Level densities of rare-earth nuclei in the shell model Monte Carlo approach

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- The shell model Monte Carlo (SMMC) approach.
- The thermodynamic approach to level densities.
- A theoretical challenge: the heavy deformed nuclei.
- Example: ^{162}Dy
- The crossover from vibrational to rotational collectivity in heavy nuclei
- Conclusion and prospects.

Introduction

Experimental methods: (i) counting (low energies). (ii) charged particles, Oslo method (intermediate energies); (iii) neutron resonances (neutron threshold); (iv) Ericson fluctuations (higher energies).

Theory: Fermi gas models ignore important correlations.

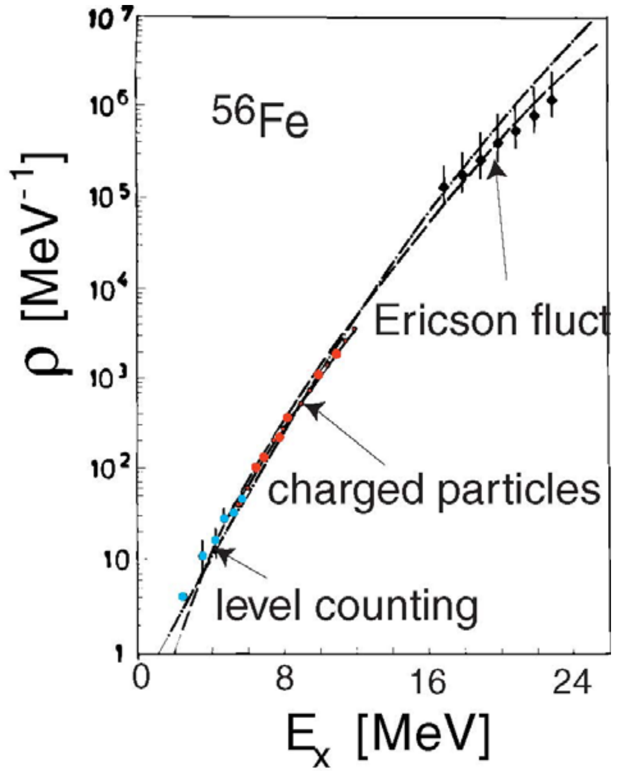
Good fits to the data are obtained using the backshifted Bethe formula (BBF):

$$\rho(E_x) = \frac{\sqrt{\pi}}{12} a^{-1/4} (E_x - \Delta)^{-5/4} e^{2\sqrt{a(E_x-\Delta)}}$$

a = single-particle level density parameter.

Δ = backshift parameter.

But: a and Δ are adjusted for each nucleus and it is difficult to predict ρ to an accuracy better than an order of magnitude.



The interacting shell model includes both shell effects and residual interactions but the required model space is prohibitively large.

Shell Model Monte Carlo (SMMC) method

Correlations beyond the mean field can be calculated by taking into account all fluctuations of the mean field:

Gibbs ensemble $e^{-H/T}$ at temperature T can be written as a superposition of ensembles U_σ of non-interacting nucleons in time-dependent fields $\sigma(\tau)$

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

(Hubbard-Stratonovich transformation).

The calculation of the integrand reduces to matrix algebra in the single-particle space.

The multi-dimensional integral is evaluated by Monte Carlo methods.

- The method has been used in the interacting shell model and is known as the shell model Monte Carlo (SMMC)

[Lang, Johnson, Koonin, Ormand, PRC 48, 1518 (1993);
Alhassid, Dean, Koonin, Lang, Ormand, PRL 72, 613 (1994)].

