Importance-Truncated No-Core Shell Model for Ab-Initio Nuclear Structure
From QCD to Nuclear Structure

Nuclear Structure

Realistic Nuclear Interactions

Low-Energy QCD

- chiral EFT interactions: consistent NN & 3N interaction derived within $\chi$EFT
- traditional NN-interactions: Argonne V18, CD Bonn,...
- reproduce experimental two-body data with high precision
- induce strong short-range central & tensor correlations
Nuclear Structure

- adapt realistic potential to the available model space
  - tame short-range correlations
  - improve convergence behavior
- conserve experimentally constrained properties (phase shifts & deuteron)
  - generate new realistic int.
- need consistent effective interaction & effective operators
- unitary transformations most convenient

Modern Effective Interactions

Realistic Nuclear Interactions

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Modern Effective Interactions

Realistic Nuclear Interactions

Low-Energy QCD

UCOM

SRG
Nuclear Structure

- Exact / Approx. Many-Body Tools
  - 'exact' solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
  - controlled approximations for heavier nuclei (HF & MBPT,...)
  - rely on restricted model spaces of tractable size
  - not suitable for the description of short-range correlations

Modern Effective Interactions

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this talk: NCSM

more on other methods in HK 83.2
special case of a **full configuration interaction (CI)** scheme

**many-body basis**: Slater determinants $|\Phi_\nu\rangle$ composed of harmonic oscillator single-particle states

$$|\psi\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$$

**model space**: spanned by basis states $|\Phi_\nu\rangle$ with unperturbed excitation energies of up to $N_{\text{max}} \hbar \omega$

- important difference to conventional CI, where model space is defined by a truncation of the single-particle basis

numerical solution of **eigenvalue problem** for the Hamiltonian $H_{\text{int}}$ within truncated model space via Lanczos methods

model spaces of **up to $10^9$ basis states** are used routinely
No-Core Shell Model: Applications

- typical domain of the NCSM are nuclei with $A \lesssim 13$
- Lee-Suzuki transformation used to enhance convergence
the **model-space dimension** is the single limiting factor for the NCSM

full $6\hbar\omega$ calculation for $^{40}\text{Ca}$ presently not feasible (basis dimension $\sim 10^{10}$)
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**Importance Truncation**

reduce NCSM space to the relevant basis states using an **a priori importance measure** derived from MBPT
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**Importance-Truncated NCSM**
Importance Truncation: General Idea

- given an initial approximation $|\Psi_{\text{ref}}\rangle$ for the target state

- **measure the importance** of individual basis state $|\Phi_\nu\rangle$ via first-order multiconfigurational perturbation theory

$$
\kappa_\nu = - \frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}
$$

- construct **importance-truncated space** spanned by basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$ and solve eigenvalue problem

- **iterative scheme**: repeat construction of importance-truncated model space using eigenstate as improved reference $|\Psi_{\text{ref}}\rangle$

- **threshold extrapolations** and **perturbative corrections** can be used to account for discarded basis states
$^4$He: Importance-Truncated NCSM

- **sequential IT-NCSM(seq):** single importance update using $(N_{\text{max}} - 2) \hbar \omega$ eigenstate as reference
- **reproduces exact NCSM result** for all $N_{\text{max}}$
- **reduction of basis by more than two orders of magnitude w/o loss of precision**

- $V_{\text{UCOM}} \hbar \omega = 40 \text{ MeV}$
- $D_{\text{max}}$ vs $N_{\text{max}}$
- $E$ vs $N_{\text{max}}$

+ full NCSM
+ IT-NCSM(seq)
$^4\text{He}$: Importance-Truncated NCSM

- reproduces exact NCSM result for all $\hbar \omega$ and $N_{\text{max}}$
- importance truncation & threshold extrapolation is robust
- no problem with center of mass

$E$ [MeV] vs. $\hbar \Omega$ [MeV]

- IT-NCSM(seq)
- full NCSM
$^{16}\text{O}$: Importance-Truncated NCSM

- IT-NCSM(seq) provides excellent agreement with full NCSM calculation
- dimension reduced by several orders of magnitude
- possibility to go way beyond the domain of the full NCSM

$V_{\text{UCOM}}\bar{\hbar}\omega = 22$ MeV

$D_{\text{max}}$ vs $N_{\text{max}}$

- full NCSM
- IT-NCSM(seq), $C_{\text{min}} = 0.0005$
- IT-NCSM(seq), $C_{\text{min}} = 0.0003$
$^{16}$O: Importance-Truncated NCSM

$V_{UCOM}$

$\hbar \omega = 22 \text{ MeV}$

- Extrapolation to $N_{\text{max}} \to \infty$
  \[ E_{\text{IT-NCSM(seq)}} = -133(3) \text{ MeV} \]
  \[ E_{\text{exp}} = -127.6 \text{ MeV} \]

- $V_{UCOM}$ predicts \textbf{reasonable binding energies} also for heavier nuclei

- Slow non-exponential convergence makes precise extrapolation difficult

\begin{itemize}
  \item Full NCSM
  \item IT-NCSM(seq), $C_{\text{min}} = 0.0005$
  \item IT-NCSM(seq), $C_{\text{min}} = 0.0003$
\end{itemize}
\[12^C: \text{IT-NCSM for Open-Shell Nuclei}\]

- Excellent agreement with full NCSM calculations
- IT-NCSM(seq) works just as well for non-magic / open-shell nuclei
- All calculations limited the available two-body matrix elements of $V_{UCOM}$ only

\[
V_{UCOM} \quad \hbar \omega = 24 \text{ MeV}
\]

\[
\begin{align*}
\text{full NCSM} & \quad C_{\text{min}} = 0.0005 \\
\text{IT-NCSM(seq), } C_{\text{min}} = 0.0003
\end{align*}
\]
Summary

- Importance-truncation scheme extends the domain of ab-initio NCSM calculations to **much larger** $N_{\text{max}}$ and $A$
  - $22\hbar\omega$ calculations for $^{12}\text{C}$ and $^{16}\text{O}$ done routinely

- IT-NCSM has **all the advantages of the full NCSM**
  - Variational principle
  - No spurious center-of-mass contamination
  - Applicable for closed and open-shell nuclei
  - Ground and excited states are treated on the same footing
  - Wave-functions for free
  - Expectation values, transition matrix elements, densities and form-factors can be computed with standard shell-model technology

- Implementation is different from standard NCSM & calculations are computationally demanding
Outlook

- further development of the **IT-NCSM technology**
- IT-NCSM as tool for **testing new interactions**
- **full spectroscopy** for low-lying states in nuclei with $A \lesssim 40$ in large $N_{\text{max}} \hbar \omega$ spaces
- **nucleon-nucleus reactions** within the RGM approach using IT-NCSM wave functions (with P. Navrátil)
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