The shell model Monte Carlo approach to level densities: from medium-mass to heavy deformed nuclei

Yoram Alhassid (Yale University)

- Introduction
- The shell model Monte Carlo (SMMC) approach.
- The thermodynamic approach to level densities.
- Level densities in medium-mass nuclei: theory versus experiment.
- Projection on good quantum numbers: parity, spin,…
- A theoretical challenge: the heavy deformed 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.

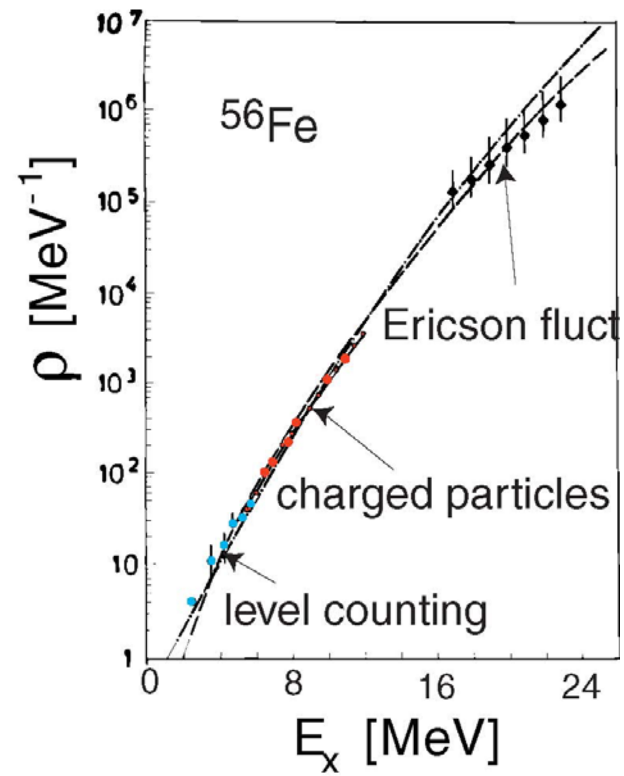
Good fits to the data are obtained using the backshifted Bethe formula (BBF):

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

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.

Auxiliary field Monte Carlo (AFMC) 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)]

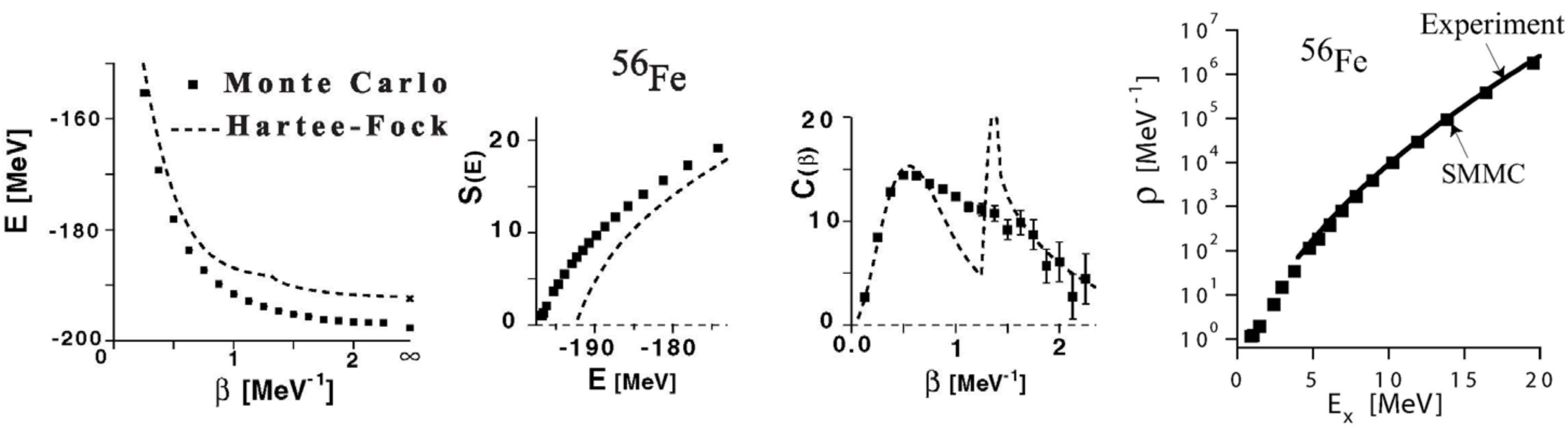
The *average* level density is given by: $\rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)}$

