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

Bruce R. Barrett
University of Arizona, Tucson

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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
\[ H \Psi = E \Psi \]

We cannot, in general, solve the full problem in the complete Hilbert space, so we must truncate to a finite model space.

\[ \Rightarrow \quad \text{We must use effective interactions and operators!} \]
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

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

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
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
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

Core Shell Model

effective interactions for valence nucleons

Diagonalization of the Hamiltonian for valence nucleons

Many-body experimental data
Ab-initio shell model with a core

A. F. Lisetskiy,1,* B. R. Barrett,1 M. K. G. Kruse,1 P. Navratil,2 I. Stetcu,3 and J. P. Vary4

1Department of Physics, University of Arizona, Tucson, Arizona 85721, USA
2Lawrence Livermore National Laboratory, Livermore, California 94551, USA
3Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
4Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

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We construct effective two- and three-body Hamiltonians for the $p$-shell by performing $12\hbar\Omega$ ab initio no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians into inert core, one- and two-body contributions (also three-body for $A = 7$) and analyze the systematic behavior of these different parts as a function of the mass number $A$ and size of the NCSM basis space. The role of effective three- and higher-body interactions for $A > 6$ is investigated and discussed.

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\[ H \Psi_\alpha = E_\alpha \Psi_\alpha \quad \text{where} \quad H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}. \]

\[ \mathcal{H} \Phi_\beta = E_\beta \Phi_\beta \]

\[ \Phi_\beta = P \Psi_\beta \]

\( P \) is a projection operator from \( S \) into \( S \)

\[ \langle \Phi_\gamma | \Phi_\beta \rangle = \delta_{\gamma \beta} \]

\[ \mathcal{H} = \sum_{\beta \in S} | \Phi_\beta > E_\beta < \Phi_\beta | \]
Effective Hamiltonian for NCSM

Solving

\[
H^\Omega_{A, a=2} \Psi_{a=2} = E^\Omega_{A, a=2} \Psi_{a=2}
\]

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

\(P + Q = 1;\) \(P - \) model space; \(Q - \) excluded space;

\[
E^\Omega_{A,2} = U_2 H^\Omega_{A,2} U_2^\dagger
\]

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

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

\[
H^{N_{\text{max}},\Omega,\text{eff}}_{A,2} = \frac{U_{2,P}^\dagger E^\Omega_{A,2,P} U_{2,P}}{\sqrt{U_{2,P}^\dagger U_{2,P}}}
\]

Two ways of convergence:

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

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

- $0^+$ states
- $1^+$ states
- $2^+$ states
- $3^+$ states

Energy levels ($E_x$ in MeV):

\[ N_a + N_b \leq N_{\text{max}} + 2 \]

\[ Q_1 = P_1 - P_2 \]
Effective Hamiltonian for SSM

Two ways of convergence:

1) For \( P \to 1 \) and fixed \( a \): \( \mathcal{H}_{A,a=2}^{\text{eff}} \to \mathcal{H}_A \); previous slide

2) For \( a_1 \to A \) and fixed \( P_1 \): \( \mathcal{H}_{A,a_1}^{\text{eff}} \to \mathcal{H}_A \)

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

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

Valence Cluster Expansion

\( N_{1,\max} = 0 \) 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;

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

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

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

- $^4$He
- $^5$He $^5$Li
- $^6$He $^6$Li $^6$Be

With effective interaction for A=6 !!!

$$\mathcal{H}_{A=6,2}^{N_{\text{max}}, \Omega, \text{eff}}$$

Core Energy

$$V_0^{6,4} = -51.644 \text{ MeV}$$

$$V_1^{6,5} = \mathcal{H}_{6,5}^{0, N_{\text{max}}} - V_0^{6,4}$$

$$\langle ab; JT | V_1^{6,5} | cd; JT \rangle = (\epsilon_a + \epsilon_b) \delta_{a,c} \delta_{b,d}$$

Single Particle Energies

$$\epsilon_{p3/2} = 14.574 \text{ MeV}$$

$$\epsilon_{p1/2} = 18.516 \text{ MeV}$$

$$V_2^{6,6} = \mathcal{H}_{6,6}^{0, N_{\text{max}}} - \mathcal{H}_{6,5}^{0, N_{\text{max}}}$$

TBMEs

$$\langle p_{3/2} p_{3/2} | V_2^{6,6} | p_{3/2} p_{3/2} \rangle_{J=3, T=0} = -1.825 \text{ MeV}$$

$$\langle p_{3/2} p_{3/2} | V_2^{6,6} | p_{3/2} p_{3/2} \rangle_{J=2, T=1} = 2.762 \text{ MeV}$$
2-body Valence Cluster approximation for $A=6$

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

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

$N_{\text{max}} = 6$

With effective interaction for $A$ !!!
2-body Valence Cluster approximation for $A=7$

\[ \mathcal{H}_A^{0,N_{\text{max}};\alpha=5} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6} \]

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 $A=7$ !!!

