Auxiliary-field Monte Carlo methods in Fock space: sign problems and methods to circumvent them

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- Introduction

- Finite-temperature auxiliary-field Monte Carlo methods in Fock space (e.g., in the framework of the nuclear configuration-interaction shell model)

- Sign rule and good-sign interactions

- Practical solution to the sign problem (in the nuclear shell model)

- Circumventing the odd particle-number sign problem

- Projection on good quantum numbers and “sign” problems

- Imaginary-time response functions

Recent review: Y. Alhassid, arXiv:1607.01870 (2016)

Introduction

Consider a system of fermions in Fock space described by the Hamiltonian

$$H = \sum_{ij} \varepsilon_i a_i^\dagger a_i + \tfrac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

where $i = 1,\ldots,N_s$ are single-particle states with energies ε_i and v_{ijkl} are two-body interaction matrix elements.

The dimensionality of the many-particle model space increases combinatorially with the number of single-particle orbitals and/or the number of fermions, and conventional diagonalization methods become intractable.

- The auxiliary-field Monte Carlo (AFMC) method for the shell model enables calculations in model spaces that are many orders of magnitude larger than those that can be treated by diagonalization methods.

Examples: configuration-interaction (CI) shell model for nuclei and cold atoms in a trap.

Hubbard-Stratonovich (HS) transformation

A general effective Hamiltonian in Fock space with a one-body part and a two-body interaction can be written as :

$$\hat{H} = \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} \sum_\alpha v_\alpha \hat{\rho}_\alpha^2$$

ϵ_i are single-particle energies and $\hat{\rho}_\alpha$ are linear combinations of one-body densities $\hat{\rho}_{ij} = a_i^\dagger a_j$.

The HS transformation describes the Gibbs ensemble $e^{-\beta H}$ at inverse temperature $\beta = 1/T$ as a path integral over time-dependent auxiliary fields $\sigma(\tau)$

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

$G_\sigma = e^{-\frac{1}{2}\int_0^\beta |v_\alpha| \sigma_\alpha^2(\tau) d\tau}$ is a Gaussian weight and U_σ is a one-body propagator of non-interacting fermions in time-dependent auxiliary fields

$$\hat{U}_\sigma = \mathcal{T} e^{-\int_0^\beta \hat{h}_\sigma(\tau) d\tau}$$

with a one-body Hamiltonian $\hat{h}_\sigma(\tau) = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha s_\alpha |v_\alpha| \sigma_\alpha(\tau) \hat{\rho}_\alpha$

$s_\alpha = 1$ for $v_\alpha < 0$, and $s_\alpha = i$ for $v_\alpha > 0$

Thermal expectation values of observables

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\,(\hat{O} e^{-\beta \hat{H}})}{\mathrm{Tr}\,(e^{-\beta \hat{H}})} = \frac{\int \mathcal{D}[\sigma] G_\sigma \langle \hat{O} \rangle_\sigma \,\mathrm{Tr}\, \hat{U}_\sigma}{\int \mathcal{D}[\sigma] G_\sigma \,\mathrm{Tr}\, \hat{U}_\sigma}$$

where $\langle \hat{O} \rangle_\sigma \equiv \mathrm{Tr}\,(\hat{O}\hat{U}_\sigma)/\mathrm{Tr}\,\hat{U}_\sigma$

Grand canonical quantities in the integrands can be expressed in terms of the single-particle representation matrix $\mathbf{U}_\sigma$ of the propagator :

$$\mathrm{Tr}\,\hat{U}_\sigma = \det(\mathbf{1} + \mathbf{U}_\sigma)$$

$$\langle a_i^\dagger a_j \rangle_\sigma \equiv \frac{\mathrm{Tr}\,(a_i^\dagger a_j \hat{U}_\sigma)}{\mathrm{Tr}\,\hat{U}_\sigma} = \left[\frac{1}{\mathbf{1} + \mathbf{U}_\sigma^{-1}} \right]_{ji}$$

- The integrand reduces to matrix algebra in the single-particle space (of typical dimension ~100).

Auxiliary-field Monte Carlo (AFMC) and the sign problem

The path integrals are done by Monte Carlo methods, sampling the fields according to a weight $W_\sigma = G_\sigma |Tr U_\sigma|$

$\Phi_\sigma = Tr U_\sigma / |Tr U_\sigma|$ is the Monte Carlo "sign" function.

