Symplectic no-core configuration interaction framework

A. E. McCoy¹, M. A. Caprio¹, and T. Dytrych²

¹University of Notre Dame
²Nuclear Physics Institute, Academy of Sciences of the Czech Republic

February 29, 2017
Dimension explosion for NCCI calculations

Standard NCCI Basis

A. E. McCoy, M. A. Caprio, and T. Dytrych

TRIUMF 2 / 31
Ab initio many-body calculations in a symplectic scheme

Outline

▶ How does the symplectic basis relate to the harmonic oscillator basis?
▶ Symplectic no-core configuration interaction (SpNCCI) framework
▶ Initial calculations

Acknowledgements

▶ David Rowe (University of Toronto)
▶ Pieter Maris (Iowa State University)
▶ Calvin Johnson (San Diego State University)
▶ Chao Yang (Lawrence Berkeley National Laboratory)
▶ Patrick Fasano (University of Notre Dame)
Harmonic oscillator basis

- States are configurations, i.e., distributions of particles over HO shells

- $N_{ex}$: total number of oscillator quanta above lowest Pauli allowed number.

- Wavefunctions are linear combinations of infinitely many HO configurations

$$|\Psi\rangle = c_0\phi_0 + c_1\phi_1 + c_2\phi_2 + ... + c_i\phi_i + ...$$

- Basis must be truncated

- How large must the basis be to contain states necessary for convergence?
$N_{\text{max}}$ truncation

- Basis includes all configurations with $N_{\text{ex}} \leq N_{\text{max}}$
- Interaction strength expected to decrease with $N$
- Kinetic energy strongly couples configurations at low $N_{\text{ex}}$ to those at high $N_{\text{ex}}$
- Basis must include these high $N_{\text{ex}}$ configurations

\[
H = V + T \\
H \approx T
\]
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-$N_{ex}$ and high-$N_{ex}$ configurations induced by kinetic energy.
Nuclear symmetries

Exact symmetries
- Spacial Translation ($p$)
- Time Translation ($E$)
- Rotation ($J$): SU(2)

Approximate symmetries
- Isospin ($T$)
- Elliot SU(3)
- Symplectic Sp(3,$\mathbb{R}$)

Why symplectic

Kinetic energy strongly connects states of different $N_{\text{ex}}$ ($\Delta N_{\text{ex}} = 2$)
- Results in strong mixing of high $N_{\text{ex}}$ configurations into many-body eigenstates

Kinetic energy conserves $\text{Sp}(3,\mathbb{R})$ symmetry!
Symplectic reorganization of the many-body space

If we reorganize the many-body space by symplectic symmetry...

- Kinetic energy does not connect different symplectic irreducible representations (irrep)
- Resulting basis states are highly-correlated linear combinations of harmonic oscillator configurations
Kinetic energy

M-scheme basis

Symplectic basis

Kinetic energy matrix

Kinetic energy matrix with Sp(3,R) selection rules
**Exact symmetry under rotation: SU(2)**

### SU(2) generators

<table>
<thead>
<tr>
<th>$J_0$</th>
<th>Weight operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J_{\pm}$</td>
<td>Raising and lowering operator</td>
</tr>
</tbody>
</table>

### Action of the lowering operator

$$J_\pm |JM\rangle = \sqrt{(J \mp M)(J \pm M + 1)} |JM \pm 1\rangle$$

$$J_- |J - J\rangle = 0$$

### Irreducible representation (irrep) $J$

$$M = -J, \ldots, J$$

### Hamiltonian matrix can be broken into $J$ spaces (J-scheme)

<table>
<thead>
<tr>
<th>$J=0$</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$J=2$</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>$J=4$</td>
</tr>
</tbody>
</table>

---

A. E. McCoy, M. A. Caprio, and T. Dytrych

TRIUMF
SU(3)-NCSM basis

### SU(3) generators

<table>
<thead>
<tr>
<th>$Q_{2M}$</th>
<th>Algebraic quadrupole operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_{1M}$</td>
<td>Orbital angular momentum</td>
</tr>
</tbody>
</table>

SU(3) ⊃ SO(3)  
$(\lambda, \mu) \kappa L \otimes SU(2) \supset J$  
SU(2) $S$

SU(3) ⊃ U(3)  
$(\lambda, \mu) \kappa \rho(\lambda \mu) S$

SU(3) symmetry of a nucleus is obtained by:

1. SU(3) coupling particles within major shells. Each particle has SU(3) symmetry $(N, 0)$ where $N = 2n + l$.

2. SU(3) coupling successive shells.

3. SU(3) coupling protons and neutrons.

### References

SU(3)-NCSM basis: $^{18}\text{O}$

SU(3) has built-in correlations
SU(3) decomposition

- Ground state wavefunction dominated by a few SU(3) irreps
- SU(3) irreps consistent with Sp(3,R) symmetry

