

# Nuclear level densities: from empirical models to microscopic methods

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## Level densities: introduction

The level density is among the most important statistical nuclear properties.

- It appears in Fermi's golden rule for transition rates.
- It is an important input to the Hauser-Feshbach theory of compound nuclear reactions: the decay of the compound nucleus in a given channel is proportional to the available phase space, i.e., the level density.
- It has many applications in diverse areas such as stellar nucleosynthesis and nuclear reactor technology.

While *qualitative* features of level densities can be understood by simple models, a *quantitative* understanding presents a major challenge, in particular when correlations beyond the mean field are important.

The state density at total energy  $E$  is defined as the number of states per unit energy

$$\rho(E) = \text{Tr} \delta(E - H)$$

where  $H$  is the system's Hamiltonian.

For a system with discrete energy levels  $E_i$ ,  $\rho(E) = \sum_i \delta(E - E_i)$  is singular.

We are interested in a smoothed version of this density, i.e., the *average* state density.

## Thermodynamic approach

We assume the nucleus to be in contact with a heat reservoir at temperature  $T$ , in which case its equilibrium configuration is described by the canonical Gibbs ensemble. The partition function at inverse temperature  $\beta = 1/T$  is defined by

$$Z(\beta) = \text{Tr} e^{-\beta H}$$

$Z(\beta)$  is the Laplace transform of the level density

$$Z(\beta) = \int_0^{\infty} dE e^{-\beta E} \rho(E)$$

The level density  $\rho(E)$  is then the inverse Laplace transform of  $Z(\beta)$

$$\rho(E) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\beta e^{\beta E} Z(\beta)$$

The inverse Laplace transform is numerically ill-defined. It can be evaluated in the saddle-point approximation and provides the *average* level density.

$$\rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)}$$

where  $\beta$  is determined as a function of  $E$  by the saddle-point condition

$$-d \ln Z / d\beta = E(\beta)$$

$S(E) = \ln Z + \beta E$  is the canonical entropy

$C = -\beta^2 \frac{dE}{d\beta}$  is the canonical heat capacity

## Non-interacting (Fermi gas) model

For non-interacting fermions, the grand canonical partition is given by

$$\ln Z = \int_0^{\infty} d\varepsilon g(\varepsilon) \ln[1 + e^{-\beta(\varepsilon - \mu)}]$$

where  $g(\varepsilon)$  is the *single-particle* level density, and  $\mu$  is the chemical potential

The excitation energy is calculated using the low-temperature expansion (Sommerfeld 1928)

$$E_x = aT^2 \quad \text{where} \quad a = \frac{\pi^2}{6} g(\varepsilon_F) \quad \text{is the single-particle level density parameter.}$$

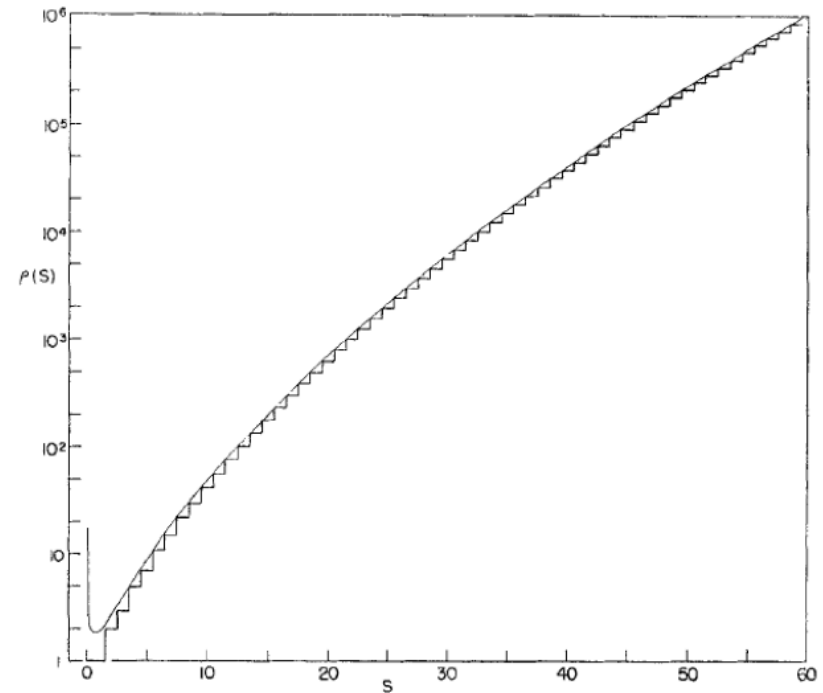
The heat capacity is  $C = dE / dT = 2aT$

Using  $C = T dS / dT$ , the entropy is  $S = 2aT = 2\sqrt{aE_x}$

The saddle-point approximation leads to Bethe's formula (1936) for one type of nucleons

$$\rho(E_x) = \frac{1}{\sqrt{48E_x}} e^{2\sqrt{aE_x}}$$

Equidistant single-particle spectrum:  
the exact solution (histogram, Euler 1753)  
is compared with Bethe's formula (line)



For both protons and neutrons with  $N \approx Z$

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

$a \approx A/15 \text{ MeV}^{-1}$  for uniform Fermi gas (in a box)

$a \approx A/10 \text{ MeV}^{-1}$  for harmonic oscillator potential

$a \approx A/10.7 \text{ MeV}^{-1}$  for Woods-Saxon potential

## Spin-cutoff model

The spin cutoff model assumes random coupling of single-particle spins (Bethe 1937, Ericson 1960). The distribution of the spin projection  $M = \sum_i m_i$

$$\frac{\rho_M}{\rho} = \frac{1}{\sqrt{2\pi\sigma}} e^{-M^2/2\sigma^2}$$

where  $\sigma^2$  is the spin-cutoff parameter. Using equipartition theorem  $\sigma^2 = IT / \hbar^2$ , where  $I$  is the moment of inertia.

