Ab Initio Shell Model with a Core: Extending the NCSM to Heavier Nuclei

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MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory
We cannot, in general, solve the full problem in the complete Hilbert space, so we must truncate to a finite model space.

\[ H \Psi = E \Psi \]

\[ \implies \] We must use effective interactions and operators!
Some current shell-model references


No Core Shell Model

“Ab Initio” approach to microscopic nuclear structure calculations, in which all $A$ nucleons are treated as being active.

Want to solve the $A$-body Schrödinger equation

$$H_A \Psi^A = E_A \Psi^A$$

P. Navratil, et al., nucl-th arXiv: 0904.0463
From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

Diagonalization of many-body Hamiltonian

Many-body experimental data
$^{4}\text{He}$

CD-Bonn
From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

Diagonalization of many-body Hamiltonian

Many-body experimental data

Core Shell Model

Phenomenological effective interactions

Diagonalization of the Hamiltonian for valence nucleons
Limits of nuclear existence

Towards a unified description of the nucleus

Ab initio few-body calculations
No-Core Shell Model

Density Functional Theory Selfconsistent Mean Field

r-process
From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

Diagonalization of many-body Hamiltonian

Many-body experimental data

Core Shell Model

effective interactions for valence nucleons

Diagonalization of the Hamiltonian for valence nucleons
No Core Shell Model

Starting Hamiltonian

\[ H = \sum_{i=1}^{A} \frac{\vec{p}_i^2}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) + \sum_{i<j<k}^{A} V_{NNN}(\vec{r}_{ijk}) \]

Realistic NN and NNN potentials

Coordinate space – Argonne V18, AV18', CD-Bonn, chiral N^3LO,
Momentum space – NNN Tucson - Melbourne,
NNN chiral N^2LO

Binding center-of-mass
HO potential (Lipkin 1958)

\[ \frac{1}{2} Am\Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^2 - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \]

Cluster Expansion:
Two-body cluster approximation

\[ H^\Omega_{2} = \sum_{i=1}^{2} \left[ \frac{\vec{p}_i^2}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^2 \right] + \sum_{i<j}^{2} \left[ V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \]
Effective Hamiltonian for NCSM

Solving

\[ H_{\Omega, a=2}^{\Psi_{a=2}} = E_{\Omega, a=2}^{\Psi_{a=2}} \]

in “infinite space” \(2n+1 = 450\) relative coordinates

\[ P + Q = 1; \quad P \rightarrow \text{model space}; \quad Q \rightarrow \text{excluded space}; \]

\[ E_{A,2}^{\Omega} = U_2 H_{A,2}^{\Omega} U_2^\dagger \]

\[ U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \]

\[ E_{A,2}^{\Omega} = \begin{pmatrix} E_{A,2,P}^{\Omega} & 0 \\ 0 & E_{A,2,Q}^{\Omega} \end{pmatrix} \]

\[ H_{A,2}^{N_{\max}, \Omega, \text{eff}} = \frac{U_2^\dagger E_{A,2,P}^{\Omega} U_{2,P}}{\sqrt{U_{2,P}^\dagger U_{2,P}}} \]

Two ways of convergence:

1) For \( P \rightarrow 1 \) and fixed \( a \):
   \[ \sim_{A,a=2}^{\text{eff}} \rightarrow H_A \]

2) For \( a \rightarrow A \) and fixed \( P \):
   \[ \sim_{A,a}^{\text{eff}} \rightarrow H_A \]
NCSM results for $^6$Li with CD-Bonn NN potential

Dimensions
- p-space: 10;
- $N_{\text{max}} = 12$: 48 887 665;
- $N_{\text{max}} = 14$: 211 286 096

$^6$Li CD-Bonn, $\hbar\Omega = 20$ MeV
Effective Hamiltonian for SSM

Two ways of convergence:

1) For \( P \to 1 \) and fixed \( a \): \( H_{A,a=2}^{\text{eff}} \to H_A \): previous slide

2) For \( a_1 \to A \) and fixed \( P_1 \): \( H_{A,a_1}^{\text{eff}} \to H_A \)

