Microscopic Shell-Model Calculations in the sd-shell

Bruce R. Barrett
University of Arizona, Tucson

ICNT/MSU&FRIB/NSCL May 21, 2015
COLLABORATORS

Erdal Dikmen, Suleyman Demirel U., Isparta, Turkey
Michael Kruse, Lawrence Livermore National Laboratory
Alexander Lisetskiy, Mintec, Inc., Tucson
Pieter Maris, Iowa State University
Petr Navratil, TRIUMF, Vancouver, BC, Canada
A. M. Shirokov, Lomonosov Moscow State U.
Ionel Stetcu, Los Alamos National Laboratory
James P. Vary, Iowa State University
Towards a unified description of the nucleus

The goal of nuclear structure theory:

exact treatment of nuclei based on NN, NNN,... interactions

⇒ need to build a bridge between:

- *ab initio* few-body & light nuclei calculations: $A \leq 24$
- $0\hbar\Omega$ Shell Model calculations: $16 \leq A \leq 60$
- Density Functional Theory calculations: $A \geq 60$
Coupled Cluster approach
GFMC formalism

Limits of nuclear existence

Towards a unified description of the nucleus

Ab initio few-body calculations
GFMC formalism

0\hbar\omega Shell Model
No-Core Shell Model
Coupled Cluster approach

Density Functional Theory
Selfconsistent Mean Field

r-process
OUTLINE

I. Brief Overview of the No Core Shell Model (NCSM)

II. Ab Initio Shell Model with a Core Approach

III. Results: sd-shell

IV. Summary/Outlook
I. Brief Overview of the No Core Shell Model (NCSM)
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

Flow chart for a standard NCSM calculation
No-Core Shell-Model Approach

- Start with the purely intrinsic Hamiltonian

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

**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

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

To \( H_A \), yielding

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

Defines a basis (i.e. HO) for evaluating \( V_{ij} \)
Effective Interaction

- Must truncate to a finite model space \( V_{ij} \rightarrow V_{ij}^{\text{effective}} \)

- In general, \( V_{ij}^{\text{eff}} \) is an \( A \)-body interaction

- We want to make an \( a \)-body cluster approximation

\[
\mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \gtrapprox \mathcal{H}^{(I)} + \mathcal{H}^{(a)} \text{ for } a < A
\]
Effective interaction in a projected model space

\[ H \Psi_\alpha = E_\alpha \Psi_\alpha \]

where

\[ H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}. \]

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

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

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

\[ < \tilde{\Phi}_{\gamma} | \Phi_\beta > = \delta_{\gamma \beta} \]

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

Solving \( \mathbf{H}_{A, a=2}^{\Omega} \mathbf{\Psi}_{a=2} = \mathbf{E}_{A, a=2}^{\Omega} \mathbf{\Psi}_{a=2} \) in "infinite space" 2n+l = 450 relative coordinates

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

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

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

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

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

Two ways of convergence:

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

2) For \( a \to A \) and fixed \( P \): \( H_{A,a}^{\Omega} \to H_{A} \)
\[ N_a + N_b \leq N_{\text{max}} + 2 \]

\[ Q_2 = P_1 - P_2 \]
- NCSM convergence test
  - Comparison to other methods

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<th>NCSM</th>
<th>FY</th>
<th>HH</th>
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<td>$^3$H</td>
<td>7.852(5)</td>
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<td>$^4$He</td>
<td>25.39(1)</td>
<td>25.37</td>
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- Short-range correlations ⇒ effective interaction
- Medium-range correlations ⇒ 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
II. Ab Initio Shell Model with a Core Approach
From few-body to many-body

Using the NCSM to calculate the shell model input

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
From few-body to many-body

Using the NCSM to calculate the shell model input

*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
We construct effective two- and three-body Hamiltonians for the $p$-shell by performing $12\hbar \Omega$ \textit{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.

DOI: 10.1103/PhysRevC.78.044302 

PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n
FORMALISM

1. Perform a large basis NCSM for a core + 2N system, e.g., 18^F.

2. Use Okubo-Lee-Suzuki transformation to project these results into a single major shell to obtain effective 2-body matrix elements.

3. Separate these 2-body matrix elements into a core term, single-particle energies and residual 2-body interactions, i.e., the standard input for a normal Shell Model calculation.