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

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

$^7\text{Li}$ CD-Bonn $h\Omega=20$ MeV
2-body Valence Cluster approximation for $A=7$

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

Need NCSM results in $N_{\text{max}}$ space for Valence Cluster Expansion for $N_{1,\text{max}}=0$ space; $a_1 = A_C + a_V$.

With effective interaction for $A=7$!!

$^7\text{Li}$ CD-Bonn $\hbar\omega=20$ MeV

![Graph](image)
3-body Valence Cluster approximation for $A>6$

$$\mathcal{H}^{0,N_{\text{max}}}_{A,a_{1}=7} = V_{0}^{A,4} + V_{1}^{A,5} + V_{2}^{A,6} + V_{3}^{A,7}$$

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

$$V^{A,7} = \mathcal{H}^{0,N_{\text{max}}}_{A,7} - \mathcal{H}^{0,N_{\text{max}}}_{A,6}$$
3-body Valence Cluster approximation for $A>6$

Valence Cluster Expansion for $N_{1,max} = 0$ space; $a_1 = A_C + a_V$;
A.F. Lisetskiy, et al., Session BM 8, Wednesday, October 14, 20:45
Effective operators from exact many-body renormalization

A. F. Lisetskiy,1,2,* M. K. G. Kruse,1 B. R. Barrett,1 P. Navratil,3 I. Stetcu,4 and J. P. Vary5

1Department of Physics, University of Arizona, Tucson, Arizona 85721, USA
2National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824-1321, USA
3Lawrence Livermore National Laboratory, Livermore, California 94551, USA
4Department of Physics, University of Washington, P. O. Box 351560, Seattle, Washington 98195-1560, USA
5Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

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We construct effective two-body Hamiltonians and $E2$ operators for the $p$ shell by performing $16\hbar\Omega$ ab initio no-core shell model (NCSM) calculations for $A = 5$ and $A = 6$ nuclei and explicitly projecting the many-body Hamiltonians and $E2$ operator onto the $0\hbar\Omega$ space. We then separate the effective $E2$ operator into one-body and two-body contributions employing the two-body valence cluster approximation. We analyze the convergence of proton and neutron valence one-body contributions with increasing model space size and explore the role of valence two-body contributions. We show that the constructed effective $E2$ operator can be parametrized in terms of one-body effective charges giving a good estimate of the NCSM result for heavier $p$-shell nuclei.

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\[ E_J = U_J \mathcal{H}_J U_J^\dagger. \]  (4)

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

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

R. Okamoto, et al., Session LL9, Oct. 17, 14:00
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

4) similar approach can be applied for calculating effective operators for other physical quantities
COLLABORATORS

Alexander Lisetskiy, U. of Arizona
Michael Kruse, U. of Arizona
Sybil de Clark, U. of Arizona
Ionel Stetcu, LANL
Petr Navratil, LLNL
James Vary, Iowa State U.
No Core Shell Model

Starting Hamiltonian

\[ H = \sum_{i=1}^{A} \frac{\tilde{p}_i^2}{2m} + \sum_{i<j}^{A} V_{NN}(\tilde{r}_i - \tilde{r}_j) + \sum_{i<j<k}^{A} V_{NNN}^{3b}(\tilde{r}_{ijk}) \]

Realistic NN and NNN potentials

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

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

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

Cluster Expansion:
Two-body cluster approximation

\[ H^\Omega_2 = \sum_{i=1}^{2} \left[ \frac{\tilde{p}_i^2}{2m} + \frac{1}{2} m \Omega^2 \tilde{r}_i^2 \right] + \sum_{i<j}^{2} \left[ V_{NN}(\tilde{r}_i - \tilde{r}_j) - \frac{m \Omega^2}{2A} (\tilde{r}_i - \tilde{r}_j)^2 \right] \]
2-body Valence Cluster approximation for $A > 6$

$$\mathcal{H}_A^{0,N_{\max},a_1=6} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$
From $4h\Omega$ NCSM to sd CSM for $^{18}\text{F}$


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

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

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

dim($P_1$) = 6706 870  

dim($P_2$) = 28  

dim($Q_2$) = 6706 842

$$U = \begin{pmatrix}
U_{PP} & U_{PQ} \\
U_{QP} & U_{QQ}
\end{pmatrix}$$

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

$$E_{k}(A=18)$$

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

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

$$H_{\text{eff}} = \frac{U_{P}^\dagger H_{\text{diag}} U_{P}}{\sqrt{U_{P}^\dagger U_{P}}}$$

- A. Lisetskly
Two-body cluster projection scheme for $A \geq 18$

4$\hbar\Omega$ space

NCSM

\begin{align*}
P\text{-space: } & N_a + N_b \leq 8 \\
\Delta (N_a + N_b) \leq 4
\end{align*}

Second (many-body) projection

\begin{align*}
P_1\text{-space: } & N_a = N_b = 2 \\
\Delta (N_a + N_b) = 0
\end{align*}