Nuclear level densities by the shell model Monte Carlo method

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- The shell model Monte Carlo (SMMC) approach and level densities

- Recent technical developments:

  Odd-even nuclei: circumventing a sign problem

  Direct SMMC calculations of *level* densities
  (spin degeneracy is not counted)

- Applications:

  Level densities in even and odd nickel isotopes

  Level densities in heavy rare-earth nuclei

- Conclusion and prospects

Shell model Monte Carlo (SMMC) method

• Most microscopic treatments of heavier nuclei are based on mean-field methods but important correlations can be missed.

• The interacting shell model accounts for correlations but diagonalization methods are limited to $\sim 10^{11}$ configurations.

The SMMC 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.

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

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

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

• The high-dimensional integration over σ is evaluated by Monte Carlo methods.

Lang, Johnson, Koonin, Ormand, Phys. Rev. C 48, 1518 (1993);
Alhassid, Dean, Koonin, Lang, Ormand, Phys. Rev. Lett. 72, 613 (1994).

Thermodynamic approach to level densities

H. Nakada and Y.A., PRL **79**, 2939 (1997)

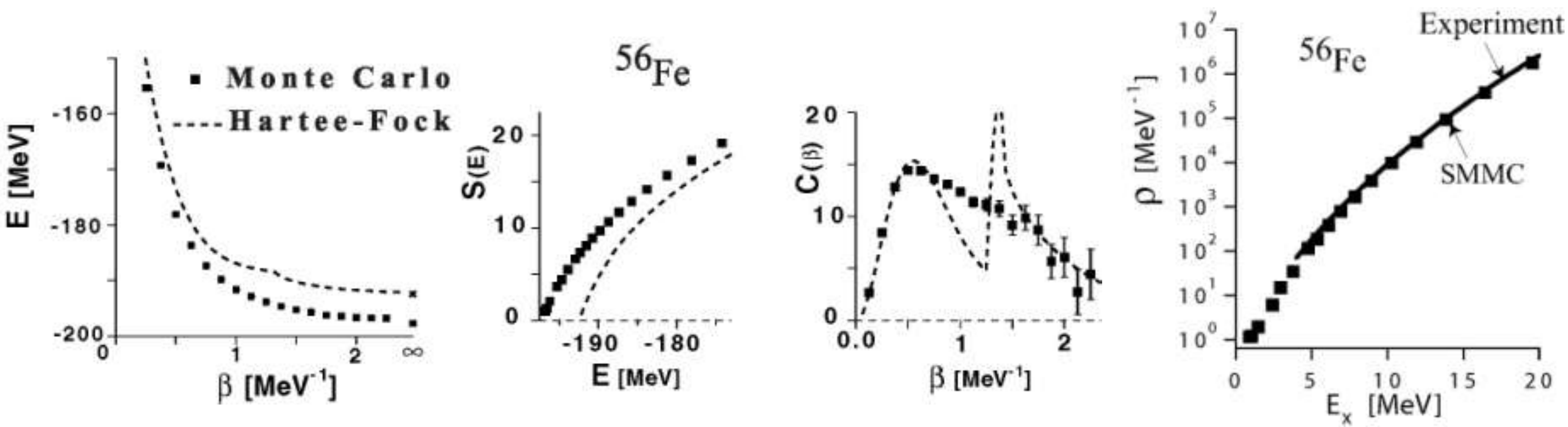
- Calculate the thermal energy $E(\beta) = \langle H \rangle$ and integrate $-\partial \ln Z / \partial\beta = E(\beta)$ to find the partition function $Z(\beta)$

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

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

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

$$S(E) = \ln Z + \beta E \qquad C = -\beta^2 \partial E / \partial\beta$$



Odd-particle-number systems in SMMC: circumventing a sign problem

A. Mukherjee and Y.Alhassid, Phys. Rev. Lett. 109, 032503 (2012)

Applications of SMMC to odd-even and odd-odd nuclei has been hampered by a sign problem that originates from the projection on odd number of particles.

