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Convergence in the ab initio symplectic no-core configuration interaction framework

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TRIUMF, Canada

Nuclear Theory in the Supercomputing Era
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Outline

- SU(3) No-core shell model (SU(3)-NCSM)
- Symplectic no-core configuration interaction (SpNCCI) framework
- Convergence in SpNCCI
- Truncations by $\mathrm{Sp}(3,\mathbb{R})$ irreps

SU(3)-NCSM

SU(3) generators

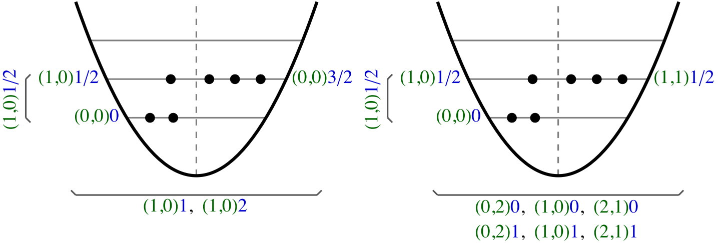
Q_{2M}	*Algebraic quadrupole*
L_{1M}	*Orbital angular momentum*

$$\begin{array}{ccccc} \mathrm{SU}(3) & \supset & \mathrm{SO}(3) & & \\ (\lambda,\mu) & \kappa & L & & \\ & & \otimes & \supset & \mathrm{SU}(2) \\ & & \mathrm{SU}(2) & & J \\ & & S & & \end{array}$$

(λ,μ) SU(3) irrep label

κ SU(3) to SO(3) branching multiplicity

L SO(3) orbital angular momentum



<u>SU(3) symmetry of a configuration</u>

- SU(3) coupling particles within major shells
  Each particle has SU(3) symmetry $(N,0)$,
  $N = 2n + \ell$.
- SU(3) coupling successive shells
- SU(3) coupling protons and neutrons

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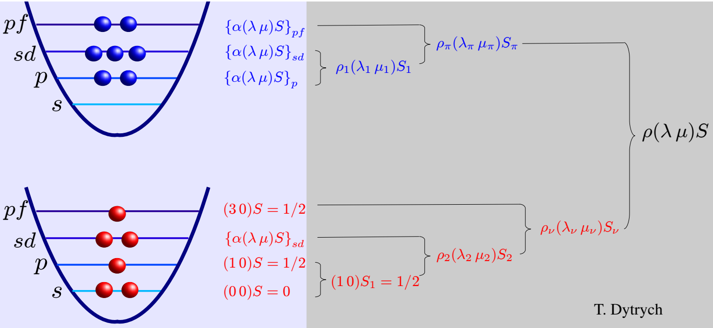


There are many $\mathrm{SU}(3)\times\mathrm{SU}(2)$ irreps in SU(3)-NCSM basis with the same $(\lambda,\mu)S$

(λ,μ)	SU(3) irrep label
κ	SU(3) to SO(3) branching multiplicity
L	SO(3) orbital angular momentum

$\mathrm{Sp}(3,\mathbb{R})$

$\mathrm{Sp}(3,\mathbb{R})$ generators can be grouped into ladder and U(3) operators

$A^{(20)}$	$\sim b^\dagger b^\dagger$	*Raises N*
$H^{(00)}, C^{(11)}$	$\sim b^\dagger b$	U(3) *generators*
$B^{(02)}$	$\sim bb$	*Lowers N*

Start from a single U(3) irrep at lowest “grade" N

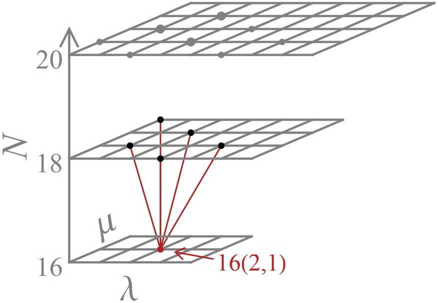
Lowest grade irrep (LGI)

Ladder upward in N using $A^{(20)}$ *No limit!*

$$B^{(02)}\,|\sigma\rangle = 0$$

$$|\psi^\omega\rangle \sim [A^{(20)}A^{(20)}\cdots A^{(20)}\,|\sigma\rangle]^\omega$$

$$\underset{\sigma}{\mathrm{Sp}(3,\mathbb{R})} \underset{\upsilon}{\supset} \underset{\omega}{\mathrm{U}(3)} \qquad \underset{\omega}{\mathrm{U}(3)} \sim \underset{N_\omega}{\mathrm{U}(1)} \otimes \underset{(\lambda_\omega,\mu_\omega)}{\mathrm{SU}(3)}$$



