Importance-Truncated Shell Model
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New effective interactions and operators derived in ab initio framework

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$T_{\text{max}}$-truncated Slater determinants $|\Phi_\nu\rangle$
built of valence-space single-particle states
Valence-Space Shell Model – Overview

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- **diagonalization of Hamilton matrix:**
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  In many cases:
  $|c_\nu| \approx 0$
Important Truncation – General Concept

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

\[ |\psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C^{(\text{ref})}_\nu |\Phi_\nu\rangle \]

- 1$^{\text{st}}$-order correction to $|\psi_{\text{ref}}\rangle$ in MCPT defines **importance measure** $\kappa_\nu$ for basis states $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$

\[ |\psi^{(1)}\rangle = - \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle \Phi_\nu | H | \psi_{\text{ref}}\rangle}{\varepsilon_\nu - \varepsilon_{\text{ref}}} |\Phi_\nu\rangle \Rightarrow \kappa_\nu = - \frac{\langle \Phi_\nu | H | \psi_{\text{ref}}\rangle}{\varepsilon_\nu - \varepsilon_{\text{ref}}} \]

- construct **IT model space** $\mathcal{M}_{\text{IT}}$: include all basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$

- solve **eigenvalue problem** in IT model space $\rightarrow$ improved approximation for target state
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  \]

- construct **IT model space $\mathcal{M}_{\text{IT}}$**:
  include all basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$

- **solve eigenvalue problem** in IT model space
  → improved approximation for target state
Importance-Truncated Shell Model

- Use importance threshold $\kappa_{\text{min}}$ as adaptive truncation criterion.
- Construct IT model space containing only most relevant basis states.
- Solve eigenvalue problem in IT model space and obtain approximation for target state.
- Dramatic reduction of model-space dimension.
- Extrapolation $\kappa_{\text{min}} \rightarrow 0$ accounts for excluded configurations.
Energy-Variance Extrapolation

- **energy variance**
  \[ \Delta E^2 = \langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2 \]
  is **measure for quality** of approximate eigenstate \(|\psi\rangle\)

- \(\Delta E^2\) vanishes in limit of exact eigenstate

- **physically motivated** and **controlled** extrapolation

- \(\Delta E^2\) extrapolation **improves** results for energies

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![Graph showing energy vs. variance extrapolation](attachment:graph.png)

56Ni
GXPF1A

\[ C_{\text{min}} = \begin{cases} 1 \times 10^{-4} \\ 2 \times 10^{-4} \\ 3 \times 10^{-4} \end{cases} \]

CS et al., PRC 93, 021301(R) (2016)
shell-model calculations for $^{60}$Zn and $^{64}$Ge not feasible in pfg$_{9/2}$-shell

slow convergence for $^{64}$Ge due to strong deformation

variance extrapolation corrects for different truncations and yields excellent agreement with MCSM
Effective Interactions from Chiral Potentials

- several ab initio approaches allow for calculation of nonperturbative effective shell-model Hamiltonians and operators from chiral potentials: NCSM, CC-EI, IM-SRG, ...

- test new effective interactions derived in IM-SRG using IT-SM and IT-NCCI in single- and multi-shell valence spaces
  
  K. Tsukiyama et al., PRC 85, 061304 (2012)
  S. Bogner et al., PRL 113, 142501 (2014)

- IM-SRG flow equation
  
  - decouples inert core from all possible excitations
  - decouples states with $A_v$ valence nucleons from excluded space
IM-SRG Interactions for sd Shell

- good agreement of SM and IT-NCCI results
- successful decoupling of valence space from core and excluded space
- quality of results comparable to phenomenological interactions
problems with multi-shell spaces: spurious intruders destroy spectrum
**IM-SRG Interactions for sdpf Shell**

- **problems** with multi-shell spaces: **spurious intruders** destroy spectrum
  - removal of intruding spurious states does not lead to stable results
Summary

- IT-SM extends valence-space shell model to larger valence spaces in excellent agreement with exact results
- Progress in derivation of nonperturbative effective interactions and operators from chiral potentials in ab initio approaches
- Derivation of nonperturbative effective interactions for multi-shell valence spaces in IM-SRG challenging

Outlook

- Systematic study of single- and multi-shell effective interactions and operators from IM-SRG and CC-EI
- IT-SM for island of inversion using new effective interactions
Thanks to my group


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Thank you for your attention!