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

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

Nuclear Level Densities: introduction

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

Theory: Fermi gas models ignore important correlations.

However, good fits to the data are obtained using the backshifted Bethe formula (BBF):

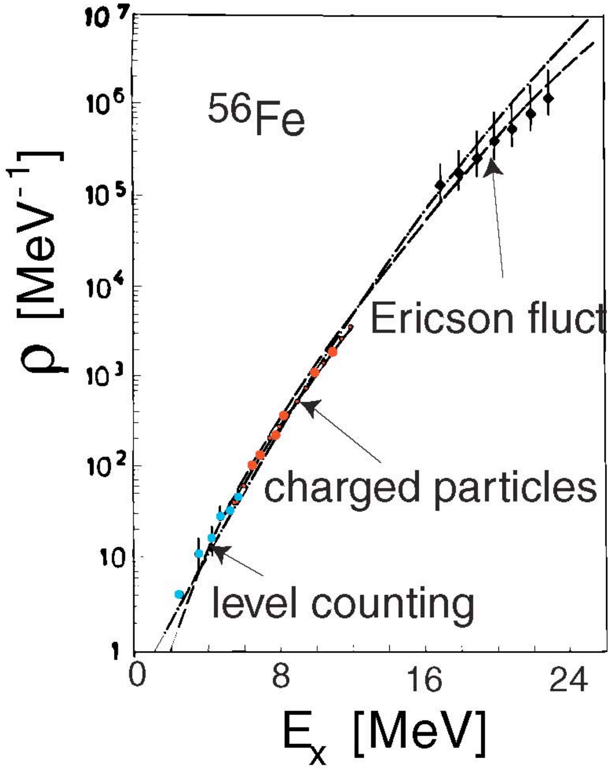
$$\rho\left(E_x\right) = \frac{\sqrt{\pi}}{12} a^{-1/4} \left(E_x - \Delta\right)^{-5/4} e^{2\sqrt{a(E_x-\Delta)}}$$

a = single-particle level density parameter.

Δ = backshift parameter.

But: a and Δ are adjusted for each nucleus.

- It is difficult to predict ρ to an accuracy bette than an order of magnitude.



⇒ Use the interacting shell model (includes both shell effects and residual interactions).

Auxiliary field Monte Carlo (AFMC) methods

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

Gibbs ensemble $e^{-\beta H} \left(\beta = 1/T\right)$ 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: shell model Monte Carlo (SMMC): Caltech + Yale

- We have recently extended AFMC to ultra-small metallic particles (nanoparticles).

Interactions

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-Saxson potential plus spin-orbit.

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

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

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

• Interaction has a good Monte Carlo sign.

Thermodynamic approach

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

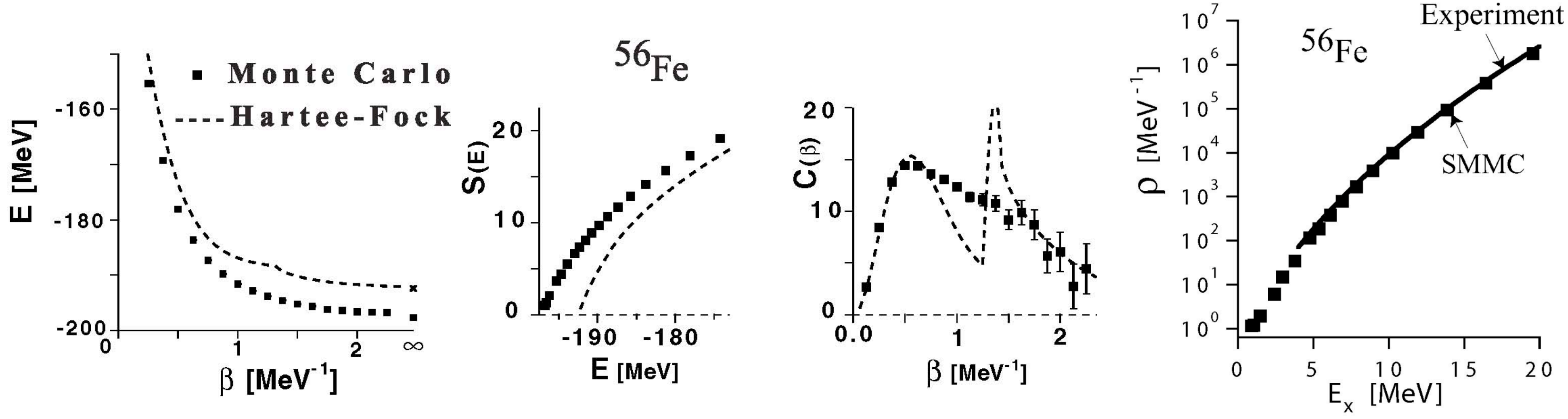
The *average* level density is given by: $\rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)}$

$S(E)$ = 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.

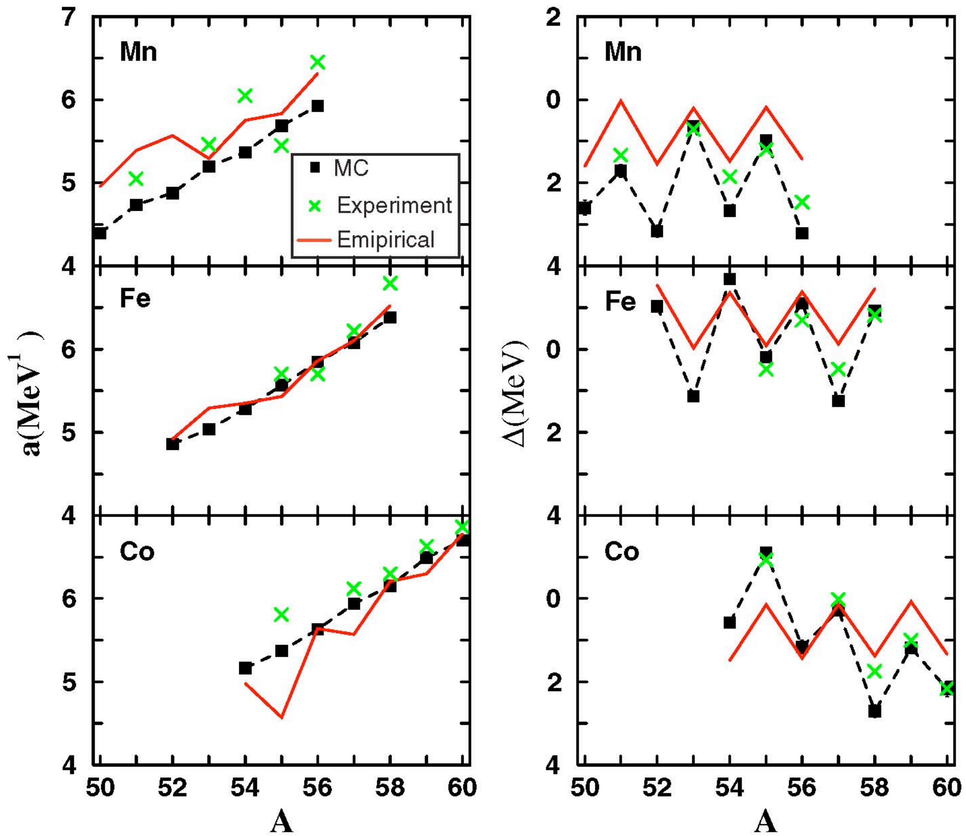
Entropy: $S(E) = \ln Z + \beta E$, Heat capacity: $C = -\beta^2 \partial E / \partial \beta$