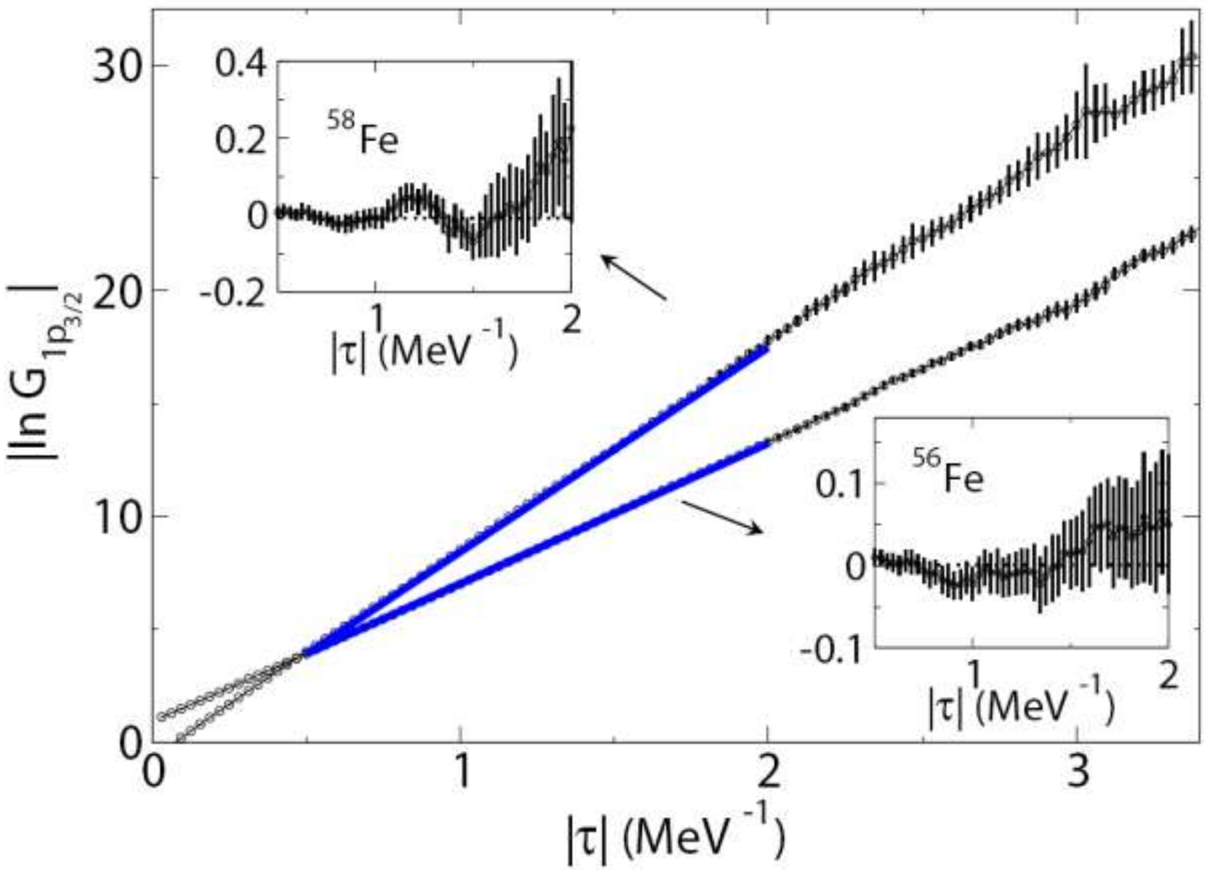
- We introduced a method to calculate the ground-state energy of the odd-particle system that avoids this sign problem.

We calculate the imaginary-time scalar single-particle Green's functions in even-even nuclei for all single-particle orbitals $\nu = n\,l\,j$:

$$G_\nu(\tau) = \Sigma_m \left\langle T\, a_{\nu m}(\tau) a^\dagger_{\nu m}(0) \right\rangle$$