Thermodynamic approach to level densities

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

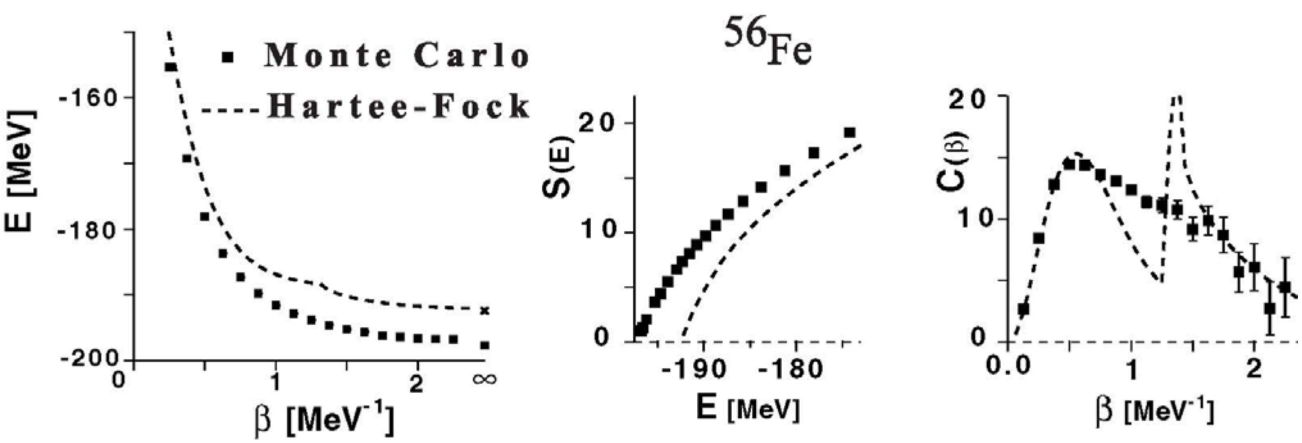
The *average* level density is given by: $\rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)}$

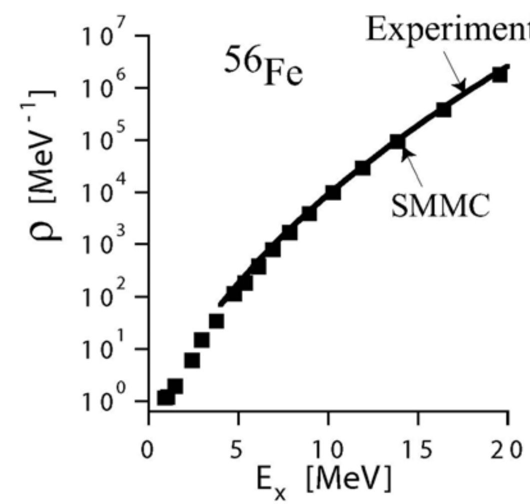
$S(E)$ = canonical entropy; C = canonical heat capacity.

We calculate the thermal energy $E(T) = \langle H \rangle$ in SMMC and integrate

$-\partial \ln Z / \partial\beta = E(\beta)$ to find the partition function $Z(\beta)$.

Entropy: $S(E) = \ln Z + \beta E$, Heat capacity: $C = -\beta^2 \partial E / \partial \beta$





The heavy deformed nuclei

[Y. Alhassid, L. Fang and H. Nakada, Phys. Rev. Lett. **101**, 082501 (2008)]

• Most SMMC calculations to date were in medium-mass nuclei:
small deformation, first excitation ~ 1- 2 MeV in even-even nuclei.

• Very different situation in heavy deformed nuclei:
large deformation, first excitation ~ 100 keV, rotational bands.

Can we describe rotational behavior microscopically in a truncated spherical shell model?

Technical challenges

• Protons and neutrons occupy *different* shells

$\Rightarrow$ SMMC extended to *pn formalism*.

• Very large shell model space (~10^{29} in rare-earth nuclei)
• Propagation to much longer imaginary time (low temperature)

$\Rightarrow$ Largest SMMC calculations to date

• The one-body propagator becomes ill-conditioned at large imaginary times

$\Rightarrow$ Introduced stabilization methods in the canonical ensemble

Model space

Determine the occupation probability $r_{\alpha j} = \langle n_{\alpha j} \rangle / (2j+1)$
of spherical orbitals of the ground-state solution in a deformed
Woods-Saxon potential.

- We choose orbitals with $0.1 < r_{\alpha j} < 0.9$
- Effect of other orbitals is taken into account by renormalization of the interaction.

In our studies of rare-earth nuclei we have used the following model space

Protons: [50-82 shell] + 1*f*7/2.

