Towards Multi-Shell Valence Spaces

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Motivation

- traditional valence-space shell model (SM):
  - model space: spanned by Slater determinants composed of single-particle states for the valence nucleons (m-scheme)
  - traditional effective interactions of phenomenological origin
  - diagonalization of the Hamilton matrix:
    → energies and eigenstates
    → observables: matrix elements of operators computed for the eigenstates
  - limitations:
    → SM calculations limited by valence-space dimensions
    → effective interactions lack consistent framework for treatment of all observables
- improvements on traditional approach:
  - importance-truncated shell model (IT-SM): simple and straightforward extension of the shell model to larger valence spaces and a wider range of nuclei [1]
  - use of new effective interactions derived in In-Medium Similarity Renormalization Group (IM-SRG) [2, 3]

Importance Truncation

Basic Idea

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

General Concept [1, 4]

- start from initial approximation for the target state in a reference space $\mathscr{M}_{\text{ref}} \subset \mathscr{M}_{\text{full}}$

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

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

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

- construct IT model space $\mathscr{M}_{\text{IT}}$ from all basis states with $|\kappa_\nu| \geq \kappa_{\min}$
- solve the eigenvalue problem in $\mathscr{M}_{\text{IT}}$
  → 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 $\mathscr{M}_{\text{ref}}$
- vary $\kappa_{\min}$ and extrapolate to account for effects of basis states excluded from $\mathscr{M}_{\text{IT}}$

Extrapolation Schemes in the IT-SM

Threshold Extrapolation

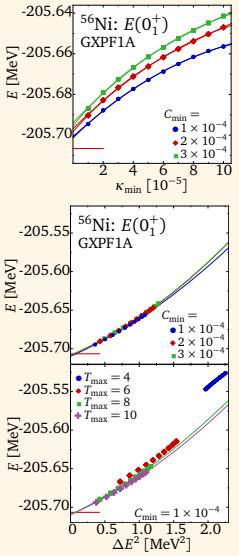
- fit polynomials to a sequence of IT-SM energies or observables and extrapolate to $\kappa_{\min} \to 0$
- no additional computational cost
- no physical motivation for fit function
  → potentially large uncertainties
- applicable to all observables on equal footing

Energy-Variance Extrapolation

- improved technique for energies
- compute energy variance

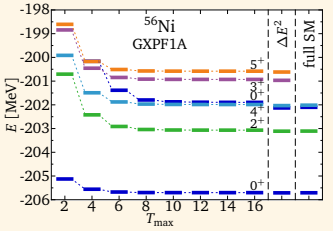
$$\Delta E^2 = \langle \Psi|\mathbf{H}^2|\Psi\rangle - \langle \Psi|\mathbf{H}|\Psi\rangle^2$$

  for the sequence of IT-SM eigenstates and extrapolate to $\Delta E^2 \to 0$ [5]
- corrects for effects of the different truncations applied ($T_{\max}, \kappa_{\min}, C_{\min}$):
  - $\kappa_{\min}$ sequences for different $C_{\min}$ fall on line
  - $\kappa_{\min}$ sequences for different $T_{\max} > 6$ fall on line
- physically motivated and controlled
- computationally demanding



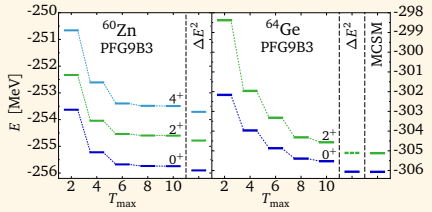
Benchmark of the IT-SM: ^{56}Ni

- threshold-extrapolated spectrum in good agreement with full SM [6]
- converged energies for $T_{\max} > 8$
- description of strongly deformed 0_2^+ state poses challenge
- energy-variance extrapolation for $T_{\max} = 8$ yields excellent agreement with full SM and correct state ordering



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

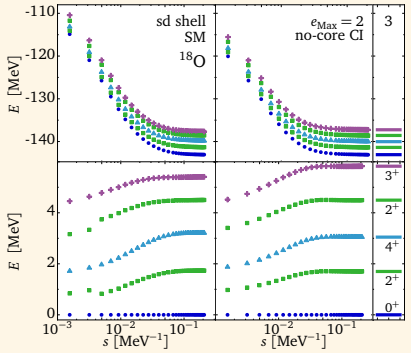
- ^{60}Zn and ^{64}Ge feasible in pfg$_{9/2}$ shell only in IT-SM
- fast convergence for ^{60}Zn
- slow convergence for ^{64}Ge due to strong deformation
- variance-extrapolated energies in excellent agreement with MCSM [7, 8]



Benchmark SM with IM-SRG Interactions for ^{18}O

Effective Interactions from IM-SRG

- extension of IM-SRG to nonperturbative derivation of effective SM Hamiltonians and operators [2, 3]
- IM-SRG flow equation
  - decouples inert core from all possible excitations
  - decouples states with A_ν particles from states containing non-valence states
- use chiral NN (N^{3}LO) [9] and 3N (N^{2}LO) [10, 11] SRG-evolved potentials ($\alpha = 0.08\text{fm}^4$) for IM-SRG evolution with imaginary-time generator [12]

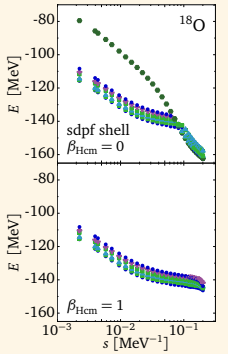


sd shell

- no-core CI results benchmark valence-space decoupling from core ($e_{\text{Max}} = 2$) and excluded space ($e_{\text{Max}} = 3$) through IM-SRG
- very similar convergence behavior of energies for SM and no-core CI
- excellent agreement of SM and no-core CI results confirms decoupling

sdpf shell

- obvious problem in IM-SRG flow for multi-shell valence spaces
- removal of intruding spurious states not sufficient to remedy IM-SRG interactions for sdpf shell



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