\( P_1 + Q_1 = P; \quad P_1 \) - small model space; \( Q_1 \) - excluded space;

\[
\mathcal{H}_{A,a_1}^{N_{1,\text{max}}, N_{\text{max}}} = \frac{U_{a_1,P_1}^A, \dagger}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}} \frac{E_{A,a_1,P_1}^{N_{\text{max}}, \Omega}}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}} \frac{U_{a_1,P_1}^A}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}}
\]

Valence Cluster Expansion

\( N_{1,\text{max}} = 0 \) space (p-space); \( a_1 = A_c + a_v; \quad a_1 \) - order of cluster;
\( A_c \) - number of nucleons in core; \( a_v \) - order of valence cluster;

\[
\mathcal{H}_{A,a_1}^{0,N_{\text{max}}} = \sum_{k}^{a_v} V_{k,A,A_c+k}
\]
Two-body VCE for $^6\text{Li}$

$$\mathcal{H}^0,N_{\text{max}}_{A=6,a_1=6} = V^{6,4}_0 + V^{6,5}_1 + V^{6,6}_2$$

Need NCSM results in $N_{\text{max}}$ space for

$^4\text{He}$  $^5\text{He}$  $^5\text{Li}$  $^6\text{He}$  $^6\text{Li}$  $^6\text{Be}$

With effective interaction for $A=6$ !!!

Core Energy

$$V^{6,4}_0 = -51.644 \text{ MeV}$$

Single Particle Energies

$$\varepsilon_{p_{3/2}} = 14.574 \text{ MeV} \quad \varepsilon_{p_{1/2}} = 18.516 \text{ MeV}$$

$$V^{6,6}_2 = \mathcal{H}^0,N_{\text{max}}_{6,6} - \mathcal{H}^0,N_{\text{max}}_{6,5}$$

$$\langle p_{3/2}p_{3/2}|V^{6,6}_2|p_{3/2}p_{3/2}\rangle_{J=3,T=0} = -1.825 \text{ MeV}$$

$$\langle p_{3/2}p_{3/2}|V^{6,6}_2|p_{3/2}p_{3/2}\rangle_{J=2,T=1} = 2.762 \text{ MeV}$$
2-body Valence Cluster approximation for $A>6$

$$\mathcal{H}_A^{0,N_{\text{max}}},a_1=6 = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

**Graphs:**
- **Graph 1:**
  - Title: $^6\text{Li}$ CD-Bonn, $\hbar\Omega=20$ MeV
  - Data points and lines representing diagonal $V_{2\nu}$ (MeV) vs. $N_{\text{max}}$.
- **Graph 2:**
  - Title: $^6\text{Li}$ CD-Bonn, $\hbar\Omega=20$ MeV
  - Data points and lines representing $E_{\text{core}} + V_{1\nu}$ (MeV) vs. $N_{\text{max}}$.
  - Key states: $p_{1/2}p_{1/2}$, $p_{1/2}p_{3/2}$, $p_{3/2}p_{3/2}$.
2-body Valence Cluster approximation for \( A = 6 \)

\[
\mathcal{H}_{A}^{0, N_{\text{max}}, a_1 = 6} = V_{6,4}^{0} + V_{6,5}^{1} + V_{6,6}^{2}
\]

Need NCSM results in \( N_{\text{max}} \) space for \( ^{4}\text{He} \), \( ^{5}\text{He} \), \( ^{5}\text{Li} \), \( ^{6}\text{He} \), \( ^{6}\text{Li} \), \( ^{6}\text{Be} \).

\( N_{\text{max}} = 6 \)

With effective interaction for \( A \) !!!

\[
H_{A}^{N_{\text{max}}, \Omega, \text{eff}, 2}
\]

\[
\begin{align*}
\text{Core} & \quad \text{Core Energy} \\
\text{1-body} & \quad \text{2-body} \\
\end{align*}
\]
2-body Valence Cluster approximation for A=7

\[ H_{A}^{0,N_{\text{max}};a_{1}=6} = V_{0}^{A,4} + V_{1}^{A,5} + V_{2}^{A,6} \]

Need NCSM results in \( N_{\text{max}} \) space for

- \( ^4\text{He} \)
- \( ^5\text{He} \)
- \( ^5\text{Li} \)
- \( ^6\text{He} \)
- \( ^6\text{Li} \)
- \( ^6\text{Be} \)