In the asymptotic regime in τ

$$G_\nu(\tau) \sim e^{-\beta [E_j(A\pm 1) - E_{gs}(A)]\ |\tau|}$$

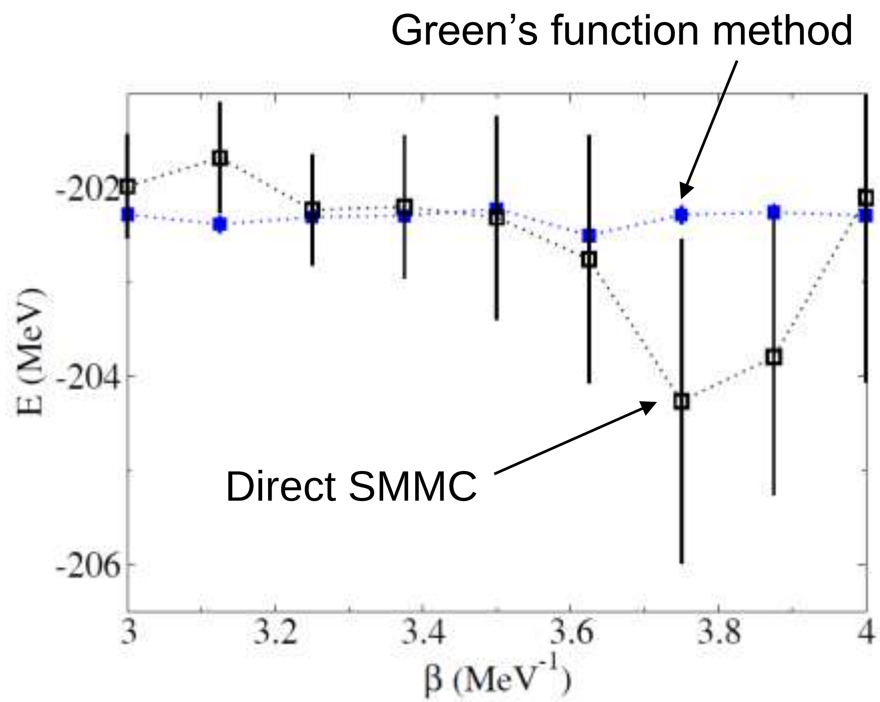


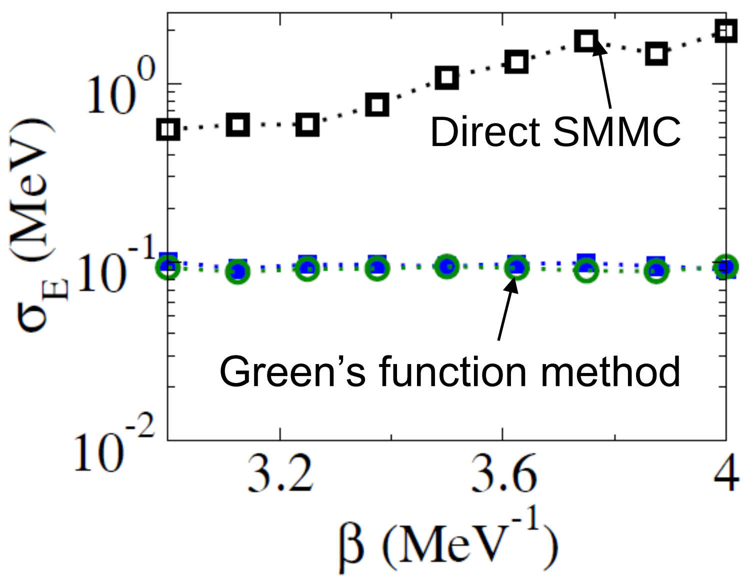
• The energy difference between the lowest energy of the odd-particle system for a given spin j and the ground-state energy of the even-particle system can be extracted from the slope of $\ln G_\nu(\tau)$

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

Statistical errors of ground-state energy:
direct SMMC versus Green's function method