4. Use these values for performing SM calculations in that shell.
\( N'_{\text{max}} = 0 \)

\[
\begin{align*}
\text{OLS} & \quad \text{OLS} \\
\text{PH}_{\text{eff}}P & = 0 \\
\text{QH}_{\text{eff}}P & = 0 \\
\text{PH}_{\text{eff}}Q & = 0 \\
\text{QH}_{\text{eff}}Q & = 0
\end{align*}
\]
\[ N_a + N_b \leq N_{\text{max}} + 2 \]

\[ Q_1 \]

\[ Q_2 = P_1 - P_2 \]

\[ P_2 \]
Effective Hamiltonian for SSM
How to calculate the Shell Model 2-body effective interaction:

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

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

$$H_{A,a_1}^{N_{1,\max},N_{\max}} = \frac{U_{a_1,P_1}^A,\dagger}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}} E_{A,a_1,P_1}^{N_{\max},\Omega} \frac{U_{a_1,P_1}^A}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}}$$

Valence Cluster Expansion
$N_{1,\max} = 0$ 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;

$$H_{A,a_1}^{0,N_{\max}} = \sum_{k}^{a_v} V_{k} A, A_c + k$$
III. Results: sd-shell nuclei
Ab initio effective interactions for sd-shell valence nucleons

E. Dikmen,1,2,* A. F. Lisetskiy,2,† B. R. Barrett,2,‡ P. Maris,3,§ A. M. Shirokov,3,4,5,¶ and J. P. Vary3, **

1Department of Physics, Suleyman Demirel University, Isparta, Turkey
2Department of Physics, University of Arizona, Tucson, Arizona 85721
3Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011
4Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia
5Pacific National University, 136 Tikhookeanskaya st., Khabarovsk 680035, Russia

(Dated: February 3, 2015)

We perform ab initio no core shell model calculations for \( A = 18 \) and 19 nuclei in a \( 4\hbar\Omega \), or \( N_{\text{max}} = 4 \), model space using the effective JISP16 and chiral N3LO nucleon-nucleon potentials and transform the many-body effective Hamiltonians into the \( 0\hbar\Omega \) model space to construct the \( A \)-body effective Hamiltonians in the \( sd \)-shell. We separate the \( A \)-body effective Hamiltonians with \( A = 18 \) and \( A = 19 \) into inert core, one- and two-body components. Then, we use these core, one- and two-body components to perform standard shell model calculations for the \( A = 18 \) and \( A = 19 \) systems with valence nucleons restricted to the \( sd \)-shell. Finally, we compare the standard shell model results in the \( 0\hbar\Omega \) model space with the exact no core shell model results in the \( 4\hbar\Omega \) model space for the \( A = 18 \) and \( A = 19 \) systems and find good agreement.

ArXiv: Nucl-th 1502.00700
Empirical Single-Particle Energies

\[ E_{0d_\frac{3}{2}} = 0.0 \text{ MeV} \]
\[ E_{1S_\frac{1}{2}} = 0.87 \text{ MeV} \]
\[ E_{0d_\frac{5}{2}} = 5.08 \text{ MeV} \]

\[ H^{sd}(P \leftrightarrow \Sigma)_{sd} = \{ \frac{\hbar^2}{2} \cdot \xi + V^{\text{eff}}_{\text{sd}} \} (P \leftrightarrow \Sigma)^{sd} \]
\[ \{ H_0 + V^{\text{eff}}_{\text{sd}} \} (P \leftrightarrow \Sigma)^{sd} = E^{sd}(P \leftrightarrow \Sigma)^{sd} \]
Input: The results of $N_{\text{max}} = 4$ and $hw = 14$ MeV NCSM calculations

TABLE II: Proton and neutron single-particle energies (in MeV) for JISP16 effective interaction obtained for the mass of $A = 18$ and $A = 19$.

<table>
<thead>
<tr>
<th>$j_i$</th>
<th>$A = 18$</th>
<th>$A = 19$</th>
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</thead>
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<tr>
<td></td>
<td>$E_{\text{core}} = -115.529$</td>
<td>$E_{\text{core}} = -115.319$</td>
</tr>
<tr>
<td>$\frac{1}{2}$</td>
<td>$\pm 3.068$</td>
<td>$\pm 3.044$</td>
</tr>
<tr>
<td>$\frac{5}{2}$</td>
<td>$\pm 2.270$</td>
<td>$\pm 2.248$</td>
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<tr>
<td>$\frac{3}{2}$</td>
<td>$\pm 6.262$</td>
<td>$\pm 6.289$</td>
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<table>
<thead>
<tr>
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<td>$E_{\text{core}} = -115.529$</td>
<td>$E_{\text{core}} = -115.319$</td>
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<tr>
<td>$\frac{1}{2}$</td>
<td>$\pm 0.603$</td>
<td>$\pm 0.627$</td>
</tr>
<tr>
<td>$\frac{5}{2}$</td>
<td>$\pm 1.938$</td>
<td>$\pm 1.419$</td>
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<tr>
<td>$\frac{3}{2}$</td>
<td>$\pm 9.748$</td>
<td>$\pm 9.774$</td>
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TABLE III: Proton and neutron single-particle energies (in MeV) for chiral N3LO effective interaction obtained for the mass of $A = 18$ and $A = 19$.

