Importance-Truncated Shell Model for Multi-Shell Valence Spaces

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IT-SM: solution of eigenvalue problem in reduced model space spanned by important basis states

Importance-Truncated Shell Model

- introduce adaptive truncation criterion:
  importance threshold κ_{min}
- construct **IT model space** containing only most relevant basis states
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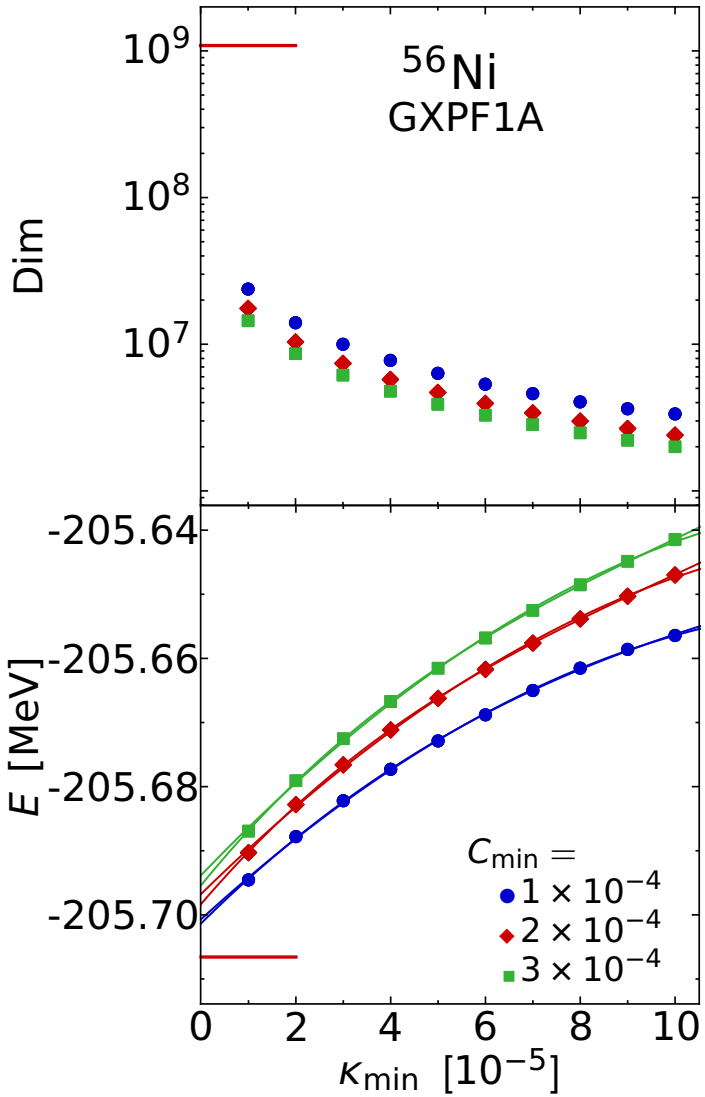
- **dramatic reduction** of model-space dimension
- **extrapolation $\kappa_{\min} \to 0$** accounts for excluded configurations

CS *et al.*, PRC 93, 021301(R) (2016)