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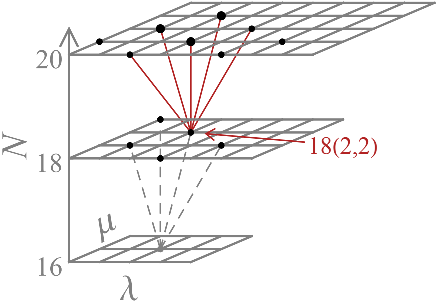

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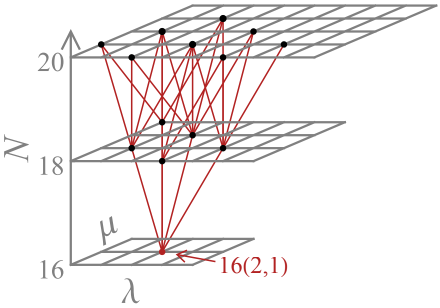
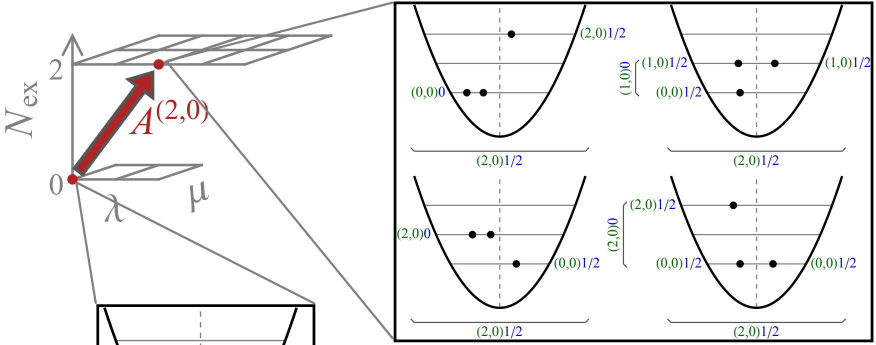
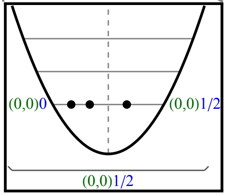


Sp(3,R) raising operator on configurations





Sp(3,R) basis states are highly correlated

States are linear combinations of many different oscillator configurations

Symplectic many-body basis

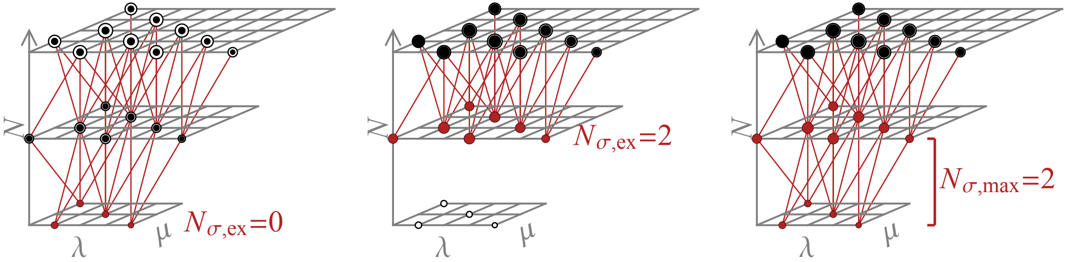
– Reorganize many-body basis into $\mathrm{Sp}(3,\mathbb{R})$ irreps

States are linear combinations of oscillator configurations

– Select a set of symplectic irreps, e.g., keep only irreps whose LGI have $N_{\mathrm{ex}} \leq N_{\sigma,\mathrm{max}}$

$N_{\sigma,\mathrm{max}}$ *truncation*

– Within each irrep, only states with total number of excitation quanta $N_{\mathrm{ex}} \leq N_{\mathrm{max}}$ are included



Calculations in a symplectic basis

- Expand $Sp(3,\mathbb{R})$ states in terms of SU(3)-NCSM states
  - Diagonalize $Sp(3,\mathbb{R})$ Casimir operator in SU(3)-coupled basis (SA-NCSM)

    T. Dytrych et al., J. Phys. G: Nucl. Part. Phys. **35** (2008) 123101.
    T. Dytrych et al., Phys. Rev. Lett.**111** (2013) 252501.
  - Expand LGI in SU(3)-coupled basis. Repeatedly apply raising operator.