Also known in nuclear physics as the shell model Monte Carlo (SMMC) method.

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).

For a generic interaction, the sign can be negative (or a phase) for some of the field configurations. When the average sign is small, the fluctuations in observables become very large $\Rightarrow$ the Monte Carlo sign problem.

Sign rule and good-sign interactions

When the Hamiltonian is time-reversal invariant, we can rewrite

$$\hat{H} = \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} \sum_\alpha v_\alpha \left(\rho_\alpha \bar{\rho}_\alpha + \bar{\rho}_\alpha \rho_\alpha \right)$$

where $\bar{\rho}_\alpha$ is the time-reversed density.

Sign rule: when all $v_\alpha < 0$ and the single-particle angular momentum is half an integer, $\mathrm{Tr}\, U_\sigma > 0$ for any configuration σ of and the interaction is known as a good-sign interaction (in the grand canonical ensemble).

Proof: when all $v_\alpha < 0$, the one-body Hamiltonian in the HS transformation

$$\hat{h}_\sigma = \sum_i \epsilon_i \hat{n}_i + \sum_\alpha \left(v_\alpha \sigma_\alpha^* \rho_\alpha + v_\alpha \sigma_\alpha \bar{\rho}_\alpha \right)$$

is time-reversal invariant $\bar{h}_\sigma = h_\sigma \Rightarrow$ U_σ is also invariant under time reversal.

If λ_i is an eigenvalue of $\mathbf{U}_\sigma$ then λ_i^* is also an eigenvalue.

If the total single-particle angular momentum is half an integer (e.g., j in nuclei), the eigenvalues appear in pairs $\{\lambda_i, \lambda_i^*\}$ (Kramer's degeneracy in the complex plane) and

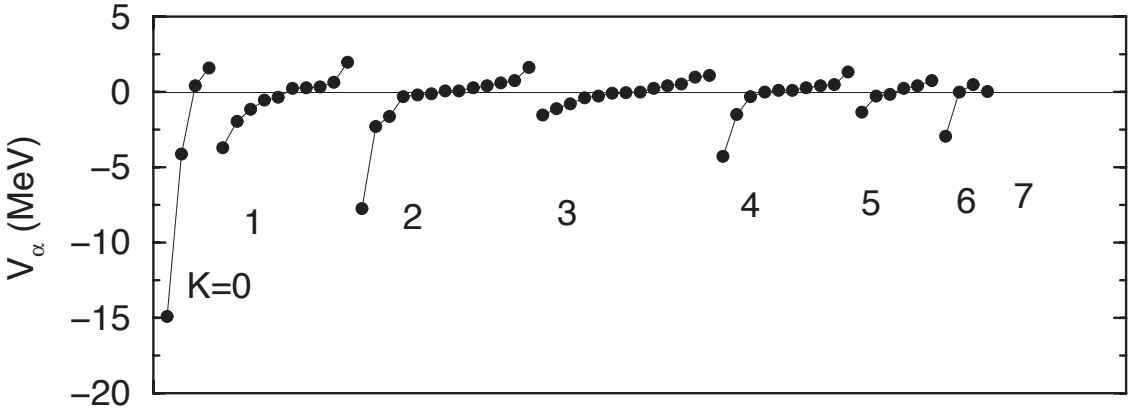
$$\mathrm{Tr}\, \hat{U}_\sigma = \prod_i |1 + \lambda_i|^2 > 0$$

$\Rightarrow$ good-sign interaction

A practical method for circumventing the sign problem in the nuclear configuration-interaction shell model

Alhassid, Dean, Koonin, Lang, Ormand, PRL **72**, 613 (1994).

The dominant collective components of effective nuclear interactions in the CI shell model have a good sign.