The spin distribution can then be calculated from

$$\rho_J = \rho_{M=J} - \rho_{M=J+1} \approx -d\rho_M / dM \big|_{M=J+1/2}$$

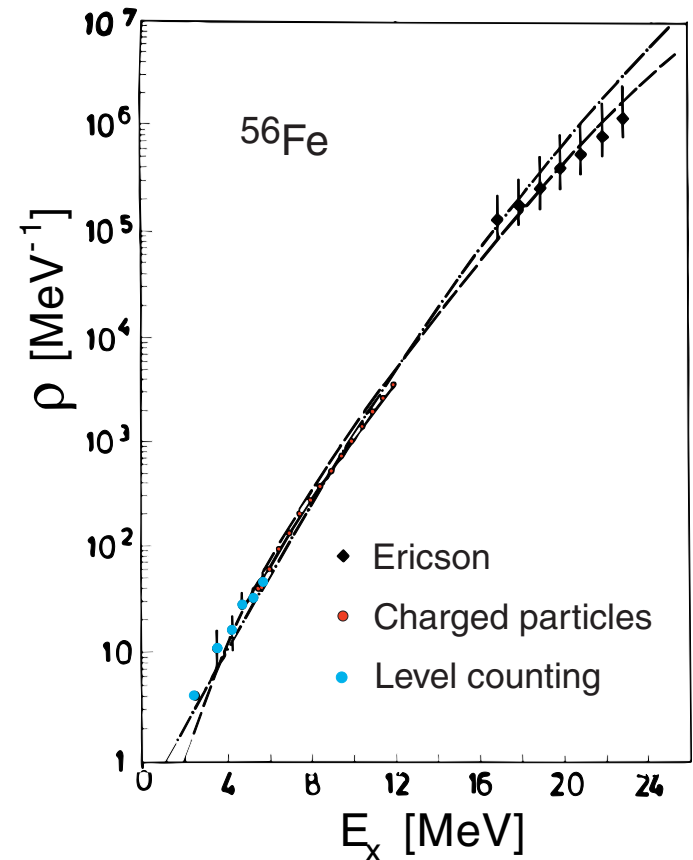
$$\frac{\rho_J}{\rho} = \frac{2J+1}{2\sqrt{2\pi\sigma^3}} e^{-J(J+1)/2\sigma^2}$$

At higher excitation energies,  $I$  approaches its rigid-body value, but it decreases at lower excitations because of pairing correlations.

## Experimental methods

The measurement of level densities is a difficult task. There are several methods but all have systematic uncertainties and are limited to certain energy regimes.

- Level counting at low energies (requires a complete set of levels)
- Neutron and proton resonance data (at threshold)
- Charged particles and evaporation spectra
- “Oslo” method (statistical analysis of primary gamma-ray spectra)
- Ericson fluctuations



Recent progress has been achieved by combining several methods.

## Empirical models

It is a challenge to calculate the level density in the presence of correlations, and several phenomenological models were introduced to describe the data.

### Back-shifted Fermi gas model

Pairing correlations and shell effects in Bethe's formula are taken into account by shifting the ground-state energy by a backshift parameter  $\Delta$

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

$a$  and  $\Delta$  are adjustable parameters determined from level counting data at low excitations and neutron resonance data (Dilg et al 1973, von Egidy et al 1988)

Global fits using energy-dependent  $a$  that includes shell effects (Ignatuk et al 1975; Koning, Hilaire and Goriely 2008)

## Constant temperature formula

At low energies it is found empirically that the level density is well described by an exponential function

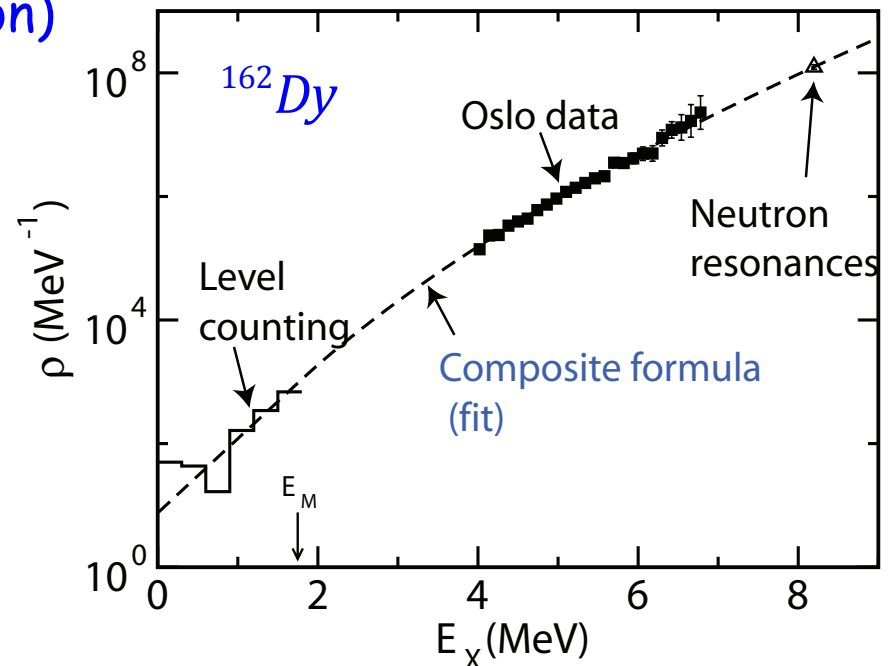
$$\rho(E_x) = e^{-(E_x - E_1)/T_1}$$

where  $E_1$  and  $T_1$  are constants.  $T_1$  is an effective temperature

$$T_1^{-1} = d \ln \rho(E_x) / dE_x$$

## Composite formula (Gilbert-Cameron)

A constant temperature formula at low energies is matched to a back-shifted Fermi gas formula at higher excitations.



# Microscopic methods

## Mean-field methods

Hartree-Fock (HF) using Skyrme or Gogny interactions at zero temperature plus finite-temperature BCS (Goriely et al).

