

Importance-Truncated Shell Model

Christina Stumpf

Institut für Kernphysik



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Motivation: Extensions of Traditional Shell Modell

- successful method for the description of spectroscopic observables using phenomenological effective interactions

Motivation: Extensions of Traditional Shell Modell


- successful method for the description of spectroscopic observables using phenomenological effective interactions
- solution of eigenvalue problem in valence space

$$\mathbf{H}_{\text{eff}}|\psi_{\text{val}}\rangle = E|\psi_{\text{val}}\rangle$$

Motivation: Extensions of Traditional Shell Modell

- successful method for the description of spectroscopic observables using phenomenological effective interactions
- solution of eigenvalue problem in valence space

no direct connection to the underlying NN interaction

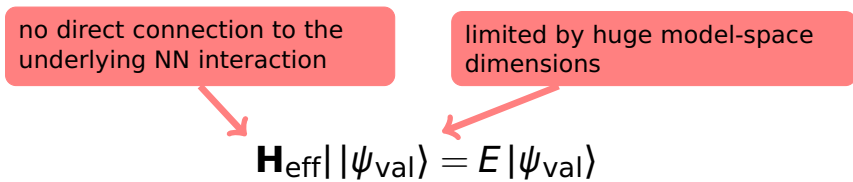

$$\mathbf{H}_{\text{eff}} |\psi_{\text{val}}\rangle = E |\psi_{\text{val}}\rangle$$

Motivation: Extensions of Traditional Shell Modell

- successful method for the description of spectroscopic observables using phenomenological effective interactions
- solution of eigenvalue problem in valence space

no direct connection to the underlying NN interaction

limited by huge model-space dimensions



The diagram consists of two red rounded rectangular boxes at the top. The left box contains the text 'no direct connection to the underlying NN interaction' and has a red arrow pointing down and to the right towards the equation. The right box contains the text 'limited by huge model-space dimensions' and has a red arrow pointing down and to the left towards the equation. The equation $\mathbf{H}_{\text{eff}}|\psi_{\text{val}}\rangle = E|\psi_{\text{val}}\rangle$ is centered below the two boxes.

$$\mathbf{H}_{\text{eff}}|\psi_{\text{val}}\rangle = E|\psi_{\text{val}}\rangle$$

Motivation: Extensions of Traditional Shell Modell

- successful method for the description of spectroscopic observables using phenomenological effective interactions
- solution of eigenvalue problem in valence space

no direct connection to the underlying NN interaction

limited by huge model-space dimensions

$$\mathbf{H}_{\text{eff}} |\psi_{\text{val}}\rangle = E |\psi_{\text{val}}\rangle$$

IT-SM: extension of shell model to larger valence spaces

Motivation: Extensions of Traditional Shell Modell

- successful method for the description of spectroscopic observables using phenomenological effective interactions
- solution of eigenvalue problem in valence space

no direct connection to the underlying NN interaction

limited by huge model-space dimensions

$$\mathbf{H}_{\text{eff}} |\psi_{\text{val}}\rangle = E |\psi_{\text{val}}\rangle$$

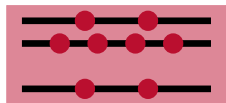
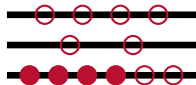
new effective interactions and operators derived in ab initio framework

IT-SM: extension of shell model to larger valence spaces

Valence-Space Shell Model – Overview

- **model space:**

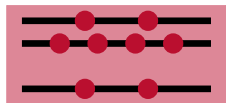
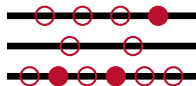
T_{\max} -truncated Slater determinants $|\Phi_{\nu}\rangle$
built of valence-space single-particle states



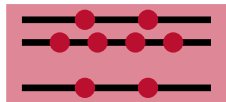
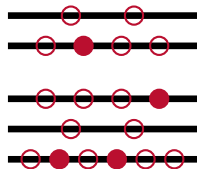
Valence-Space Shell Model – Overview

- **model space:**

T_{\max} -truncated Slater determinants $|\Phi_{\nu}\rangle$
built of valence-space single-particle states