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

In SMMC, we calculate the thermal energy $E(T) = \langle H \rangle$ 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: $C = -\beta^2 \partial E / \partial\beta$



Medium mass nuclei (A ~ 50 -70)

We have used SMMC to calculate the statistical properties of nuclei in the iron region in the complete $fpg_{9/2}$-shell.

- Single-particle energies from Woods-Saxon potential plus spin-orbit.

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

  Pairing interaction is determined to reproduce the experimental gap (from odd-even mass differences).

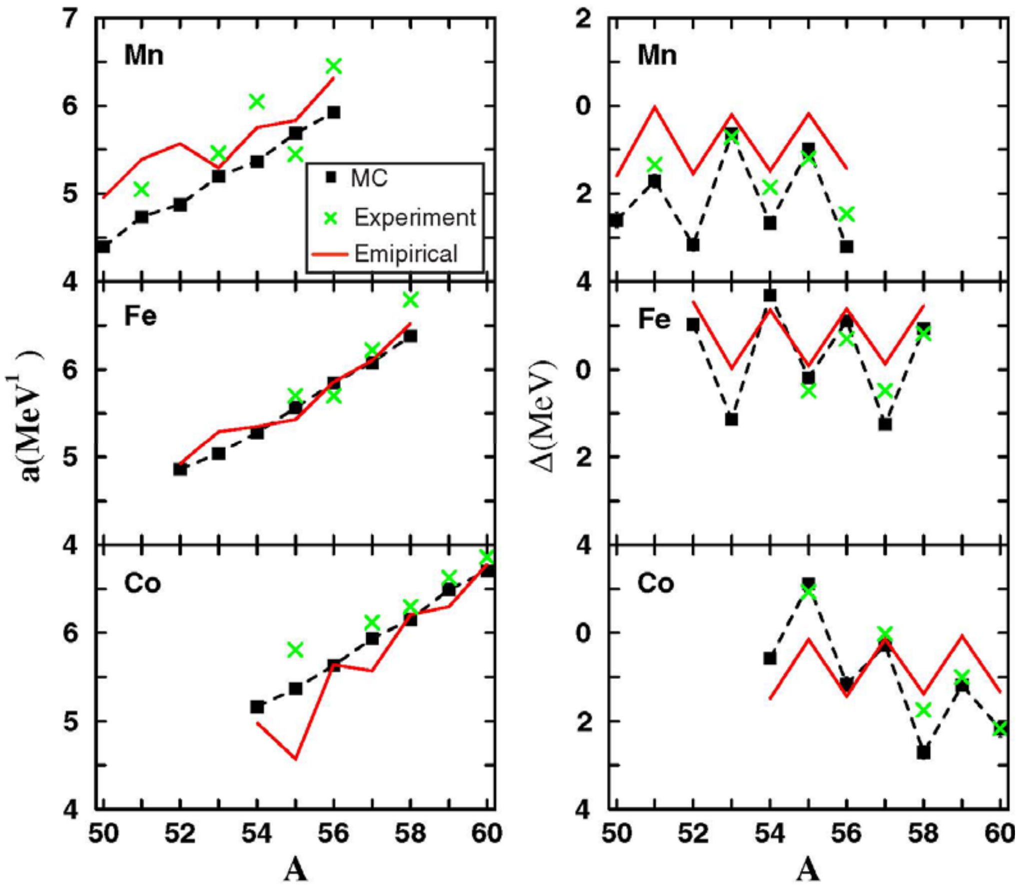
  Multipole-multipole interaction is determined *self-consistently* and *renormalized*.

- Interaction has a good Monte Carlo sign.

Systematics of the level density parameters

[Y.Alhassid, S. Liu, and H. Nakada, PRL 83, 4265 (1999)]

SMMC level densities are well fitted to the backshifted Bethe formula



$\Rightarrow$ Extract a and Δ

- a is a smooth function of A.