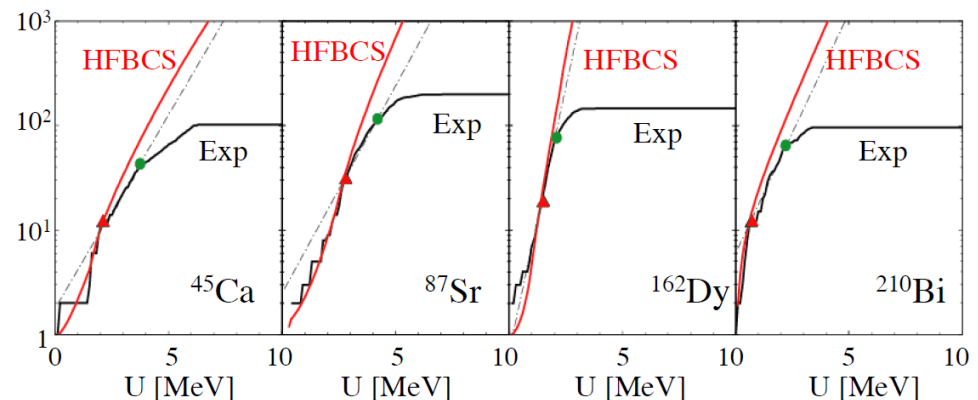
A mean-field theory provides the intrinsic level density  $\rho_{\text{int}}(E_x)$  and has to be augmented by *collective enhancement factors* (vibrational and rotational)

$$\rho(E_x) = K_{\text{vib}}(E_x) K_{\text{rot}}(E_x) \rho_{\text{int}}(E_x)$$

The energy dependence of these factors (and in particular their decay with  $E_x$ ) is one of the least understood issues in the studies of level densities - most available expressions are phenomenological.

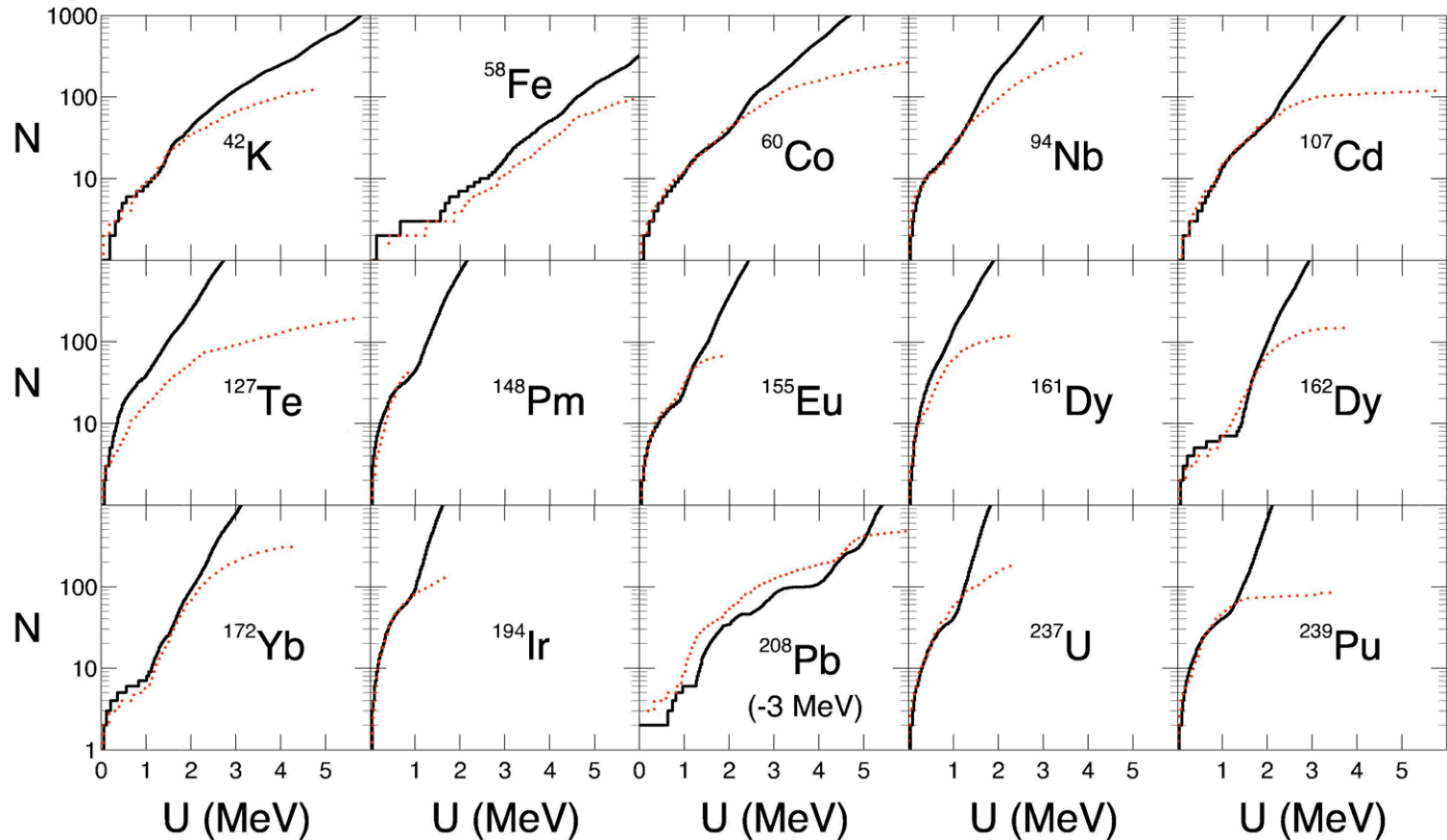
Cumulative HF+BCS  
level densities (Goriely et al)