(i) In the calculation of statistical and collective properties of nuclei, we have used successfully good-sign interactions (pairing + multipole-multipole terms)

(ii) To circumvent the sign problem for the complete interaction, a family of good-sign interactions is constructed by multiplying the bad-sign components $v_\alpha > 0$ by a negative parameter g (making $g v_\alpha < 0$):

$$H = H_G + g H_B$$

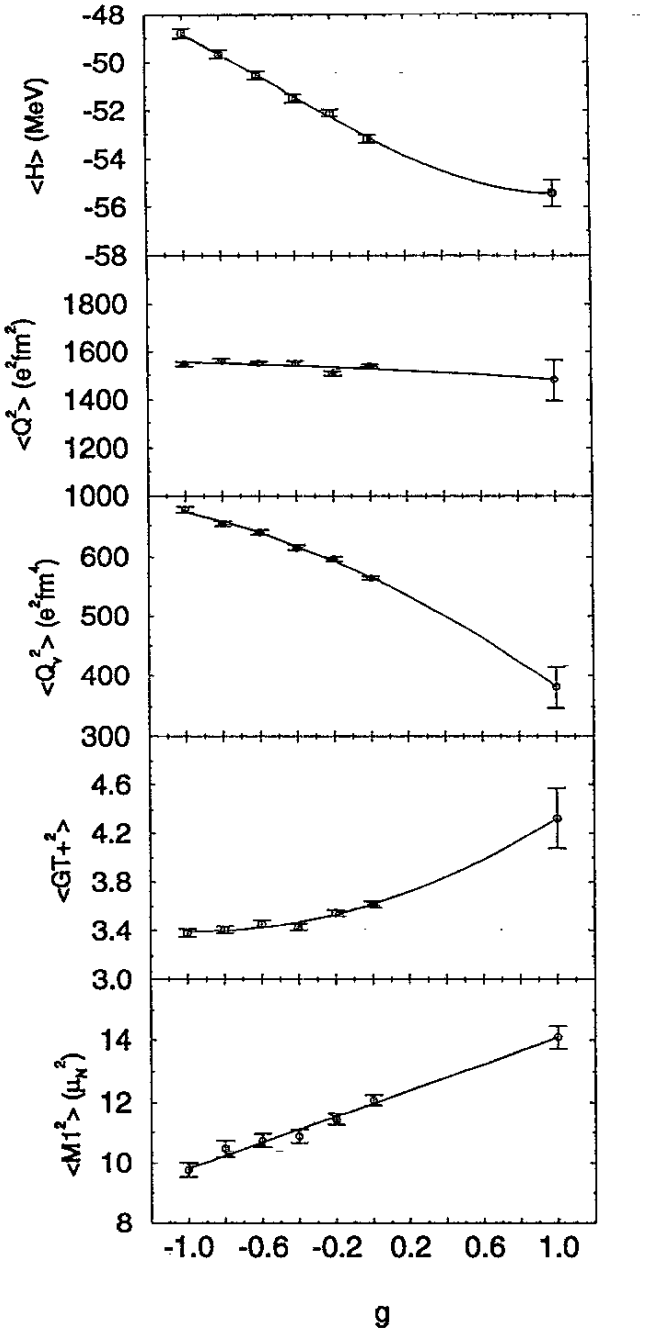
Observables are calculated with accurately for $g < 0$ and extrapolated to $g = 1$

Example: thermal observables in ^{54}Fe using an effective nuclear interaction in the pf shell, extrapolated from g <0 to g=1:

Energy <H>, total strengths of quadrupole Q, Gamow-Teller, and M1 operators

g=0 is not a singular point and simple linear or quadratic extrapolations are sufficient: find the lowest order polynomial such that χ^2 per dof < 1.

The extrapolation method was validated in nuclei for which conventional diagonalization is possible.



Particle-number projection

In a finite-size system, it is necessary to project on the canonical ensemble of fixed particle number $\mathcal{A}$. In the Fock space spanned by N_s single-particle orbitals, this can be done by an exact discrete Fourier transform.

Canonical partition (for $\mathcal{A}$ particles):

$$\mathrm{Tr}_{\mathcal{A}} U_\sigma = \frac{e^{-\beta\mu\mathcal{A}}}{N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m \mathcal{A}} \det\left(\mathbf{1} + e^{i\varphi_m} e^{\beta\mu} \mathbf{U}_\sigma\right)$$

where $\varphi_m = 2\pi m/N_s \;\; (m = 1, \ldots, N_s)$ are quadrature points.