Valence-Space Shell Model – Overview



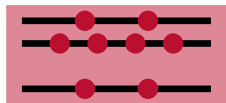
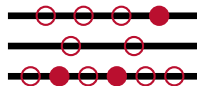
- **model space:**

T_{\max} -truncated Slater determinants $|\Phi_{\nu}\rangle$
built of valence-space single-particle states

- **effective interaction:**

interaction between valence nucleons
accounting for core and excluded space

Valence-Space Shell Model – Overview



- **model space:**

T_{\max} -truncated Slater determinants $|\Phi_\nu\rangle$
built of valence-space single-particle states

- **effective interaction:**

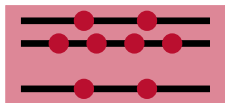
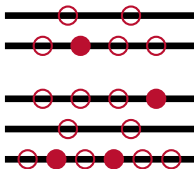
interaction between valence nucleons
accounting for core and excluded space

- **diagonalization of Hamilton matrix:**

obtain energies and eigenstates

$$|\Psi_{\text{val}}\rangle = \sum_{\nu} c_{\nu} |\Phi_{\nu}\rangle$$

Valence-Space Shell Model – Overview



- **model space:**

T_{\max} -truncated Slater determinants $|\Phi_\nu\rangle$
built of valence-space single-particle states

- **effective interaction:**

interaction between valence nucleons
accounting for core and excluded space

- **diagonalization of Hamilton matrix:**

obtain energies and eigenstates

$$|\Psi_{\text{val}}\rangle = \sum_{\nu} c_{\nu} |\Phi_{\nu}\rangle$$

in many cases:
 $|c_{\nu}| \approx 0$

Importance Truncation – General Concept

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

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

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

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

- construct **IT model space \mathcal{M}_{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 Truncation – General Concept

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

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

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

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

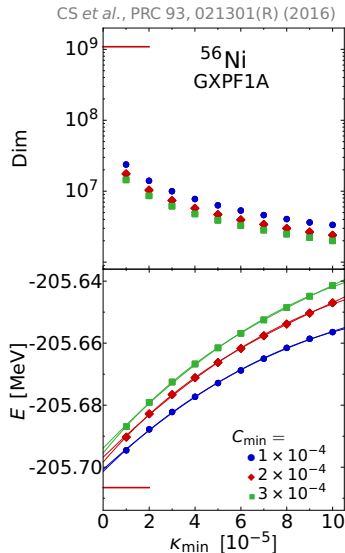
- construct **IT model space \mathcal{M}_{IT}** :
include all basis states with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$

embed into iterative scheme to access high Tmax

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

Importance-Truncated Shell Model

- use **importance threshold κ_{\min}** as adaptive truncation criterion
- carry out **sequence of IT-SM calculations**
- **extrapolation $\kappa_{\min} \rightarrow 0$** accounts for excluded configurations
- **dramatic reduction** of model-space dimension



Energy-Variance Extrapolation

- **energy variance**

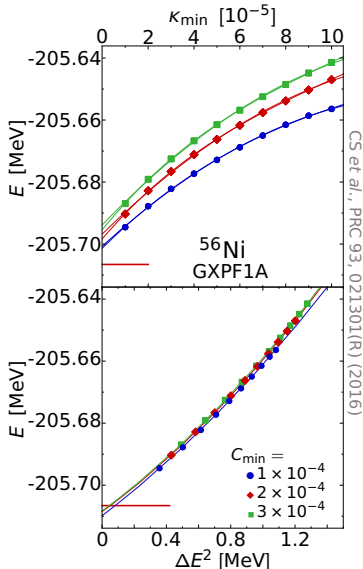
$$\Delta E^2 = \langle \psi | \mathbf{H}^2 | \psi \rangle - \langle \psi | \mathbf{H} | \psi \rangle^2$$