    F. Q. Luo, Ph.D. thesis, University of Notre Dame (2014).
- Expand matrix elements between excited states in terms of matrix elements between less excited states using operator commutators
  - Reduce calculation to sum over coefficients and LGI matrix elements

    Y. Suzuki and K. T. Hecht, Nuc. Phys. A **455** (1986) 315.
    E. Reske, Ph. D. thesis, University of Michigan (1984).
  - Recurrence relation between one-body matrix elements.

    J. Escher and J. P. Draayer, J. Math. Phys. **39** (1998) 51223.

SpNCCI framework

1. Decompose Hamiltonian in terms of fundamental relative operators $\boldsymbol{\mathcal{U}(a,b)}$

$$H = \sum \underbrace{\langle a \| H \| b \rangle}_{\text{Relative RMEs}} \mathcal{U}(a,b)$$

A unit tensor $\mathcal{U}(a,b)$ is an operator with a single “unit" non-zero reduced matrix element defined with respect to a basis. *Two- or three-body relative harmonic oscillator basis*

$$\langle a' \| \mathcal{U}(a,b) \| b' \rangle = \delta_{a',a}\delta_{b',b}$$

SpNCCI framework

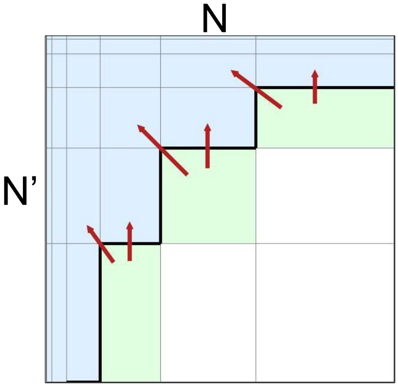
2. Compute the matrix elements of the unit tensors $\mathcal{U}(a,b)$ in the symplectic many-body basis

$$\langle \psi'_{N'} | \mathcal{U}(a,b) | \psi_N \rangle = \sum_{\bar{\psi}'_{\bar{N}'}, \bar{\psi}_{\bar{N}} cd} \langle \bar{\psi}'_{\bar{N}} | \mathcal{U}(c,d) | \bar{\psi}_{\bar{N}} \rangle$$

Recall : $\psi_N \propto A\psi_{N-2}$

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

Express commutator in terms of other unit tensors $[\mathcal{U}, A] \propto \sum \mathcal{U}$



SpNCCI framework

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2. Compute the matrix elements of the unit tensors $\mathcal{U}(a,b)$ in the symplectic many-body basis

$$\langle\psi'_{N'}|\mathcal{U}(a,b)|\psi_N\rangle = \sum_{\bar{\psi}'_{\bar{N}'},\bar{\psi}_{\bar{N}}cd} \langle\bar{\psi}'_{\bar{N}}|\mathcal{U}(c,d)|\bar{\psi}_{\bar{N}}\rangle$$

3. Construct the Hamiltonian matrix by combing the decomposition of the Hamiltonian in terms of unit tensor with matrix elements of relative unit tensors.

$$\langle\psi'_{N'}|H|\psi_N\rangle = \sum_{ab} \langle a\|H\|b\rangle \langle\psi'_{N'}|\mathcal{U}(a,b)|\psi_N\rangle$$

Symplectic many-body basis

- Reorganize many-body basis into $\mathrm{Sp}(3,\mathbb{R})$ irreps

  States are linear combinations of oscillator configurations

- Select a set of symplectic irreps, e.g., keep only irreps whose LGI have $N_{\mathrm{ex}} \le N_{\sigma,\mathrm{max}}$