Energy versus β

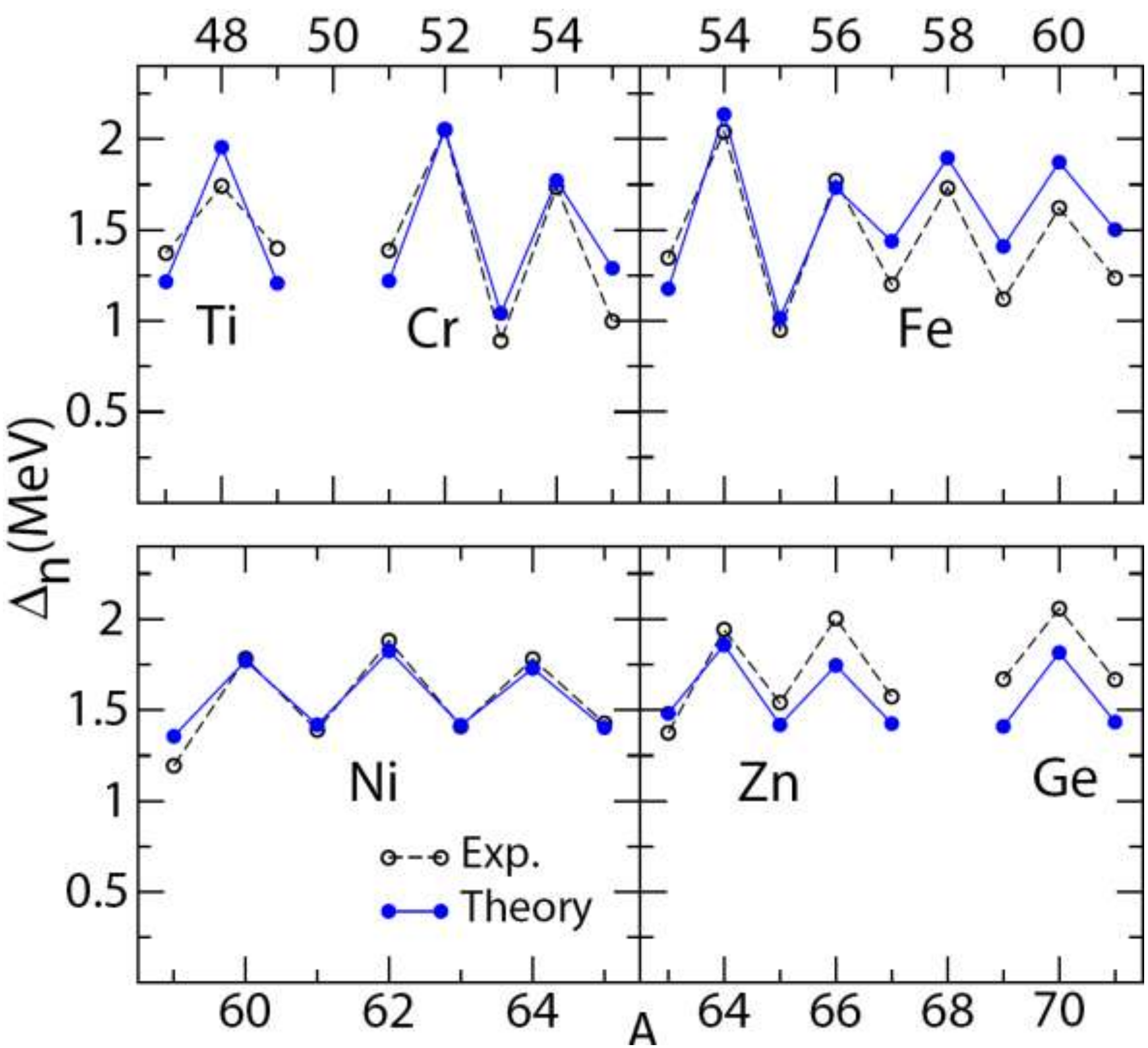




Standard deviation of energy

Application: pairing gaps in iron-region nuclei from odd-even mass differences

- Complete *fpg*9/2-shell.



Direct SMMC calculations of level densities (do not include spin degeneracy)

Y. Alhassid, M. Bonett-Matiz, S. Liu and H. Nakada, arXiv:1304.7258

- In SMMC, the thermal energy is calculated by tracing over the complete Hilbert space.

$\Rightarrow$ The calculated SMMC density ρ is the *state* density, in which the 2J+1 spin degeneracy of level with spin J is counted.

- However, experiments often measure the *level* density $\tilde{\rho}$, in which each level is counted once irrespective of its spin degeneracy.

Can we calculate the level density directly in SMMC ?

For each level, the state with the lowest non-negative spin projection M Appears exactly once.

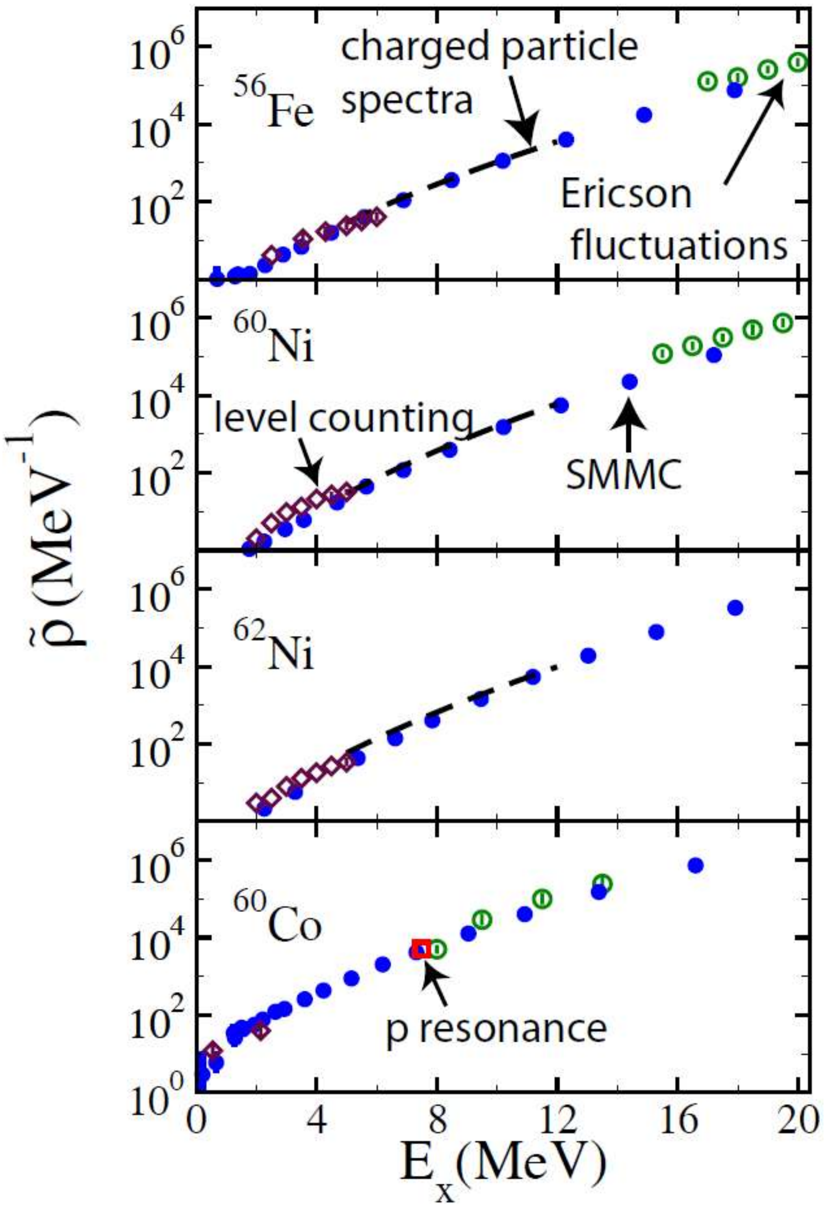
We denote by ρ_M the density at fixed spin projection M. Then:

$\tilde{\rho} = \rho_{M=0}$ for even-mass nuclei

$\tilde{\rho} = \rho_{M=1/2}$ for odd-mass nuclei

SMMC level densities in iron region nuclei

- Close agreement with experimental data



Spin cutoff parameter from state-to-level density ratio

Spin cutoff model

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

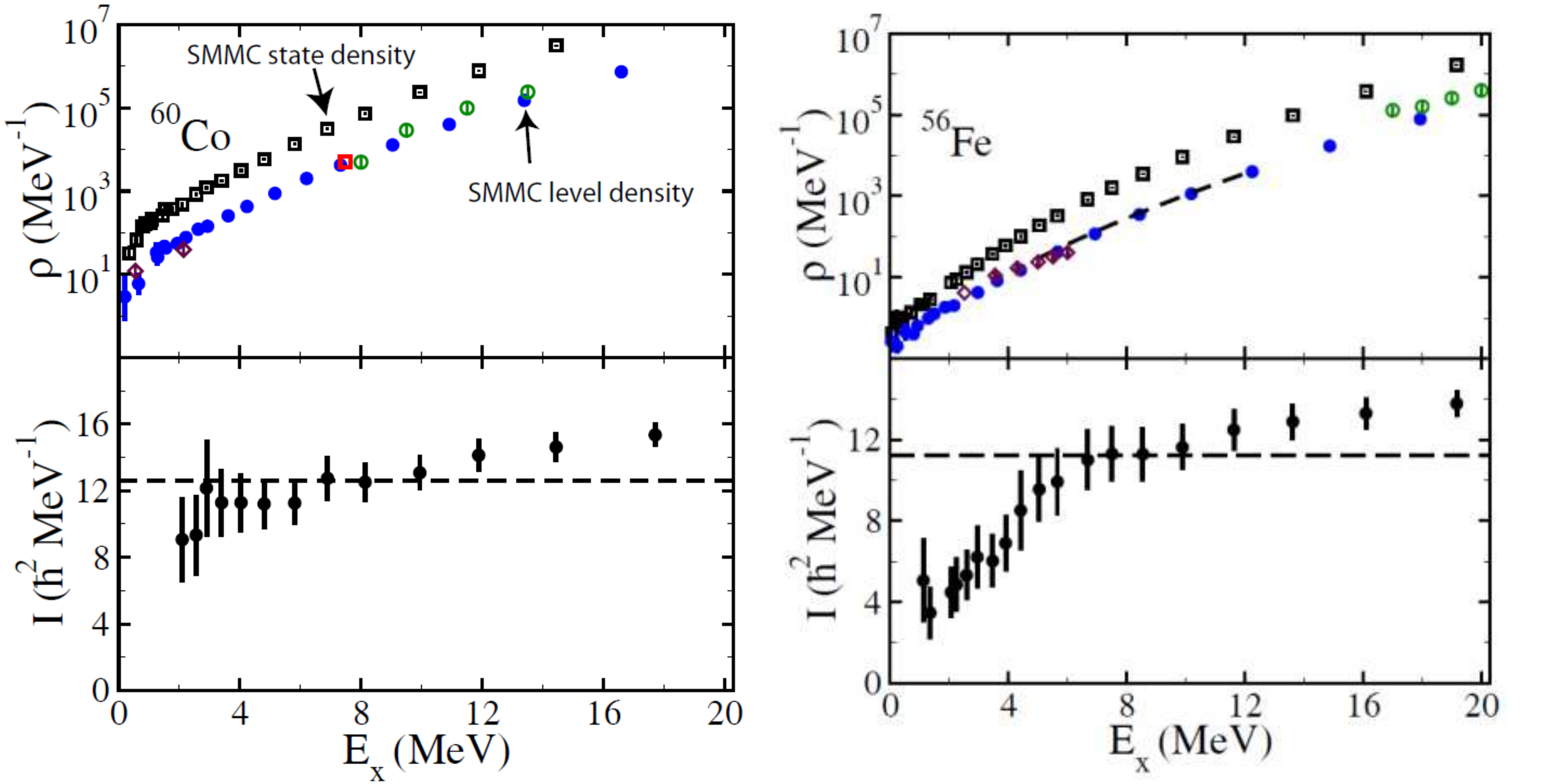
where $\sigma = \sigma(E_x)$ is the spin cutoff parameter.