Neutrons: 0*h*11/2 + [82-126 shell] + 1*g*9/2.

Effective Hamiltonian

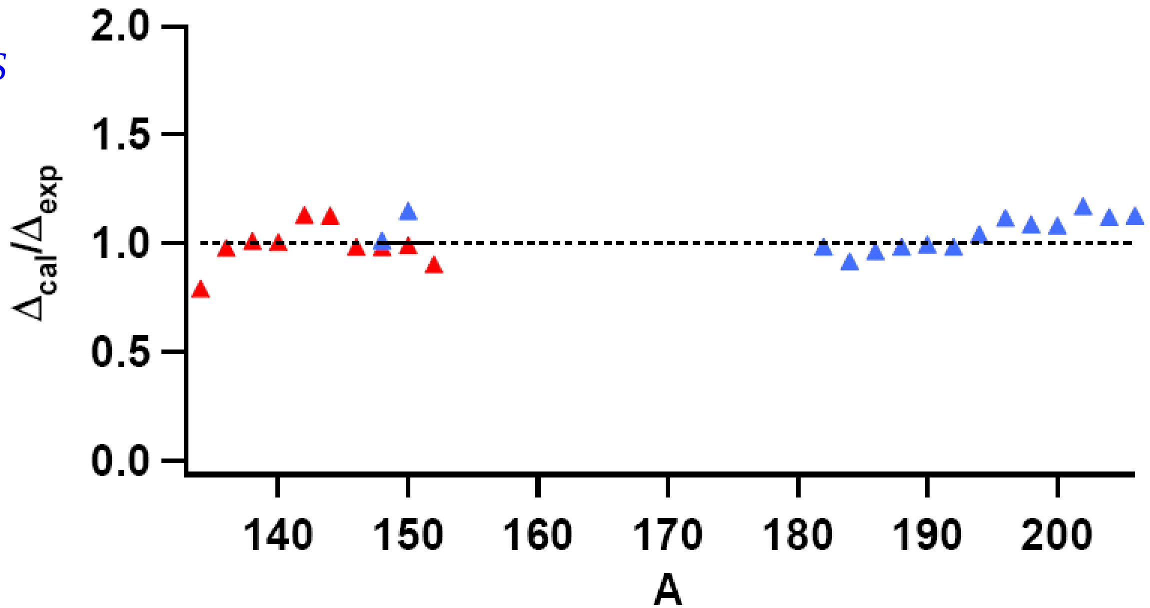
- Single-particle energies: reproduce (in spherical HF) the s.p. energies of a Woods-Saxon potential plus spin-orbit coupling.

- The interaction includes the *dominant* components of *realistic* effective interactions: pairing + multipole-multipole interactions (quadrupole, octupole, and hexadecupole).

Pairing interaction: $g = \gamma g^{BCS}$

g^{BCS} reproduces in particle-projected BCS the experimental gap (from odd-even mass differences):

$g_p^{BCS} = 10.9 / Z; \quad g_n^{BCS} = 10.9 / N$.



γ is a suppression factor (accounts for pairing field fluctuations)

- Multipole-multipole interaction is determined *self-consistently* and *renormalized* (core polarization) $k_2 \sim 2; \; k_3 = 1.5; \; k_4 = 1.$
- This interaction has a good Monte Carlo sign.

Stabilization of propagator

The propagator $U_\sigma = \prod e^{-\Delta\beta h_\sigma}$ mixes large and small scales and becomes ill-conditioned for large number of time slices.