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

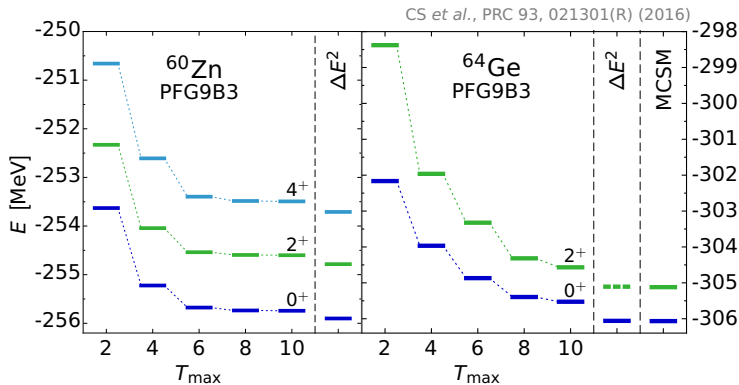
- ΔE^2 vanishes in limit of exact eigenstate

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

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



Highlights: pfg_{9/2}-shell nuclei ⁶⁰Zn and ⁶⁴Ge



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

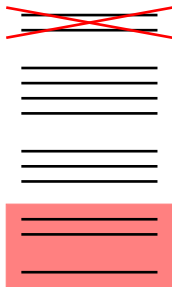
Effective Interactions from Chiral Potentials

- 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

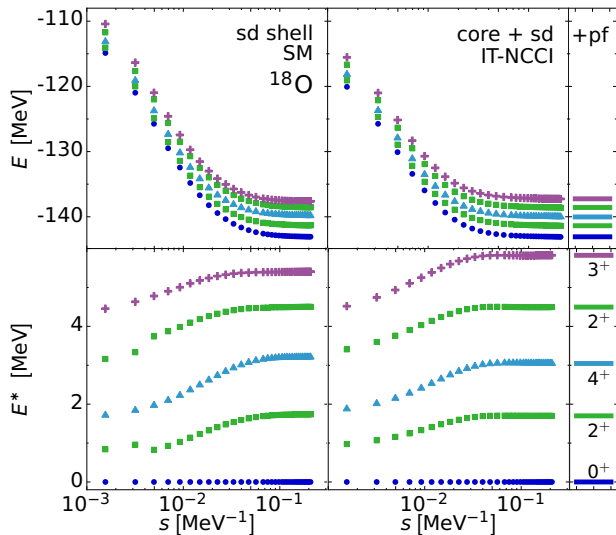
K. Tsukiyama *et al.*, PRC 85, 061304 (2012)

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

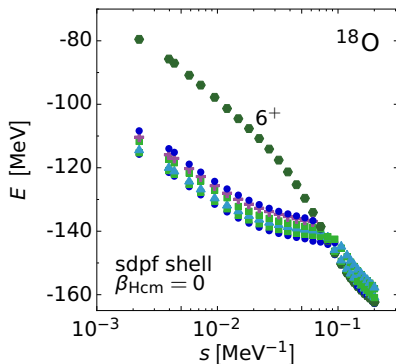


IM-SRG Interactions for sd Shell



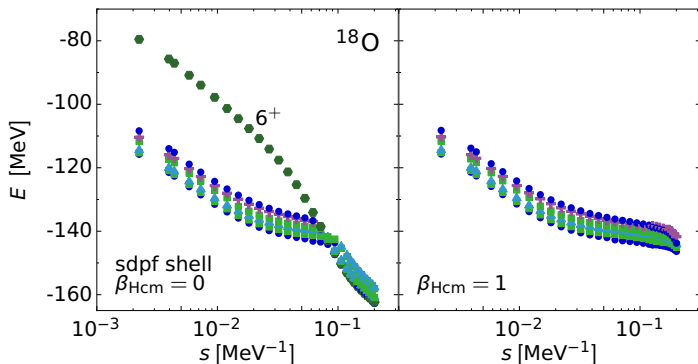
- **good agreement** of SM and IT-NCCI results
- **successful decoupling** of valence space from core and excluded space
- **quality of results** comparable to phenomenological interactions

IM-SRG Interactions for sdpf Shell



- **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 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

■ Thanks to my group

- S. Alexa, S. Dentinger, E. Gebrerufael, T. Hüther, L. Kreher, L. Mertes, **R. Roth**, S. Schulz, H. Spielvogel, H. Spiess, A. Tichai, R. Trippel, **K. Vobig**, R. Wirth, T. Wolfgruber
Institut für Kernphysik, TU Darmstadt

■ Thank you for your attention!



Deutsche
Forschungsgemeinschaft

DFG



COMPUTING TIME



Bundesministerium
für Bildung
und Forschung