Comparison with experimental low-lying levels



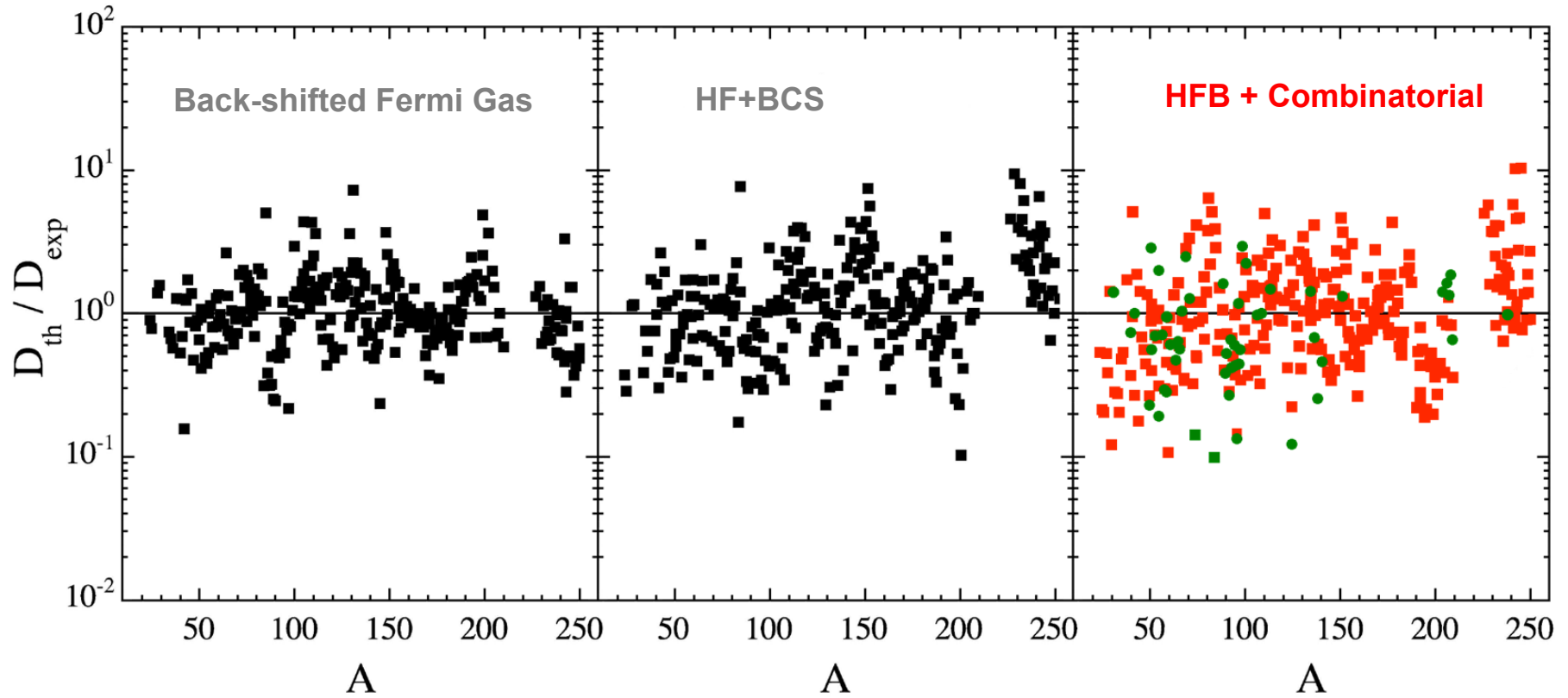
## Combinatorial methods

Count the number of ways to distribute the nucleons among single-particle levels at a given total excitation energy (Hilaire and Goriely 2006; Goriely, Hilaire and Koning 2008; Aberg, Dossing et al 2013).



Cumulative level densities (Hilaire and Goriely)

# Average neutron resonance spacing at threshold – theory vs. experiment



Courtesy of S. Hilaire

## Configuration-interaction (CI) shell model methods

Particularly suitable for precise calculations of level densities  
- includes correlations beyond the mean field and shell effects.

The combinatorial growth of the dimensionality of the model space with number of nucleons and/or number of valence orbitals has hindered its applications in mid-mass and heavy nuclei.

## Spectral averaging theory (moment method)

Mon and French 1975; Grimes et al; Kotta et al;

Horoï and Zelevinsky 2004; Senkov and Zelevinsky 2016

Superposition of Gaussian densities for various partitions of the single-particle levels with widths determined by the interaction.

- Requires a reliable calculation of the ground-state energy
- Calculation of second moments is time consuming in large CI spaces

## The shell model Monte Carlo (SMMC) method

Gibbs ensemble  $e^{-\beta H}$  at temperature  $T$  ( $\beta = 1/T$ ) can be written as a superposition of ensembles  $U_\sigma$  of *non-interacting* nucleons moving in time-dependent fields  $\sigma(\tau)$

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

- The integrand reduces to matrix algebra in the single-particle space (of typical dimension 50 – 100).
- The high-dimensional  $\sigma$  integration is evaluated by Monte Carlo methods

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).

**State density in SMMC** [Nakada and Alhassid, PRL **79**, 2939 (1997)]

- Calculate the canonical thermal energy  $E(\beta) = \langle H \rangle$  versus  $\beta$  and integrate  $-d \ln Z / d\beta = E(\beta)$  to find the canonical partition function  $Z(\beta)$ .

The *average* level density is found from  $Z(\beta)$  in the saddle-point approximation:

$$\rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)}$$

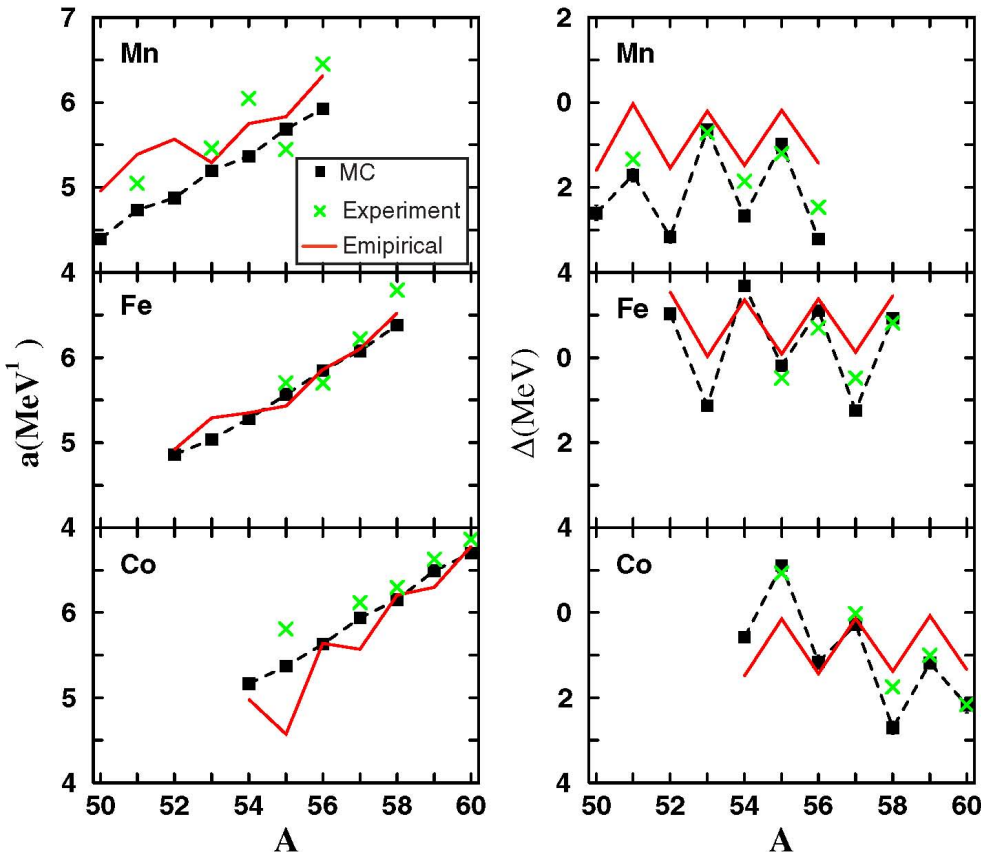
where  $S = \ln Z + \beta E$  and  $C = dE / dT$