- Use a modified Gram-Schmidt for each factor $M = ADB$ where D is diagonal and A,B are well behaved to stabilize the product

- Stabilize each term in the particle-number projection sum

Example: ^{162}Dy

Interaction: $\gamma = 0.77; \ k_2 = 2.12$

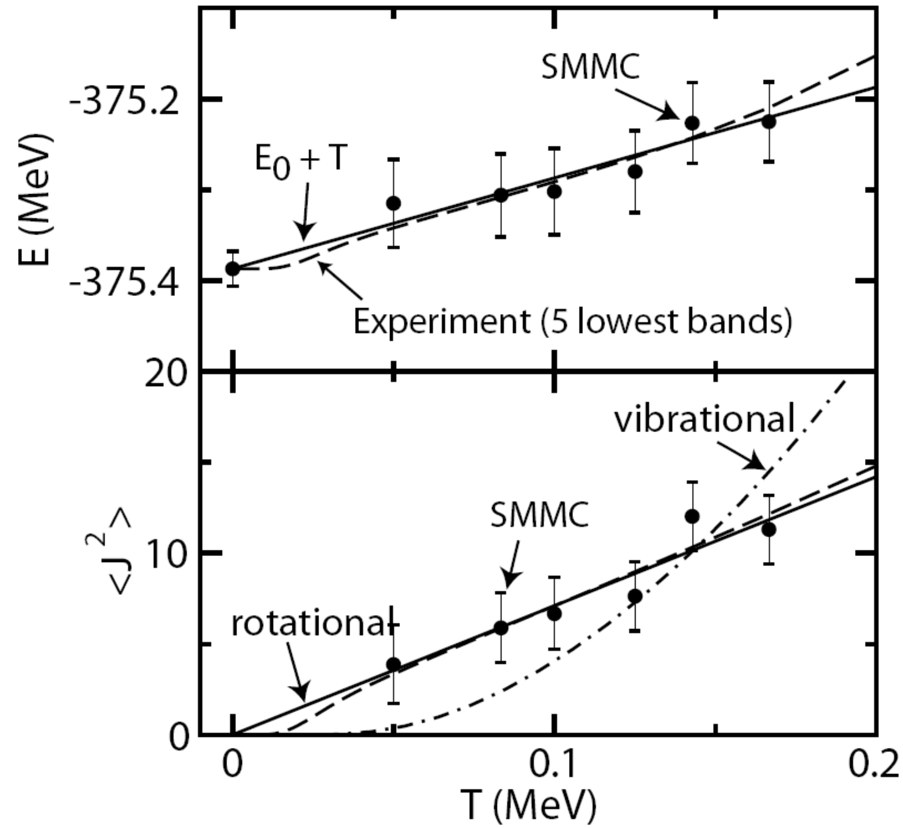
- E versus T in agreement with a ground-state *rotational* band:

$$E \approx E_0 + T$$

- $<J^2>$ versus T confirms rotational character with a moment of inertia:

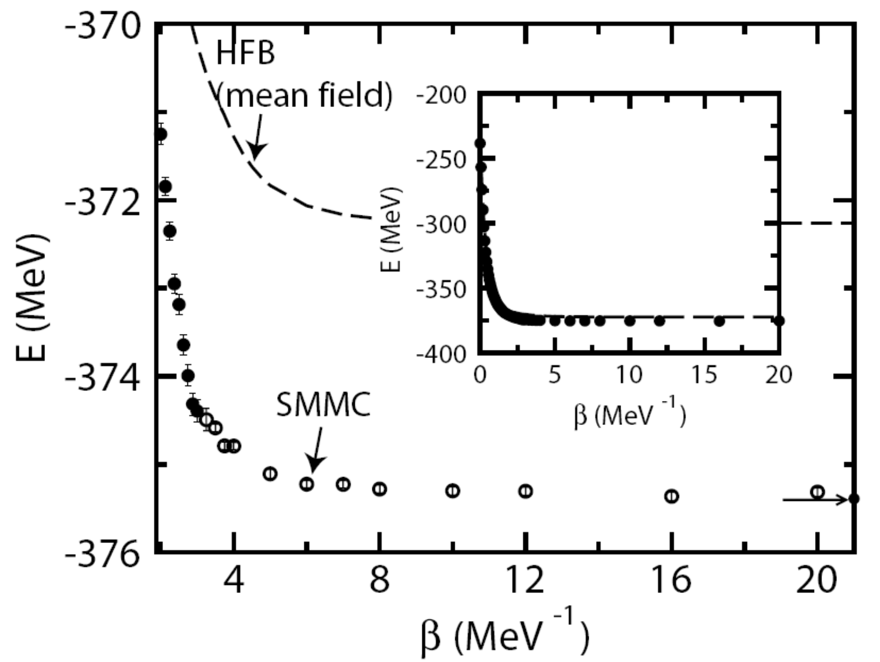
$$< J^2 > \approx 2IT$$

with $I = 35.5 \pm 3.3\, MeV^{-1}$
(experimental value is $37.2\, MeV^{-1}$).

