Nuclear level densities by the shell model Monte Carlo method

Yoram Alhassid (Yale University)

- 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 $U_\sigma$ 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 $\sigma$ is evaluated by Monte Carlo methods.

Thermodynamic approach to level densities


• 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:
  \[ \rho(E) \approx \frac{1}{\sqrt{2\pi T^2 C}} e^{S(E)} \]

\( S(E) = \text{canonical entropy} \); \( C = \text{canonical heat capacity} \).

\[ S(E) = \ln Z + \beta E \]

\[ C = -\beta^2 \partial E / \partial \beta \]
Technical developments

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


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 $\nu = n\ell j$:

$$G_{\nu}(\tau) = \sum_m \langle T a_{vm}(\tau) a_{vm}^\dagger(0) \rangle$$

In the asymptotic regime in $\tau$

$$G_{\nu}(\tau) \sim e^{-\beta [E_j(A\pm1) - E_{gs}(A)] |\tau|}$$

• 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 $\ln G_{1p_{3/2}}(\tau)$.

• Minimize $E_j(A \pm 1)$ 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 $\beta$

Standard deviation of energy

Green’s function method

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

- Complete $f_{pg9/2}$-shell.
Direct SMMC calculations of level densities (do not include spin degeneracy)


• In SMMC, the thermal energy is calculated by tracing over the complete Hilbert space.
  ⇒ The calculated SMMC density $\rho$ 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 $\rho_M$ the density at fixed spin projection $M$. Then:

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

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

\[
\tilde{\rho}(E_x) = \sum_J \rho_J(E_x) = \frac{1}{\sqrt{2\pi}\sigma} \rho(E_x)
\]

\( \Rightarrow \) \( \sigma \) 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 $E^{2+}_x$ of the first J=2 state can be determined from $\langle J^2 \rangle$ and thermal energy $E$

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

$$E = E_0 + \frac{5E^{2+}_x}{5 + e^{\beta E^{2+}_x}}$$
Odd-mass isotopes

Use Green’s function method:

\[ E_0 = -259.87 \pm 0.03 \text{ MeV} \]

\[ E_{x^2}^2 = 1.20 \pm 0.07 \text{ MeV} \]

(Exp 1.33 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

- $^{59}\text{Ni}$
- $^{61}\text{Ni}$
- $^{63}\text{Ni}$
- $^{60}\text{Ni}$
- $^{62}\text{Ni}$
- $^{64}\text{Ni}$

$n$ resonance from $p$ evaporation (Ohio U.)

SMMC

level counting
State density versus level density in heavy nuclei ($^{162}\text{Dy}$)


- 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.