Importance-Truncated Shell Model

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Motivation

- valence-space shell model:
  successful method for the description of a large variety of spectroscopic observables
  - model space: spanned by Slater determinants composed of single-particle states for the valence nucleons (m-scheme)
  - effective interactions:
    → traditional interactions of phenomenological origin
    → new ab initio interactions from In-Medium Similarity Renormalization Group [?]
  - diagonalization of the Hamilton matrix:
    → energies and eigenstates
    → observables: matrix elements of operators computed for the eigenstates
- shell-model calculations limited by valence-space dimension
  → truncated valence spaces used (t truncation)
- importance-truncated shell model (IT-SM): simple and straightforward extension of the shell model to larger valence spaces and a wider range of nuclei

Importance Truncation

Basic Idea

- introduce importance threshold $\kappa_{\min}$ as adaptive truncation criterion
- solve eigenvalue problem in reduced model space tailored to a given Hamiltonian and target state

General Concept [? ?]

- start from initial approximation for the target state in a subspace of $\mathcal{M}_{\text{full}}$

$$|\Psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_\nu \, |\Phi_\nu\rangle$$

- define importance measure κ_ν for basis states $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$ from 1st order correction to $|\Psi_{\text{ref}}\rangle$ in perturbation theory

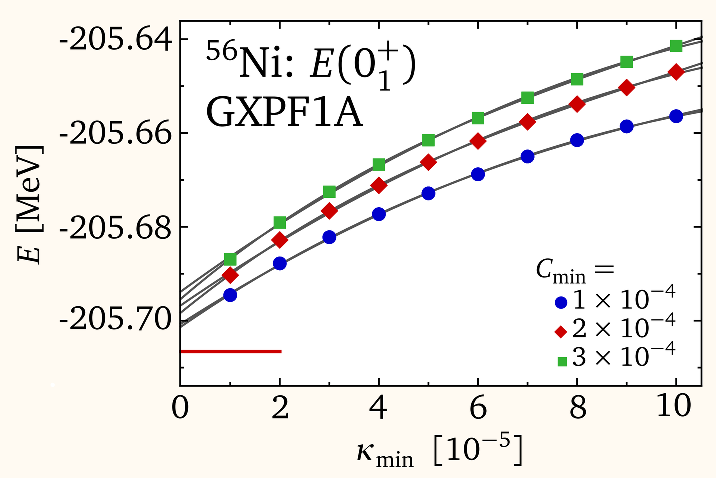
$$|\Psi^{(1)}\rangle = -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle \Phi_\nu | \mathbf{H} | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}} |\Phi_\nu\rangle \quad \Rightarrow \quad \kappa_\nu = -\frac{\langle \Phi_\nu | \mathbf{H} | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- construct importance-truncated model space $\mathcal{M}_{\text{IT}}$ from all basis states with $|\kappa_\nu| \geq \kappa_{\min}$
- solve the eigenvalue problem in $\mathcal{M}_{\text{IT}}$
  → obtain improved approximation for the target state
- define eigenstate as new $|\Psi_{\text{ref}}\rangle$ and use iterative scheme to account for all possible ph excitations on top of the initial approximation for the target state
- accelerate iteration by introducing a reference threshold $C_{\min}$: include only basis states with $|C_\nu| \geq C_{\min}$ in $\mathcal{M}_{\text{ref}}$
- vary $\kappa_{\min}$ and extrapolate to account for effects of basis states excluded from $\mathcal{M}_{\text{IT}}$

Extrapolation Schemes in the IT-SM [?]

Threshold Extrapolation

- fit polynomials to a sequence of IT-SM energies or observables and extrapolate to $\kappa_{\min} \to 0$
- no additional computational cost
- no physical motivation for fit function
  ⇒ potentially large uncertainties

