Symplectic no-core configuration interaction framework for _ab initio_ nuclear structure

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From Bound States to the Continuum
East Lansing, MI
June 14, 2018
Overview

Symplectic symmetry for \textit{ab initio} calculations

The ultimate goal of diagonalising a realistic many-nucleon Hamiltonian in a $\text{Sp}(3, \mathbb{R}) \supset \text{SU}(3)$ shell model basis, to obtain a fully microscopic description of collective states from first principles, and then to use the $\text{Sp}(3, \mathbb{R})$ model \ldots to expose the underlying dynamical content of the states obtained is, as we hope to show, very near at hand \ldots


Symplectic no-core configuration interaction (SpNCCI) framework

– Intrinsic frame (center-of-mass free) formalism
– Antisymmetric by construction
– Builds on SU(3)-NCSM machinery
– Recursive evaluation of matrix elements

$Laddering and commutators$

https://github.com/nd-nuclear-theory/spncci
Outline

– Symplectic symmetry and the SpNCCI framework
– A first look at symplectic structure of light nuclei $^6\text{Li}$
– A simple example of convergence $^3\text{He}$
Working with symmetries

States are classified into “irreducible representations” (irreps)

*Set of states connected by laddering action of generators*

\[ J_{\pm} |JM\rangle \propto |J(M \pm 1)\rangle \quad \text{Ladder} \]
\[ J_0 |JM\rangle = M |JM\rangle \quad \text{Weight (label)} \]

Irrep is uniquely defined by extremal state (lowest or highest “weight”)

*E.g., for SU(2), irrep with \( M = -J, \ldots, J \) is labeled by \( M_{\text{max}} \equiv J \)*

Operators classified by tensorial properties

Evaluation of matrix elements using group structure

- Selection rules (block structure)
- Wigner-Eckart theorem \( Clebsch-Gordan \)
- Commutators \( \Rightarrow \) Recurrence relations

\[ \begin{array}{cccc}
J=0 & 0 & 0 \\
0 & J=2 & 0 \\
0 & 0 & J=4
\end{array} \]
Why $\text{Sp}(3, \mathbb{R})$ for the many-body problem?

Generators $(i,j = 1,2,3)$

- $Q_{ij} = x_i x_j$ “Quadratic”
- $P_{ij} = x_i p_j + p_i x_j$ Scaling/deformation
- $K_{ij} = p_i p_j$ “Kinetic-like”
- $L_{ij} = x_i p_j - x_j p_i$ Rotation

Or, in terms of creation/annihilation operators, and as $\text{SU}(3)$ tensors...

$$b^\dagger = \frac{1}{\sqrt{2}} (x^{(1)} - i p^{(1)}) \quad \tilde{b} = \frac{1}{\sqrt{2}} (\tilde{x}^{(1)} + i \tilde{p}^{(1)})$$

- $A^{(20)} \sim b^\dagger b^\dagger$ “Raising” $\Delta N = +2$
- $H^{(00)}, C^{(11)} \sim b^\dagger b$ $\text{U}(3)$ generators $\Delta N = 0$
- $B^{(02)} \sim b b$ “Lowering” $\Delta N = -2$

Kinetic energy is linear combination of generators

*Kinetic energy conserves $\text{Sp}(3, \mathbb{R})$ symmetry, i.e., stays within an irrep*

$$T = H^{(00)}_{00} - \sqrt{\frac{3}{2}} A^{(20)}_{00} - \sqrt{\frac{3}{2}} B^{(20)}_{00}$$
Symplectic reorganization of the many-body space

- **Recall**: Kinetic energy connects configurations with $N'_{\text{ex}} = N_{\text{ex}} \pm 2$

- But kinetic energy does not connect different $\text{Sp}(3, \mathbb{R})$ irreps

\[
T = H^{(00)}_{00} - \sqrt{\frac{3}{2}} A^{(20)}_{00} - \sqrt{\frac{3}{2}} B^{(20)}_{00}
\]

- Nucleon-nucleon interaction will still connect $\text{Sp}(3, \mathbb{R})$ irreps at low $N_{\text{ex}}$

*By how much? How high in $N_{\text{ex}}$ will irrep mixing be significant?*
Elliott SU(3) symmetry

Generators of SU(3) ⊇ SO(3)

\[ L_M^{(1)} \sim (b^\dagger \times \tilde{b})_M^{(1)} \quad Q_M^{(2)} \sim (b^\dagger \times \tilde{b})_M^{(2)} \]