- Odd-even staggering effects in Δ (a pairing effect).

- Good agreement with experimental data without adjustable parameters.

- Improvement over empirical formulas.

Extending the theory to higher temperatures

[Alhassid, Bertsch and Fang, PRC **68**, 044322 (2003)]

- It is time consuming to include higher shells in the Monte Carlo approach.

We have combined the fully correlated partition in the truncated space with the independent-particle partition in the *full space* (all bound states plus continuum):

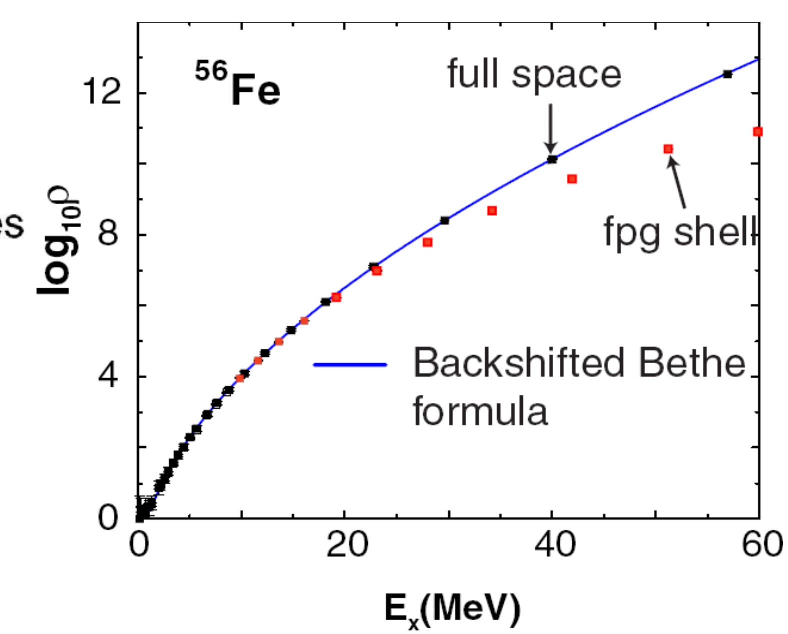
correlated

independent particles

$$\ln Z_v = \ln Z_{v,tr} + \ln Z_{sp} - \ln Z_{sp,tr}$$

correlated in truncated space

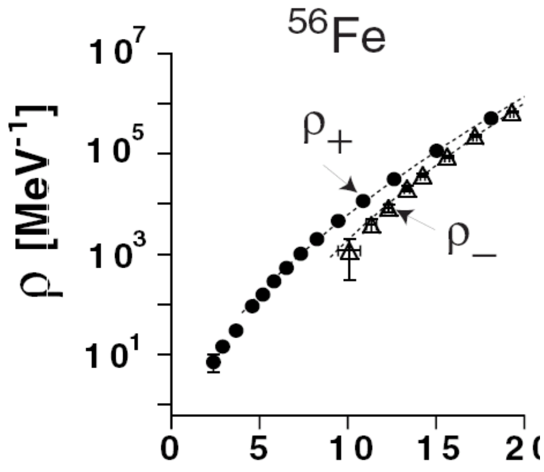
independent particles in tuncated space



Parity dependence of level densities

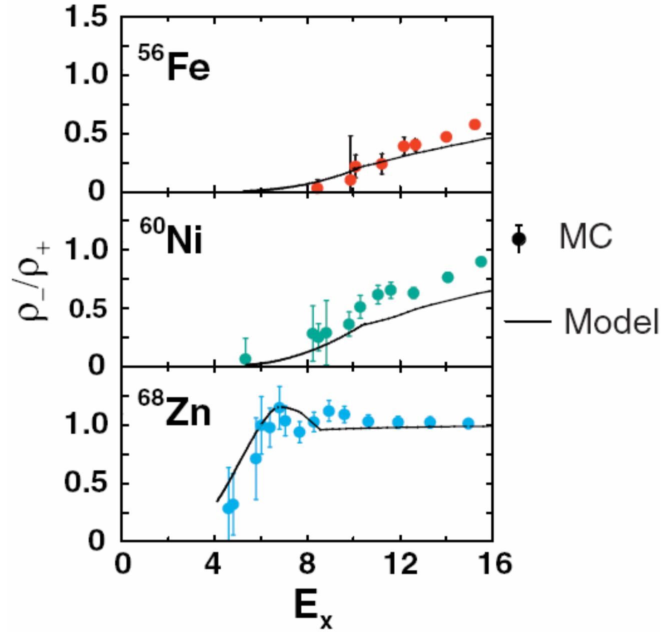
Alhassid, Bertsch, Liu, Nakada [Phys. Rev. Lett. 84, 4313 (2000)]