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



Extract a and Δ

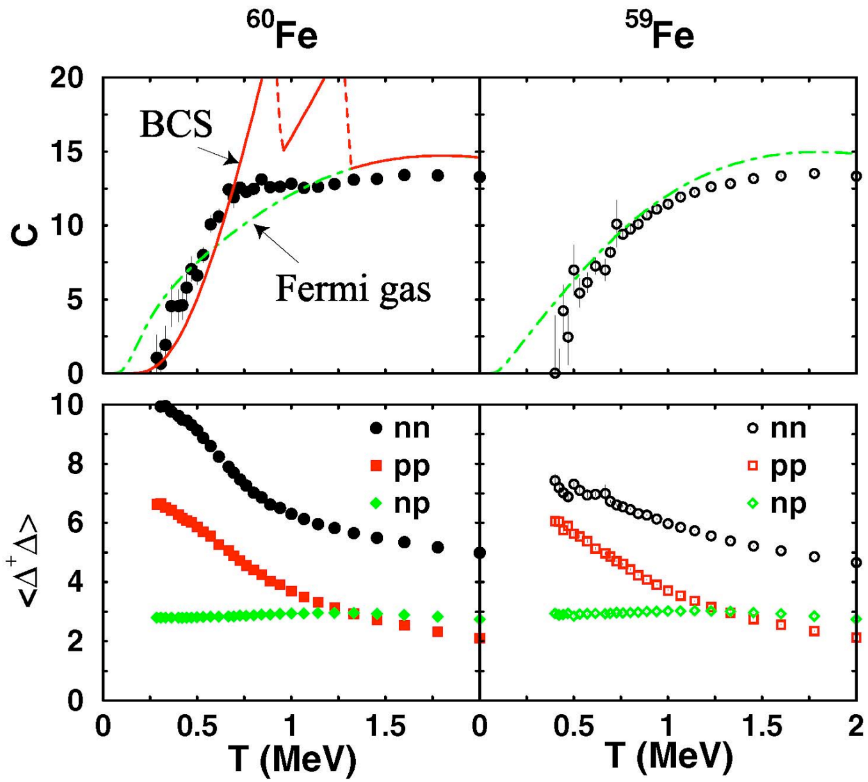
- a is a smooth function of A.
- Odd-even staggering effects in Δ (a pairing effect).

- Good agreement with experimental data without adjustable parameters.
- Improvement over empirical formulas.

Heat capacity

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

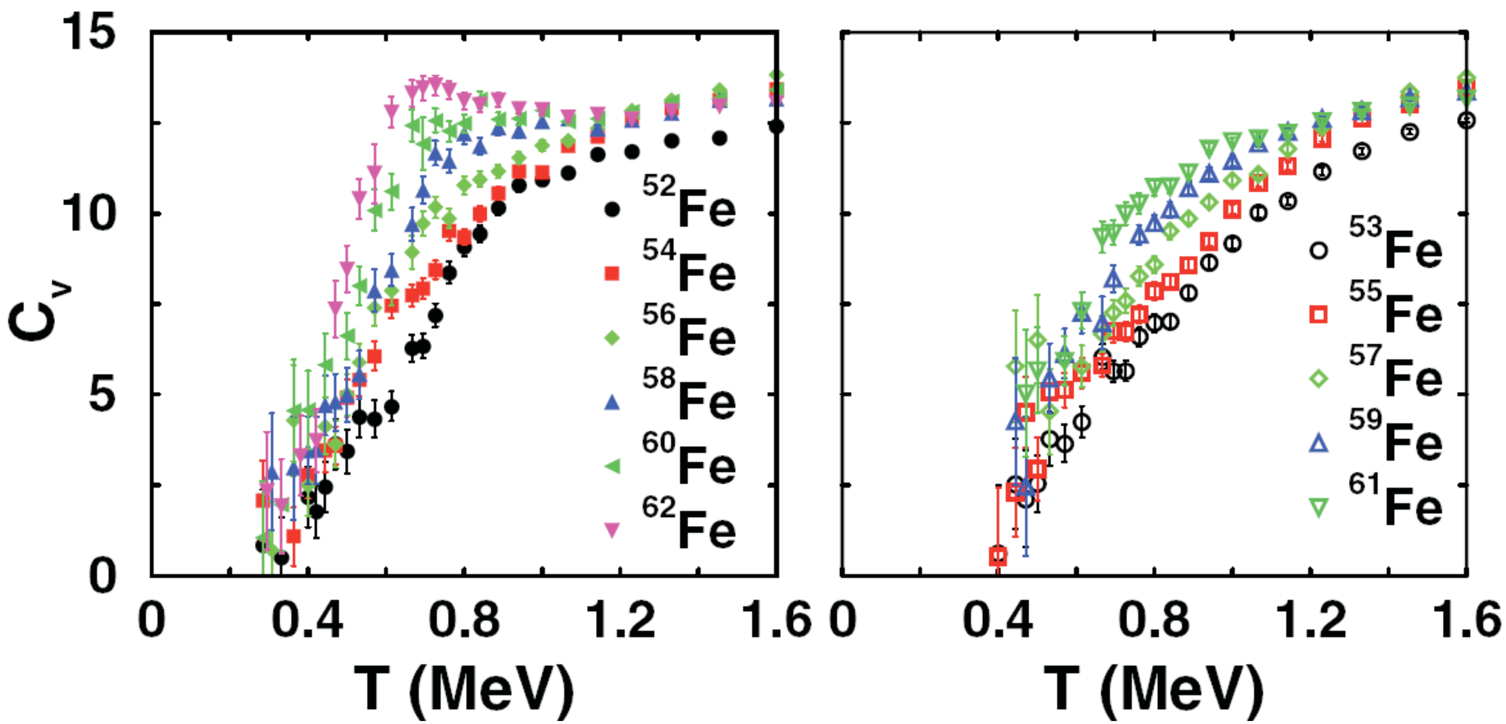
- Strong suppression of the BCS peak.
- A 'bump' remains for ^{60}Fe around the neutron pairing transition temperature.



- Correlated with $<\Delta^{\dagger}\Delta>$. for $J=0$ neutron pairs

But: since only one major shell is taken, the heat capacity saturates in the vicinity of the 'bump'.

Systematic of the heat capacity in neutron-rich iron isotopes



A bump develops in the heat capacity of even-even nuclei with increasing number of neutron pairs.