States classified into SU(3) irreps \((\lambda, \mu)\)

- States are correlated linear combinations of configurations over \(\ell\)-orbitals
- Branching of SU(3) \(\rightarrow\) SO(3) gives rotational bands (in \(L\))

[Diagram showing \(^{18}\text{O} N_{\text{ex}} = 0\) and states classified into SU(3) irreps]
SU(3) no-core shell model

Build up many-body NCCI basis states with good SU(3) symmetry
- A single nucleon in shell $N = 2n + \ell$ has SU(3) symmetry $(N, 0)$
- Choose a distribution of protons and neutrons over oscillator shells
- Couple all protons or nucleons in single shell to good SU(3) $U(\nu) \supset U(3)$
- Couple successive oscillator shells to total SU(3) symmetry

Then apply the SU(3) group theoretical tensor “machinery” for matrix elements

SU(3) coupling and recoupling techniques, SU(3) Wigner-Eckart theorem

Antisymmetry: Implemented in second quantization $(c^\dagger_{(0,0)} \cdots c^\dagger_{(N,0)}) \omega S |\rangle$

Center-of-mass: Factorizes within each $U(3) \times SU(2)$ subspace $\omega S \equiv N(\lambda \mu S)$
Building an Sp(3, R) irrep

Sp(3, R) generators can be grouped into ladder and weight-like operators

\[ A^{(20)} \sim b^\dagger b^\dagger \quad \text{“Raising”} \quad \Delta N = +2 \]
\[ H^{(00)}, C^{(11)} \sim b^\dagger b^\dagger \quad \text{U(3) generators} \quad \Delta N = 0 \]
\[ B^{(02)} \sim bb \quad \text{“Lowering”} \quad \Delta N = -2 \]

Start from single SU(3) irrep at lowest “grade” \( N \)

\textit{Lowest grade irrep (LGI)}

Ladder upward in \( N \) using \( A^{(20)} \quad \text{No limit!} \)

\[ B^{(02)} |\sigma\rangle = 0 \]
\[ |\psi^\omega\rangle \sim [A^{(20)}A^{(20)}\cdots A^{(20)} |\sigma\rangle]^\omega \]

\[ \text{Sp}(3, \mathbb{R}) \supset \text{U}(3) \quad \text{U}(3) \sim \text{U}(1) \otimes \text{SU}(3) \]

\[ n^\sigma \omega^\omega N_{\omega} (\lambda_{\omega}, \mu_{\omega}) \]
Building up the SpNCCI many-body space

\[ N_{\sigma,\text{max}} = 4 \]

\[ N_{\sigma,\text{ex}} = 0 \]

\[ N_{\sigma,\text{ex}} = 2 \]

\[ N_{\sigma,\text{ex}} = 2 \]
SpNCCI dimensions in $N_{\sigma,\text{max}}$ truncation

- Take all $\text{Sp}(3, \mathbb{R})$ irreps with $U(3) \times SU(2)$ LGIs through $N_{\sigma,\text{max}}$
- Truncate each of these irreps at $N_{\text{max}}$ excitation quanta
- For $N_{\sigma,\text{max}} = N_{\text{max}}$: Maps to the center-of-mass free subspace of the traditional NCCI $N_{\text{max}}$ space  

Benchmark!

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![Graphs for $^3\text{He}$ and $^6\text{Li}$](image-url)
Construction of LGIs for SpNCCI Sp(3, \(\mathbb{R}\)) irreps

How do we identify linear combinations of SU(3)-NCSM configurations which form SpNCCI LGIs?

- LGIs are annihilated by Sp(3, \(\mathbb{R}\)) lowering operator \(B^{(0,2)}\)
- Center-of-mass free LGIs also have zero eigenvalue of \(N_{c.m.}\)
- Within each SU(3)-NCSM \(\omega S\) subspace, LGIs span the simultaneous null space of \(B^{(0,2)}\) and \(N_{c.m.}\)
- Solve for simultaneous null vectors of \(B^{(0,2)}\) and \(N_{c.m.}\)
  
  \[= N - N_{\text{intr}}\] within \(\omega S\) subspace
- Linear combinations obtained using null solver are *arbitrary*
- Within each Sp(3, \(\mathbb{R}\)) \(\times\) SU(2) subspace, can we identify LGIs of most important irreps, as linear combinations of original LGIs, and then truncate to those Sp(3, \(\mathbb{R}\)) irreps?