# Medium mass nuclei ( $A \sim 50 - 70$ )

Alhassid, Liu, and Nakada, PRL 83, 4265 (1999)

- Complete  $fpg9/2$ -shell: single-particle levels from Woods-Saxon +spin-orbit

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



SMMC densities are well fitted to the backshifted Bethe formula (BBF)

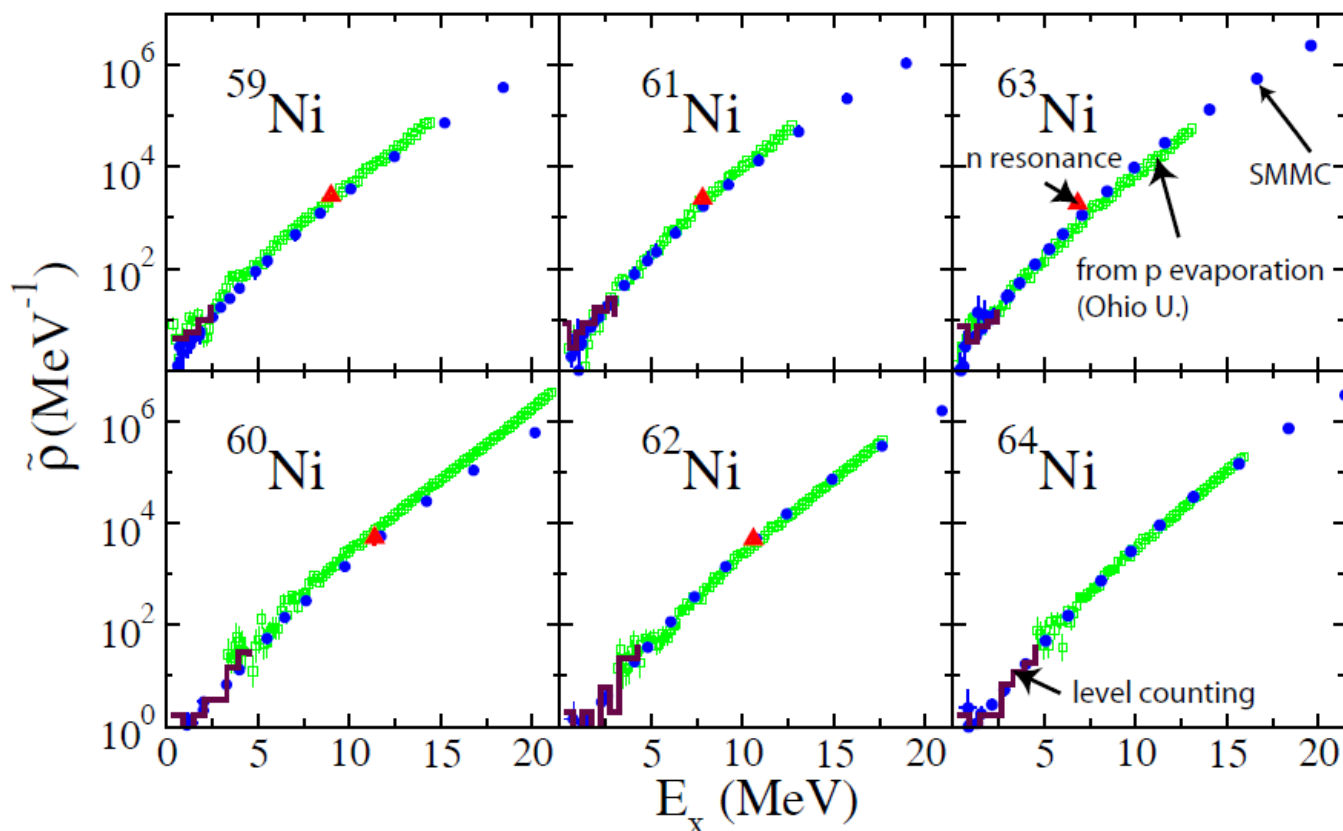
$\Rightarrow$  Extract  $a$  and  $\Delta$

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

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

# Level densities in nickel isotopes (including odd mass)

Bonett-Matiz, Mukherjee, Alhassid, PRC 88, 011302 R (2013)