Extending the theory to higher temperatures

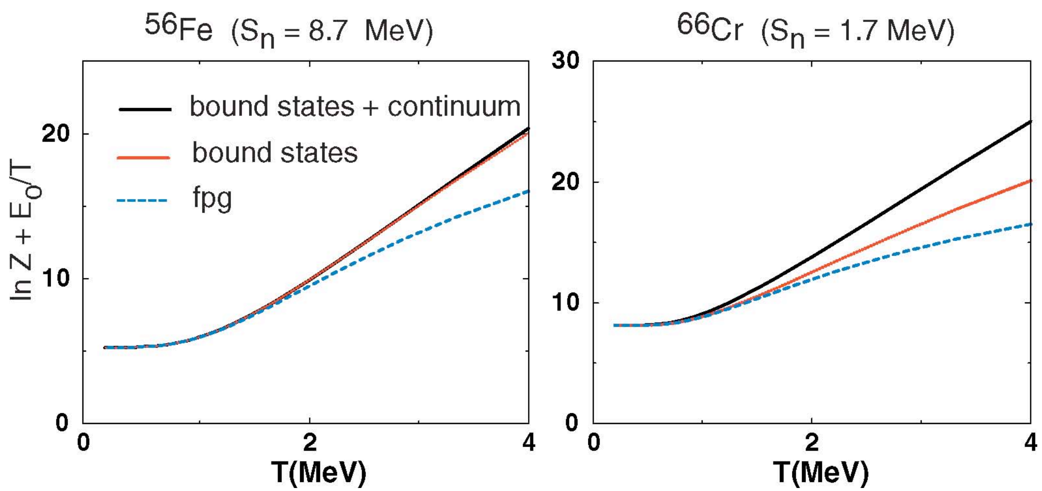
[Y.Alhassid., G.F. Bertsch, and L. Fang, Phys. Rev. C **68**, 044322 (2003)]

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):

(i) Independent-particle model

- Include both bound states and *continuum*:



- Truncation to one major shell is problematic for $T > 1.5$ MeV.
- The continuum is important for a nucleus with a small neutron separation energy (^{66}Cr).

(ii) With interactions

Combine the fully correlated partition in the truncated space with the independent-particle partition in the full space

correlated ↓ — independent particles ↓

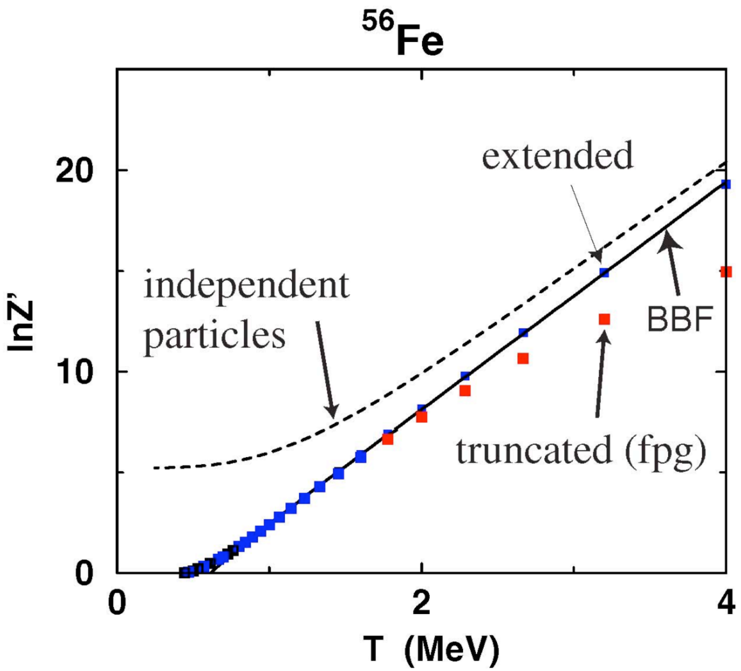
$$\ln Z_v = \ln Z_{v,tr} + \ln Z_{sp} - \ln Z_{sp,tr}$$

