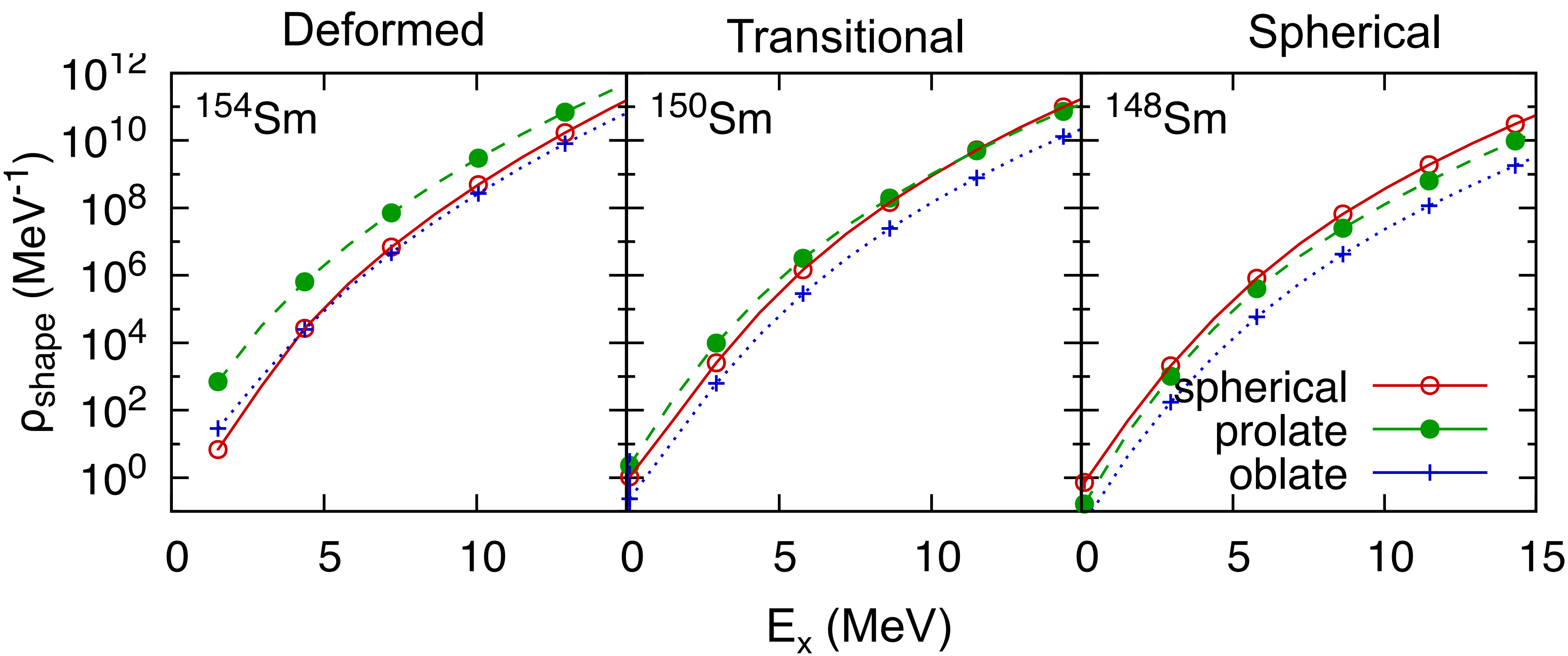


- Compare deformed (^{154}Sm), transitional (^{150}Sm) and spherical (^{148}Sm) nuclei



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)

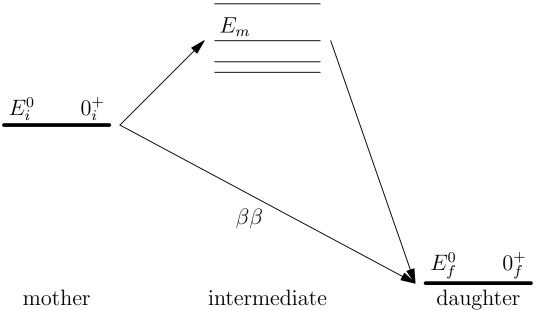


In strongly deformed nuclei, the contributions from prolate shapes dominate the level density below the shape transition energy.