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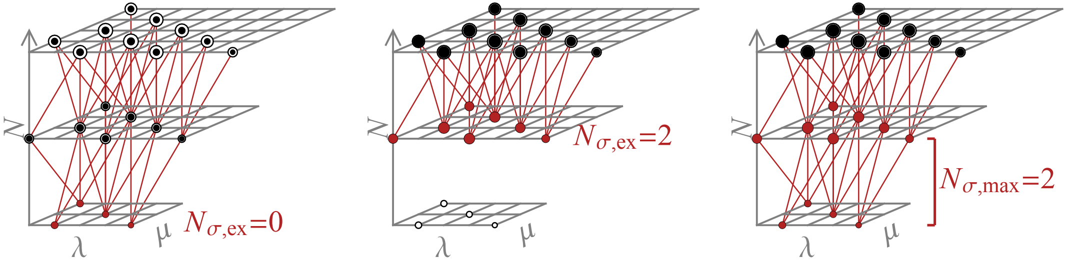
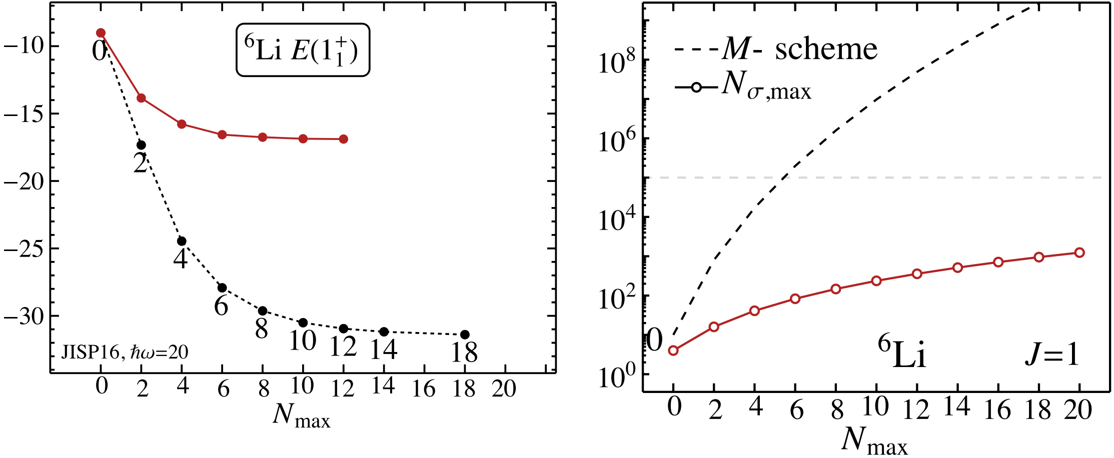


Convergence in the SpNCCI framework



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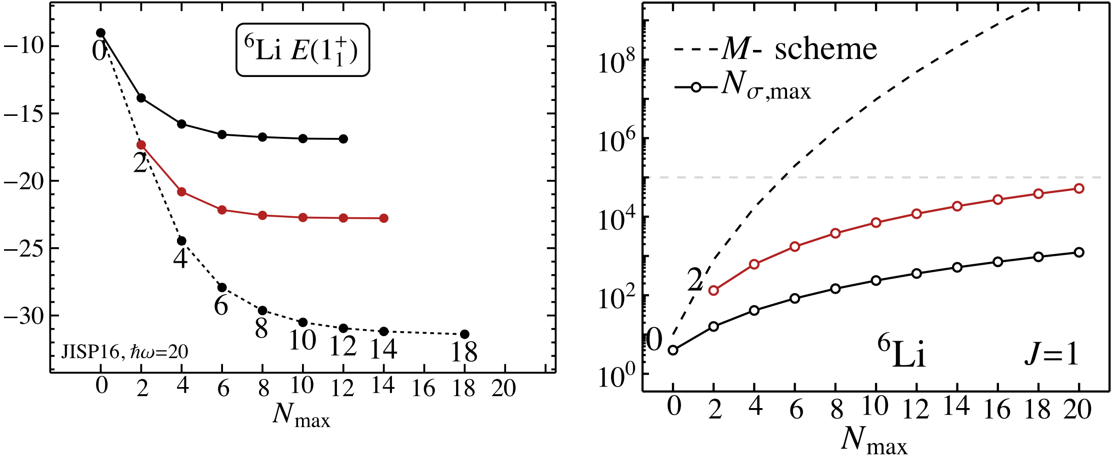
Convergence in the SpNCCI framework