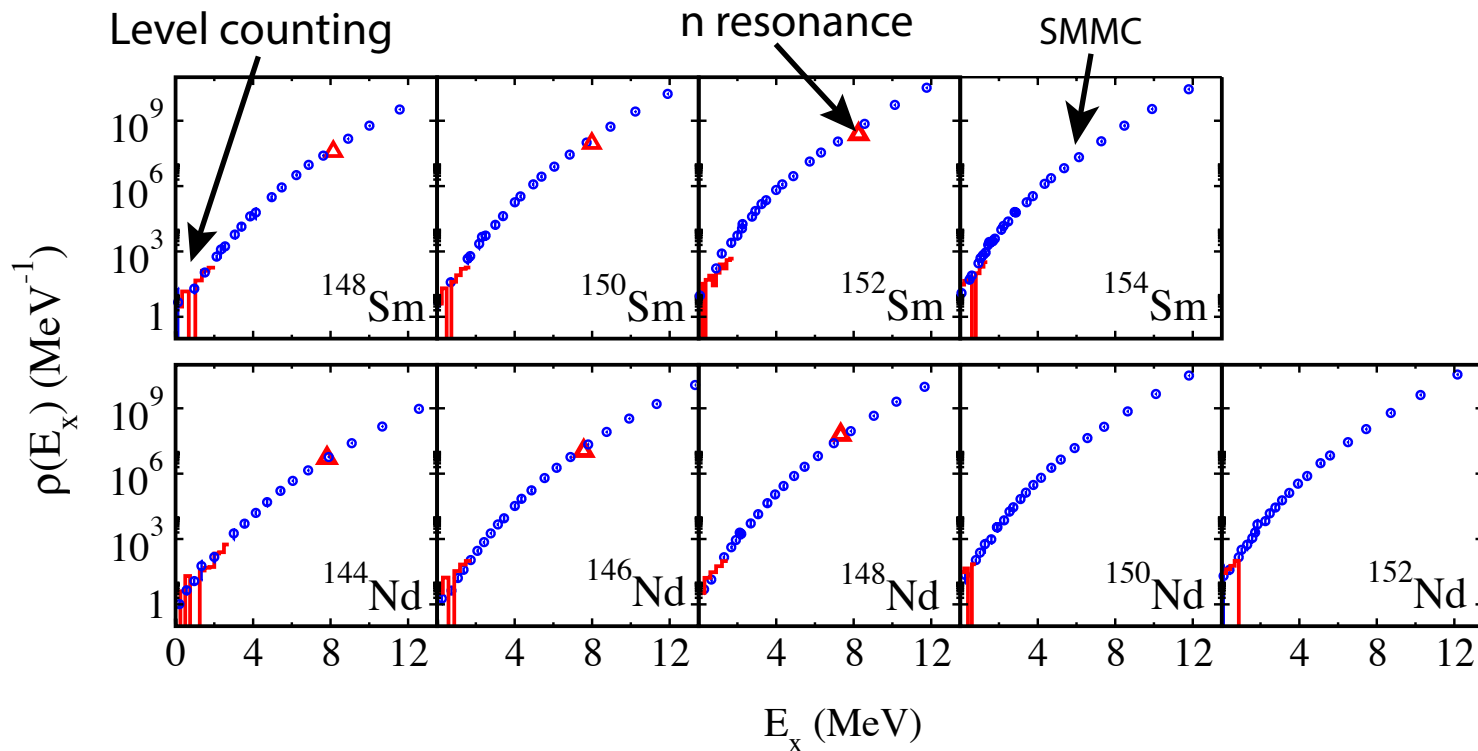
Excellent agreement with experiments:

- (i) level counting
- (ii) proton evaporation spectra (Ohio U., 2012)
- (iii) neutron resonance data

# Heavy nuclei: lanthanides

Ozen, Alhassid, and Nakada, PRL 110 (2013)

CI shell model space - protons: 50-82 shell plus  $1f_{7/2}$ ; neutrons: 82-126 shell plus  $0h_{11/2}$  and  $1g_{9/2}$



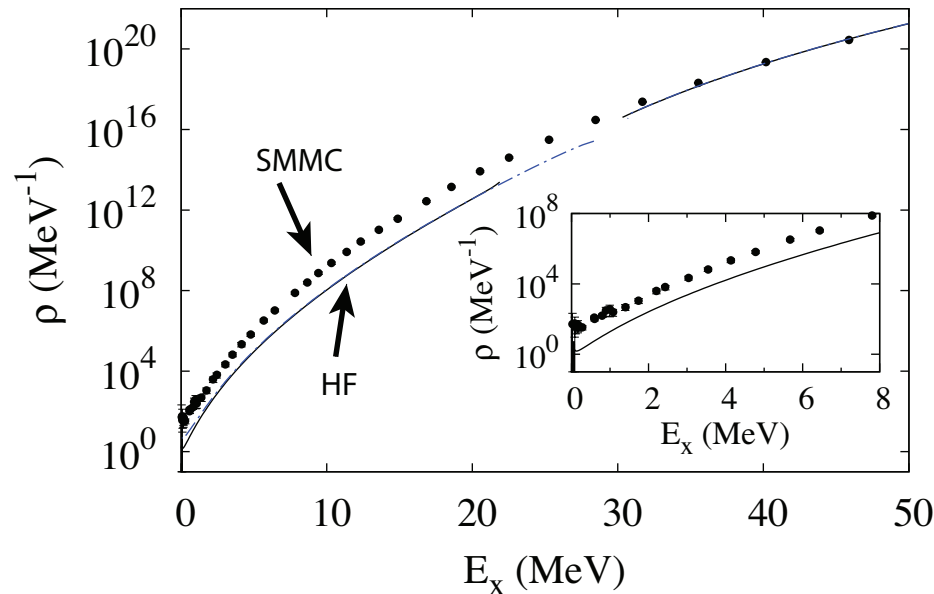
- Good agreement of SMMC densities with various experimental data sets (level counting, neutron resonance data when available).

# Rotational enhancement in deformed nuclei

Alhassid, Bertsch, Gilbreth and Nakada, PRC 93, 044320 (2016)

A deformed nucleus ( $^{162}\text{Dy}$ ): Hartree-Fock (HF) vs SMMC

- Particle-number projection is carried out in the saddle-point approximation
- Exact particle-number projection: [Fanto, Alhassid, Bertsch, PRC 96, 014305 \(2017\)](#)



- The enhancement of the SMMC density (compared with HF) is due to rotational bands built on top of the intrinsic bandheads.
- The rotational enhancement gets damped above the shape transition.

We can define the collective enhancement factor as the ratio between the SMMC density and mean-field intrinsic density.