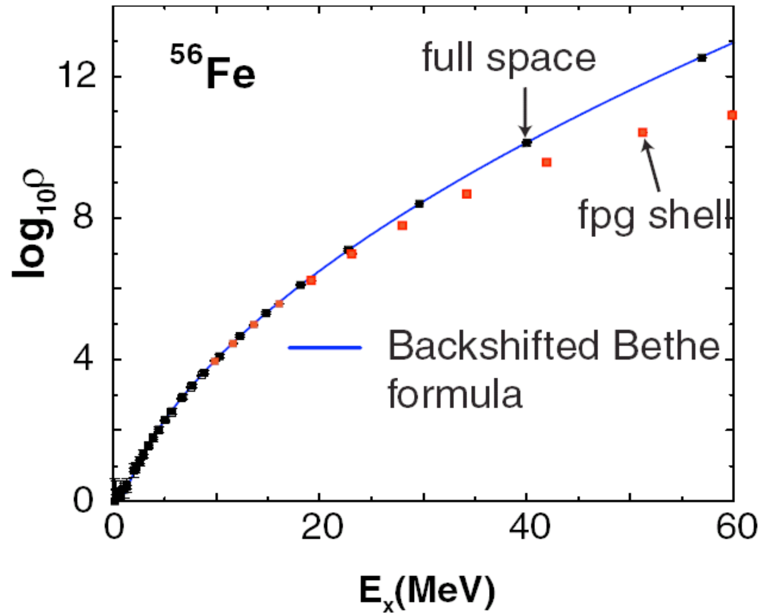
$\ln Z_v$: correlated

$\ln Z_{v,tr}$: correlated in truncated space

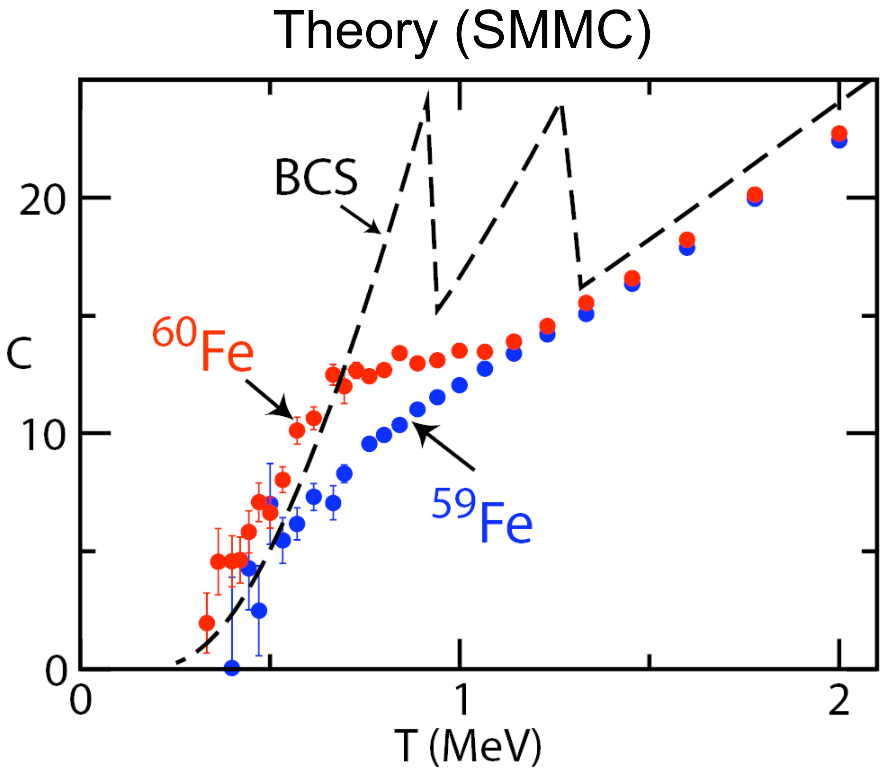
$\ln Z_{sp}$: independent particles

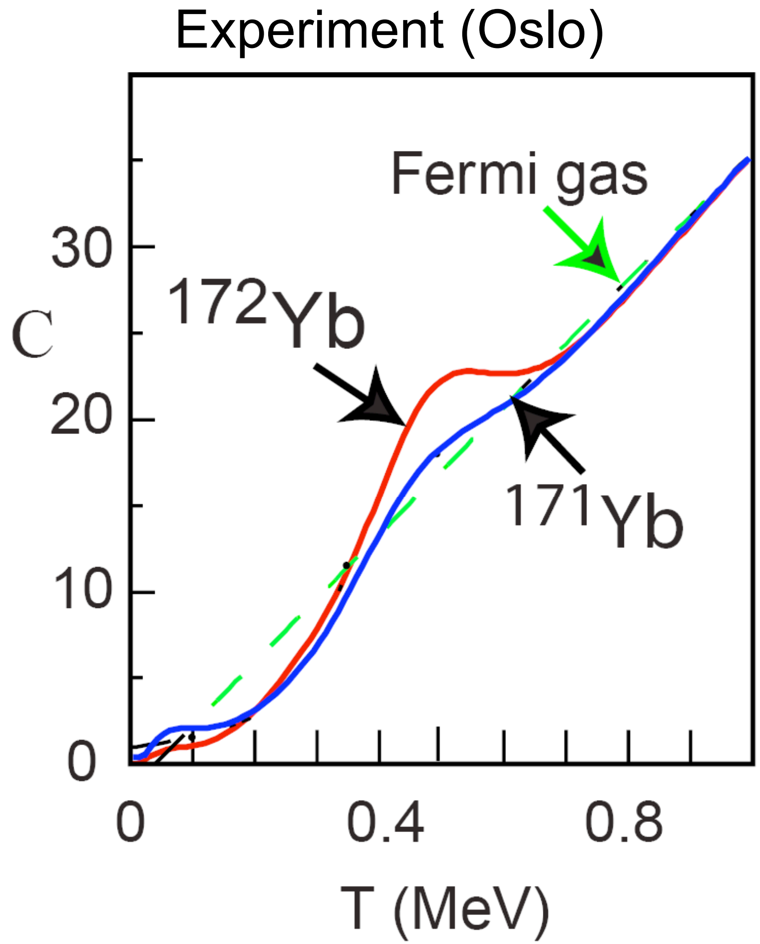
$\ln Z_{sp,tr}$: independent particles in tuncated space





Extended heat capacity (up to $T \sim 4$ MeV)





- Strong odd/even effect: a signature of pairing phase transition

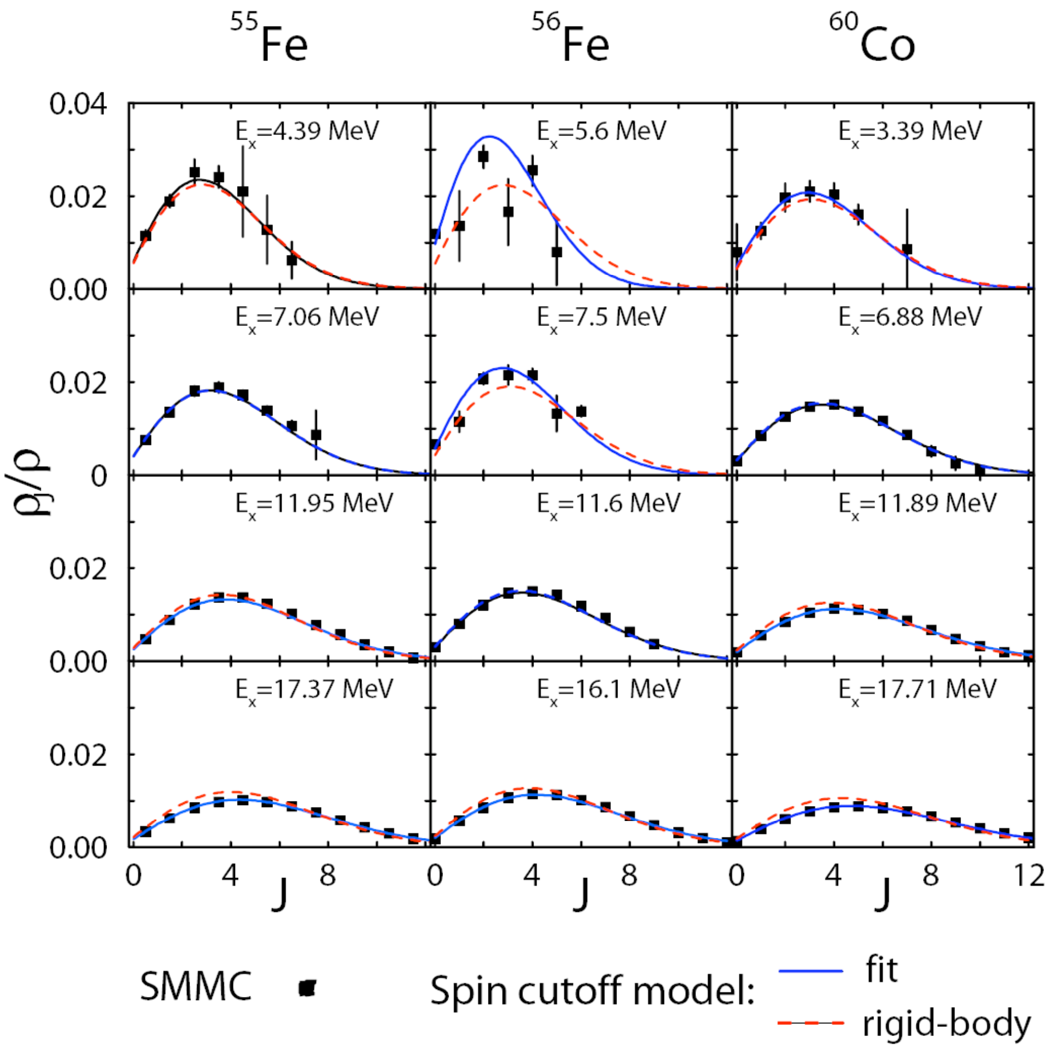
Spin distribution and moment of inertia

[Y. Alhassid, S. Liu and H. Nakada, nucl-th/0607062]

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

Spin cutoff model
(random coupling of s.p. spins):

