Fluorine isotope systematics: *ab initio* vs phenomenological analyses

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Coupled Cluster approach
GFMC formalism

Limits of nuclear existence

Towards a unified description of the nucleus
OUTLINE

I. Overview of the *Ab Initio* Shell Model with a Core Approach

II. Results:
   a.) General sd-shell
   b.) Fluorine isotopes

III. Summary/Outlook
I. Overview of the *Ab Initio* Shell Model with a Core Approach
Ab-initio shell model with a core

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(Received 20 June 2008; published 10 October 2008)

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

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
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 \( S \)

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

\[ \mathcal{H} = \sum_{\beta \in S} |\Phi_\beta\rangle \quad E_\beta \quad \langle \bar{\Phi}_\beta| \]
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.
$N_a + N_b \leq N_{\text{max}} + 2$

$Q_1$

$Q_2 = P_1 - P_2$

$P_2$
II. Results: a.) sd-shell nuclei
Ab initio effective interactions for sd-shell valence nucleons

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(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

\[ E_{0d_{5/2}} = 0.0 \text{ MeV} \]
\[ E_{15s_{1/2}} = 0.87 \text{ MeV} \]
\[ E_{0d_{3/2}} = 5.08 \text{ MeV} \]

\[ H^{sd}(P_{3/2})^{sd} = \{ \frac{\vec{z}^2}{2} \cdot \vec{\varepsilon} + \nu^{sd}_{\text{eff}} \} (P_{3/2})^{sd} \]

\[ [H_0 + \nu^{sd}_{\text{eff}}] (P_{3/2})^{sd} = E^{sd}(P_{3/2})^{sd} \]
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>
<tbody>
<tr>
<td></td>
<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>3.068</td>
<td>-3.044</td>
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<tr>
<td>$\frac{5}{2}$</td>
<td>-2.270</td>
<td>-2.248</td>
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<td>$\frac{3}{2}$</td>
<td>6.262</td>
<td>6.289</td>
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<tr>
<td>$e_{f_{ji}}^p$</td>
<td>0.603</td>
<td>0.627</td>
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<tr>
<td>$e_{f_{ji}}^n$</td>
<td>1.398</td>
<td>1.419</td>
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<tr>
<td>$e_{f_{ji}}^p$</td>
<td>9.748</td>
<td>9.774</td>
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</table>

**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>
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<th>$A = 19$</th>
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</thead>
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<td>$E_{\text{core}} = -118.469$</td>
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<td>3.763</td>
<td>3.770</td>
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<td>$e_{f_{ji}}^n$</td>
<td>0.044</td>
<td>0.057</td>
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<tr>
<td>$e_{f_{ji}}^p$</td>
<td>0.690</td>
<td>0.700</td>
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<td>$e_{f_{ji}}^n$</td>
<td>7.299</td>
<td>7.307</td>
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</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

**A = 18**

**A = 19**

-130.056 from G.R. Jansen et al. PRL 113, 142502 (2014)
-129.637 from H. Hergert private comm.
No-Core Shell-Model Approach

Next, add CM harmonic-oscillator Hamiltonian

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

To \( H_A \), yielding

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

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

\[ f(x) = ax + b \]

- \( a = 0.999329 \)
- \( b = 1e-30 \)
- RMS = 0.00235272
Preliminary Results
II. Results: b) Fluorine isotopes
Survey of the Fluorine isotopes

1. Calculate the Fluorine isotopes using the same set of effective TBMEs, which are very weakly A-dependent, e.g., those determined from the JISP16 NN interaction, to test how well they reproduce data trends.

2. Assume that the effects of 3NFs can be approximated by replacing the theoretical single-particle energies with the empirical ones used by Brown & Richter* for their USDB effective interaction.

3. Compare our results for 18,20,22,24 F with those obtained with the USDB effective interaction and with those obtained with the IM-SRG approach** using an EFT N3LO NN plus N2LO NNN interaction.

Preliminary Results

| TABLE I: The single-particle energies (in MeV) used in the standard shell model calculations of F isotopes. (n) and (p) represent neutron and proton, respectively. |
|---|---|---|---|
| $j_i$ | $\frac{1}{2}$ | $\frac{5}{2}$ | $\frac{3}{2}$ |
| JISP16$_{A=18}$ ($^{17}$O) : (n) | -3.068 | -2.270 | 6.262 |
| JISP16$_{A=18}$ ($^{17}$F) : (p) | 0.603 | 1.398 | 9.748 |
| USDA | -3.0612 | -3.9436 | 1.9798 |
| USDB | -3.2079 | -3.9257 | 2.1117 |
| IM-SRG ($^{17}$O) : (n) | -3.089 | -4.643 | 2.940 |
| IM-SRG ($^{17}$F) : (p) | 0.255 | -0.909 | 6.035 |