<table>
<thead>
<tr>
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<td></td>
<td>$E_{\text{core}} = -118.469$</td>
<td>$E_{\text{core}} = -118.306$</td>
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<tr>
<td>$\frac{1}{2}$</td>
<td>$\pm 3.638$</td>
<td>$\pm 3.625$</td>
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<tr>
<td>$\frac{5}{2}$</td>
<td>$\pm 3.042$</td>
<td>$\pm 3.031$</td>
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<td>$\frac{3}{2}$</td>
<td>$\pm 3.763$</td>
<td>$\pm 3.770$</td>
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<table>
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<th>$j_i$</th>
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<th>$A = 19$</th>
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<td></td>
<td>$E_{\text{core}} = -118.469$</td>
<td>$E_{\text{core}} = -118.306$</td>
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<tr>
<td>$\frac{1}{2}$</td>
<td>$\pm 0.044$</td>
<td>$\pm 0.057$</td>
</tr>
<tr>
<td>$\frac{5}{2}$</td>
<td>$\pm 0.690$</td>
<td>$\pm 0.700$</td>
</tr>
<tr>
<td>$\frac{3}{2}$</td>
<td>$\pm 7.299$</td>
<td>$\pm 7.307$</td>
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</tbody>
</table>

Coupled Cluster, $E_{\text{core}}$: -130.462
Idaho NN N3LO + 3N N2LO

IM-SRG, $E_{\text{core}}$: -130.132
Idaho NN N3LO + 3N N2LO

from G.R. Jansen et al. PRL 113, 142502 (2014)

A = 18

A = 19

-130.056
from H. Hergert
private comm.
No-Core Shell-Model Approach

- Next, add CM harmonic-oscillator Hamiltonian

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

To \( H_A \), yielding

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

Defines a basis (i.e. \( HO \)) for evaluating \( V_{ij} \)
Preliminary Results

TBME with $T=0$
TBME with $T=1$

$y=x$ line

$f(x)=ax+b$

$a=0.999329$
$b=1e-30$

RMS=0.00235272
Preliminary Results

TBME with $T=0$

$y=x$ line

TBME with $T=1$

$f(x)=ax+b$

$a=0.98073$

$b=1\times10^{-30}$

RMS=0.202564
TABLE III: The NCSM energies (in MeV) of the lowest 28 states \( J^T \) of \(^{18}\)F calculated in \( 4\hbar\Omega \) model space using JISP16 and chiral N3LO NN interactions with \( \hbar\Omega = 14 \) MeV.

<table>
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<tr>
<th>( J^T )</th>
<th>T</th>
<th>JISP16</th>
<th>( J^T )</th>
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</table>
Comparison of effective TBMEs in the sd-shell: JISP16 vs USDA by Alex Brown et al.

Preliminary Results
PRELIMINARY RESULTS

JISP16

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

-131
-132
-133
-134
-135
-136
-137
-138

\( ^{20}\text{F} \)

NCSM

SSM

\(-137.663\)

\(-138.099\)

\(-137.791\)

\(-137.517\)

A=20
A=18
A=19
A=20

\( ^{20}\text{F} \)

\( ^{20}\text{F} \)

\( ^{20}\text{F} \)

\( ^{20}\text{F} \)

5\(^+\)

3\(^+\)

3\(^+\)

3\(^+\)

0\(^+\)

0\(^+\)

5\(^+\)

5\(^+\)

1\(^+\)

1\(^+\)

2\(^+\)

2\(^+\)

4\(^+\)

4\(^+\)

2\(^+\)

2\(^+\)

3\(^+\)

3\(^+\)
Preliminary Results
Summary

Perform a converged NCSM calculation with a NN or NN+NNN interaction for a closed core + 2 valence nucleon system.

An OLS transformation of the results of the above NCSM calculation into a single major shell allows one to obtain core and single-particle energies and two-body residual matrix elements appropriate for shell model calculations in that shell, which have only a weak A-dependence.

The core and single-particle energies and two-body residual matrix elements obtained by this procedure can be used in Standard Shell Model calculations in the sd-shell, yielding results in good agreement with the full space NCSM results. The core and s.p. energies + 2-body effective interactions for A=18 give also good results for A=19 and 20.

Additional calculations are being performed with other NN interactions and for heavier nuclei in the sd-shell.
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 $A=6$ !!!

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

\[ V_3^{A,7} = \mathcal{H}_{A,7}^{0,N_{\text{max}}} - \mathcal{H}_{A,6}^{0,N_{\text{max}}} \]
Chiral effective field theory (EFT) for nuclear forces

Separation of scales: low momenta \( \frac{1}{\lambda} = Q \ll \Lambda_b \) breakdown scale \( \Lambda_b \)

explanes pheno hierarchy:

\( \text{NN} > 3\text{N} > 4\text{N} > \ldots \)

\( \text{NN-3N, } \pi\text{N, } \pi\pi\text{, electro-weak,…} \)

consistency

3N,4N: 2 new couplings to \( \text{N}^3\text{LO}! \)

theoretical error estimates

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Meissner, Nogga, Machleidt,…

A. Schwenk