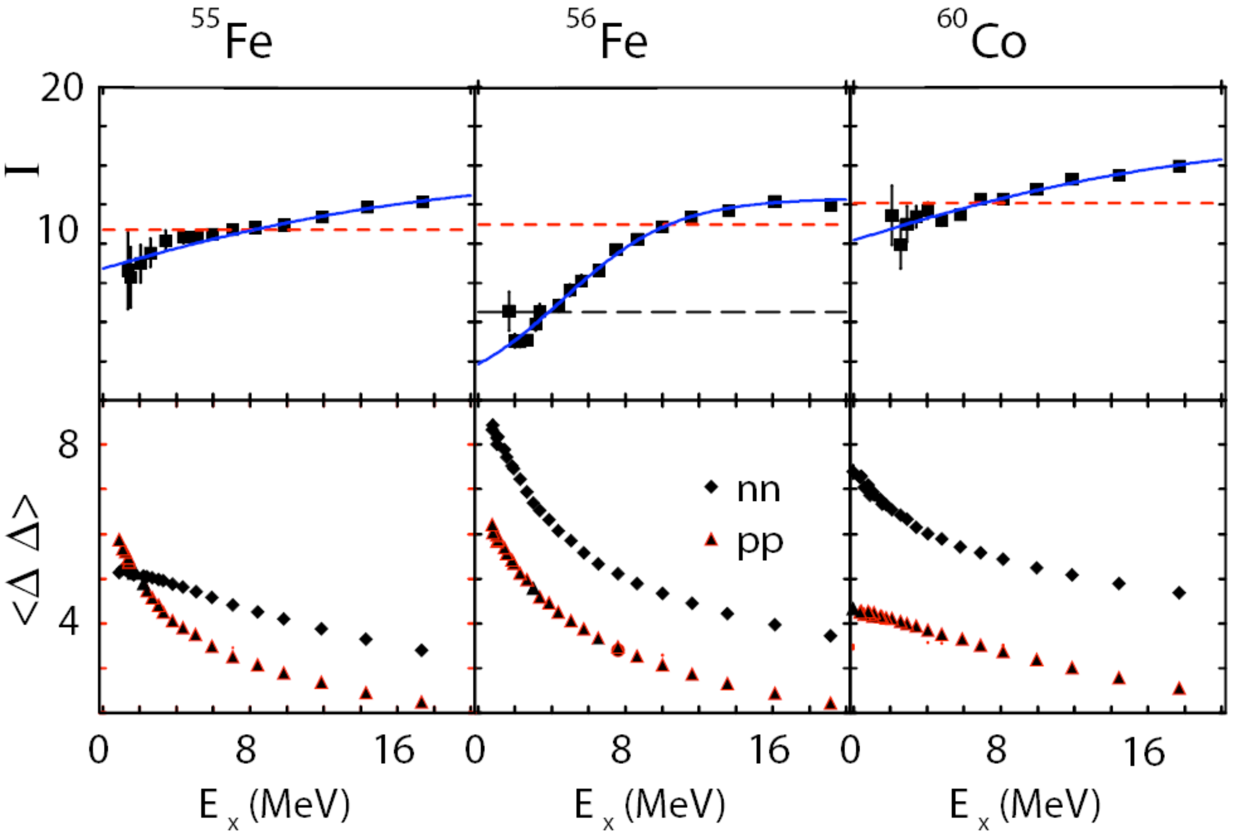
$$\frac{\rho_J}{\rho} = \frac{2J+1}{2\sqrt{2\pi}\sigma^3} e^{-J(J+1)/2\sigma^2}$$



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

- Staggering effect in spin for even-even nuclei.

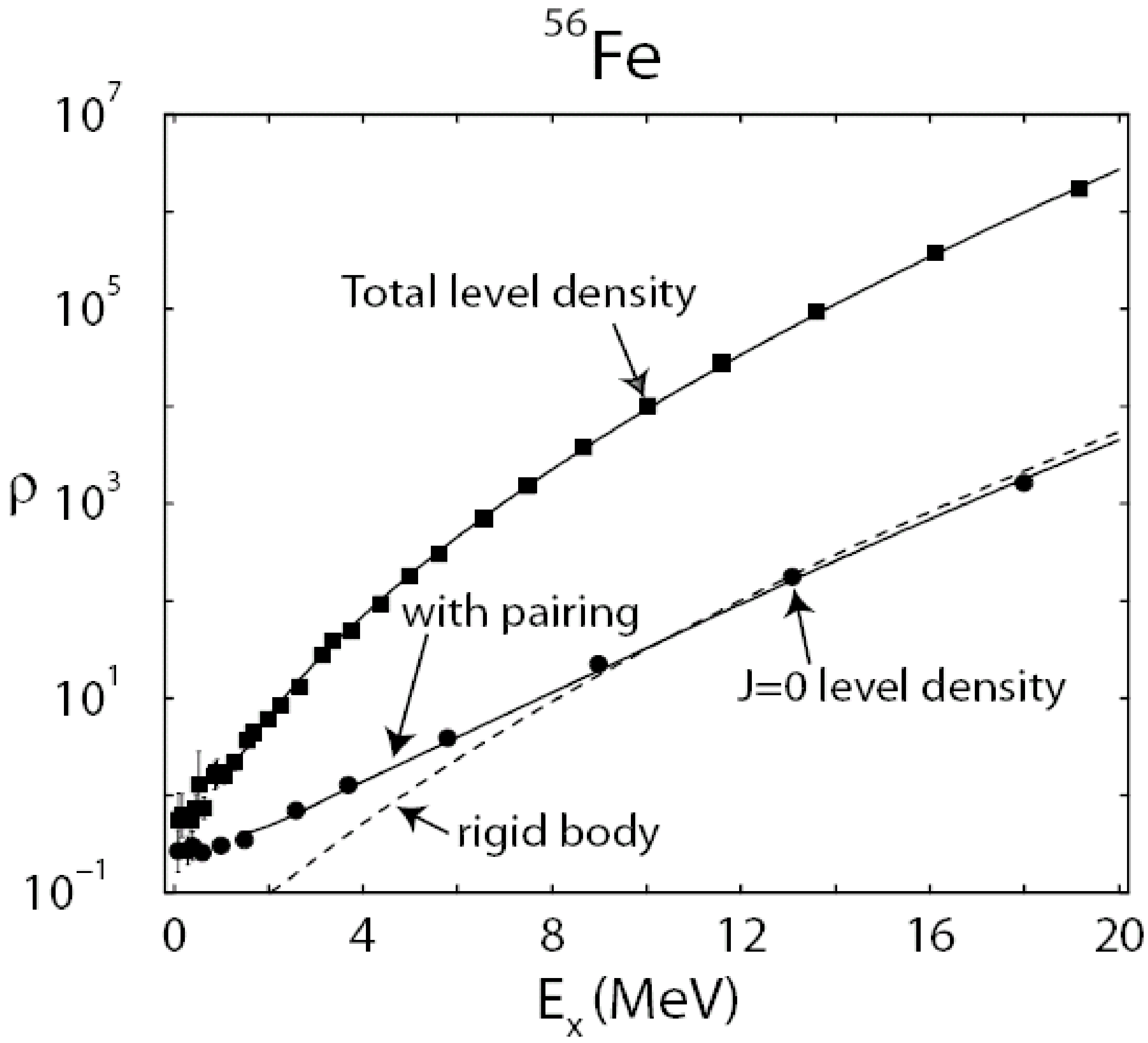
Thermal moment of inertia can be extracted from: $\sigma^2 = \frac{IT}{\hbar^2}$



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.

Energy-dependent enhancement of J=0 level density (pairing effect)



A simple model for the moment of inertia

[Alhassid, Bertsch, Fang, and Liu; Phys. Rev. C **72**, 064326 (2005)]

Model: *deformed* Woods-Saxon potential plus *pairing* interaction.

(i) Number-parity projection : the major odd-even effects are described by a number-parity projection

$$P_\eta = \frac{1}{2}\left(1 + \eta e^{i\pi \hat{N}}\right)$$

- Projects on even ($\eta = 1$) or odd ($\eta = -1$) number of particles.