With effective interaction for A=7 !!!

\[ H_{A}^{N_{\text{max}},\Omega,\text{eff}},2 \]

**Graph:**

- Exact NCSM
- SSM with A-dependent core
- SSM with inert core

**Equation:**

\[ E_{\text{Binding}} (\text{MeV}) \]

- \( ^7\text{Li} \) CD-Bonn \( \hbar \Omega = 20 \text{ MeV} \)

**Axes:**

- \( N_{\text{max}} \)
- \( E_{\text{Binding}} (\text{MeV}) \)
2-body Valence Cluster approximation for A=7

\[ H_A^{0, N_{\text{max}}}, a_1 = 6 = V_0^{A,4} + V_1^{A,5} + V_2^{A,6} \]
3-body Valence Cluster approximation for $A > 6$

\[ \mathcal{H}_{A,a_1=7}^{0,N_{\text{max}}} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6} + V_3^{A,7} \]

Need NCSM results in $N_{\text{max}}$ space for

- $^4\text{He}$
- $^5\text{He}$, $^5\text{Li}$
- $^6\text{He}$, $^6\text{Li}$, $^6\text{Be}$
- $^7\text{He}$, $^7\text{Li}$, $^7\text{B}$, $^7\text{Be}$

With effective interaction for $A$!!!

Construct 3-body interaction in terms of 3-body matrix elements: Yes
3-body Valence Cluster approximation for $A > 6$

Valence Cluster Expansion for $N_{1,\text{max}} = 0$ space; $a_1 = AC + a_V$;
\[ E_J = \mathcal{U}_J \mathcal{H}_J \mathcal{U}_J^\dagger. \] 

(4)

This same eigenstate matrix \( \mathcal{U}_J \) can also be used to calculate the matrix elements of other effective operators, \( \mathcal{O}^\text{eff}_{A,a_1} (\lambda k; J J') \), between basis states with spins \( J \) and \( J' \) in the \( 0\hbar \Omega \) space:

\[ \mathcal{M}^\text{eff}_{A,a_1} (\lambda k; J J') = \mathcal{U}_J \mathcal{O}^\text{eff}_{A,a_1} (\lambda k; J J') \mathcal{U}_J^\dagger, \] 

(5)
FIG. 6: The quadrupole moment of the ground state for $^6$Li ($1^+ (T = 0)$) is shown in terms of one- and two-body contributions as a function of increasing model space size.
FIG. 2: Low-lying energy levels of the positive-parity states in $^{18}$O.

Summary

3-step technique to construct effective Hamiltonian for SSM with a core:

#1 2-body UT of bare NN Hamiltonian (2-body cluster approximation)

#2 NCSM diagonalization in large $N_{\text{max}}$ space for $A = 4, 5, 6, 7$

#3 many-body UT of NCSM Hamiltonian (up to 3-body valence cluster approximation)

Results:

1) strong mass dependence of core & one-body parts of $H_{\text{eff}}$

2) 3-body effective interaction plays crucial role

3) negligible role of 4-body and higher-order interactions for identical nucleons
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From $4h\Omega$ NCSM to sd CSM for $^{18}$F


Step 2: Projection of 18-body $4h\Omega$ Hamiltonian onto $0h\Omega$ 2-body Hamiltonian for $^{18}$F

$$H_{\text{eff}}([sd]^2) = \sum_k |k, N_{\text{max}} = 4, A=18 > \cdot E_k (A=18) < k, N_{\text{max}} = 4, A=18|$$

$$|k, N_{\text{max}} = 4, A=18 > = U_{k,kp2}|k_{pz}[0h\Omega, 18] > + U_{k,kq2}|k_{qz}[2+4h\Omega, 18] >$$

$$\text{dim}(P_1) = 6\ 706\ 870 \quad \text{dim}(P_2) = 28 \quad \text{dim}(Q_2) = 6\ 706\ 842$$

$$H_{\text{diag}} = U H U^\dagger$$

$$E_k(A=18) \quad H(N_{\text{max}} = 4, A=18)$$

$$H_{\text{eff}} = H_{\text{eff}}(1b) + H_{\text{eff}}(2b) + H_{\text{eff}}(3b) + H_{\text{eff}}(4b) + \ldots$$