Toward a Unified Description of 4n N=Z Light Nuclei in the “Ab initio” Symplectic No Core Shell Model

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Outline

1. Motivation

2. Overview of symplectic symmetry
   - Relation to $\alpha$-cluster model wave functions
   - Inclusion of highly deformed particle-hole configurations within symplectic space
   - Discussion on center of mass spuriousity

3. Expansion of symplectic states in shell model basis

4. “proof-of-principle” results
**Scale Explosion:** combinatorial growth in dimensionality of basis for heavier nuclei and increasing $N\hbar \Omega$ model spaces.

High $N\hbar \Omega$ configurations essential for:

- improving overall convergence of the spectrum
- reproducing B(E2) without effective charges
- modelling deformed and cluster modes

Yet even larger model spaces are needed!
Solution to Scale Explosion

Symplectic $Sp(3, \mathbb{R})$ symmetry-adapted basis

G. Rosensteel and D. J. Rowe, Phys. Rev. Lett. 38, 10 (1977)

Properties of symplectic basis:

✔ Complete
✔ Translationally invariant
✔ Natural for description of many-body collective dynamics
  - quadrupole and monopole vibrations
  - microscopic realization of Bohr-Mottelson model is embedded within $Sp(3,\mathbb{R})$
  - rotational dynamics in continuous range from rigid rotor to irrotational flow
✔ Appropriate for description of $\alpha$-clusters

In the classical limit symplectic symmetry underpins rotation of deformed stars and galaxies!

Reduction of Model Space

spherical harmonic oscillator basis

symplectic symmetry-adapted basis

space splits into infinite number of vertical slices

Only fraction of vertical slices are expected to be important
Sp-NCSM approach

\[ 0\hbar\Omega - 8\hbar\Omega \]

full space

m-scheme basis

\[ 10\hbar\Omega - 16\hbar\Omega \]

reduced space

\( \text{Sp}(3,\mathbb{R}) \) basis
Overview of Symplectic Sp(3,R) Symmetry

\[
\sum_n x_{ni} x_{nj} \quad \text{mass quadrupole moments}
\]
\[
\sum_n x_{ni} p_{nj} \pm x_{nj} p_{ni} \quad (-) \text{angular momentum}
\]
\[
\sum_n p_{ni} p_{nj} \quad \text{many particle kinetic energy}
\]

Collective model chain \( \text{Sp}(3, \mathbb{R}) \supset \text{GCM}(3) \supset \text{ROT}(3) \)

- impractical for expansion in terms of shell model basis

Shell model chain \( \text{Sp}(3, \mathbb{R}) \supset \text{SU}(3) \supset \text{SO}(3) \)

- expandable in harmonic oscillator basis
- labeled by Elliot's SU(3) quantum numbers \((\lambda, \mu) \leftrightarrow (\beta, \gamma)\)
Translationally invariant generators of \( \text{Sp}(3,\mathbb{R}) \) can be expressed in terms of harmonic oscillator raising and lowering operators:

\[
\begin{align*}
    b^\dagger_{ni} &= \frac{1}{\sqrt{2}} (x_{ni} - ip_{ni}) \\
    b_{ni} &= \frac{1}{\sqrt{2}} (x_{ni} + ip_{ni})
\end{align*}
\]

**2\(\hbar\Omega\) - raising operators**

\[
A_{ij} = \frac{1}{2} \sum_{n=1}^{A} b^\dagger_{ni} b^\dagger_{nj} - \frac{1}{2A} \sum_{s,t=1}^{A} b^\dagger_{si} b^\dagger_{tj}
\]

**2\(\hbar\Omega\) - lowering operators**

\[
B_{ij} = \frac{1}{2} \sum_{n=1}^{A} b_{ni} b_{nj} - \frac{1}{2A} \sum_{s,t=1}^{A} b_{si} b_{tj}
\]

**U(3) operators**

\[
C_{ij} = \frac{1}{2} \sum_{n=1}^{A} (b^\dagger_{ni} b_{nj} + b_{nj} b^\dagger_{ni}) - \frac{1}{2A} \sum_{s,t=1}^{A} (b^\dagger_{si} b_{tj} + b_{tj} b^\dagger_{si})
\]

Symplectic \( \text{Sp}(3, \mathbb{R}) \supset \text{SU}(3) \supset \text{SO}(3) \) basis is generated using raising operators \( A_{ij} \)
Construction of Shell Model Chain Basis

Basis states in symplectic “slice” are built over symplectic bandhead by action of raising operators

\[
|\lambda_\sigma \mu_\sigma\rangle \equiv (\lambda_\mu)\kappa L_\sigma J M_J \rangle = \left[\mathcal{P}^n(A_{ij}) \times |\lambda_\sigma \mu_\sigma\rangle\right]_{\kappa L_\sigma J M_J}^{\lambda_\mu}.
\]