- There is a relation between the level density and state density:

$$\tilde{\rho}(E_x) = \Sigma_J \rho_J(E_x) = \frac{1}{\sqrt{2\pi}\sigma} \rho(E_x)$$

$\Rightarrow$ σ can be determined from the state-to-level density ratio.

Moment of inertia I is determined from $\sigma^2 = \frac{IT}{\hbar^2}$



- In even-even nuclei we observe suppression of the moment of inertia at low excitation energies (effect of pairing correlations).

Microscopic level densities of nickel isotopes: theory versus experiment

M. Bonett-Matiz, A. Mukherjee and Y. Alhassid, arXiv:1305.0250,
PRC Rapid Comm, in press

- Recent determination of level densities in nickel isotopes from proton evaporation spectra by the Ohio University group (A. Voinov, S. Grimes et al.).
- We can now calculate accurate ground-state energies for both even-even and even-odd isotopes.

Even-mass isotopes

At low temperatures we can use a two-level model: only J=0 ground state and first excited state contribute to thermal observables.

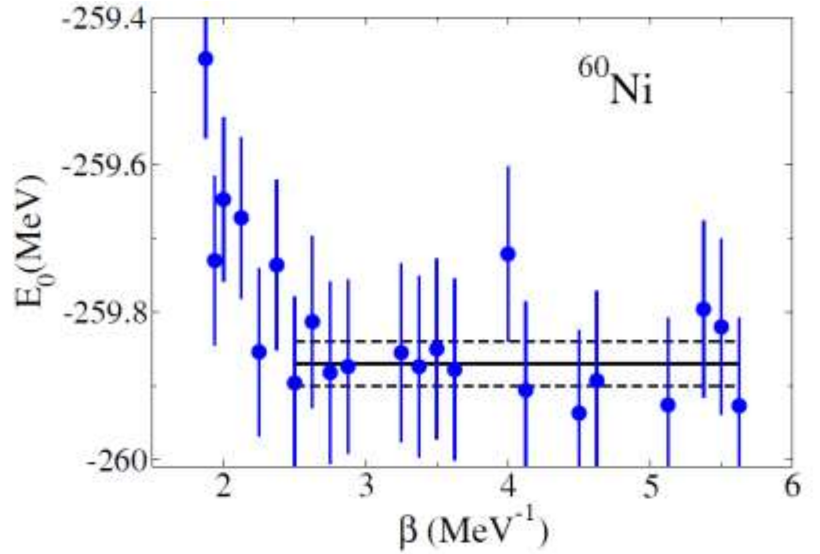
The ground-state energy E_0 and excitation energy $E_x^{2^+}$ of the first J=2 state can be determined from $\langle J^2 \rangle$ and thermal energy E

$$\langle J^2 \rangle = \frac{30}{5 + e^{\beta E_x^{2^+}}} \qquad E = E_0 + \frac{5E_x^{2^+}}{5 + e^{\beta E_x^{2^+}}}$$

$E_0 = -259.87 \pm 0.03$ MeV

$E_x^{2^+} = 1.20 \pm .07$ MeV

(Exp 1.33 MeV)