Energy-Variance Extrapolation

- **energy variance**

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

  is **measure for quality** of approximate eigenstate $|\psi\rangle$

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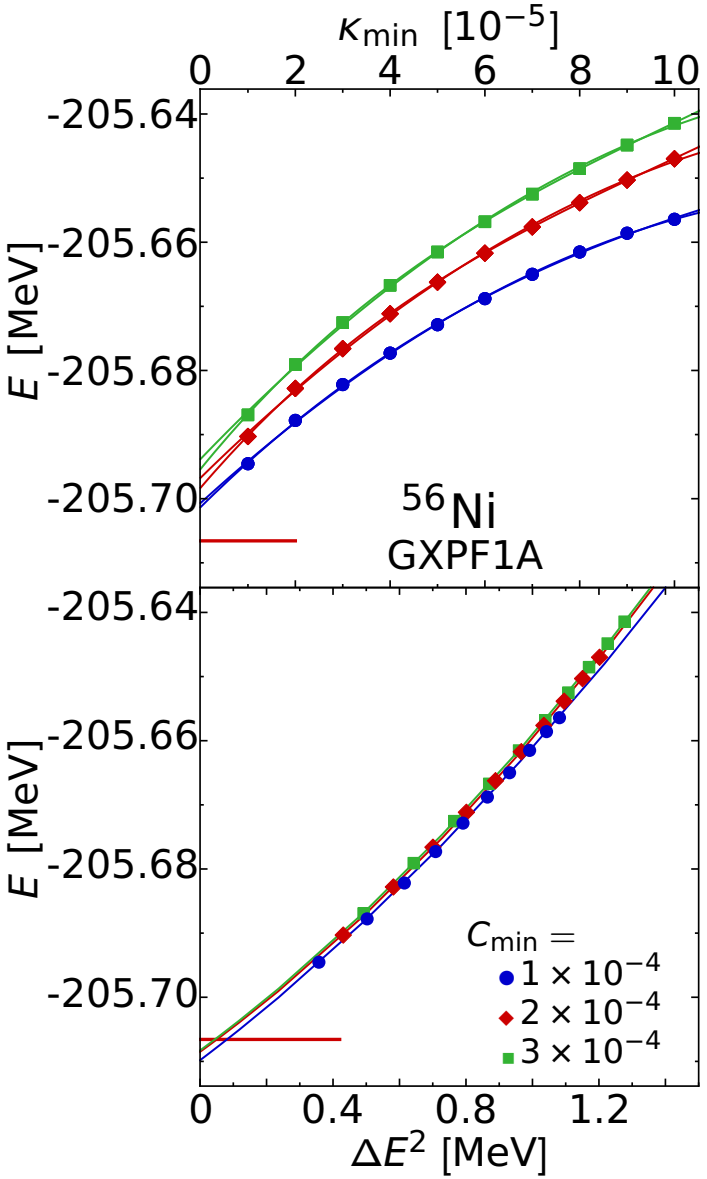
- ΔE^2 extrapolation **improves results** for energies



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

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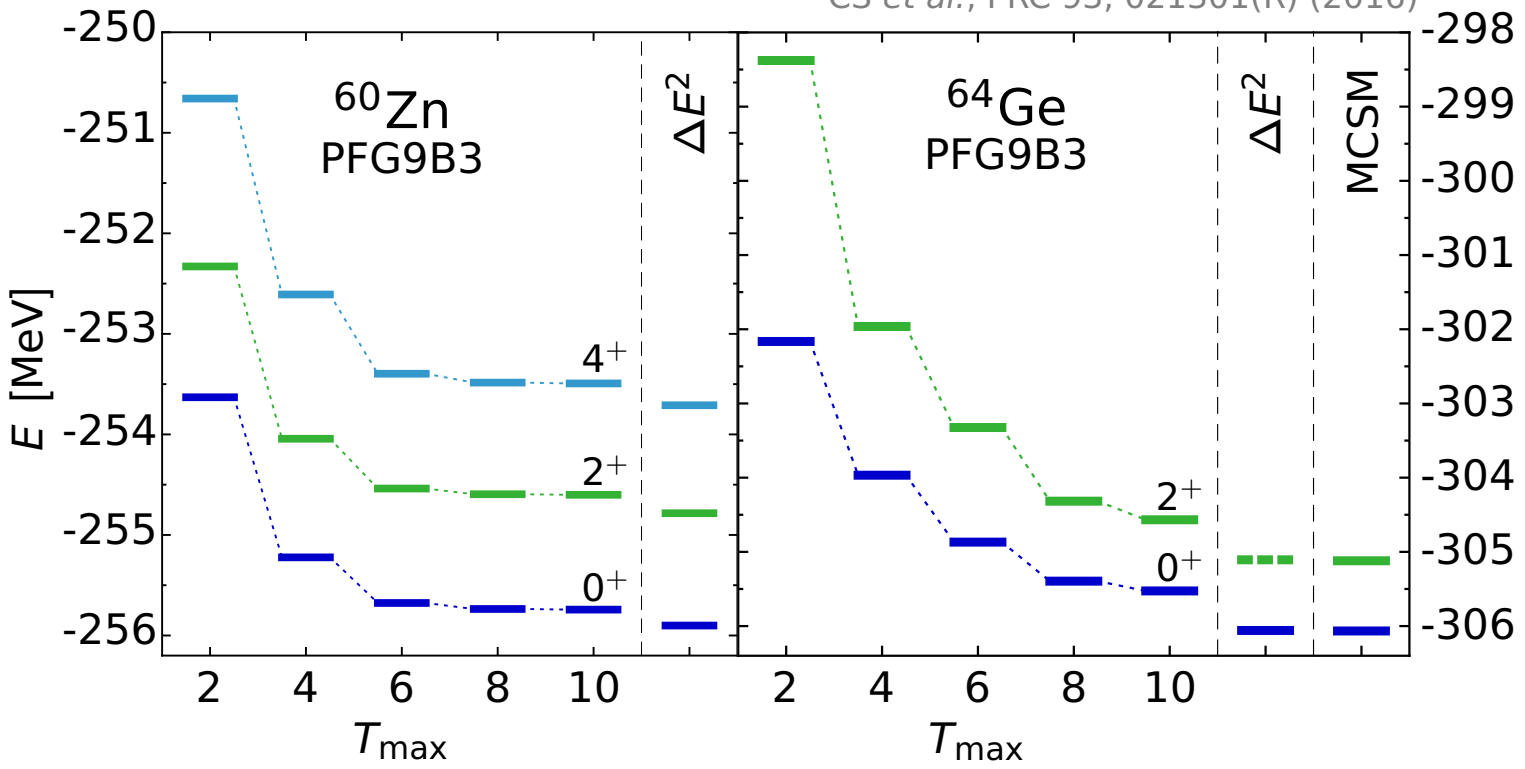