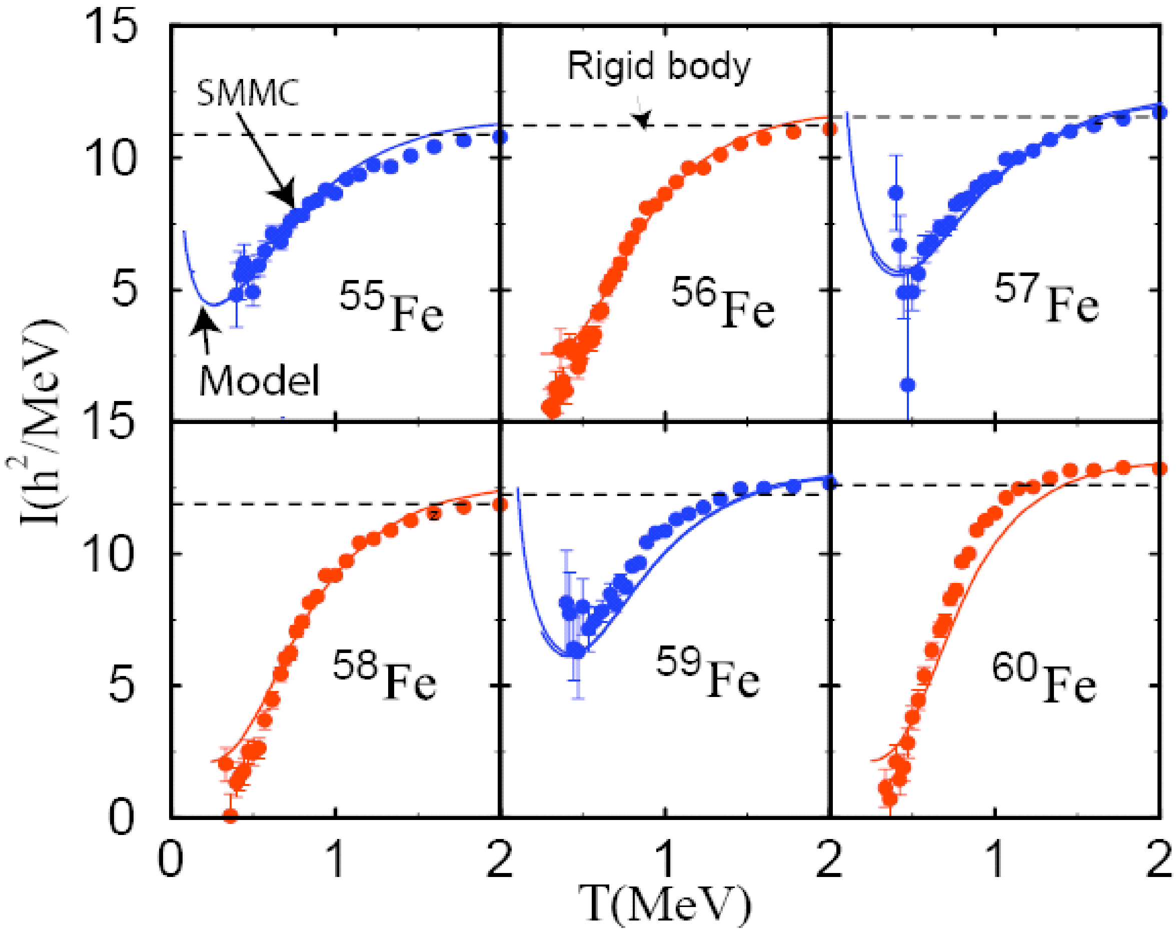
$\langle \ldots \rangle_\pi$ is obtained from $\langle \ldots \rangle$ by the the replacement

$$f_k \to \tilde{f}_k = \left(1 - e^{E_k / T}\right)^{-1}$$ (negative occupations !)

(ii) Static path approximation (SPA)

- include static fluctuations of the pairing order parameter.

iron isotopes (even-even and even-odd nuclei)



• Good agreement with SMMC

• Strong odd/even effect

A simple model for parity distribution

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

The distribution to find n particles in single-particle states with parity π is a Poisson distribution:

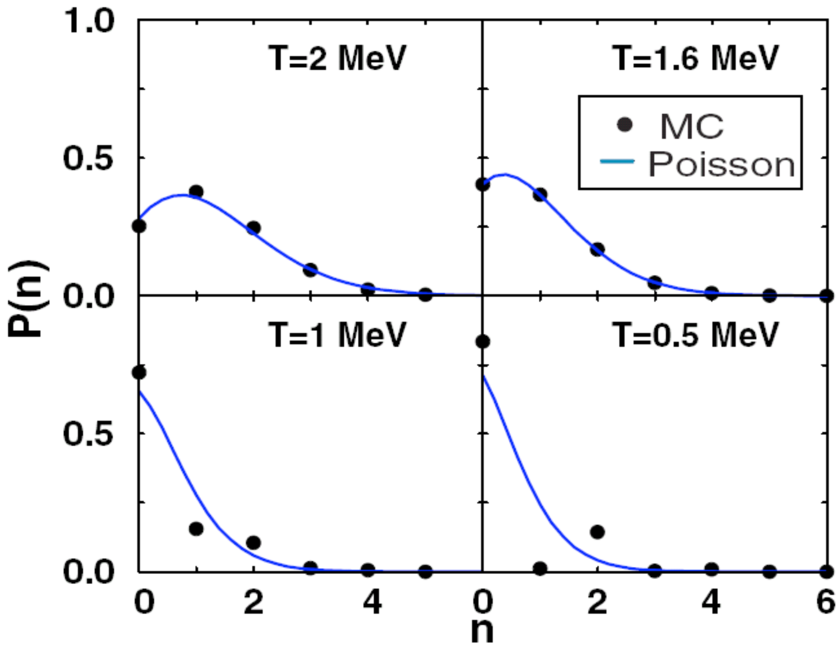
$$P(n) = \frac{f^n}{n!} e^{-f}$$

For an even-even nucleus:

$$\frac{Z_-(\beta)}{Z_+(\beta)} = \frac{\sum_{n\_odd} P(n)}{\sum_{n\_even} P(n)} = \tanh f$$

Where $f = \sum_{a \in \pi} \frac{1}{1 + e^{\beta(E_a - \mu)}}$ is the total Fermi- Dirac occupation in all states with parity π

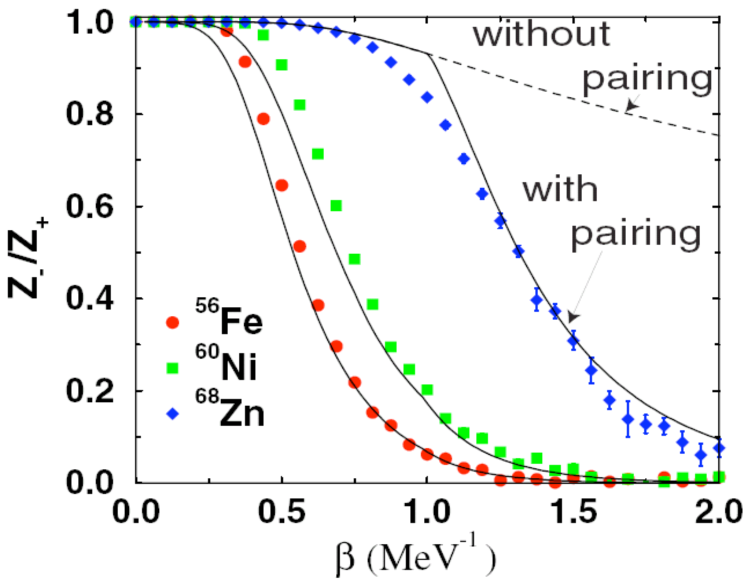
Occupation distribution of the even-parity orbits ($g_{9/2}$) in ^{60}Ni