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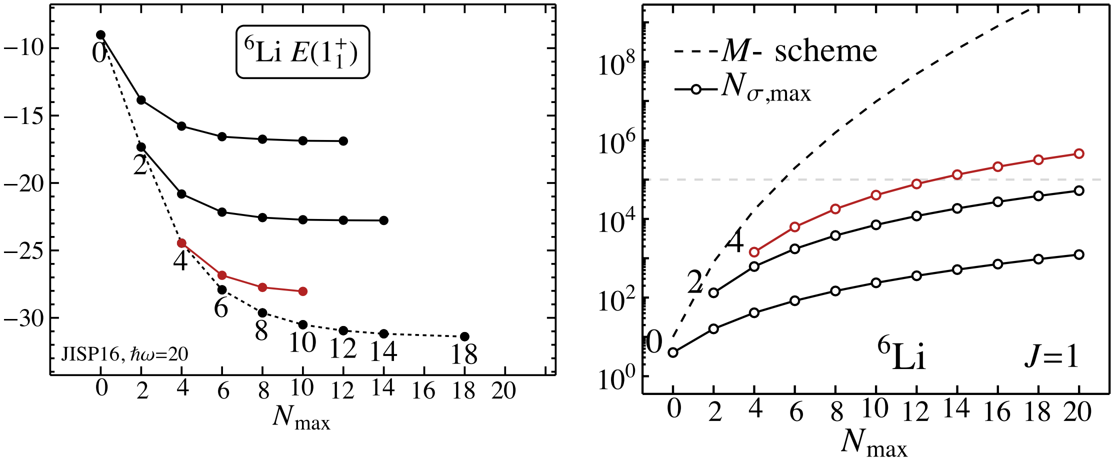

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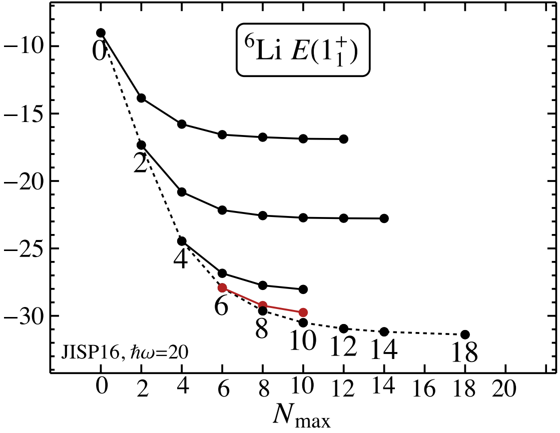

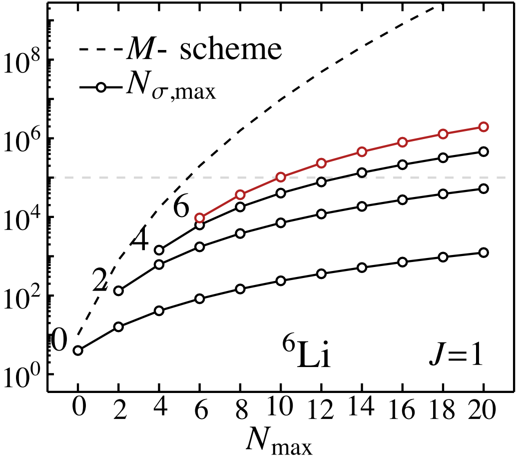

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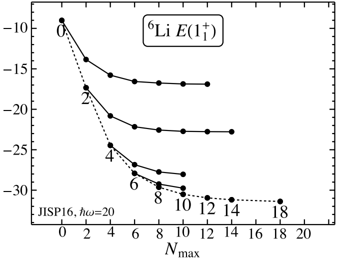