Canonical expectation of an observable O:

$$\mathrm{Tr}_{\mathcal{A}}\left(\hat{O}\hat{U}_\sigma\right) = \frac{e^{-\beta\mu\mathcal{A}}}{N_s} \sum_{m=1}^{N_s} e^{-i\varphi_m \mathcal{A}} \det\left(\mathbf{1} + e^{i\varphi_m + \beta\mu} \mathbf{U}_\sigma\right) \times \mathrm{tr}\left(\frac{1}{\mathbf{1} + e^{-i\varphi_m - \beta\mu} \mathbf{U}_\sigma^{-1}} \mathbf{O}\right)$$

The $\mathcal{A}$-projected partition is used in the Monte Carlo weight function

$$W_\sigma \equiv G_\sigma |\mathrm{Tr}_{\mathcal{A}}\, \hat{U}_\sigma|$$

For a good-sign interaction, the projection on an even number of particles keeps the sign good but the odd-particle projection leads to a new sign problem.

Circumventing the odd-particle sign problem in AFMC

Mukherjee and Alhassid, PRL **109**, 032503 (2012)

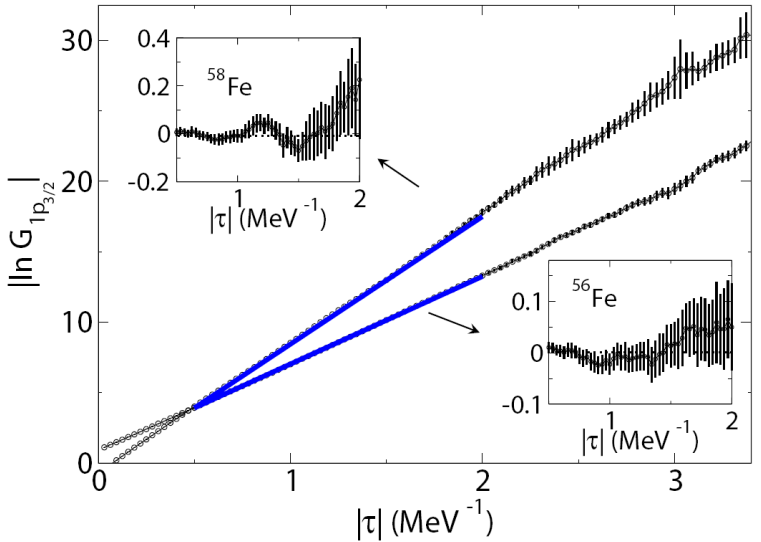
Applications of AFMC to odd-even and odd-odd nuclei has been hampered by a sign problem that originates from the projection on odd number of particles.

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

Consider the imaginary-time single-particle Green's functions for even-even nuclei: $G_\nu(\tau) = \Sigma_m \left\langle T\, a_{\nu m}(\tau) a^\dagger_{\nu m}(0) \right\rangle$ for orbitals $\nu = n\,l\,j$

In the asymptotic regime in $(1 < \tau \ll \beta)$ $\quad G_\nu(\tau) \sim e^{-[E_j(A\pm1) - E_{gs}(A)]\,|\tau|}$

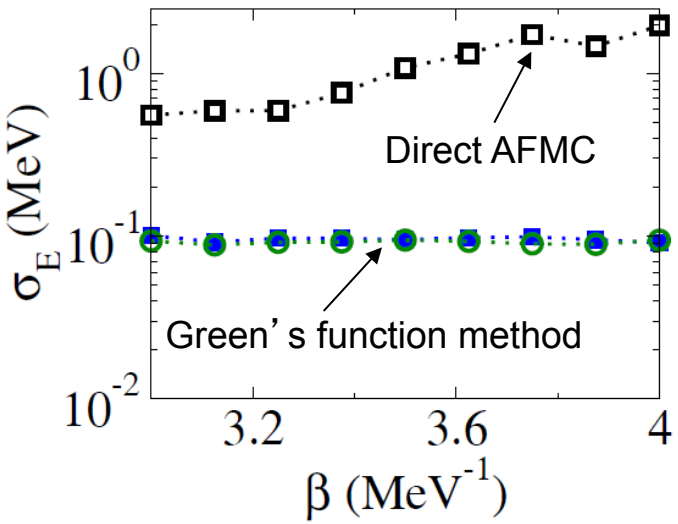
- The energy difference between the lowest energy of the odd-particle system for a given spin j and the ground-state energy of the even-particle system can be extracted from the slope of $\ln G_\nu(\tau)$.