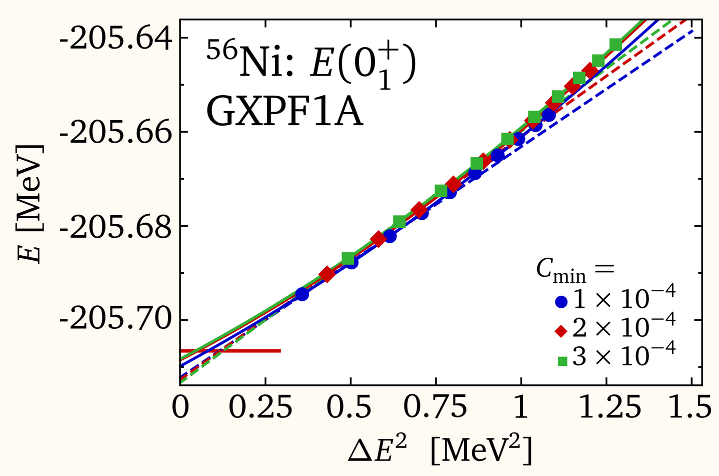


Energy-Variance Extrapolation

- improved technique for energies
- compute energy variance

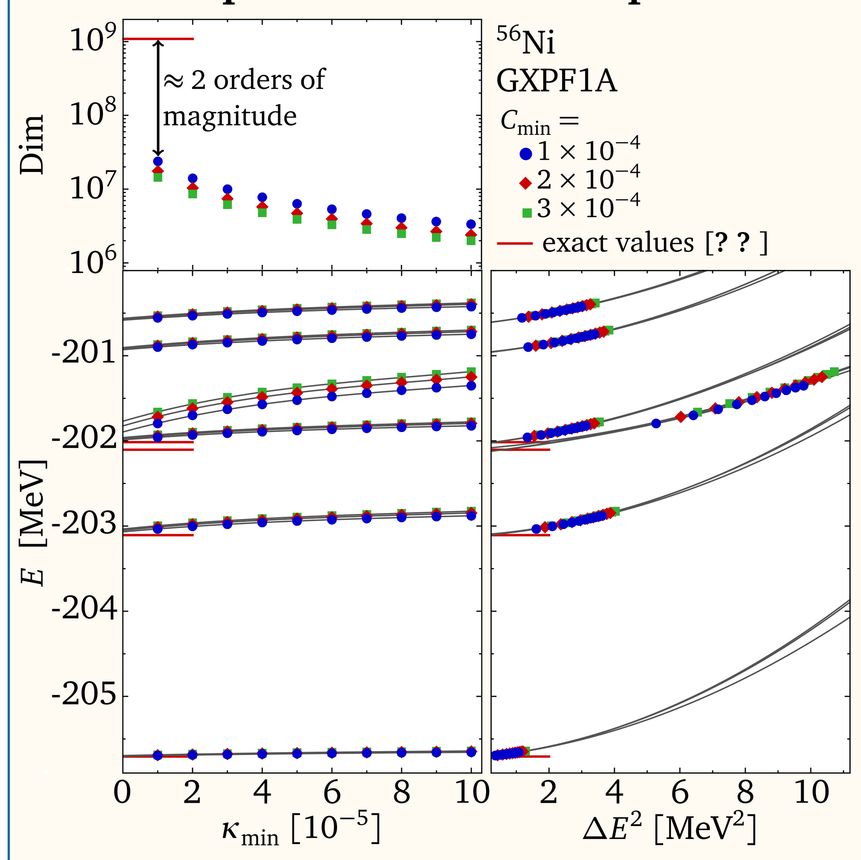
$$\Delta E^2 = \langle \Psi | \mathbf{H}^2 | \Psi \rangle - \langle \Psi | \mathbf{H} | \Psi \rangle^2$$

  for the sequence of IT-SM eigenstates and extrapolate to $\Delta E^2 \to 0$ [?]
- corrects for effects of the different truncations applied ($t, \kappa_{\min}, C_{\min}$)
- physically motivated and controlled
- computationally demanding