We use parity projection to calculate exactly even- and odd-parity level densities $\rho_{\pm}$



$\rho_+ \neq \rho_-$ even at neutron resonance energy (contrary to a common assumption used in nucleosynthesis).

Ratio of odd-to-even parity level densities versus excitation energy.



Spin distribution of level densities and moment of inertia

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

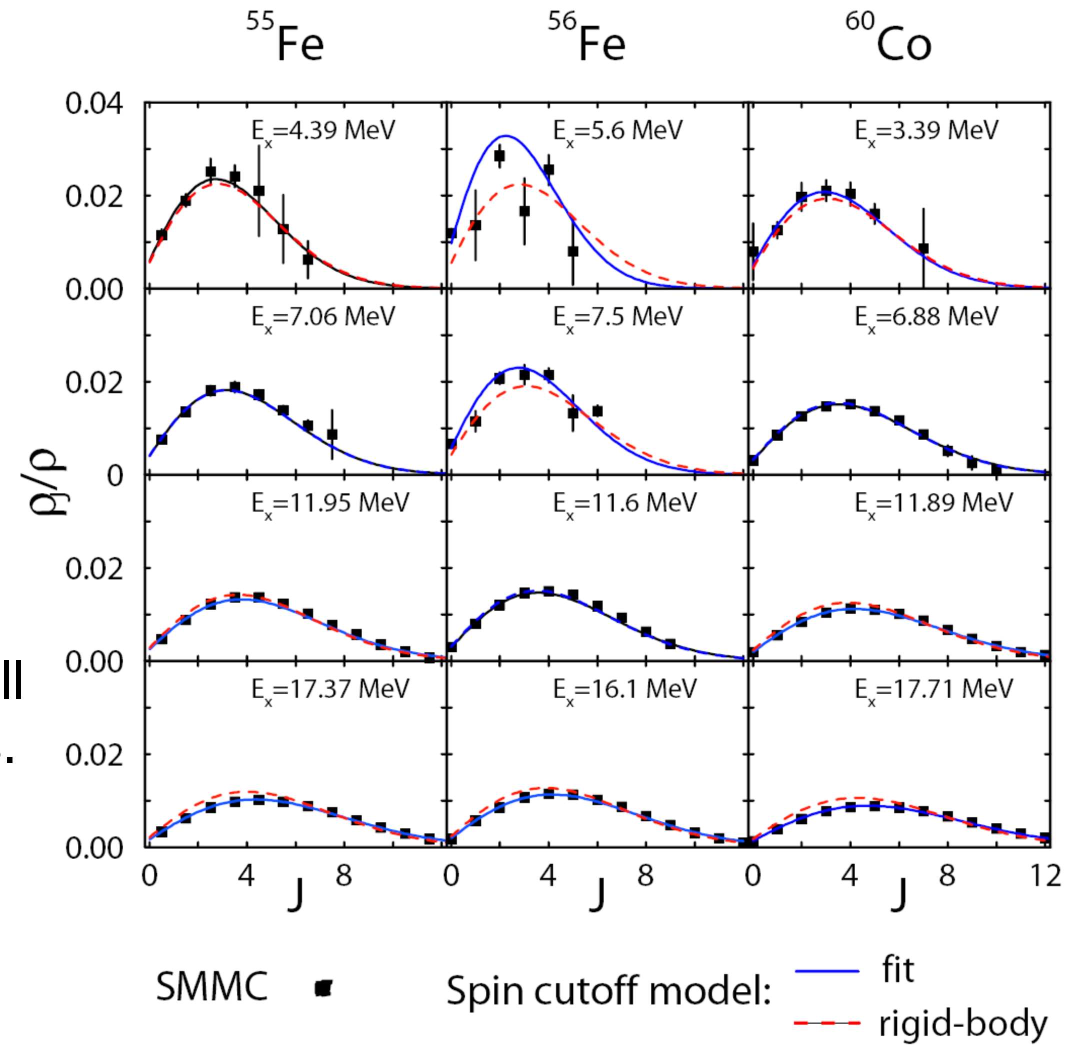
Spin distributions in even-odd, even-even and odd-odd nuclei