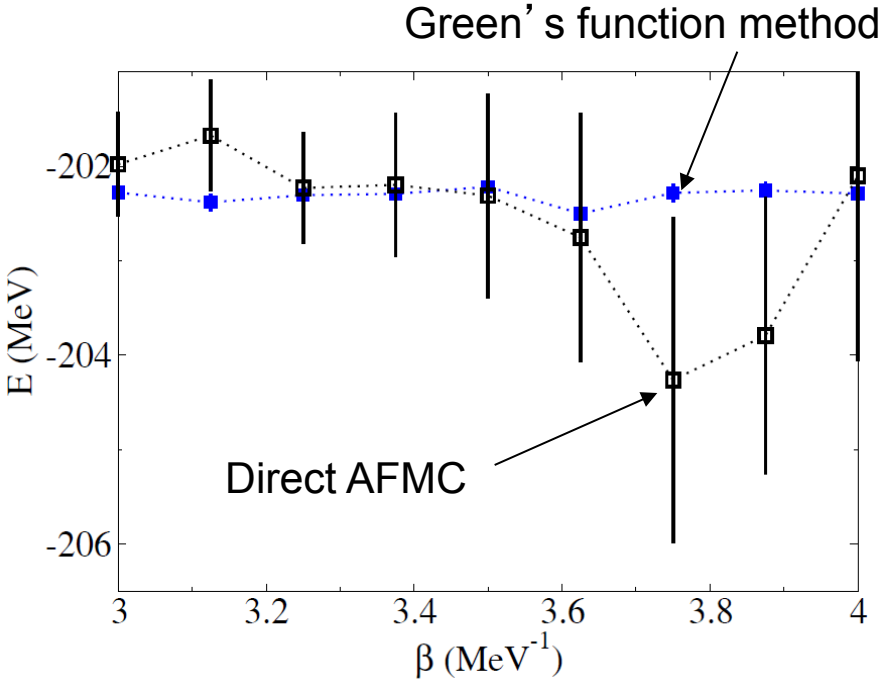


^{57}Fe

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

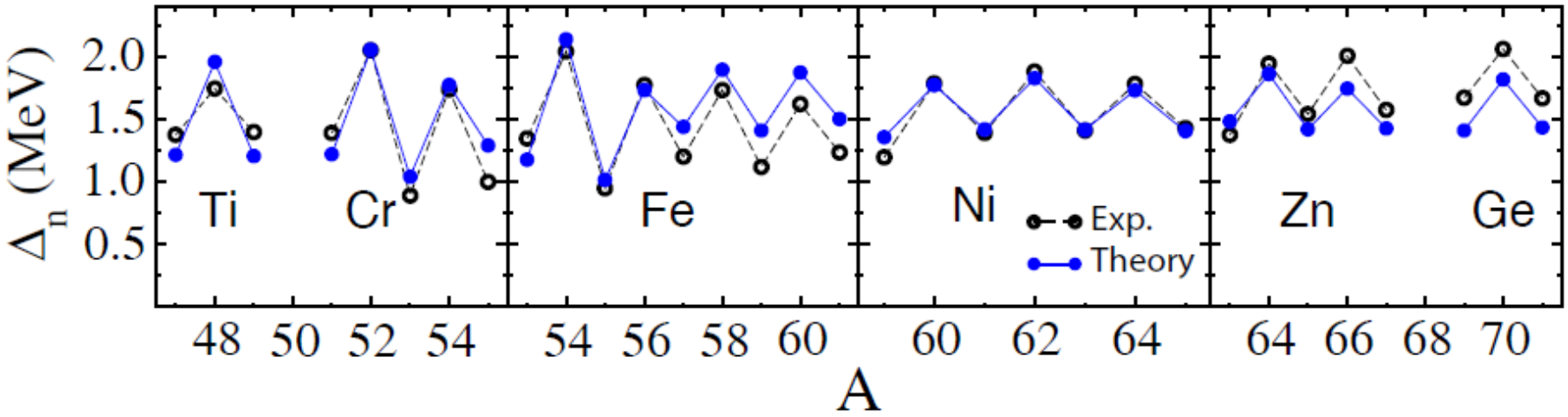
Statistical errors of ground-state energy of direct SMMC versus Green's function method





Pairing gaps in mid-mass nuclei from odd-even mass differences

- AFMC in the complete $fpg_{9/2}$ shell (in good agreement with experiments)