*E.g.*, Sp(3, \(\mathbb{R}\)) *importance truncation*?
Recursive scheme for SpNCCI matrix elements

Expand Hamiltonian in terms of fundamental SU(3) “unit tensor” operators $U_{N0}^{N0(\lambda_0,\mu_0)}(a,b)$

Analogous to second-quantized expansion of two-body operators in terms of two-body matrix elements:

$$H \propto \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | H | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

$$H = \sum \langle a| H_{N0(\lambda_0,\mu_0)} | b \rangle U_{N0(\lambda_0,\mu_0)}(a,b)$$

Find expansion for LGIs in SU(3)-NCSM basis

Compute matrix elements of $U$ between LGIs using SU(3)-NCSM

Compute matrix elements of $U$ between all higher-lying $Sp(3,\mathbb{R})$ irrep members via recurrence on $N$

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

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

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

– Symplectic symmetry and the SpNCCI framework
– A first look at symplectic structure of light nuclei
  $^6\text{Li}$
– A simple example of convergence
  $^3\text{He}$
Structure of the NCCI spectrum of $^6\text{Li}$

JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\text{max}} = N_{\text{max}} = 6$, $\hbar\omega = 20\text{ MeV}$
Decomposition of $^6$Li states by $N_{\text{ex}}$ and $N_{\sigma,\text{ex}}$

- Panel (a): $2(4,0)\,1$
- Panel (b): $0(2,0)\,1$

**Graphs:**
- **Panel (a):** $N_{\text{ex}}$ distribution
- **Panel (b):** $N_{\sigma,\text{ex}}$ distribution

**Formulas:**
- $JISP16$ (no Coulomb), SpNCCI, $N_{\sigma,\text{max}} = N_{\text{max}} = 6$, $\hbar \omega = 20$ MeV
What we might expect for $^{6}\text{Li}$ from Elliott SU(3)

Schematic Hamiltonian $E = \alpha_1 Q \cdot Q + \alpha_2 L \cdot S + \alpha_3 \delta_{T=1}$, fit to experiment
Decomposition by \textbf{U}(3) content

Expected “valence space” \textbf{U}(3) families are indeed found ($N_{\text{ex}} = 0$)

These are “dressed” with $N_{\text{ex}} = 2, 4, \ldots$ excitations

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure.png}
\end{figure}

$^6\text{Li}$

$N_{\text{ex}}(\lambda, \mu) = 0(2, 0)$

$S = 1$ $T = 0$

JISP16 (no Coulomb), SpNCCI, $N_{\sigma, \text{max}} = N_{\text{max}} = 6$, $\hbar\omega = 20\text{MeV}$

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Decomposition by U(3) content

Expected “valence space” U(3) families are indeed found (\(N_{\text{ex}} = 0\))

These are “dressed” with \(N_{\text{ex}} = 2, 4, \ldots\) excitations

\[\begin{align*}
\text{\(6\)}\text{Li} \\
N_{\text{ex}}(\lambda, \mu) &= 0(2, 0) \\
S &= 0 \quad T = 1
\end{align*}\]
Decomposition by $U(3)$ content

Expected “valence space” $U(3)$ families are indeed found ($N_{\text{ex}} = 0$)

These are “dressed” with $N_{\text{ex}} = 2, 4, \ldots$ excitations

$\frac{6}{6} Li$

$N_{\text{ex}}(\lambda, \mu) = 0(0,1)$

$S = 1 \quad T = 1$

$E(\text{MeV})$

$J$

$JISP16$ (no Coulomb), SpNCCI, $N_{\sigma, \text{max}} = N_{\text{max}} = 6$, $\hbar \omega = 20$ MeV

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Decomposition by U(3) content

Expected “valence space” U(3) families are indeed found \((N_{\text{ex}} = 0)\)

These are “dressed” with \(N_{\text{ex}} = 2, 4, \ldots\) excitations

\[\begin{align*}
6\text{Li} \\
N_{\text{ex}}(\lambda, \mu) &= 0(0, 1) \\
S &= 0 \quad T = 0
\end{align*}\]

JISP16 (no Coulomb), SpNCCI, \(N_{\sigma,\text{max}} = N_{\text{max}} = 6, \hbar\omega = 20\text{MeV}\)
Decomposition by $\text{Sp}(3, \mathbb{R})$ content