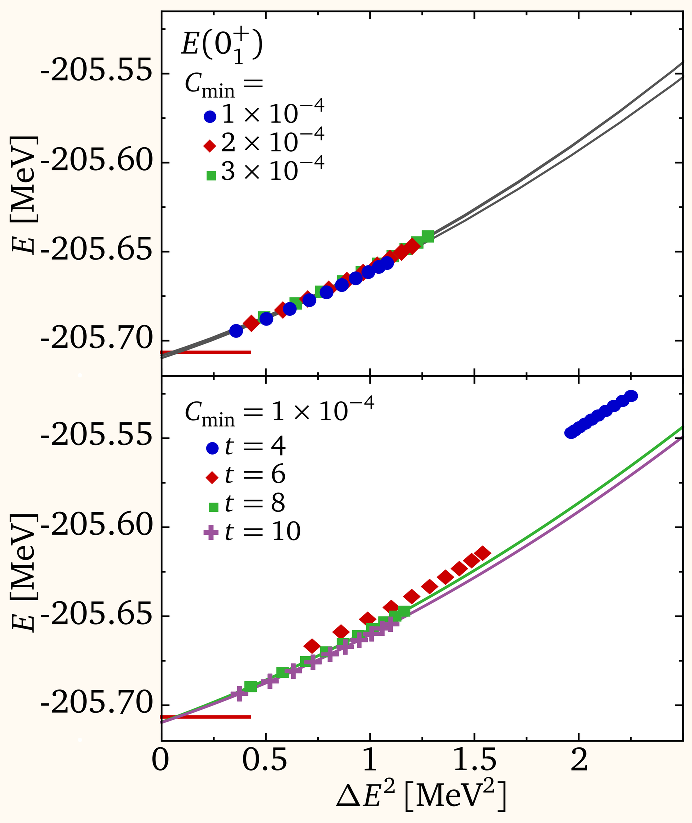
Benchmark of the IT-SM: ^{56}Ni in the pf shell

Threshold and Energy-Variance Dependence and Extrapolation



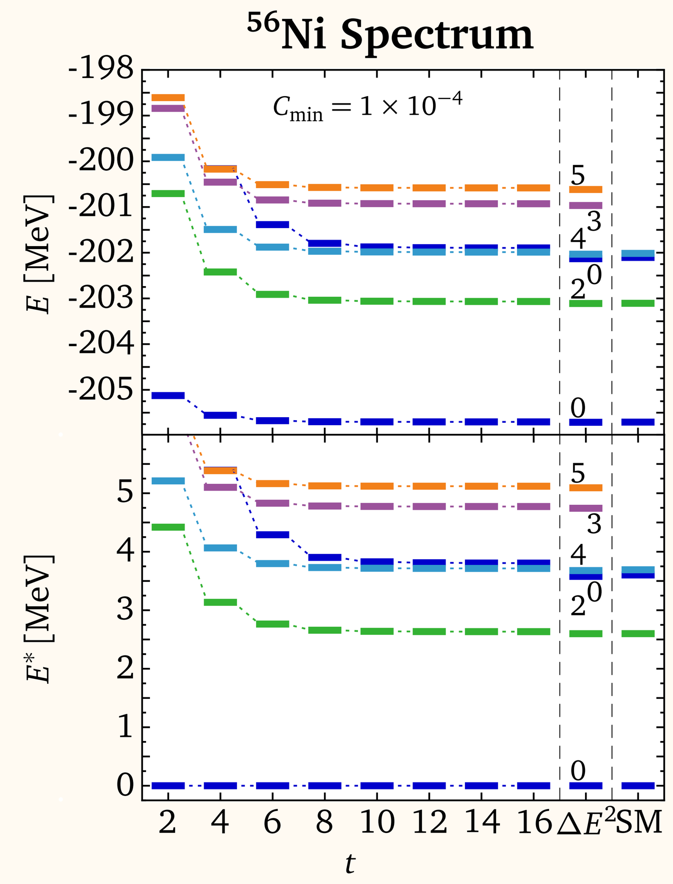
- reduced model-space dimension
- very weak $C_{\min}$ and $\kappa_{\min}$ dependence
- both extrapolation techniques yield excellent agreement with exact values

