Ab Initio NS Studies
Underpinned and Enhanced
by
Symmetry Considerations

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NCSM versus ‘Symmetry Adapted’ NCSM

NCSM (multi-\(\hbar\omega\))
- Horizontal discs (all configurations)
- (0\(\hbar\omega\)) limit

SA-NCSM*
(multi-\(\hbar\omega\))
- Vertical slices (monopole & quadrupole collective excitations)
- 0\(\hbar\omega\) SU(3) limit

*Complete (= NCSM) if/when all irreps are included, but down select to physically relevant subset …

\(N_{\text{max}}\)
Historical Backdrop (60s - 90s) –
* Majority of algebraic (group theoretical) work done
* Modest applications restricted to 0hω model space
* Single irrep results get E2 with no effective charge

Most Recent History (90s - 00s) –
* Group theory / data structures are complementary
* NCSM suggested / enabled proof-of-principle tests
* Parallel architecture natural to irrep decomposition
* Balanced use of Fast CPUs and massive storage

Next Generation Plans (10s - ??) –
* Fast CPUs, massive storage, advanced languages
* Balanced use of fast CPUs and massive storage
* Clever “kids” - physics / computer scientist unite
Symmetry-Adapted Configuration
Interaction Developments

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Motivation:
- utilize nuclear collective correlations in ab initio approaches

SU(3)-scheme basis
- relevant for description of spatially deformed nuclei
- $(\lambda \mu)$ related to shape variables $\beta$ and $\gamma$ of the collective model
- embedded in the symplectic model of the nuclear collective motion
- SU(3) contains rotational group SO(3) as a subgroup

**SU(3) classification scheme**

$SU(3) \supset SO(3)$

$(\lambda \mu) \rightarrow L$ orbital angular momentum

k multiplicity label – needed to distinguish multiple occurrence of L

SU(3) quantum numbers

**Example:** $(4 2)$
- $\kappa = 0$  $L = \{0, 2, 4, 5, 6\}$
- $\kappa = 1$  $L = \{2, 4\}$
**Construction of SU(3) symmetry-adapted basis in NCSM**

**Step 1**
- Generate distributions of nucleons over HO shells for a given Nmax model space

\[ N_{\text{max}} = \begin{array}{c}
  p & f \\
  s & d \\
  p & s
\end{array} \]

**Step 2**
- for each set of nucleons in a HO shell determine antisymmetric representations of U(N)xU(2)

\[ U(2) \otimes U(10) \]

**Step 3**
- decompose each U(N) irrep into a complete set of SU(3) irreps

\[ \lambda \mu \]

**Example:**
- 4 nucleons in pf

\[ S=0 \]

\[ S=1 \]

\[ S=2 \]

"seeds"
Step 4

- Complete Nmax basis constructed by inter-shell SU(3) & spin coupling of "seeds"

![Graph of Number of "seeds" representations vs Nmax for various elements]

Step 5

- LS-coupling → J-coupled proton-neutron basis labeled by spin \( S_p \) \( S_n \) \( S \) and deformations \((\lambda, \mu)\)

- SU(3)-scheme basis is not translationally invariant
SU(3)-scheme decomposes model space into subspaces of states labeled by $S_p S_n S$ ($\lambda \mu$)

The center-of-mass HO can not mix $S_p S_n S$ ($\lambda \mu$)

c.m. spurious states can be removed from each subspace exactly

Truncation according to intrinsic spin $S_p S_n S$

Spin-decomposition of ground state band wavefunctions in $^{12}$C [Nmax=6 model space]
Many-body Collective Dynamics in SU(3)-scheme

- Sp(3,R): symmetry of the nuclear collective dynamics

\[ 6 \rightarrow \sum_n x_{ni}x_{nj} \quad \text{mass monopole and quadrupole moments} \]

\[ 9 \rightarrow \sum_n x_{ni}p_{nj} \pm x_{nj}p_{ni} \quad (-) \text{angular momentum} \]

\[ 6 \rightarrow \sum_n p_{ni}p_{nj} \quad (+) \text{monopole and quadrupole deformations} \]

\[ 21 \text{ generators} \]

- quadrupole and monopole vibrations and deformations

- rotational dynamics from rigid rotor to irrotational flow

SU(3) is a subgroup of Sp(3,R) symplectic basis states are labeled by \((\lambda \mu)\) and also by \(S_pS_nS\)

Symplectic Sp(3,R) symmetry matches deformed geometry [SU(3)] with the various modes of the nuclear collective dynamics
Many-body Collective Dynamics in SU(3)-scheme