Spin cutoff model (random coupling of single-particle spins):

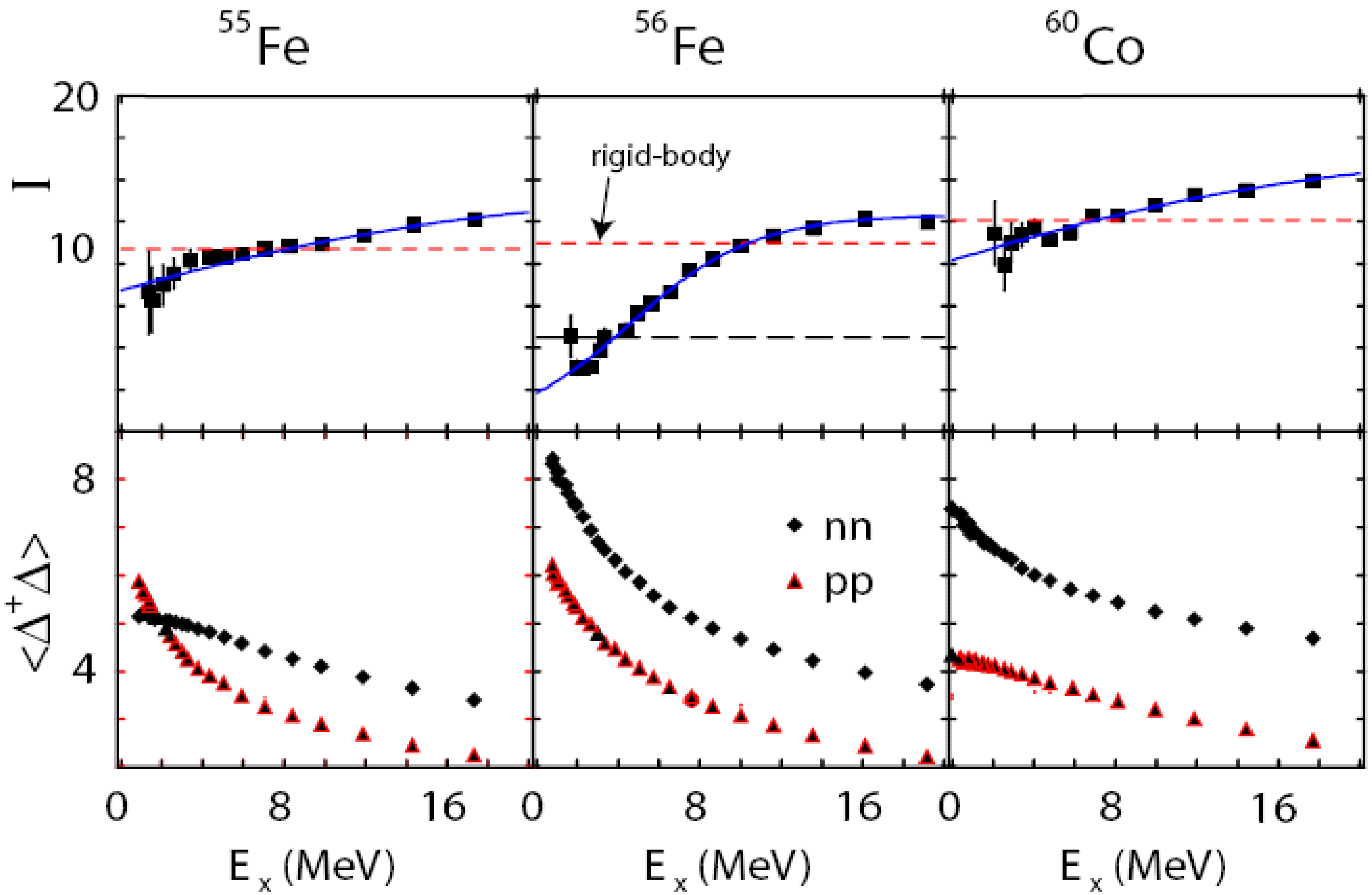
$$\frac{\rho_J}{\rho} = \frac{2J+1}{2\sqrt{2\pi}\sigma^3} e^{-J(J+1)/2\sigma^2}$$