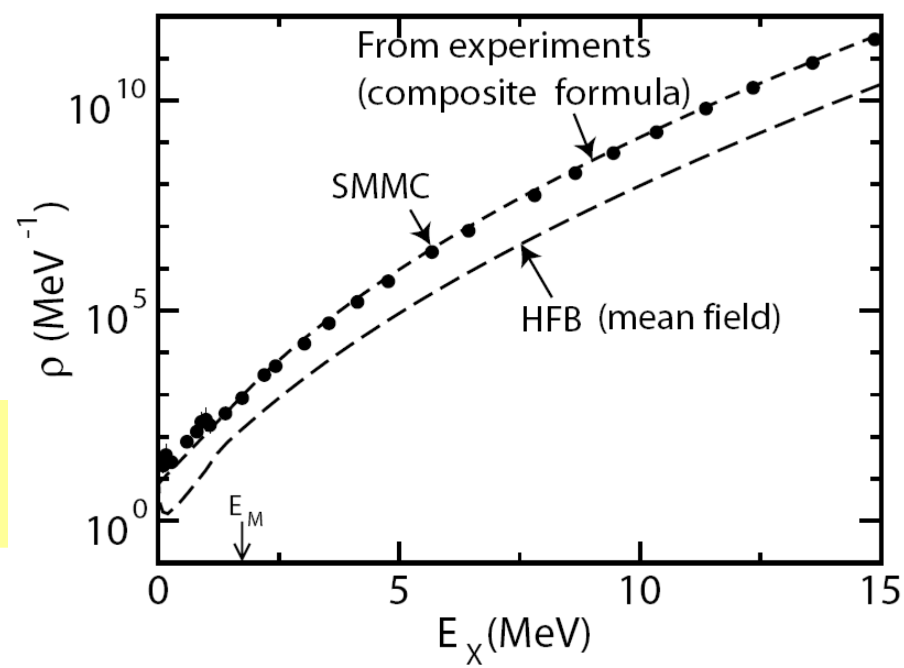


Rotational character can be reproduced in a truncated spherical shell model !

Thermal energy vs. inverse temperature



- Ground-state energy in SMMC has additional ~ 3 MeV of correlation energy as compared with Hartree-Fock-Boguliubov (HFB).



- Results from several experiments are fitted to a *composite formula*: constant temperature below E_M and BBF above.

- SMMC level density is in excellent agreement with experiments.