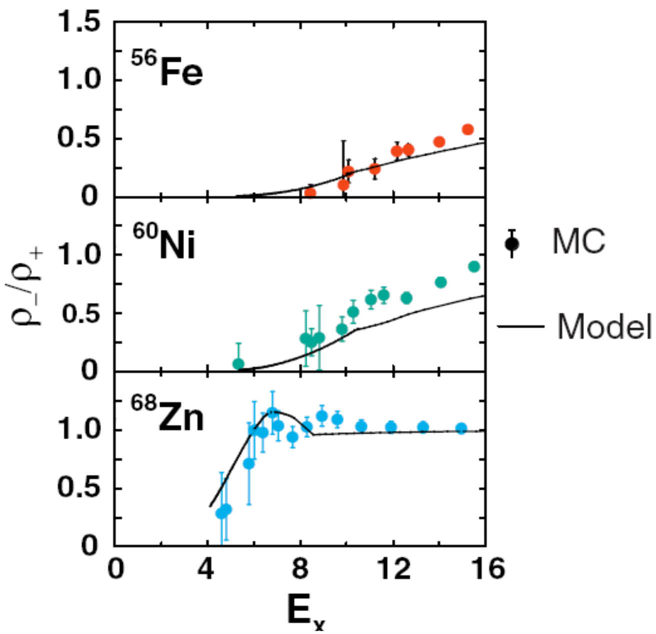


- Deviations from Poisson distribution for T < 1 MeV (pairing effect)

The model should be applied for the quasi-particles:

$$f = \sum_{a \in \pi} f_a = \sum_{a \in \pi} \frac{1}{1 + e^{\beta E_a}}$$





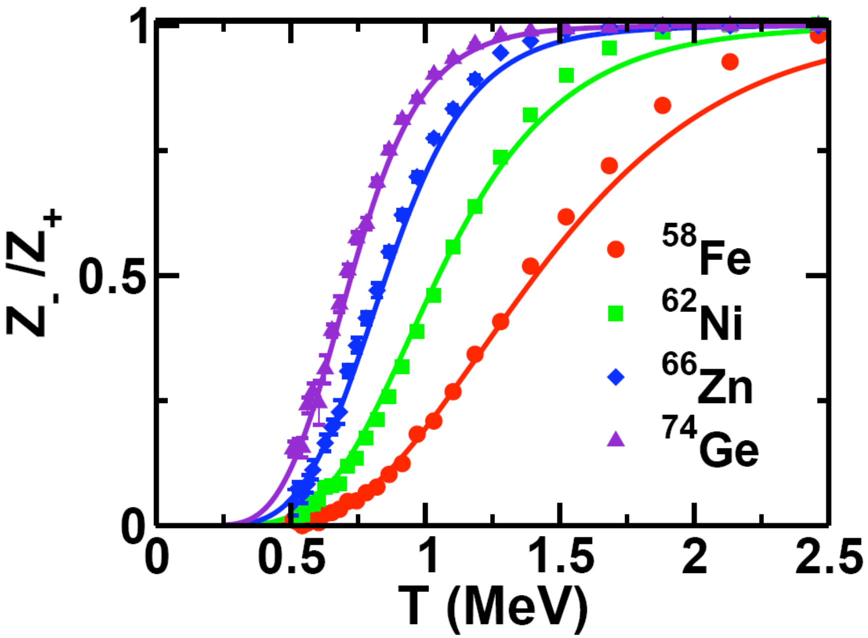
An improved model for the parity dependence

(H. Chen and Y. Alhassid)

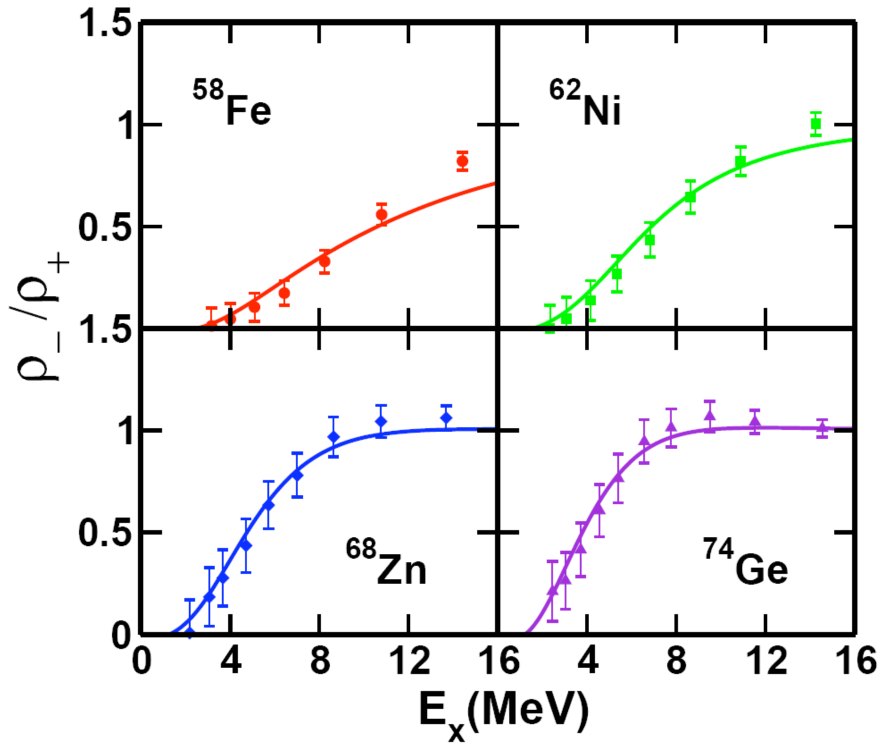
• Improvement of the previous model.

• *Deformed WS plus pairing*.
• Solve using number-parity projection, SPA plus *parity* projection.