- Spin cutoff model works very well except at low excitation energies.

- Staggering effect in spin for even-even nuclei.



Thermal moment of inertia can be extracted from: $\sigma^2 = \frac{IT}{\hbar^2}$



Signatures of pairing correlations:

- Suppression of moment of inertia at low excitations in even-even nuclei.
- Correlated with pairing energy of J=0 neutrons pairs.

The heavy deformed nuclei

[Y. Alhassid, L. Fang and H. Nakada, arXive:0710.1656 (2007)]

• 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 nuclei:
large deformation, first excitation ~ 100 keV, rotational bands.

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

Technical challenges

• Choice of single-particle model space: inclusion of *intruder* states.

• Protons and neutrons occupy *different* shells: SMMC extended to *pn formalism*.

• The one-body propagator become ill-conditioned at large imaginary times: apply *stabilization* methods in the *canonical* ensemble.

First example: ^{162}Dy

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

• Model space includes 10^{29} configurations ! (largest SMMC calculation to date).

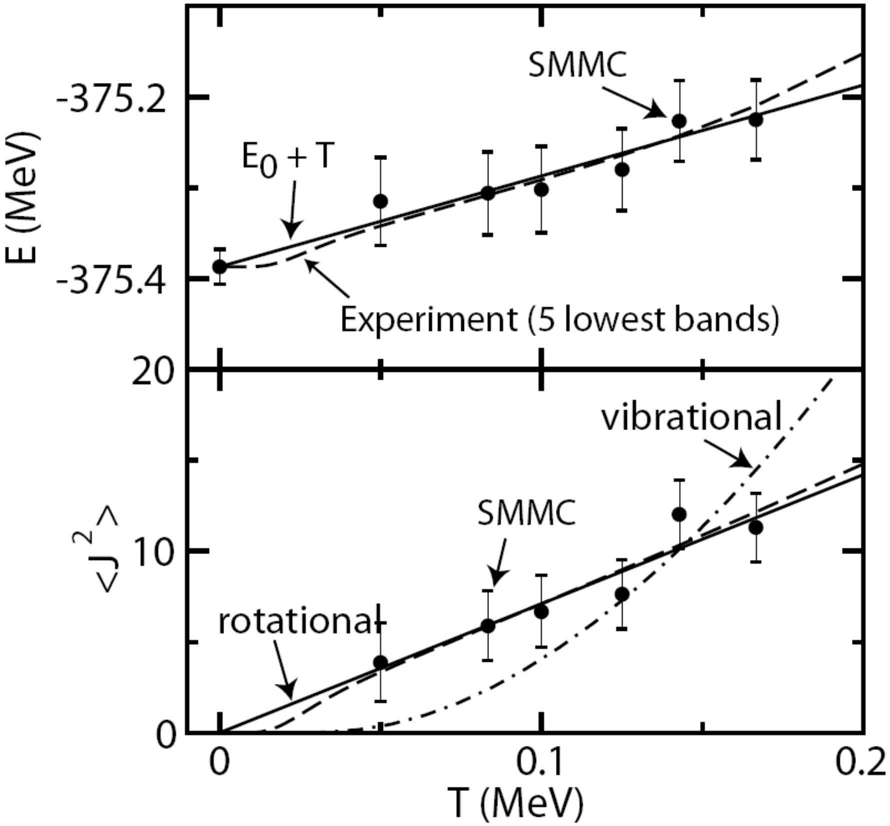
• E versus T in agreement with a ground-state *rotational* band:

$$E \approx E_0 + T$$

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

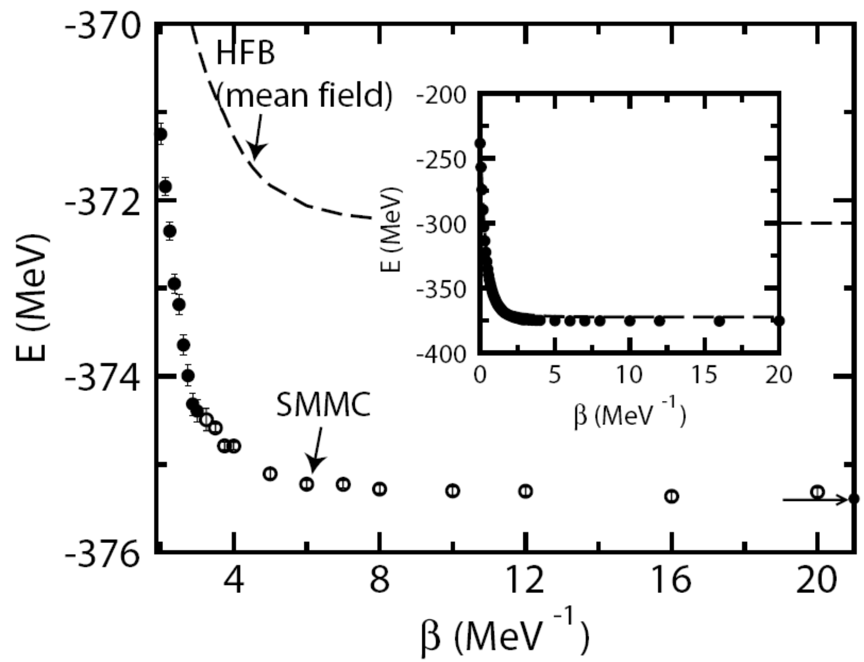
$$< J^2 > \approx 2IT$$

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 !

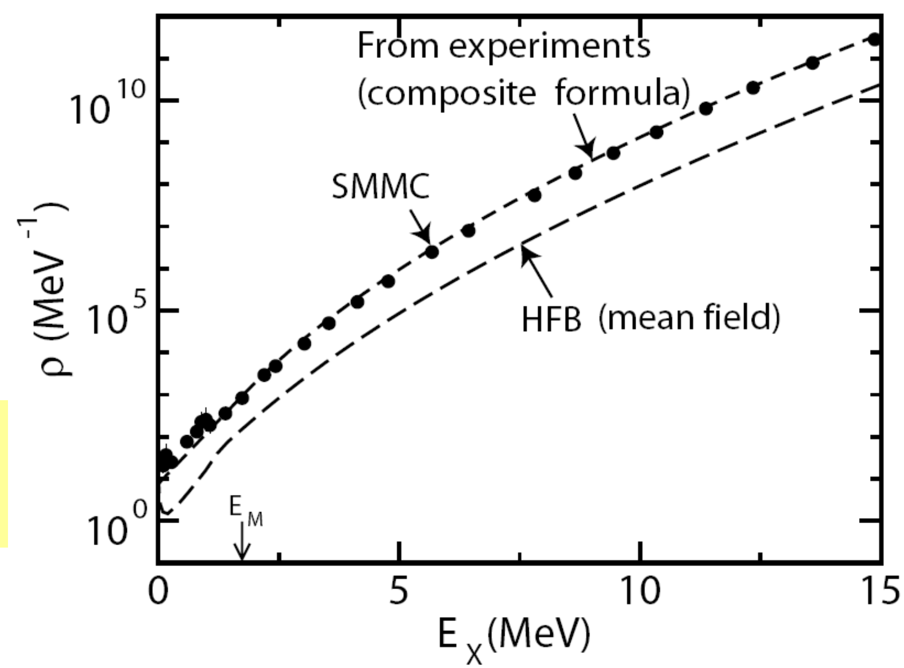
Thermal energy vs. inverse temperature



• 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.