## Spin distributions: mid-mass nuclei

Y. A., S. Liu and H. Nakada, Phys. Rev. Lett. **99**, 162504 (2007)

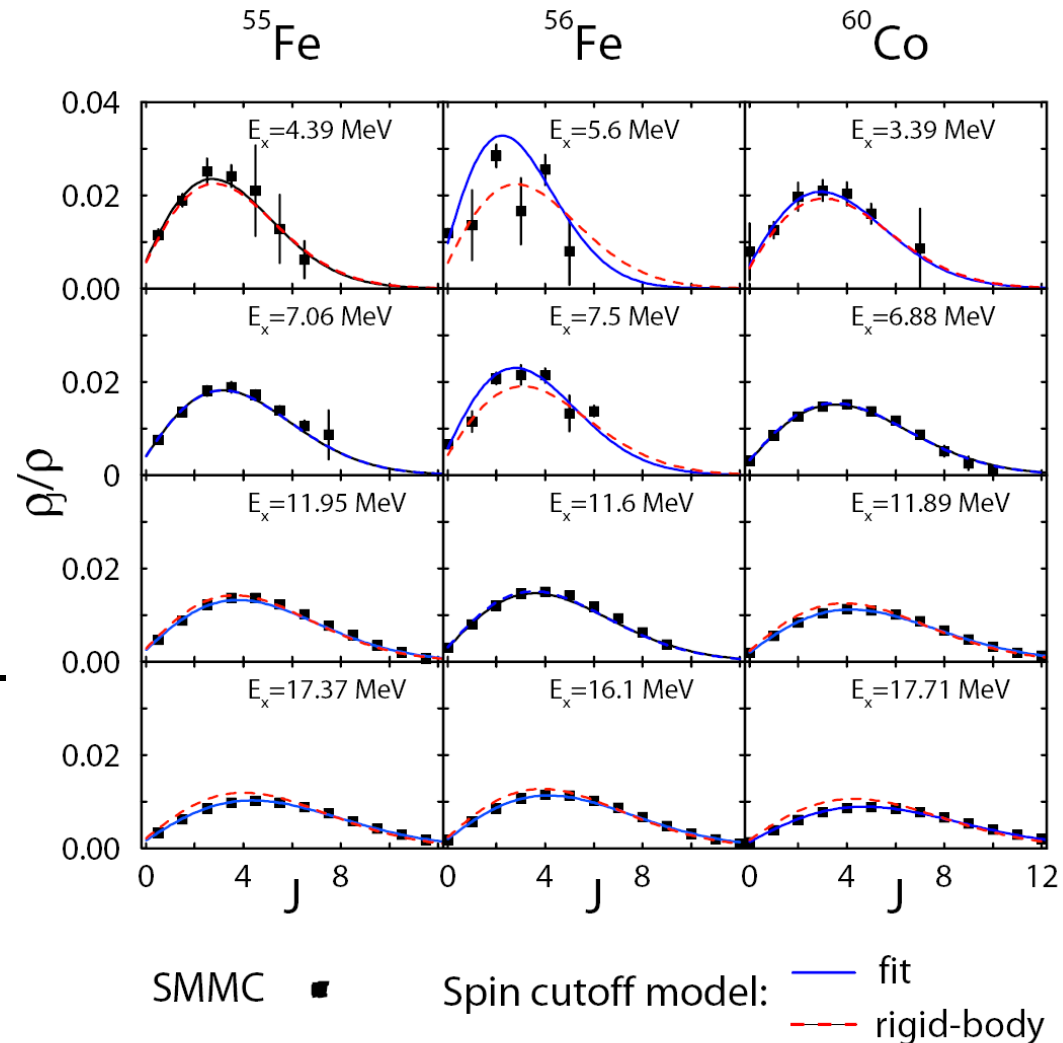
- Use exact spin projection to calculate spin distributions

Spin cutoff model:

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

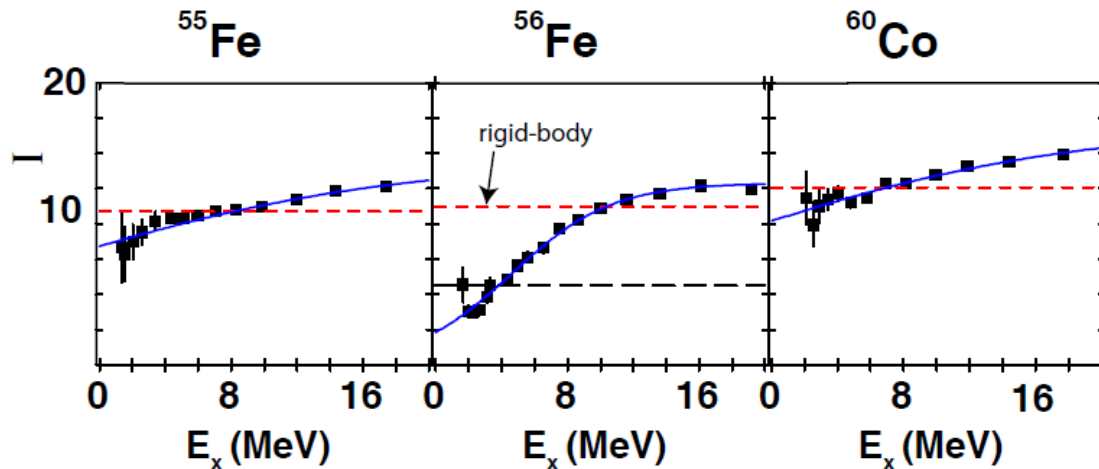
- Spin cutoff model works well except at low excitation energies.

- Staggering effect in spin for even-even nuclei.