Symplectic symmetry reorganizes SU(3) & spin subspaces

Validation runs: JISP16, \( N_{\text{max}}=6 \), \( h\omega=10\text{MeV} \)

- resulting binding energies agree with \( m \)-scheme based MFDn calculations
- ground states of \( 6\text{Li}, 7\text{Li}, 12\text{C} \) dominated by the spin & SU(3) subspaces of the leading Sp(3,\( \mathbb{R} \)) representations

Biggest run: \( J=0 \) in \( 12\text{C} \), \( N_{\text{max}}=6 \)
12C ground state leading configurations

\[ S_p = 0 \quad S_n = 0 \quad S = 0 \]

collective dynamics & geometry

spin guided selection rules

symplectic Sp(3, R) symmetry guided selection rules

SU(3) symmetry guided selection rules

\( (\lambda \mu) : \lambda \geq \mu \)

\( 0 \hbar \Omega \quad 2 \hbar \Omega \quad 4 \hbar \Omega \quad 6 \hbar \Omega \)

50.29% 24.05% 15.00% 10.66%
$^{12}$C ground state next-to-leading configurations

- Spin guided selection rules:
  - $Sp=1 \; Sn=0 \; S=1$
  - $Sp=1 \; Sn=0 \; S=1$

- Symplectic $Sp(3, R)$ symmetry guided selection rules:

- SU(3) symmetry guided selection rules:

$$\begin{pmatrix} \lambda & \mu \end{pmatrix} : \lambda \geq \mu$$
\( \lambda \mu : \lambda \geq \mu \)

Spin

\[ S_p = 1 \quad S_n = 1 \quad S = 2 \]

Collective dynamics & geometry

Mixed

12C ground state next-to-next-to-leading configurations
$^{12}\text{C}: J = 0^+_2$

- **All six spin components highly mixed**
- **Not a Hoyle state**

### Energy Levels

- $0^+_2$: $47.69\%$
- $2^+_2$: $25.54\%$
- $4^+_2$: $15.53\%$
- $6^+_2$: $11.24\%$
$^{12}$C: $J = 0^+$

Spin:
- $S_p = 0$ $S_n = 1$ $S = 1$
- $S_p = 1$ $S_n = 0$ $S = 1$

Collective dynamics & geometry:

Symplectic (1 2) representation:

- $S_p = 0$ $S_n = 1$ $S = 1$
- $S_p = 1$ $S_n = 0$ $S = 1$
- $S_p = 1$ $S_n = 1$ $S = 1$
- $S_p = 1$ $S_n = 2$ $S = 3$
- $S_p = 2$ $S_n = 1$ $S = 3$

Remaining $S_p$ $S_n$ $S$:

- $S_p = 0$ $S_n = 1$ $S = 1$
- $S_p = 1$ $S_n = 0$ $S = 1$
- $S_p = 1$ $S_n = 1$ $S = 1$
- $S_p = 1$ $S_n = 2$ $S = 3$
- $S_p = 2$ $S_n = 1$ $S = 3$

Frequency distribution:

- $0\hbar\Omega$: 54.77%
- $2\hbar\Omega$: 20.57%
- $4\hbar\Omega$: 13.40%
- $6\hbar\Omega$: 10.26%
some $Sp\ Sn\ S (\lambda \mu)$ spaces contain $\alpha$-cluster correlations

Example: $^{12}\text{C}$

\[
\phi^{(4,0)}(r_1, \ldots , r_8) \quad \phi^{(0,0)}(r_9, \ldots , r_{12})
\]

Relative motion

$\phi_{cm}^{(n,0)}(R)$

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cluster correlations
$^{12}\text{C} \ J = 0^+_6$: leading configurations

Spin

$S_p = 0 \ S_n = 0 \ S = 0$

Collective dynamics & geometry

Symplectic (0 4) representation

Cluster correlations

$^8\text{Be} + ^4\text{He}$
$E_{N_{\text{max}}=4}^{0^+} - E_{N_{\text{max}}=6}^{0^+} = 13$ MeV

$E_{N_{\text{max}}=4}^{2^+} - E_{N_{\text{max}}=6}^{2^+} = 9$ MeV

Nmax = 4: 0$_7$$_7$

Nmax = 6: 0$_6$$_6$
methods for evaluation of a realistic NN interaction in SU(3)-scheme developed and validated

SU(3) & spin truncation keeps ability to factorize the center-of-mass motion exactly

SU(3)-scheme has a potential to include important many-body correlations spanning high Nmax model spaces

Outlook:
- Code(s) improvements: data structures, hybrid MPI/openMP version, etc ...
- three-body interactions in SU(3)-scheme
- inclusion of the symplectic configurations for large model spaces