SU(3) decomposition of $^8\text{Be}$ $0^+_\text{gs}$

$N_{\text{max}}=10$

$\hbar\Omega = 20$ MeV

Chiral $N^3LO$

A. E. McCoy, M. A. Caprio, and T. Dytrych

Sp(3, ℜ) algebra

| Sp(3, ℜ) generators | \[
A_{LM}^{(20)} = \frac{1}{\sqrt{2}} \sum_i (b_i^\dagger \times b_i)^{(20)}_{LM} \]
| B_{LM}^{(02)} = \frac{1}{\sqrt{2}} \sum_i (b_i \times b_i)^{(02)}_{LM} | Sp(3, ℜ) raising
| C_{LM}^{(11)} = \sqrt{2} \sum_i (b_i^\dagger \times b_i)^{(11)}_{LM} | Sp(3, ℜ) lowering
| H_{00}^{(00)} = \sqrt{3} \sum_i (b_i^\dagger \times b_i)_{00} | SU(3) generators
| \]

The kinetic energy
\[ T_{00} = \frac{1}{2} (2H_{00}^{(0,0)} - \sqrt{6}A_{00}^{(2,0)} - \sqrt{6}B_{00}^{(0,2)}) \]

Sp(3, ℜ) states with spin: |σνωκLSJM⟩

| Sp(3, ℜ) ⊆ U(3) ⊆ SO(3) | \[
\sigma \quad \nu \quad \omega \quad \kappa \quad L
\]
| ⊗ ⊆ SU(2) | \[
SU(2) \quad J
\]

σ Lowest grade U(3) irrep (LGI), labels the Sp(3, ℜ) irrep
ν Sp(3, ℜ) to U(3) branching multiplicity
ω U(3) symmetry of state in Sp(3, ℜ) irrep
κ U(3) to SO(3) branching multiplicity
L Orbital angular momentum
S Spin
J Total angular momentum

U(3) = U(1) ⊗ SU(2)
\[ \sigma = N_\sigma(\lambda_\sigma, \mu_\sigma) \]
\[ \omega = N_\omega(\lambda_\omega, \mu_\omega) \]
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-$N_{ex}$ and high-$N_{ex}$ configurations induced by kinetic energy.

- SpNCCI basis states incorporate $\text{Sp}(3,\mathbb{R})$, $\text{SU}(3)$ and $\text{SU}(2)$ symmetries.
$Sp(3, \mathbb{R})$ raising operator

$Sp(3, \mathbb{R})$ raising operator relates states with different number of oscillator excitation quanta $N_{\text{ex}}$.

$A_{LM}^{(20)} = \frac{1}{\sqrt{2}} \sum_i (b_i^\dagger \times b_i^\dagger)^{(20)}_{LM}$

- Symplectic states have built in correlations across distributions of particles over major oscillator shells.

At $N_{\text{ex}}=0$, $Sp(3,\mathbb{R})$ states correspond to a single configuration, or distribution over major shells. At higher $N_{\text{ex}}$, $Sp(3,\mathbb{R})$ states are linear combinations of configurations.
Symplectic basis

Symplectic irrep

- Start from lowest $N_{\text{ex}}$ $U(3)$ irrep: lowest grade irrep (LGI)

- Repeatedly act on the LGI with the $\text{Sp}(3, \mathbb{R})$ raising operator

  $$|\psi\rangle = A A \cdots A |\text{LGI}\rangle$$

- Truncate each $\text{Sp}(3, \mathbb{R})$ irrep by total number of oscillator excitations $N_{\text{max}}$

Defining SpNCCI basis

- Select a set of symplectic irreps

- $E.g.$, select only irreps whose LGI have $N_{\text{ex}} \leq N_{\sigma, \text{max}}$
Basis dimensions with increasing $N_{\sigma,\text{max}}$

\[ \text{Dimension} \]

- $M$-scheme
- $N_{\sigma,\text{max}} = 0$
- $N_{\sigma,\text{max}} = 2$
- $N_{\sigma,\text{max}} = 4$
- $N_{\sigma,\text{max}} = 6$

\[ N_{\text{max}} \]

$^6\text{Li} \ 1^+$

$N_{\text{ex}}$

$N_{\sigma,\text{max}} = 0$

A. E. McCoy, M. A. Caprio, and T. Dytrych

TRIUMF
Basis dimensions with increasing $N_{\sigma,\text{max}}$

- M-scheme
- $N_{\sigma,\text{max}}=0$
- $N_{\sigma,\text{max}}=2$
- $N_{\sigma,\text{max}}=4$
- $N_{\sigma,\text{max}}=6$

$^6\text{Li} \ 1^+$

$N_{\text{ex}}$

$N_{\sigma,\text{max}}=2$
Basis dimensions with increasing $N_{\sigma,\text{max}}$
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-$N_{ex}$ and high-$N_{ex}$ configurations induced by kinetic energy.

- SpNCCI basis states incorporate $Sp(3, \mathbb{R})$, SU(3) and SU(2) symmetries.