Symplectic bandhead:
- Expandable in m-scheme basis; labeled by \((\lambda_\sigma \mu_\sigma)S_\sigma\)
- Spurious center of mass excitation free
- Annihilated by the symplectic lowering operators \(B_{ij}|\lambda_\sigma \mu_\sigma\rangle_{S_\sigma} = 0\)
Expanding Symplectic Bandheads in $m$-scheme Basis

Single fermion creation operator is $SU(3) \times SU(2)$ irreducible tensor:

$$a_{\eta_{ljm}}^\dagger = a_{ljm}^\dagger(\eta)$$

$$\left[a_{\pi}^\dagger(\eta_1 0) \times \cdots \times a_{\pi}^\dagger(\eta_Z 0)\right]^{(\lambda_\pi \mu_\pi)}_{S_\pi} \times \left[a_{\nu}^\dagger(\eta_1' 0) \times \cdots \times a_{\nu}^\dagger(\eta_N' 0)\right]^{(\lambda_\nu \mu_\nu)}_{S_\nu} \rightarrow \mathcal{P}^{(\lambda_\sigma \mu_\sigma)}_{\kappa(L_\sigma S_\sigma)J_\sigma M_\sigma}
$$

... Act with $\mathcal{P}$ on vacuum state:

$$|\left(\lambda_\sigma \mu_\sigma\right)_{\kappa(L_\sigma S_\sigma)J_\sigma M_\sigma}\rangle = \mathcal{P}^{(\lambda_\sigma \mu_\sigma)}_{\kappa(L_\sigma S_\sigma)J_\sigma M_\sigma} |0\rangle$$

to obtain a “candidate” on symplectic bandhead ... test whether:

$$B_{ij} |(\lambda_\sigma \mu_\sigma) S_\sigma\rangle = 0$$
Expanding Symplectic Bandheads in $m$-scheme Basis

This procedure does not generate translationally invariant $SU(3) \times SU(2)$ bandheads!

$$\sum_{n=0}^{N} \psi_{cm}(n) \otimes \psi_{int}(N - n)$$

Quick Fix: project out center of mass spuriosity excitations by symmetry preserving operator.

$$\hat{P}(N) = \prod_{k=1}^{N} \left( 1 - \mathcal{B}_{cm}^{\dagger} \cdot \mathcal{B}_{cm}^{k} \right)$$

center-of-mass HO raising and lowering operators

Result: center-of-mass spuriosity free bandhead ... $\psi_{cm}(0) \otimes \psi_{int}(N)$

with the same symmetry
Calculations performed in symplectic basis achieved good description of low-lying spectra and B(E2) values ... **BUT** ... with simplistic or symmetry preserving phenomenological interactions.

How badly will symplectic symmetry be broken when realistic interactions are employed?

Project NCSM eigenstates onto symplectic $Sp(3, R) \supset SU(3) \supset SO(3)$ basis.

Trivial task if we find expansion of symplectic states in terms of m-scheme basis

Example: $^4$He

\[ |2\hbar\Omega \ (2 \ 0) L=2 \ j=2 \rangle \]

\[
\begin{align*}
\frac{1}{2} | \begin{array}{cccc}
0 & 0 & \frac{1}{2} & -\frac{1}{2} \\
0 & 0 & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & -\frac{1}{2} & \frac{1}{2} \\
0 & 0 & -\frac{1}{2} & -\frac{1}{2}
\end{array} \rangle & \quad \text{proton single particle states} \\
-\sqrt{\frac{1}{5}} | \begin{array}{cccc}
0 & 0 & \frac{1}{2} & -\frac{1}{2} \\
0 & 0 & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & -\frac{1}{2} & \frac{1}{2} \\
0 & 0 & -\frac{1}{2} & -\frac{1}{2}
\end{array} \rangle & \quad \text{neutron single particle states}
\end{align*}
\]
Example: $^4\text{He}$

Start with symplectic bandhead $(0\ 0)S=0$

$$| (0\ 0) L=0J=0M_J=0 \rangle = \left[ \begin{array}{cccc} 0 & 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 1/2 & 0 & 1/2 \end{array} \right]$$

Construction formula is trivial:

$$| (2\ 0) L=2J=2M_J=2 \rangle = A_{2\ 2}^{(2\ 0)} \ | (0\ 0) L=0J=0M_J=0 \rangle$$

$$\vdots$$

$$| (2\ 0) L=0J=0M_J=0 \rangle = A_{0\ 0}^{(2\ 0)} \ | (0\ 0) L=0J=0M_J=0 \rangle$$

