The No Core Shell Model: with and without a core (Extensions to Heavier Nuclei)

Bruce R. Barrett
University of Arizona, Tucson
MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory
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
No-Core Shell-Model Approach

• Start with the purely intrinsic Hamiltonian

\[ H_A = T_{rel} + V = \frac{1}{A} \sum_{i<j=1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j=1}^{A} V_{NN} + \sum_{i<j<k}^{A} V_{ijk}^{3b} \]

Note: There are no phenomenological s.p. energies!

Can use any NN potentials

Coordinate space: Argonne V8', AV18
Nijmegen I, II

Momentum space: CD Bonn, EFT Idaho
No-Core Shell-Model Approach

- Next, add CM harmonic-oscillator Hamiltonian

\[
H_{CM}^{HO} = \frac{\vec{P}^2}{2Am} + \frac{1}{2}Am\Omega^2 \vec{R}^2; \quad \vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i, \quad \vec{P} = Am\vec{\dot{R}}
\]

To \( H_A \), yielding

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

Defines a basis (i.e. \( HO \)) for evaluating \( V_{ij} \)
\[ H \Psi = E \Psi \]

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

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

- Must truncate to a finite model space
- In general, $V_{ij}^{\text{eff}}$ is an $A$-body interaction
- We want to make an $a$-body cluster approximation

$$\mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \approx \mathcal{H}^{(I)} + \mathcal{H}^{(a)}$$

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

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

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

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

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

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

Solving \( \mathbf{H}_A, a=2 \mathbf{\Psi}_{a=2} = \mathbf{E}_A, a=2 \mathbf{\Psi}_{a=2} \) in “infinite space” \( 2n+1 = 450 \) relative coordinates

\( P + Q = 1; \quad P - \text{model space}; \quad Q - \text{excluded space}; \)

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

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

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

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

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 \( P \): \( H_{A,a}^{\text{eff}} \to H_A \)
$N_a + N_b \leq N_{\text{max}} + 2$

$Q_1$

$Q_2 = P_1 - P_2$

$P_2$
- NCSM convergence test
  - Comparison to other methods

<table>
<thead>
<tr>
<th></th>
<th>N$^3$LO</th>
<th>NCSM</th>
<th>FY</th>
<th>HH</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3$H</td>
<td>7.852(5)</td>
<td>7.854</td>
<td>7.854</td>
<td></td>
</tr>
<tr>
<td>$^4$He</td>
<td>25.39(1)</td>
<td>25.37</td>
<td>25.38</td>
<td></td>
</tr>
</tbody>
</table>

- Short-range correlations $\Rightarrow$ effective interaction
- Medium-range correlations $\Rightarrow$ multi-$h\Omega$ model space
- Dependence on
  - size of the model space ($N_{\text{max}}$)
  - HO frequency ($h\Omega$)
- Not a variational calculation
- Convergence OK
- NN interaction insufficient to reproduce experiment

P. Navratil, INT Seminar, November 13, 2007, online
Limits of nuclear existence

Density Functional Theory
Selfconsistent Mean Field

Towards a unified description of the nucleus

Ab initio few-body calculations

$0\hbar\omega$ Shell Model

No-Core Shell Model

protons

neutrons

A=10
A=12
A=60

r-process
Beyond the No Core Shell Model

1. The NCSM in an Effective Field Theory (EFT) Framework

2. Importance Truncation

3. The *ab initio* Shell Model with a core
1. The NCSM in an Effective Field Theory Framework (talk by Bira van Kolck on Monday, June 6, 2001)
2. Importance Truncation
The idea of Importance Truncation

Small model space you can do a full NCSM calculation in

4hΩ space

Full large space – not accessible to NCSM

Truncated space—still accessible

Contains some basis states from 6hΩ space + all of 4hΩ

6hΩ space
Formalism of Importance truncation.

- First order multi-configurational perturbation theory gives...

\[
|\Psi^{(1)}\rangle = - \sum_{\nu \notin M_{\text{ref}}} \frac{\langle \Phi_\nu | W | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}} |\Phi_\nu\rangle
= - \sum_{\nu \notin M_{\text{ref}}} \frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}} |\Phi_\nu\rangle.
\]

\[
W = H - H_0
\]
Importance truncation schematically

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

- N=0 (s-shell)
  - \( 0p_{3/2} \)
  - \( 0p_{1/2} \)

- N=1 (p-shell) \( \rightarrow 0p_{3/2} 0p_{1/2} \)

- N=2 (sd-shell)
  - \( M_z = -1/2, 1/2, -1/2, 1/2 \)

O16 – one possible configuration

O16 - 0\( \hbar \Omega \) configuration

Kept states

Discarded states
Corrections to the energy

• 2nd order perturbation theory gives you an estimate of the correction to the energy from the discarded state. The first order result is equal to zero.