- shell-model calculations for ^{60}Zn and ^{64}Ge not feasible in pfg$_{9/2}$-shell
- slow convergence for ^{64}Ge due to **strong deformation**
- variance extrapolation **corrects for different truncations** and yields **excellent agreeement** with MCSM

Effective Interactions from Chiral Potentials

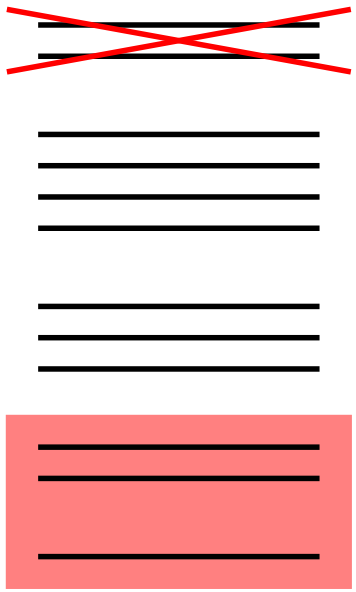
- several ab initio approaches allow for calculation of nonperturbative effective shell-model Hamiltonians and operators from chiral potentials: NCSM, CC-EI, IM-SRG, ...

- test new effective interactions derived in IM-SRG using IT-SM and IT-NCCI in single- and multi-shell valence spaces

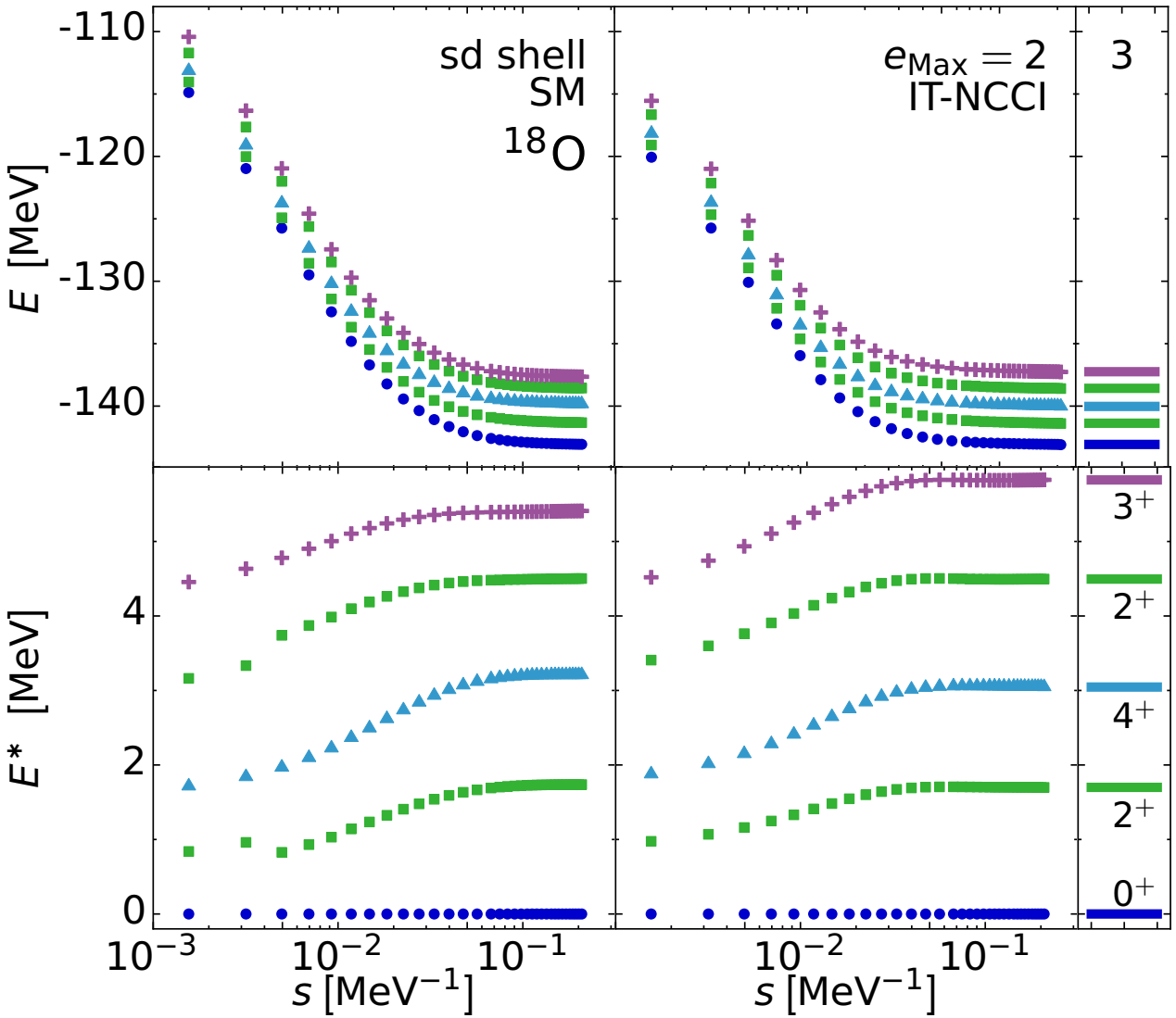
  K. Tsukiyama *et al.*, PRC 85, 061304 (2012)