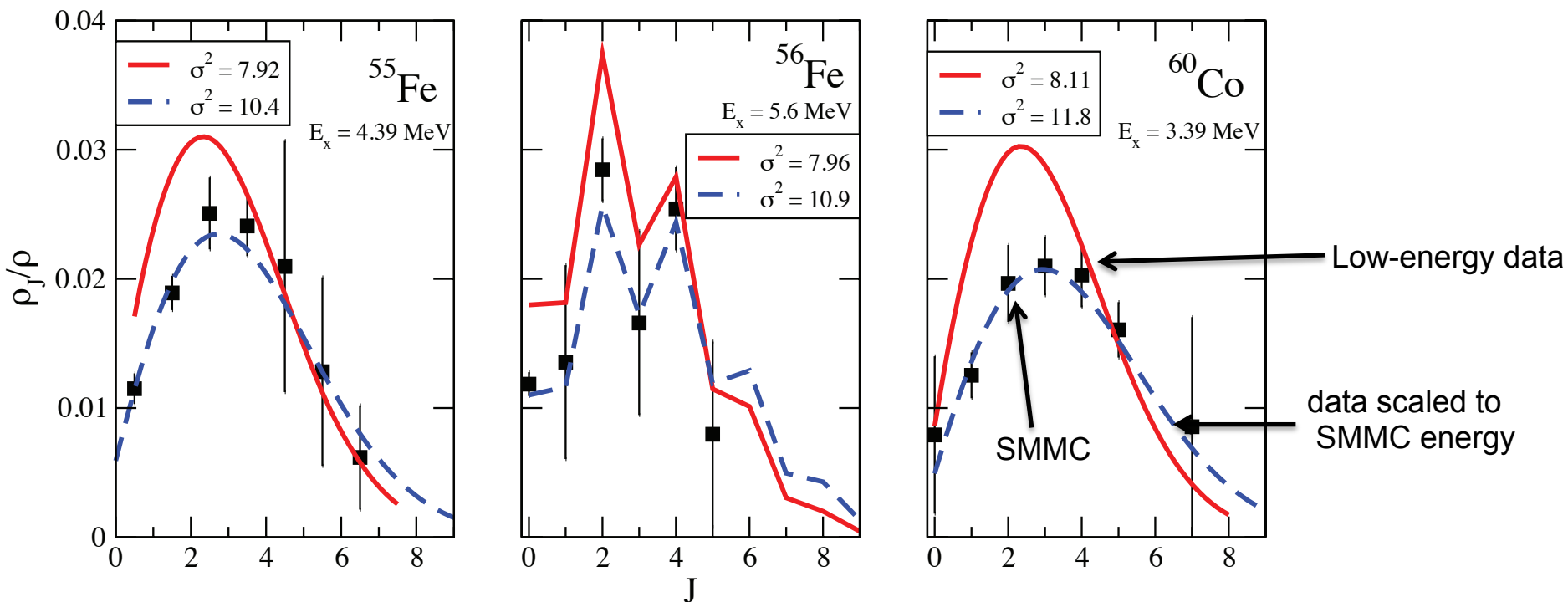


Thermal moment of inertia  
I can be extracted from:

$$\sigma^2 = IT / h^2$$



- Analysis of experimental data [von Egidy and Bucurescu, PRC 78, 051301 R (2008)] confirmed our prediction.



## The deformation dependence of level densities

Alhassid, Gilbreth, and Bertsch, PRL **113**, 262503 (2014)

Gilbreth, Alhassid and Bertsch, PRC **97**, 014315 (2018)

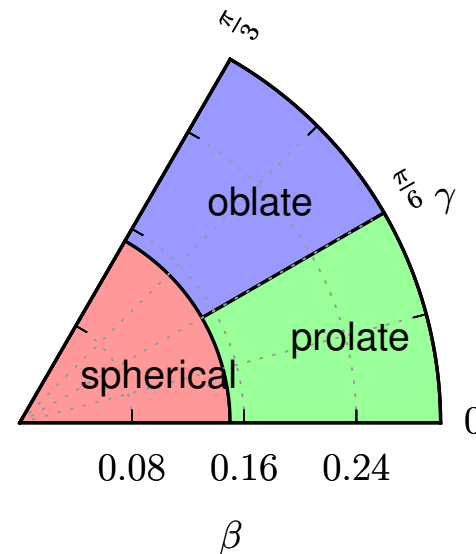
Mustonen, Gilbreth, Alhassid, Bertsch, PRC **98**, 034317 (2018)  
- Editor's Suggestion

Modeling of shape dynamics, e.g., fission, requires the knowledge of level density as a function of deformation.

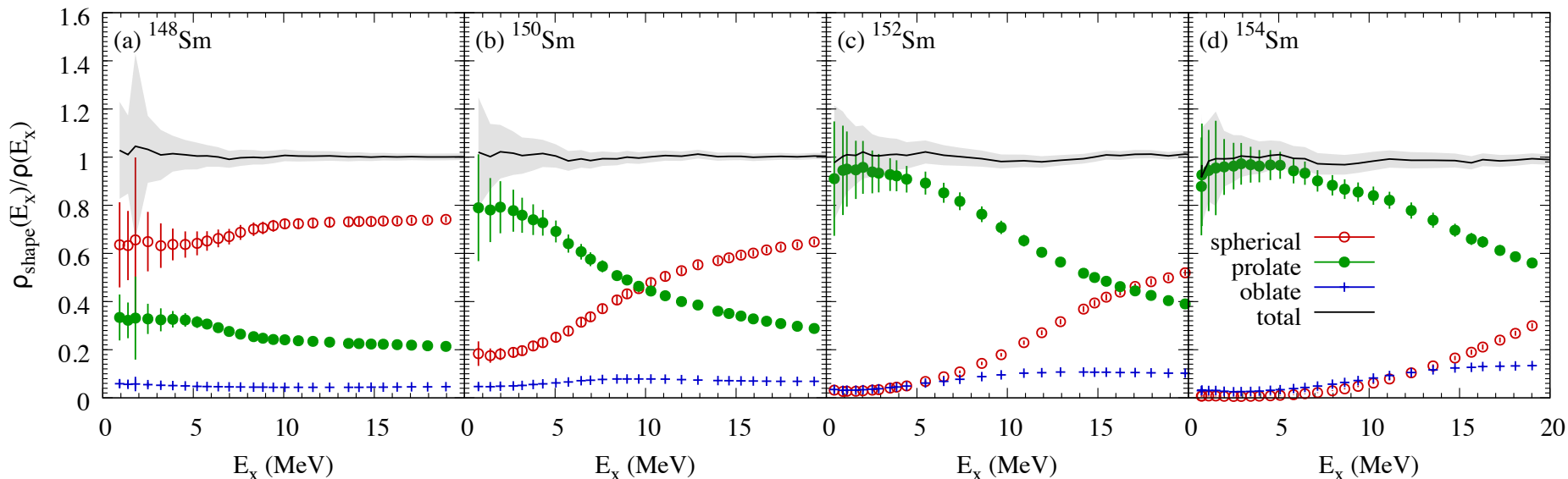
We have introduced a novel model-independent method to calculate the exact distributions of intrinsic deformation within the rotationally invariant framework of the CI shell model without invoking a mean-field approximation.

The method uses a projection on the axial quadrupole operator in the lab frame, and is based on a Landau-like expansion of the logarithm of the quadrupole distribution.

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



Fraction of the level density in each shape region vs. excitation energy for deformed ( $^{154}\text{Sm}$ ,  $^{152}\text{Sm}$ ), transitional ( $^{150}\text{Sm}$ ) and spherical ( $^{148}\text{Sm}$ ) nuclei



## Conclusion

- The calculation of level densities in the presence of correlations is a challenging many-body problem.
- Phenomenological models of level densities are often based on empirical modifications of the Fermi gas model and on the constant temperature formula. They lack predictive power.
- Mean-field and combinatorial models of level densities have been applied across the nuclear chart but often have to be augmented by empirical collective enhancement factors.
- The moment method and the shell model Monte Carlo (SMMC) method have been formulated in the context of the CI shell model approach, and include correlations beyond the mean field approximation.
- The moment method has been applied to light and mid-mass nuclei, while SMMC has been applied to nuclei as heavy as the lanthanides.