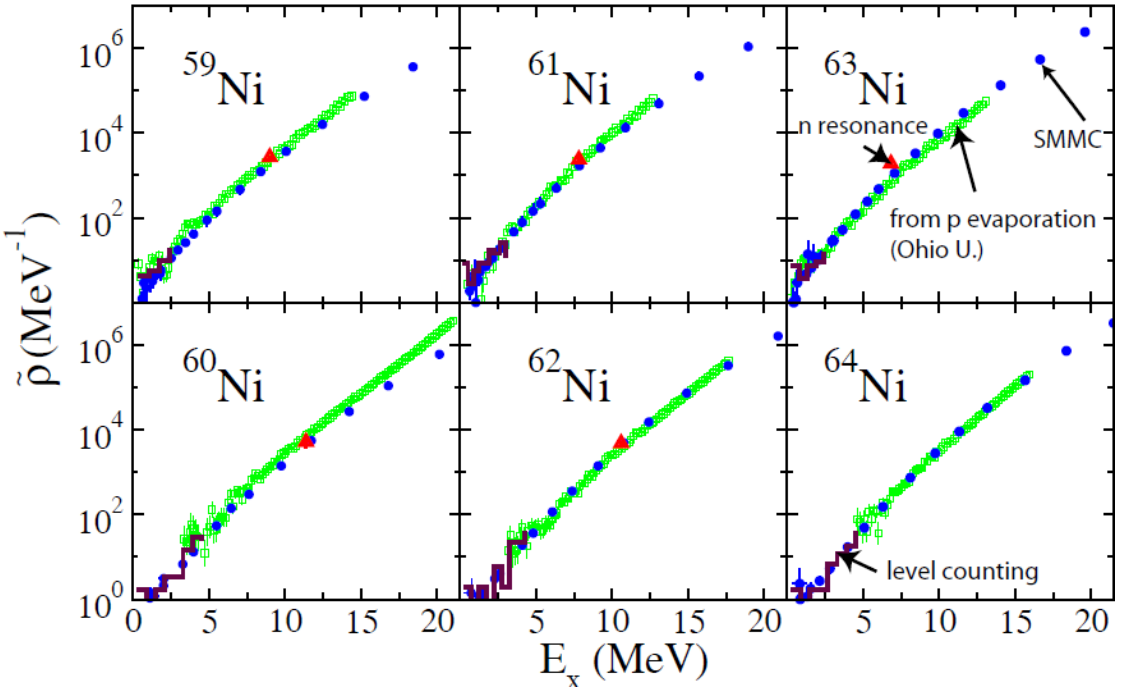
Application: statistical properties of nuclei

Statistical properties, and, in particular, level densities, are important input in the theory of statistical nuclear reactions, but are not always accessible to direct measurements.

AFMC is the state-of-the-art method for the microscopic calculation of statistical properties of nuclei.

Example: level densities in nickel isotopes

Excellent agreement with experiments:
(i) level counting,
(ii) proton evaporation Spectra,
(iii) neutron resonance data



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

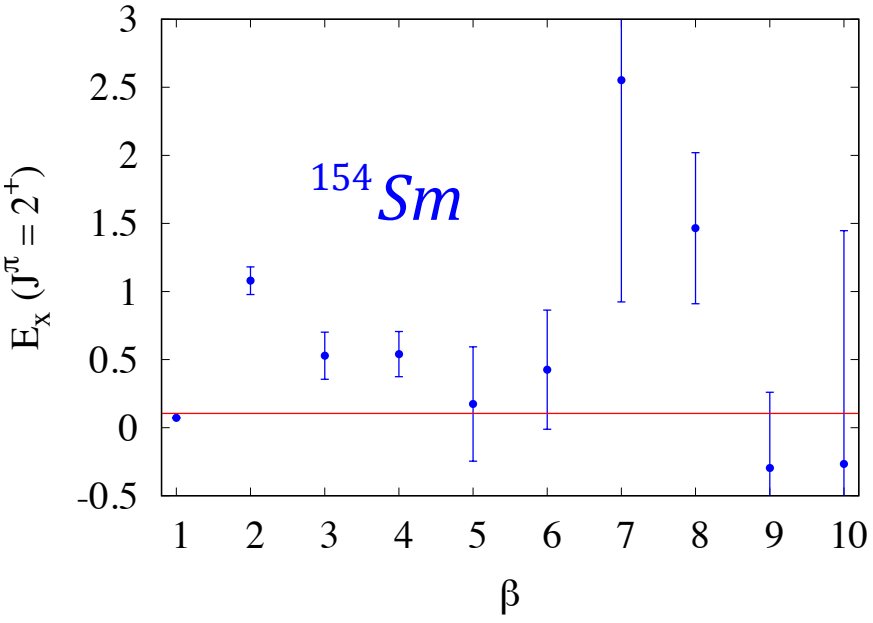
Projection on good quantum numbers and "sign" problems

The traces in thermal expectation values sum over all values of the good quantum numbers (e.g., spin, parity, …).