- A symplectic irrep is generated by starting with the lowest $N_{ex}$ configuration and repeatedly acting with the symplectic raising operator $A$.
  \[ A |N\rangle \rightarrow |N + 2\rangle \]
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-$N_{ex}$ and high-$N_{ex}$ configurations induced by kinetic energy.

- SpNCCI basis states incorporate $\text{Sp}(3, \mathbb{R})$, SU(3) and SU(2) symmetries.

- A symplectic irrep is generated by starting with the lowest $N_{ex}$ configuration and repeatedly acting with the symplectic raising operator $A$.
  \[
  A |N\rangle \rightarrow |N + 2\rangle
  \]

- Truncation by symplectic irrep allows us to include relevant high $N_{ex}$ configurations in basis without needing to include full $N_{ex}$ subspace.
Calculations in a symplectic basis


- Expand $\text{Sp}(3, \mathbb{R})$ states in terms of SU(3)-NCSM states
  - Diagonalize $\text{Sp}(3, \mathbb{R})$ Casimir operator in SU(3)-coupled basis
  - Obtain expansion of LGIs in SU(3)-coupled basis, then repeatedly apply symplectic raising operator to LGIs

- Expand matrix elements in terms of LGI matrix elements using operator commutators (Suzuki and Hecht approach)
SpNCCI recurrence scheme

- Expand Hamiltonian in terms of fundamental “unit tensor” operators $\mathcal{U}(a, b)$ (analogous to TBME expansion of two-body operators in terms of $c_a^\dagger c_b^\dagger c_c c_d$)

$$H = \sum \langle a\|H\|b \rangle \mathcal{U}(a, b)$$

- Expand only LGIs in SU(3)-NCSM basis
- Compute seed matrix elements ($\text{LSU3shell}$)
- Compute matrix elements of $\mathcal{U}(a, b)$ via recurrence

$$\langle N'\|\mathcal{U}\|N \rangle = \langle N'\|UA\|N - 2 \rangle$$

$$= \langle N'\|A\mathcal{U}\|N - 2 \rangle + \langle N'\|[\mathcal{U}, A]\|N - 2 \rangle$$

$$= \langle N' - 2\|\mathcal{U}\|N - 2 \rangle + \langle N'\|[\mathcal{U}, A]\|N - 2 \rangle$$
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-$N_{ex}$ and high-$N_{ex}$ configurations induced by kinetic energy.

- SpNCCI basis states incorporate $Sp(3,\mathbb{R})$, SU(3) and SU(2) symmetries.

- A symplectic irrep is generated by starting with the lowest $N_{ex}$ configuration and repeatedly acting with the symplectic raising operator $A$.

\[ A |N\rangle \rightarrow |N + 2\rangle \]

- Truncation by symplectic irrep allows us to include relevant high $N_{ex}$ configurations in basis without needing to include full $N_{ex}$ subspace.

- Matrix elements are computed recursively and so explicit construction of full basis is not necessary.
Initial results

\[ ^{6}\text{Li}, \text{JISP16 (no Coulomb)} \]

- Examine convergence with \( N_{\sigma,\text{max}} \)
- Need to include all irreps strongly connected by interaction

\textit{At what }N_{\text{max}}\text{ does the interaction fade away and the kinetic energy dominate?}

\[ ^{6}\text{Li} E(1^{+}) \]

\[ h\Omega=20 \text{ MeV} \]
Initial results

$^6\text{Li}$, JISP16 (no Coulomb)

- Examine convergence with $N_{\sigma,\text{max}}$
- Need to include all irreps strongly connected by interaction

*At what $N_{\text{max}}$ does the interaction fade away and the kinetic energy dominate?*

![Graph showing the energy levels of $^6\text{Li}$ as a function of $N_{\text{max}}$ with $\hbar \Omega = 20$ MeV.]
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-$N_{\text{ex}}$ and high-$N_{\text{ex}}$ configurations induced by kinetic energy.

- SpNCCI basis states incorporate $\text{Sp}(3, \mathbb{R})$, SU(3) and SU(2) symmetries.

- A symplectic irrep is generated by starting with the lowest $N_{\text{ex}}$ configuration and repeatedly acting with the symplectic raising operator $A$.

  $$ A |N\rangle \rightarrow |N + 2\rangle $$

- Truncation by symplectic irrep allows us to include relevant high $N_{\text{ex}}$ configurations in basis without needing to include full $N_{\text{ex}}$ subspace.

- Matrix elements are computed recursively and so explicit construction of full basis is not necessary.

- We have initial results as of 5 days, 5 hours and 43 minutes ago.
Going forward

- Significant improvement can be made to SpNCCI code (memory usage and parallelization) to extend calculations to higher $N_{\sigma,\text{max}}$ and $N_{\text{max}}$ (and heavier nuclei).

- Exploration of basis truncations: restrict basis to physically preferred LGI’s
  
  - Extract physically preferred transformed LGI set from wave functions in low $N_{\text{max}}$ reference calculation
  
  - Determine preferred LGI set from self consistency approach

- ...