In spherical nuclei, both spherical and prolate shapes make significant contributions.

Double Beta Decay in AFMC

- We can do heavy nuclei in the pn-formalism using AFMC
- AFMC shell-model estimates for open-shell and heavy nuclei
- Estimate contribution of the model space truncation to the g_A quenching



Matrix elements from response functions in AFMC

- $\hat{O}(\tau) = e^{\tau H} \hat{O} e^{-\tau H}$

$$\langle \hat{O}^\dagger(\tau)\hat{O}(0)\rangle = \frac{1}{\sum_i e^{-\beta E_i}} \sum_{fi} e^{-\beta E_i} e^{-\tau(E_f - E_i)} |\langle f|\hat{O}|i\rangle|^2$$

- At the limit $\beta \to \infty$, $\tau \ll \beta$, and large τ, only the lowest possible $E_f = E_f^0$ and $E_i = E_i^0$ contribute:

$$\langle \hat{O}^\dagger(\tau)\hat{O}(0)\rangle = e^{-\tau(E_f^0 - E_i^0)} |\langle f_0|\hat{O}|i_0\rangle|^2$$

- If $\hat{O}$ is the mass quadrupole $\hat{Q}_2$, for an even-even nucleus

$$\langle \hat{O}^\dagger(\tau)\hat{O}(0)\rangle = e^{-\tau E_x^{2^+}} |\langle 2_1^+|\hat{Q}_2|0^+_{\mathrm{g.s.}}\rangle|^2$$

where 2_1^+ is the lowest 2^+ state (C.N. Gilbreth *et al.*)

$2\nu\beta\beta$ in AFMC

- Closure approximation:

$$M^{2\nu} = \sum_m \frac{\langle 0_f^+|\vec{G}|m\rangle \cdot \langle m|\vec{G}|0_i^+\rangle}{E_m - \frac{1}{2}(E_f^0 + E_i^0)} \approx \frac{\langle 0_f^+|\vec{G}\cdot\vec{G}|0_i^+\rangle}{\bar{E} - \frac{1}{2}(E_f^0 + E_i^0)}$$

where $G = \sum_a \vec{\sigma}_a \tau_a^-$.

- With $\hat{O} = \vec{G}\cdot\vec{G}$ (a separable two-body operator):

$$\langle \hat{O}^\dagger(\tau)\hat{O}(0)\rangle = e^{-\tau(E_f^0 - E_i^0)}|\langle 0_f^+|\vec{G}\cdot\vec{G}|0_i^+\rangle|^2$$

- To go beyond the closure approximation, a more complicated approach is needed (P.B. Radha *et al.*, PRL **76**, 2642 (1996) for ^{48}Ca, ^{76}Ge)

$0\nu\beta\beta$ in AFMC

- Can be calculated in the closure approximation
- The Gamow-Teller part:

$$\hat{O} = \frac{2R}{1.25^2\pi}\int_0^\infty dq\, q\, \frac{\sum_{ab} j_0(qr_{ab})h_{\mathrm{GT}}(q)\vec{\sigma}_a\cdot\vec{\sigma}_b\tau_a^-\tau_b^-}{q+\bar{E}+\frac{1}{2}(E_i^0+E_f^0)}$$

- Non-separable two-body operator
- AFMC could then be used to evaluate

$$\langle \hat{O}^\dagger(\tau)\hat{O}(0)\rangle = e^{-\tau(E_f^0-E_i^0)}|\underbrace{\langle 0_f^+|\hat{O}|0_i^+\rangle}_{M'^{0\nu}_{\mathrm{GT}}}|^2$$

- The method used for calculating response functions of one-body operators can be generalized to two-body operators

Conclusion

Finite-temperature AFMC is a powerful method for the microscopic calculation of statistical and collective properties of nuclei in very large model spaces; applications in nuclei as heavy as the lanthanides.

- Microscopic description of collectivity in heavy nuclei

- Statistical properties as a function of intrinsic deformation in a rotationally invariant framework (CI shell model) without the use of a mean-field approximation

Outlook

- Applications to other mass regions (actinides, unstable nuclei,…).

- Matrix elements for neutrinoless double beta decay in very large shell model spaces