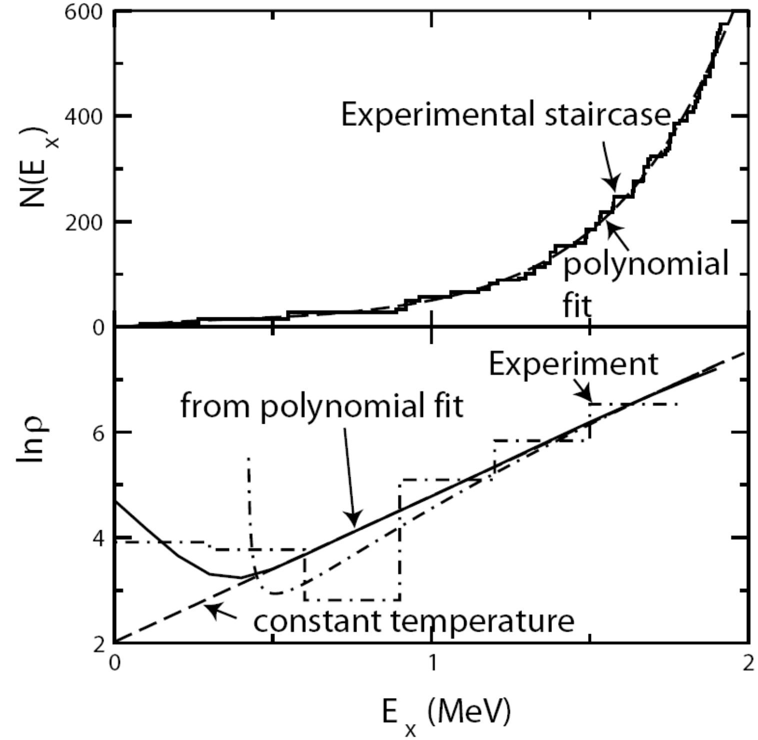
Experimental state density

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

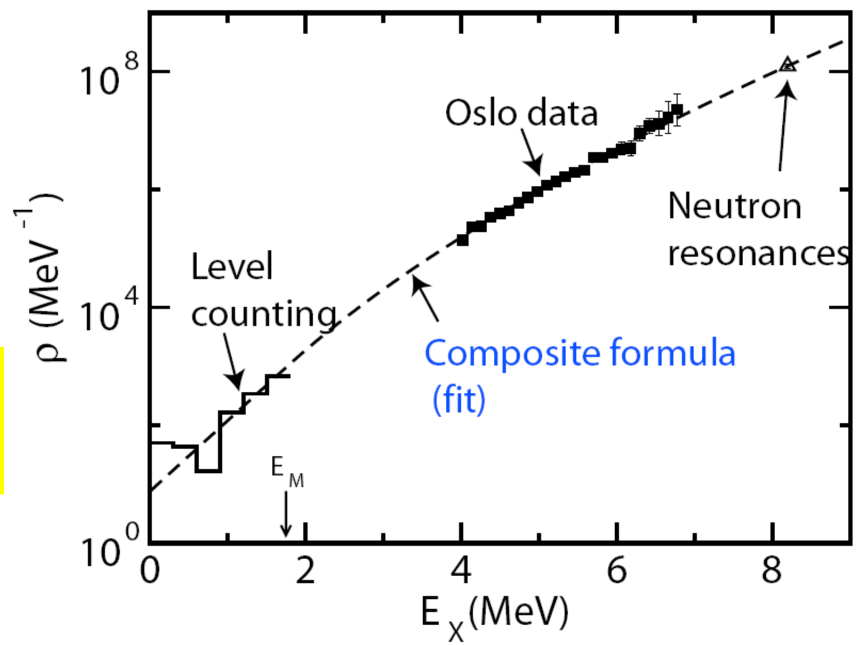
(i) A constant temperature formula is fitted to level counting.

(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 an excellent fit to all three experimental data.

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.

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

Prospects

• Mitigate the sign problem in SMMC: Stoitcheva, Ormand, Neuhauser, Dean, arXive:07082945.

• 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, arXive:0709.0508 (2007).