Apply raising operator on symplectic states generated at $2\hbar\Omega$ subspace

$$| (4\ 0) L=2J=2M_J=2 \rangle = \sqrt{\frac{4\ 0}{63}} A_{2\ 2}^{(2\ 0)} \ | (2\ 0) L=2J=2M_J=2 \rangle$$

$$+ \sqrt{\frac{2}{21}} A_{2\ 1}^{(2\ 0)} \ | (2\ 0) L=2J=2M_J=1 \rangle$$

$$+ \sqrt{\frac{7}{18}} A_{0\ 0}^{(2\ 0)} \ | (2\ 0) L=2J=2M_J=2 \rangle$$

$$+ A_{2\ 2}^{(2\ 0)} \left( \sqrt{\frac{4\ 0}{63}} \ | (2\ 0) L=2J=2M_J=0 \rangle + \sqrt{\frac{7}{18}} \ | (2\ 0) L=0J=0M_J=0 \rangle \right)$$

Symplectic states within $N\hbar\Omega$ subspace are generated using $(N-2)\hbar\Omega$ symplectic states
Constituent clusters “frozen” to ground states.

Relative motion of clusters carries $Q$ oscillator quanta.

Few facts about symplectic states and $\alpha$-cluster model wave functions:

- Deformed symplectic states possess appreciable overlaps with cluster wave functions.
- Overlap 100% for the most deformed symplectic bandheads.
- “0p-0h” $Sp(3,\mathbb{R})$ "slices" are not sufficient to reproduce $\alpha$–cluster modes.

We need to incorporate $Sp(3,\mathbb{R})$ "slices" build over highly deformed symplectic bandheads.

Results

**NCSM eigenstates:** obtained with JISP16 interaction, $N_{\text{max}}=6$ model space; $^{16}\text{O}$ and $^{12}\text{C}$

1. The ground-state band in $^{12}\text{C}$
   - reasonably well converged
   - $0\hbar\Omega$ configurations dominate

2. The ground state of $^{16}\text{O}$
   - not converged yet
   - $2\hbar\Omega$ configurations dominate
   - only a test of symplectic symmetry

3. The first $0^+$ excited state of $^{16}\text{O}$

**Sp(3,\mathbb{R}) model space includes:**

- All symplectic "slices" built over $0\hbar\Omega$ (0p-0h) and $2\hbar\Omega$ (2p-2h) bandheads
- "Slice" built over the most deformed $4\hbar\Omega$ (4p-4h) bandhead

Generated up to $N_{\text{max}}=6$ model space
Probability Distribution: Ground State 85%-90%

Only 3 “slices” built over 0p-0h bandheads: 80%
“slices” built over 2p-2h bandheads: 5%

Single (0 0) “slice”: 75%
“slices” built over 2p-2h bandheads: 10%
Probability Distribution: $2^+$ and $4^+$

Only 3 “slices” built over 0p-0h bandheads: 80%

“slices” built over 2p-2h bandheads: 4%
Spin Distribution in NCSM eigenstates

(a) $J=0$

(b) $J=2$

(c) $J=4$

(d) $J=0$
Independence of Oscillator Strength

- 6 spin S=0 symplectic “slices” compose 95% of S=0 component of NCSM eigenstates
- Independent of oscillator strength
- Same results for the bare interaction

Symplectic symmetry is not altered by Lee-Suzuki transformations
Major Reduction in Model Space

Reduction of model space size:

10^{-5} for $^{12}$C

10^{-6} for $^{16}$O

... and gets even better for higher model spaces....
the most dominant $Sp(3,R)$ slices reproduce NCSM results
Deformations present within NCSM eigenstates

Near oblate deformed shapes dominate:
(0 4), (1 2), (0 2), (2 4)

Area $\propto$ probability of given symplectic states
Deformations present within NCSM eigenstates

Spherical shape dominates: (0 0)

Prolate deformation present: (2 0), (4 0) and (6 0)

Area $\propto$ probability of given symplectic states
Deformations present within NCSM eigenstates

First $0^+$ excited state of $^{16}$O

Interplay between $0\hbar\Omega$ (blue) and $2\hbar\Omega$ symplectic “slices” (red)

4p-4h symplectic slices negligible

Area $\propto$ probability of given symplectic states
Ab-initio No Core Shell Model: successfully reproduces (low-lying) features of the deuteron, alpha particle, $^{12}\text{C}$ and even $^{12}\text{O}$

Comparison of converged NCSM eigenstates with Sp(3,R)-symmetric states shows:

- Reproduction of NCSM results by a few Sp(3,R) states
  - ✔ 85%-90% overlaps
  - ✔ 100% $\text{B}(\text{E2}; 2_1^+ \rightarrow 0_1^+)$

- Dramatic reduction in model space (several orders of magnitude)

Symplectic-NCSM: effective model space reduction scheme.