Overview

- Reminder: Modern Effective Interactions
- No-Core Shell Model
- Importance Truncated NCSM
- Conclusions & Perspectives
Modern Nuclear Structure Theory

Nuclear Structure

- Many-Body Approximations
- Modern Eff. Interactions
- Density Functional Models
- Realistic Potentials
- Chiral EFT Interactions

ab initio Approaches

Low-Energy QCD
Correlation Operator

define an unitary operator $C$ to describe the effect of short-range correlations

$$C = \exp[-i G] = \exp[-i \sum_{i<j} g_{ij}]$$

Correlated States

imprint short-range correlations onto uncorrelated many-body states

$$|\tilde{\psi}\rangle = C |\psi\rangle$$

Correlated Operators

adapt Hamiltonian and all other observables to uncorrelated many-body space

$$\tilde{O} = C^\dagger O C$$

$$\langle \tilde{\psi} | O | \tilde{\psi}' \rangle = \langle \psi | C^\dagger O C | \psi' \rangle = \langle \psi | \tilde{O} | \psi' \rangle$$
Correlated States: The Deuteron

- Central correlations
- Tensor correlations

Only short-range tensor correlations treated by $C_\Omega$
No-Core Shell Model

Roth & Navrátíl — in preparation
$^4\text{He}: \text{Convergence}$

**$V_{AV18}$**

**$V_{UCOM}$**

$N_{\text{max}}$

- 0
- 2
- 4

$E_{\text{AV18}}$

- 0
- 20
- 40

$E_{\text{UCOM}}$

- 0
- 20
- 40

$E [\text{MeV}]$

- $\hbar \omega [\text{MeV}]$

**residual state-dependent long-range correlations**

$^4$He: Convergence

\begin{align*}
V_{\text{AV18}} \\
V_{\text{UCOM}}
\end{align*}

- omitted three- and four-body contributions
Three-Body Interactions — Tjon Line

- $E(\text{^3H})$ vs. $E(\text{^4He})$

Tjon-line: $E(\text{^4He})$ vs. $E(\text{^3H})$ for phase-shift equivalent NN-interactions
Three-Body Interactions — Tjon Line

**Tjon-line:** $E(\text{^4He})$ vs. $E(\text{^3H})$

for phase-shift equivalent NN-interactions

- change of $C_\Omega$-correlator range results in shift along Tjon-line

minimize net three-body force by choosing correlator with energies close to experimental value

this $V_{\text{UCOM}}$ is used in the following

CD Bonn

Exp.
$^6\text{Li}$: NCSM throughout the p-Shell

$^6\text{Li}$

$V_{\text{UCOM}}$

$\hbar \omega = 26\text{MeV}$

systematic NCSM studies throughout p-shell with $V_{\text{UCOM}}$ (+ Lee-Suzuki)
$^{10}\text{B}: \text{ Hallmark of a 3N Interaction?}$

$V_{\text{UCOM}}$ gives correct level ordering without any 3N interaction
Importance Truncated No-Core Shell Model

Roth & Navrátil — arXiv: 0705.4069
Importance Truncated NCSM

- Converged NCSM calculations essentially restricted to p-shell
- Full $6\hbar\omega$ calculation for $^{40}$Ca presently not feasible (basis dimension $\sim 10^{10}$)

**Importance Truncation**

Reduce NCSM space to relevant states using an a priori importance measure derived from MBPT

![Graph showing energy levels](image)
■ given an intrinsic Hamiltonian
\[ H_{\text{int}} = T - T_{\text{cm}} + V = H_0 + H' \]
and an unperturbed Hamiltonian \( H_0 \) with eigenstates \( |\Phi_\nu\rangle \)

■ consider lowest-order **perturbation theory** to construct a correction \( |\Psi^{(1)}\rangle \) to the unperturbed reference state \( |\Psi^{(0)}\rangle \)

\[
|\Psi^{(0)}\rangle = |\Psi_{\text{ref}}\rangle = |\Phi_0\rangle \quad |\Psi^{(1)}\rangle = \sum_{\nu \neq \text{ref}} \kappa_\nu |\Phi_\nu\rangle
\]

■ perturbative estimate of amplitudes serves as **measure for importance of individual basis states** \( |\Phi_\nu\rangle \)

\[
\kappa_\nu = -\frac{\langle \Phi_\nu | H' | \Psi_{\text{ref}} \rangle}{E^{(0)}_\nu - E^{(0)}_{\text{ref}}}
\]