Ratio of odd-to-even parity partition functions



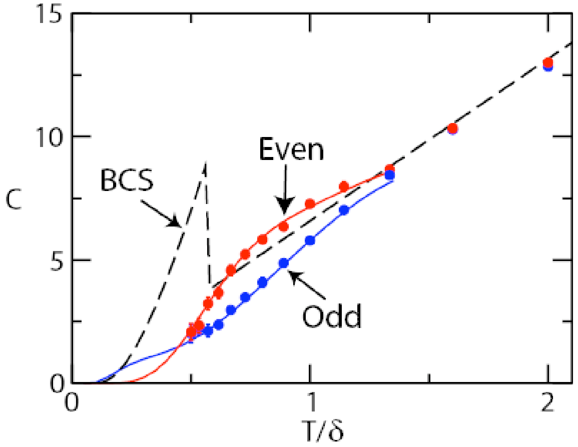
Ratio of odd-to-even parity level densities

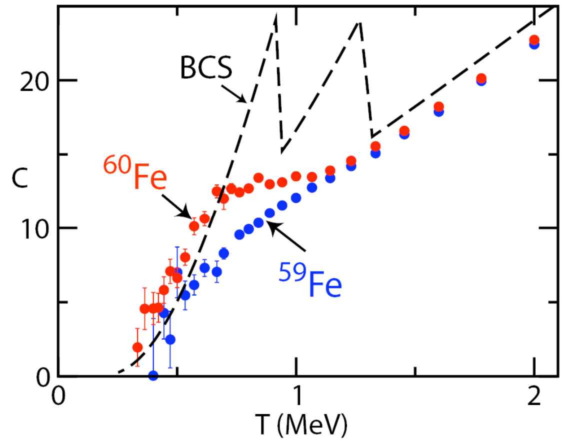


Thermal signatures of pairing correlations: summary

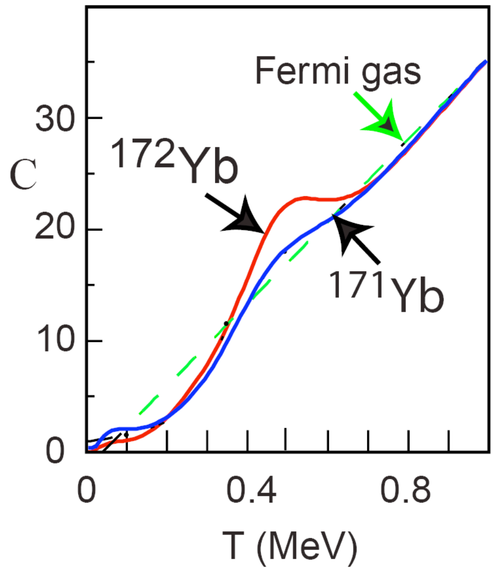
Nanoparticles $(\Delta/\delta = 1)$ versus nuclei

Heat capacity

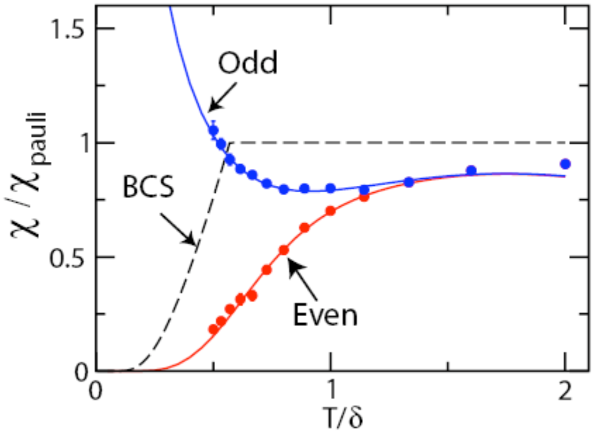




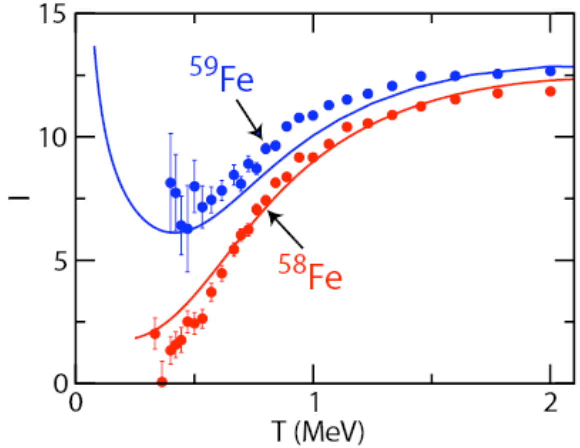
Experiment (Oslo)



Spin susceptibility



Moment of inertia



- Pairing correlations (for $\Delta/\delta \sim 1$) manifest through strong odd/even effects.

The heavy deformed nuclei

(Y. Alhassid, L. Fang and H. Nakada)

• 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

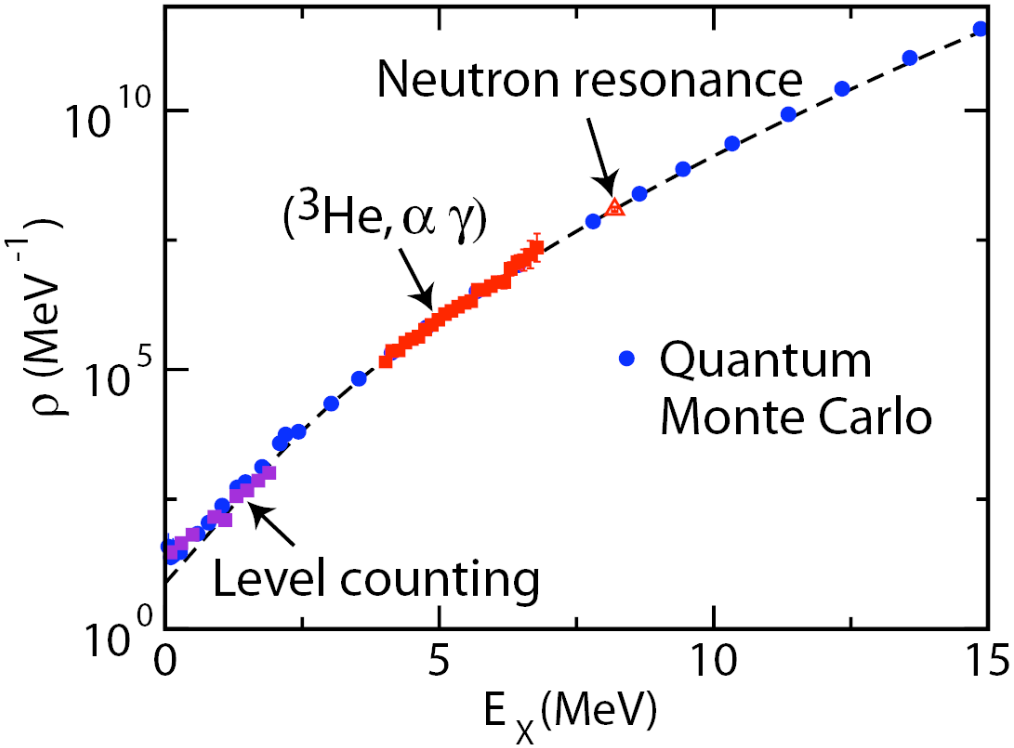
• Choice of single-particle model space: inclusion of intruder states.

• 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.

^{162}Dy

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



• Level density is in good agreement with experiments.

Conclusion

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

• Nuclei probe the fluctuation-dominated regime of pairing correlations. Thermal signatures of pairing correlations (heat capacity, moment of inertia,…) manifest through their dependence on number parity.

• The spin and parity distributions can be calculated using projection methods (see also talk by K. Van Houcke).

• SMMC successfully extended to heavy deformed nuclei (A ~ 160).

A long-range goal:

Derive global effective shell model interactions from density functional theory.

Quadrupole-quadrupole effective interaction:

Alhassid, Bertsch, Fang and Sabbey, Phys. Rev. C 74, 034301 (2006)