  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

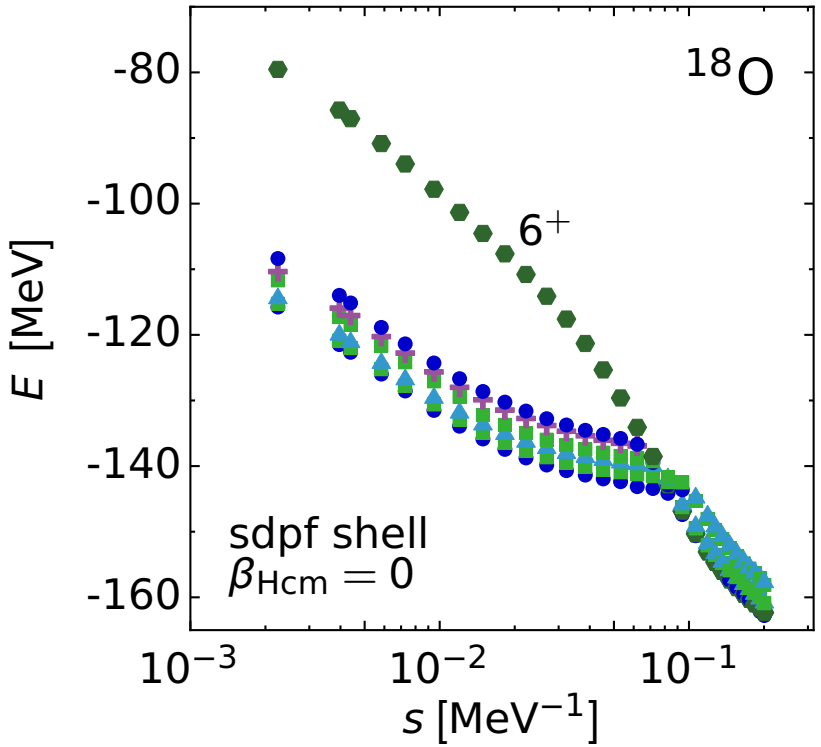


IM-SRG Interactions for sd Shell



- **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

IM-SRG Interactions for sdpf Shell



- **problems** with multi-shell spaces: **spurious intruders** destroy spectrum

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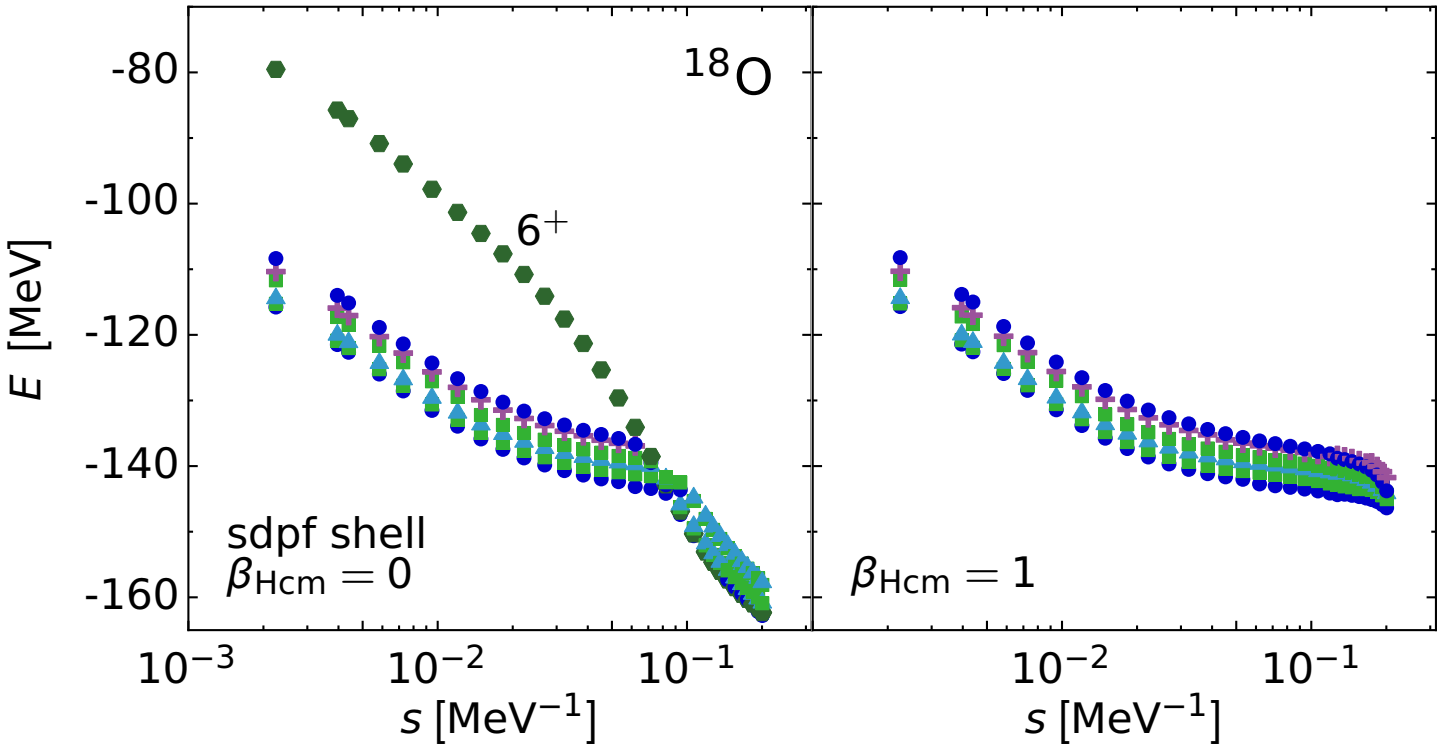


- **problems** with multi-shell spaces: **spurious intruders** destroy spectrum
- removal of intruding spurious states does not lead to stable results

Summary and Outlook

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

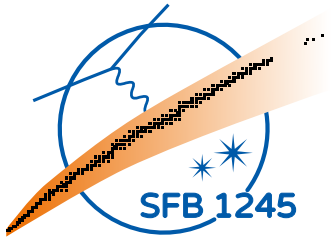
- systematic study of single- and multi-shell effective interactions and operators from IM-SRG and CC-EI
- IT-SM for island of inversion using new effective interactions

Epilog

- **Thanks to my group**
  - S. Alexa, S. Dentinger, E. Gebrerufael, T. Hüther, L. Kreher, L. Mertes, **R. Roth**, S. Schulz, H. Spiess, A. Tichai, R. Trippel, **K. Vobig**, R. Wirth

    Institut für Kernphysik, TU Darmstadt

- **Thank you for your attention!**



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DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

COMPUTING TIME

JURECA
JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC
Center for Scientific Computing Frankfurt

LICHTENBERG
HRZ Hochschulrechenzentrum

Some more details...

Backup

Importance Truncation – General Concept

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

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

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

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

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  include all basis states with $|\kappa_\nu| \geq \kappa_{\min}$

- **solve eigenvalue problem** in IT model space
  → improved approximation for target state

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- construct $\mathcal{M}$ in an iterative scheme to include all

embed into iterative scheme to access higher T_{max}

- **solve eigenvalue** in model space
  → improved approximation for target state