But excited contributions primarily from same $\text{Sp}(3, \mathbb{R})$ irrep

$^6\text{Li}$

$N_{\text{ex}}(\lambda, \mu) = 0(2,0)$

$S = 1 \quad T = 0$

JISP16 (no Coulomb), SpNCCI, $N_{\sigma, \text{max}} = N_{\text{max}} = 6$, $\hbar\omega = 20\text{MeV}$
Decomposition by U(3) content

Next excitations recognizably form “2ℏω” U(3) families ($N_{ex} = 0$)

$^{6}$Li

$N_{ex}(\lambda,\mu)=2(4,0)$

$S=1 \ T=0$

JISP16 (no Coulomb), SpNCCI, $N_{\sigma,max} = N_{max} = 6$, $\hbar \omega = 20\text{MeV}$
Decomposition by \( U(3) \) content

The \( U(3) \) contents of the \( 0\hbar\omega \) and \( 2\hbar\omega \) states are quite different

\( ^6\text{Li} \)

\( N_{\text{ex}}(\lambda,\mu)=0(2,0) \)

\( S=1 \) \( T=0 \)

JISP16 (no Coulomb), SpNCCI, \( N_{\sigma,\text{max}} = N_{\text{max}} = 6, \hbar\omega = 20\text{MeV} \)
Decomposition by $\text{Sp}(3, \mathbb{R})$ content

The $\text{U}(3)$ contents of the $0\hbar\omega$ and $2\hbar\omega$ states are quite different…

But the $2\hbar\omega$ excited states lie within ground state’s $\text{Sp}(3, \mathbb{R})$ irrep.
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  $^3\text{He}$

\[ N_{\text{ex}} = 0 \quad N_{\text{ex}} = 2 \quad N_{\text{ex}} = 4 \]

Sp(3,R) $\times$ SU(2) \[ 1^+ \]

$^3\text{He} E(1/2^+)$
Convergence in the SpNCCI framework

\[ \text{\(^3\)He } E(1/2^+) \]

\[ J = \frac{1}{2} \]

\[ M\text{-scheme} \]

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

\[ N_{\text{ex}} \]

\[ A \]

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

\[ \text{JISP16, } h\omega=20 \]

\[ 0 \quad 2 \quad 4 \quad 6 \quad 8 \quad 10 \quad 12 \quad 14 \quad 16 \quad 18 \quad 20 \]

\[ 0 \quad 2 \quad 4 \quad 6 \quad 8 \quad 10 \quad 12 \quad 14 \quad 16 \quad 18 \quad 20 \]

\[ 10^0 \quad 10^1 \quad 10^2 \quad 10^3 \quad 10^4 \quad 10^5 \quad 10^6 \]
Convergence in the SpNCCI framework

\( ^3\text{He} \ E(1/2^+) \)
Convergence in the SpNCCI framework

- For $N_{\sigma,\text{max}}=2$: 
  - $^3\text{He } E(1/2^+_1)$
  - $^3\text{He } r(1/2^+_1)$

- For $N_{\sigma,\text{max}}=6$:

- For $N_{\sigma,\text{max}}=10$:

  - Highest $N_{\text{max}}$
  - $N_{\sigma,\text{max}}=N_{\text{max}}$
  - $(M$–scheme$)N_{\text{max}}$
  - Converged value
Symplectic symmetry: Summary and outlook

Framework for *ab initio* nuclear NCCI calculation in $\text{Sp}(3, \mathbb{R})$ basis

- Identify lowest-grade $U(3)$ irreps (LGIs) in $SU(3)$-NCSM space
- $SU(3)$-NCSM gives “seed” matrix elements for LGIs
- Use commutator structure to recursively calculate matrix elements

https://github.com/nd-nuclear-theory/spncci

Some very preliminary observations in light nuclei

- Confirm $\text{Sp}(3, \mathbb{R})$ as approximate symmetry
  *Mixing of a few dominant irreps*
- Families of states with similar $\text{Sp}(3, \mathbb{R})$ structure

Computational scheme to be explored and developed

- How high must we go in $N_{\sigma, \text{ex}}$ for $\text{Sp}(3, \mathbb{R})$ irreps?
- Importance truncation of basis by $\text{Sp}(3, \mathbb{R})$ irrep?
  *I.e., going beyond first baseline implementation, to take full advantage of the approximate symmetry*