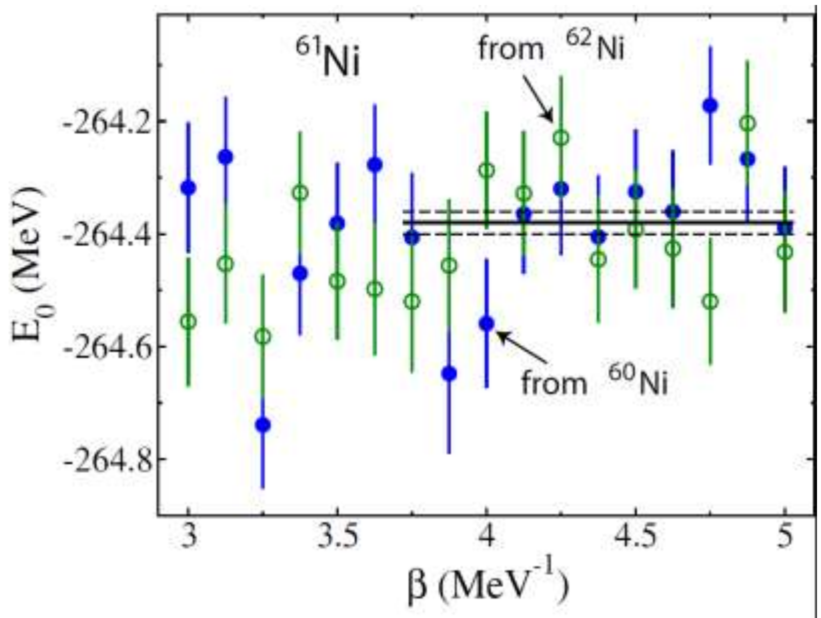
Odd-mass isotopes

Use Green's function method:

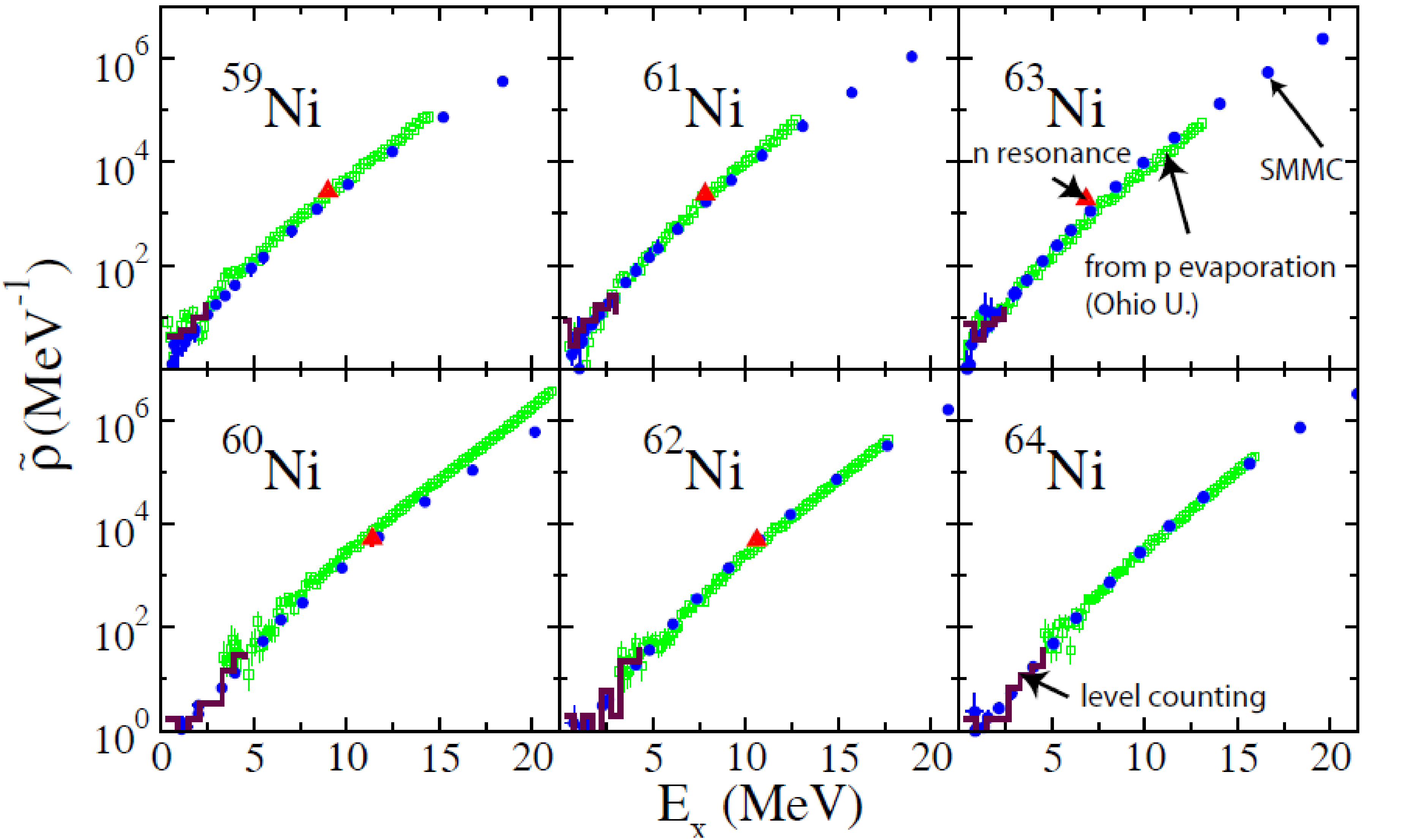
$E_0 = -264.38 \pm 0.01$ MeV

Statistical error comparable
to the error for the even nucleus

Excitation energy $E_x = E - E_0$
(to compare with experiments)