To recover the dependence on these quantum numbers, it is necessary to introduce exact projections in the HS transformation. These projections can lead to a "sign" problem even for good-sign interactions.

$Tr_J U_\sigma > 0$ for J=0 and $E_{J=0}(\beta)$ can be calculate accurately at large β.

However, $E_J(\beta)$ for $J \neq 0$ has large fluctuations at large β and it is difficult to extract the excitation energy of the lowest level with spin J.



Using the imaginary-time response function of the mass quadrupole, the lowest J=2 energy is 0.0819(7) MeV (preliminary)

Imaginary-time response functions

The lowest energy level for a given spin can be accurately extracted from imaginary-time response functions of one-body observables.

Example: for large β and sufficiently large $\tau << \beta$

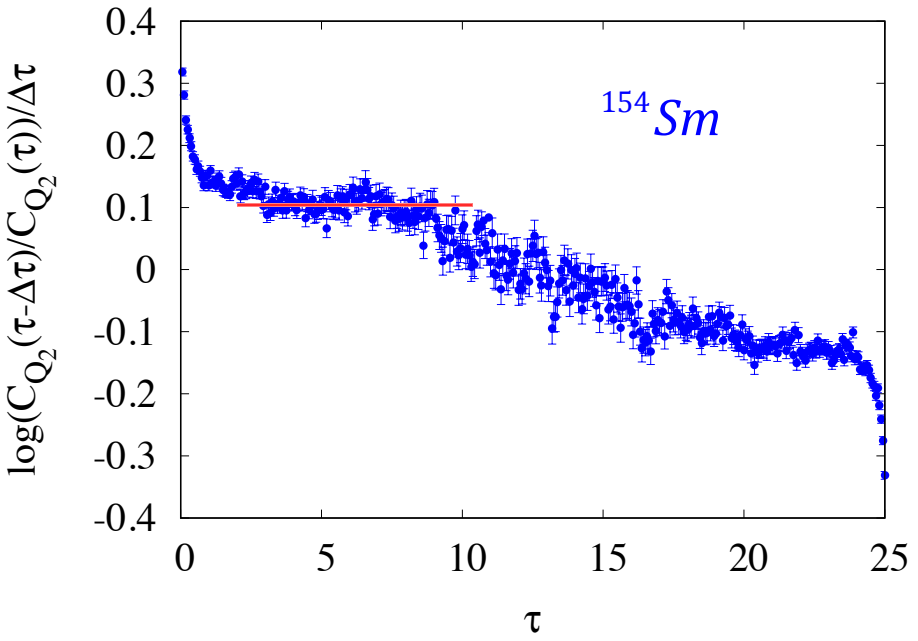
$$C_{Q_2}(\tau) = \langle Q_2(\tau) Q_2(0) \rangle \sim e^{-\tau(E_{2+} - E_0)}$$

where Q_2 is the mass quadrupole operator

The lowest J=2 level is determined from the plateau in

$$\ln[C_{Q_2}(\tau - \Delta\tau)/C_{Q_2}(\tau)]/\Delta\tau$$

C.N. Gilbreth (INT)



Conclusion

• Finite-temperature AFMC in Fock space is a powerful method in the framework of the configuration-interaction shell model (e.g., for nuclei and trapped cold atoms)

• Sign rule determines a broad class of good sign interactions

• Practical solution to the sign problem in the nuclear shell model: simple extrapolations from a family of good sign interactions

• The odd particle-number sign problem was circumvented by using the imaginary-time Green's functions in the even particle-number systems

• Projection on good quantum numbers (e.g., spin and parity) can lead to large fluctuations in the projected observables at low temperatures

Outlook

• Explore other HS decompositions (the sign problem depends on the decomposition)

• Use imaginary-time response functions of one-body observables to extract the lowest excitation energy for given values of good quantum numbers