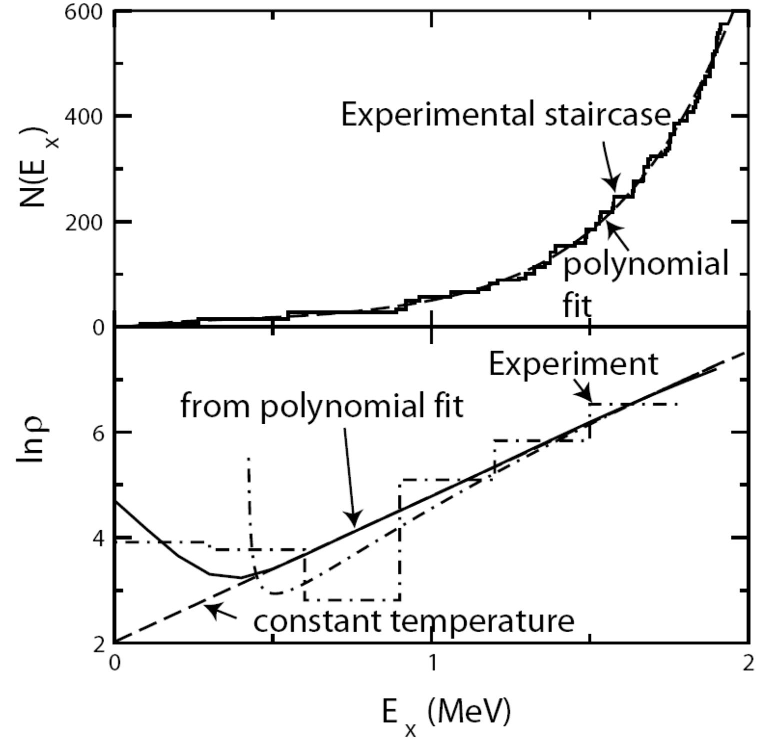
Experimental state density

- An almost complete set of levels (with spin) is known up to ~ 2 MeV.

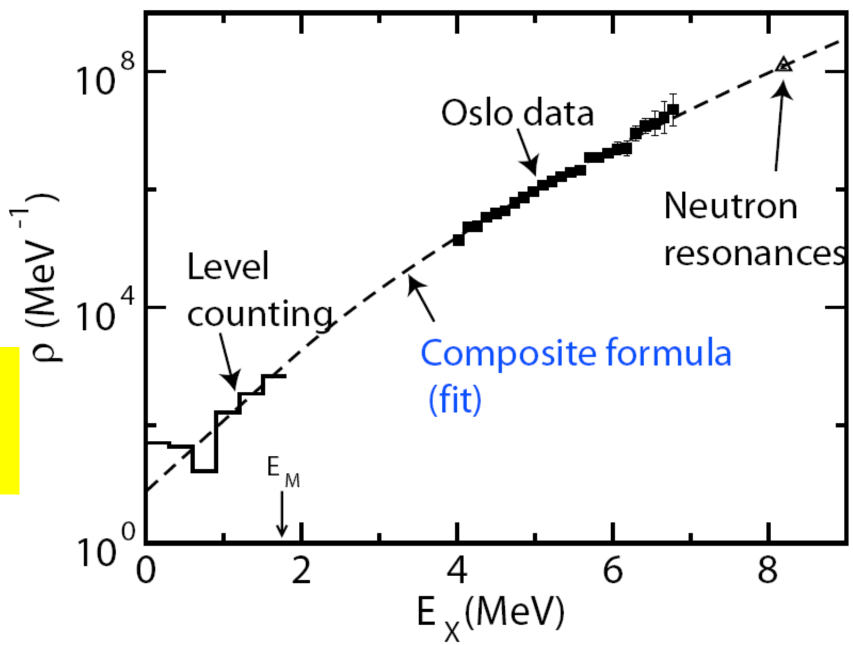
(i) A constant temperature formula is fitted to level counting.

(ii) A BBF above E_M is determined by matching conditions at E_M

$\Rightarrow$ A *composite* formula



(iii) Renormalize Oslo data by fitting their data and neutron resonance to the composite formula



The composite formula is a good fit to all three sets of experimental data.

Crossover from vibrational to rotational collectivity in heavy nuclei

(C. Ozen, Y.A., H. Nakada)

Heavy nuclei exhibit various types of collectivity: vibrational, rotational, … and crossovers between them.

Successfully described by empirical models.

However, a microscopic description is still lacking.

Can we describe the crossover from vibrational to rotational collectivity in heavy nuclei using the framework of the interacting shell model ?

The required large model space necessitates the use of SMMC.

The various types of collectivity can be 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 and can be calculated in SMMC.

Conclusion

• Fully microscopic calculations of level densities are now possible by shell model quantum Monte Carlo methods.

• The spin, isospin and parity distributions can be calculated using projection methods (see talk by H. Nakada).

• SMMC successfully extended to heavy deformed nuclei: rotational character can be reproduced in a truncated spherical shell model.

Prospects

• Study collective transitions in heavy nuclei.

• Derive global effective shell model interactions from density functional theory

[Quadrupole: Alhassid, Bertsch, Fang and Sabbey, Phys. Rev. C 74, 034301 (2006); Quadrupole + pairing: Rodriguez-Guzman, Alhassid, Bertsch, Phys. Rev. C 77, 064308 (2008)].