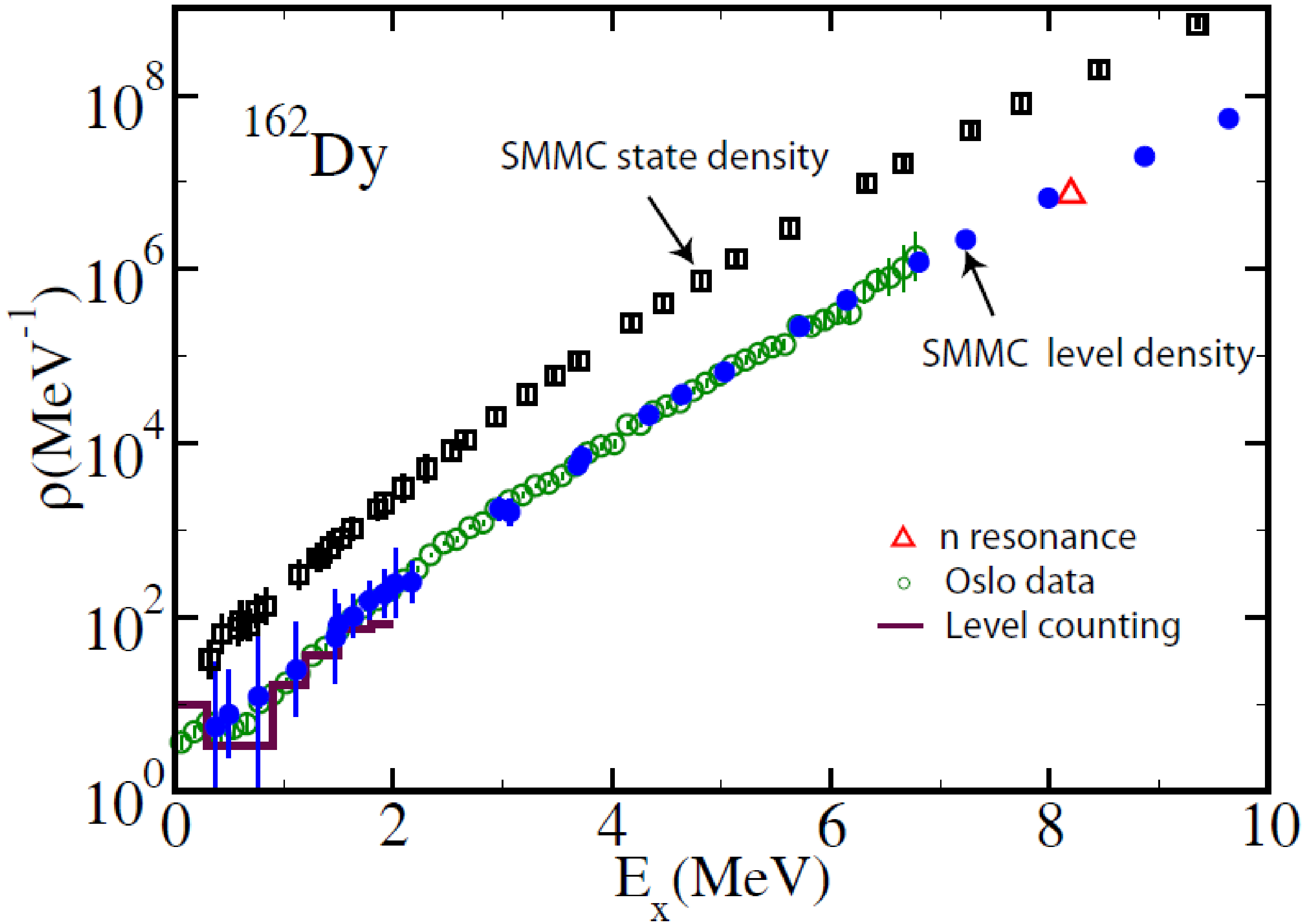


Level densities of nickel isotopes



State density versus level density in heavy nuclei (^{162}Dy)

Y. Alhassid, M. Bonett-Matiz, S. Liu and H. Nakada, arXiv:1304.7258



- Excellent agreement of the SMMC level density with experimental data

Conclusion

• Microscopic calculation of nuclear *state* and *level* densities are now possible in very large model spaces using the shell model Monte Carlo method.

• Odd-particle systems: circumventing a Monte Carlo sign problem.

• Close agreement with recent experimentally determined level densities in mid-mass and heavy nuclei.

Prospects

• Direct comparison of spin-parity projected densities with neutron resonance data

• Applications to unstable and exotic nuclei.