Truncation Removal in the Energy-Variance Extrapolation



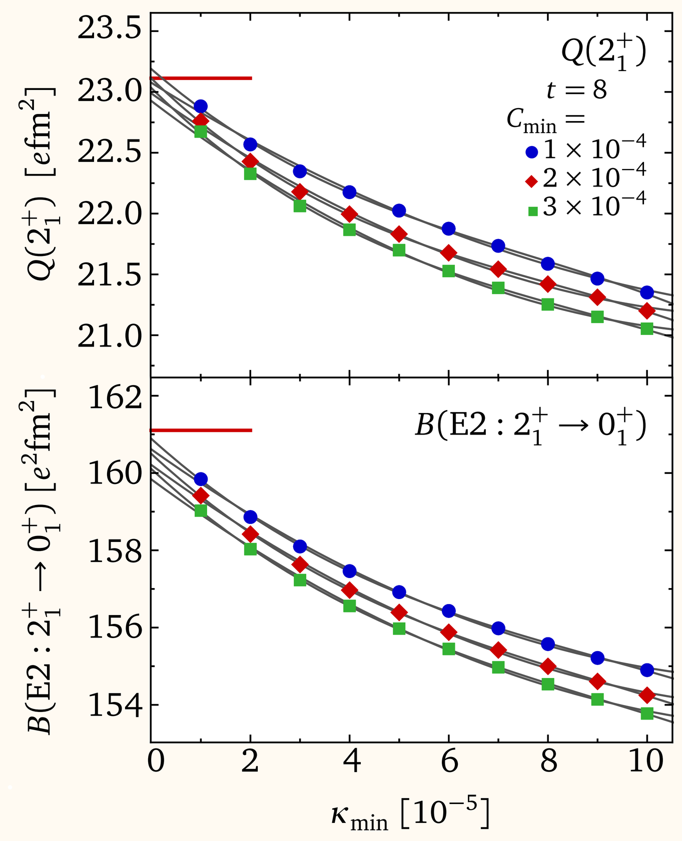
- ΔE^2 extrapolation corrects for effects of truncations applied
- reliable extrapolation

^{56}Ni Spectrum



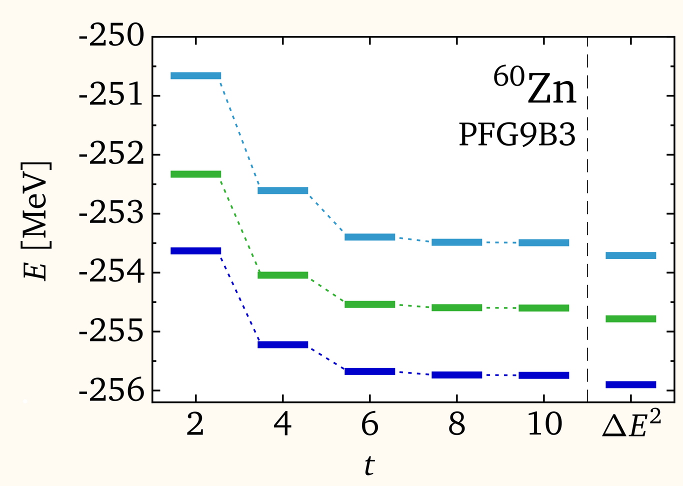
- converged from $t = 10$ on
- ΔE^2 extrapolation reproduces state ordering and energy of degenerate 0^+_2 state

Electromagnetic Observables

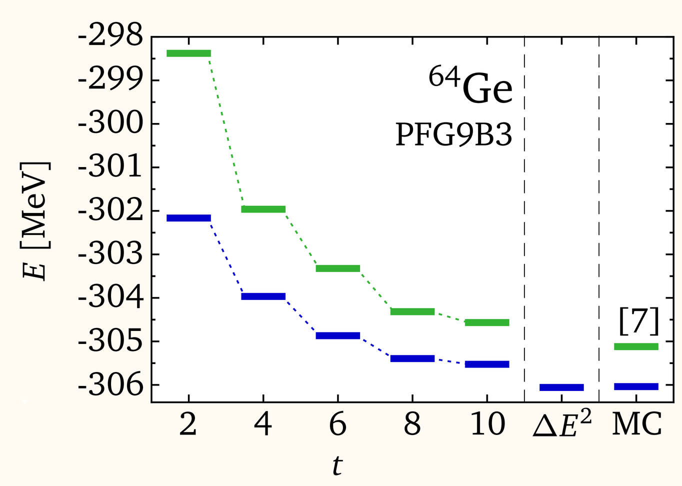


- observables equally well described
- example: quadrupole moment and $B(E2)$ transition strength

Highlights of the IT-SM: pfg$_{9/2}$-shell nuclei ^{60}Zn and ^{64}Ge



- full dimension: 2.2×10^{13}
- fast convergence w.r.t. t



- full dimension: 1.7×10^{14}
- deformation → slow convergence

Outlook

- application of valence-space interactions from IM-SRG
- IT-SM calculations for island-of-inversion nuclei in full sdpf valence spaces

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