\[ \Delta_{\text{excl}}(\kappa_{\text{min}}) = - \sum_{\nu \notin M(\kappa_{\text{min}})} \frac{|\langle \Phi_{\nu} | H | \Psi_{\text{ref}} \rangle|^2}{\epsilon_{\nu} - \epsilon_{\text{ref}}} \]
$^8$He: It started at $N_{\text{max}} = 6$, final space $N_{\text{max}} = 8$

Interaction: $^8$He SRG N3LO
3. The *ab initio* Shell Model with a Core
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. Vary 4

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
(Received 20 June 2008; published 10 October 2008)

We construct effective two- and three-body Hamiltonians for the p-shell by performing 12ℏΩ ab initio no-core shell model (NCSM) calculations for A = 6 and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the 0ℏΩ 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.

DOI: 10.1103/PhysRevC.78.044302 PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n
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
NCSM results for $^6$Li with CD-Bonn NN potential

Dimensions

<table>
<thead>
<tr>
<th>p-space</th>
<th>$N_{\text{max}} = 12$:</th>
<th>$N_{\text{max}} = 14$:</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>48,887,665</td>
<td>211,286,096</td>
</tr>
</tbody>
</table>
$N_a + N_b \leq N_{\text{max}} + 2$

$Q_1 = P_1 - P_2$

$Q_2 = P_1 - P_2$
Effective Hamiltonian for SSM

Two ways of convergence:
1) For $P \rightarrow 1$ and fixed $a$: $H_{A,a=2}^{\text{eff}} \rightarrow H_A$: previous slide
2) For $a_1 \rightarrow A$ and fixed $P_1$: $H_{A,a_1}^{\text{eff}} \rightarrow H_A$

$P_1 + Q_1 = P$; $P_1$ - small model space; $Q_1$ - excluded space;

$H_{A,a_1}^{N_1,\text{max},N_{\text{max}}} = \frac{U_{a_1,P_1}^A,\dagger}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}} E_{A,a_1,P_1}^{N_{\text{max}},\Omega} \frac{U_{a_1,P_1}^A}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}}$

Valence Cluster Expansion

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

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

\[ \mathcal{H}_{A=6, \alpha_1=6}^{0, N_{\text{max}}} = V_0^{6,4} + V_1^{6,5} + V_2^{6,6} \]

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

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

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

Core Energy

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

Single Particle Energies

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

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 $A=6$

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

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

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

With effective interaction for $A$ !!!
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:

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

With effective interaction for $A=7$!!!

Exact NCSM

SSM with $A$-dependent core

SSM with inert core
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

$$V_3^{A,7} = \mathcal{H}^{0,N_{\text{max}}}_{A,7} - \mathcal{H}^{0,N_{\text{max}}}_{A,6}$$
FIG. 9. Comparison of spectra for $^{8}\text{He}$, $^{9}\text{He}$, and $^{10}\text{He}$ from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\text{max}} = 6$ and $\hbar \Omega = 20$ MeV using the CD-Bonn interaction.
FIG. 8. Comparison of spectra for $^8$He, $^9$He, and $^{10}$He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\text{max}} = 6$ and $\hbar \Omega = 14$ MeV using the INOY interaction.
\[ \Delta E = E_{\text{NCSM}} - E_{\text{SSM}} \quad A = 16 \]

CD-Bonn

\[ h\omega = 20 \text{ MeV} \]

\[ \Delta E \text{ (MeV)} \]

\[ 2T_\pi = N - Z \]
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

(Received 15 June 2009; published 28 August 2009)

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.

DOI: 10.1103/PhysRevC.80.024315 PACS number(s): 27.20.+n, 21.10.Hw, 21.60.Cs, 23.20.Lv
\[ E_J = \mathcal{U}_J \mathcal{H}_J \mathcal{U}_J^\dagger. \] (4)

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

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

1. Extend the \textit{ab initio} Shell Model with a core approach to nuclei in the sd-shell (and later to pf-shell nuclei).

2. This will require converged results for nuclei with $A = 16, 17, 18$ and $19$.

3. The Importance Truncation method will be used to obtain the converged results for these sd-shell nuclei.

4. SSM calculations will then be performed using the core and 1-, 2- and 3-body terms determined by the \textit{ab initio} Shell Model with a core approach.
COLLABORATORS

Sybil de Clark, University of Arizona
Michael Kruse, University of Arizona
Alexander Lisetskiy, Mintec Inc.
Petr Navratil, TRIUMF, Vancouver, B.C., Canada
Jimmy Rotureau, University of Arizona
Ionel Stetcu, University of Washington
Ubirajara (Bira) van Kolck, University of Arizona
James P. Vary, Iowa State University
C.-J. (Jerry) Yang, University of Arizona
2-body Valence Cluster approximation for $A=7$

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