■ restrict model space to **important configurations with** \( |\kappa_\nu| \geq \kappa_{\text{min}} \) and solve eigenvalue problem
Iterative Construction of Model Space

1. start with reference state $|\Psi_{\text{ref}}\rangle = |\Phi_0\rangle$ (simplest case)

2. create 1p1h and 2p2h excitations of $|\Psi_{\text{ref}}\rangle$ and keep important basis states $|\Phi_\nu\rangle$ with $|\kappa_\nu| \geq \kappa_{\text{min}}$

3. solve the eigenvalue problem of $H_{\text{int}}$ in this model space (up to 2p2h); ground state yields new reference state (dominant components)

4. create 1p1h and 2p2h excitations of new $|\Psi_{\text{ref}}\rangle$ and keep the important basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$

5. solve the eigenvalue problem of $H_{\text{int}}$ in resulting model space (up to 4p4h)

...and so on...
Importance Measure

- importance measure $\kappa_\nu$ provides **reliable a priori estimate** of the a posteriori amplitude $C_\nu$ obtained from diagonalization

\[ \hbar \omega = 20 \text{ MeV} \]
\[ N_{\text{max}} = 6 \]

$^{16}\text{O}$

$v_{\text{UCOM}}$
Benchmark: $^4$He

- reproduces exact NCSM result with an importance truncated basis that is 2 orders of magnitude smaller than the full $\mathcal{N}_{\text{max}} \hbar \omega$ space

$^4$He

$V_U \mathrm{COM}$

$\hbar \omega = 20 \text{ MeV}$

$\log_{10} D$ vs. $\mathcal{N}_{\text{max}}$

- full NCSM (Antoine)
  - IT-NCSM 2p2h
  - IT-NCSM 3p3h
  - IT-NCSM 4p4h
Benchmark: $^{16}\text{O}$

- Excellent agreement with full NCSM calculation although configurations beyond 4p4h are not included.
- Dimension reduced by several orders of magnitude; possibility to go way beyond the domain of the full NCSM.

$V_{	ext{UCOM}}\ h\omega = 20\ \text{MeV}$
Benchmark: $^{40}\text{Ca}$

$^{40}\text{Ca}$

$V_{\text{UCOM}}$

$\hbar \omega = 20 \text{ MeV}$

$^{40}\text{Ca}$

$V_{\text{UCOM}}$

$\hbar \omega = 17 \text{ MeV}$

- $16\hbar \omega$ calculations for $^{40}\text{Ca}$ are feasible
- extrapolation of ground state energy (3p3h, $\hbar \omega = 17 \text{ MeV}$) yields
  
  \begin{align*}
  E_\infty & \approx -316 \text{ MeV} \\
  E_{\text{exp}} & = -342.05 \text{ MeV}
  \end{align*}

- + full NCSM (Antoine)
- IT-NCSM 2p2h
- IT-NCSM 3p3h
- IT-NCSM 4p4h
Benchmark Results for $V_{\text{low-k}}$

$V_{\text{low-k}}$  
(AV18, $\Lambda = 2.1 \text{ fm}^{-1}$)

$^{16}\text{O}$  
(up to 4p4h)

$^{40}\text{Ca}$  
(up to 3p3h)

$E_\infty(\text{4p4h}) \approx -138 \text{ MeV}$

$R_{\text{rms}}(\text{4p4h}) = 2.03 \text{ fm}$

$E_\infty(\text{3p3h}) \approx -463 \text{ MeV}$

$R_{\text{rms}}(\text{3p3h}) = 2.27 \text{ fm}$

Conclusions

- Importance truncation provides a **conceptually simple and universal tool** for large-scale eigenvalue problems.

- **Fully variational**: can be viewed as a variational calculation with an adaptive trial state.

- Very efficient in **reducing the model space** (by several orders of magnitude) to relevant states without losing precision.

- **No center-of-mass contaminations** ($< 100 \text{ keV}$): Importance truncation preserves properties of full $N_{\text{max}} \hbar \omega$ space.

- Eigenstates in **shell-model representation** for free: Convenient starting point for calculation of densities, form factors, etc.

- **Computationally efficient** (need only a few processors).
Perspectives

- explicit inclusion of **configurations beyond 4p4h**
- **perturbative estimate** for contribution of configurations beyond 4p4h
- **alternative schemes** for construction of importance truncated space
- study of **excited states** with generalized reference states
- use of **Hartree-Fock single-particle states**
- use of **Lee-Suzuki transformed interactions**

**exciting new tool** for ab initio calculations beyond the p-shell
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