Preliminary Results

\[ \varepsilon_{\text{theo}} \quad \varepsilon_{\text{USDB}} \quad \varepsilon_{\text{USDB}} \]

\[ {^18F} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]

\[ \begin{array}{c}
0^+ \\
1^+ \\
2^+ \\
3^+ \\
4^+ \\
5^+ \\
\end{array} \]
Preliminary Results

\[ ^{22}_{\text{F}} \]

\[ \varepsilon_{\text{theo}} \quad \varepsilon_{\text{USDB}} \quad \varepsilon_{\text{USDB}} \]

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

\[ 0^+ \quad 1^+ \quad 2^+ \quad 3^+ \quad 4^+ \]

\[ JISP16_{A=18} \quad JISP16_{A=18} \quad \text{USDB}_{A=18} \quad \text{Experiment} \]
Preliminary Results
Preliminary Results
Preliminary Results

Graphs showing energy levels for isotopes of fluorine and uranium.
RMS deviation of 471 keV

Preliminary Results

* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802
* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802
Preliminary Results
SUMMARY AND OUTLOOK

1. All three interactions and approaches used in this study reproduced the gross trends and features of the experimental data for the 18,20,22,24 F isotopes.

2. Replacing the theoretical s.p. energies with the empirical ones for the USDB interaction, perhaps approximating the effects of a NNN interaction, improved, in general, the agreement with experiment.

3. The overall, reasonable agreement with experiment obtained using the IM-SRG approach with an EFT N3LO NN and N2LO NNN suggests that it is worthwhile to further improve our interactions and increase the size of the model space for our NCSM calculations.

4. The current results support the hypothesis that a single A-independent set of effective TBMEs can explain the trends in the F isotopes.

OUTLOOK: Plan to perform further calculations implementing the changes outlined above.
Flow chart for a standard NCSM calculation

**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

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

**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
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

\[ \mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \gtrsim \mathcal{H}^{(I)} + \mathcal{H}^{(a)} \]

\[ a < A \]
Effective Hamiltonian for NCSM

Solving
\[ \hat{H}^\Omega_{A, a=2} \psi_{a=2} = E^\Omega_{A, a=2} \psi_{a=2} \]

in “infinite space” \( 2n+1 = 450 \)

relative coordinates

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

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

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

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

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

Two ways of convergence:

1) For \( P \rightarrow 1 \) and fixed \( a \): \( \hat{H}_{A, a=2}^{\text{eff}} \rightarrow H_A \)

2) For \( a \rightarrow A \) and fixed \( P \): \( \hat{H}_{A, a}^{\text{eff}} \rightarrow H_A \)
- NCSM convergence test
  - Comparison to other methods

<table>
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<tr>
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<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
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 $a$: $H_{A,a=2}^{\text{eff}} \rightarrow H_A$: previous slide
2) For $a_1 \rightarrow A$ and fixed $P_1$: $H_{A,a1}^{\text{eff}} \rightarrow H_A$

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

$$H_{A,a1}^{N_{1,max},N_{max}} = \frac{U_{a_1,P_1}^A,\dagger}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}} E_{A,a_1,P_1}^{N_{max},\Omega} \frac{U_{a_1,P_1}^A}{\sqrt{U_{a_1,P_1}^A U_{a_1,P_1}^A}}$$

Valence Cluster Expansion

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

$$H_{A,a1}^{0,N_{max}} = \sum_{k}^{a_v} V_{A,A_c+k}$$
\[ N_{\text{max}}' = 0 \]

\[ P'H'_{\text{eff}}P' \]

\[ PH_{\text{eff}}P = 0 \]

\[ QH_{\text{eff}}P = 0 \]

\[ PH_{\text{eff}}Q = 0 \]

\[ QH_{\text{eff}}Q \]
Preliminary Results

TBME with $T=0$  
y=x line  
TBME with $T=1$  
f(x) = ax + b  
a = 0.98073  
b = 1e-30  
RMS = 0.202564
TABLE III: The NCSM energies (in MeV) of the lowest 28 states $J^T_\pi$ of $^{18}$F calculated in $4\hbar\Omega$ model space using JISP16 and chiral N3LO $NN$ interactions with $\hbar\Omega = 14$ MeV.

<table>
<thead>
<tr>
<th>$J^T_\pi$</th>
<th>T</th>
<th>JISP16</th>
<th>$J^T_\pi$</th>
<th>T</th>
<th>N3LO</th>
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<tr>
<td>0$^+_3$</td>
<td>1</td>
<td>-99.848</td>
<td>2$^+_8$</td>
<td>1</td>
<td>-107.473</td>
</tr>
<tr>
<td>2$^+_8$</td>
<td>1</td>
<td>-99.607</td>
<td>0$^+_3$</td>
<td>1</td>
<td>-107.436</td>
</tr>
</tbody>
</table>
PRELIMINARY RESULTS

JISP16

$^{20}\text{F}$

NCSM

SSM

SSM

SSM

$E$ (MeV)

$A=20$

$A=18$

$A=19$

$A=20$

$(-137.663)$

$(-138.099)$

$(-137.791)$

$(-137.517)$