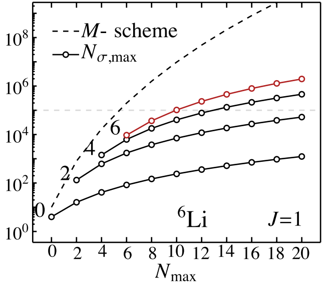

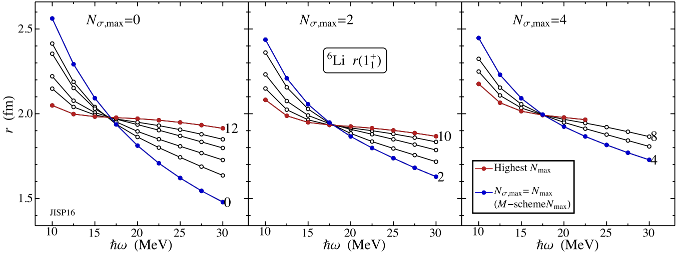

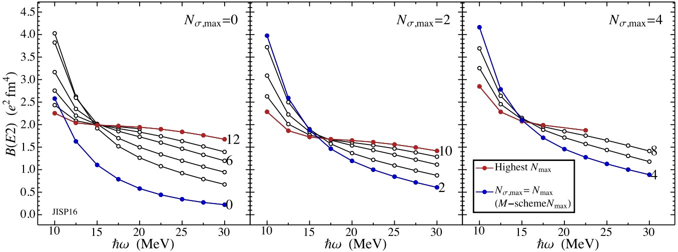

Convergence in the SpNCCI framework

- Results converge with respect to $N_{\max}$ and $\hbar\omega$ within each $N_{\sigma,\max}$ space but not necessarily to actual value

- To get convergence with respect to $\mathrm{Sp}(3,\mathbb{R})$ irreps included, we need higher $N_{\sigma,\max}$

- Convergence is achieved when results do not change as more irreps are included

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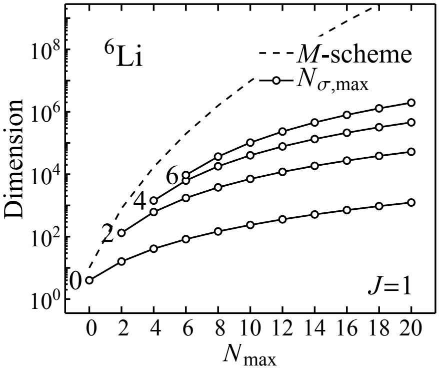
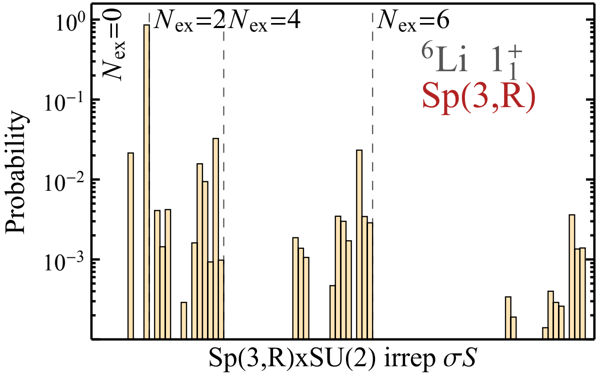
Sp(3, ℝ) decomposition

- The ^{6}Li ground state is dominantly a single irrep Sp(3, ℝ) (≈ 86%)
- Only a subset of the Sp(3, ℝ) irreps contribute at more than 0.01%
- SpNCCI basis can be further truncated by specific irreps





Trucating by Sp(3,$\mathbb{R}$) irreps

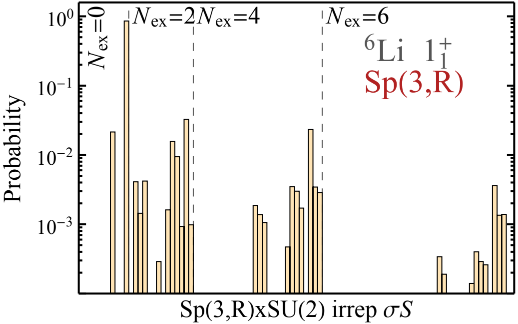
Truncation by Sp(3,$\mathbb{R}$) **subspaces**: Accumulate wavefunction amplitudes over states with same Sp(3,$\mathbb{R}$) labels σS. (SA-NCSM, SpNCCI)

Keep all Sp(3,$\mathbb{R}$) *irreps with the same labels σS.*

Truncation by Sp(3,$\mathbb{R}$) irrep: Accumulate amplitudes over states belonging to a single Sp(3,$\mathbb{R}$) irrep (SpNCCI)

Truncate within σS subspaces

May need to transform to "Hamiltonian preferred" basis



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Generating the recurrence seeds *LSU3Shell*

Expand LGI in terms of SU(3)-NCSM basis states:

$$\underbrace{B^{(0,2)}_{\text{intr}}\,|\sigma S\rangle}_{\text{Identify LGI}} = 0 \qquad \underbrace{N^{(0,0)}_{\text{cm}}\,|\sigma S\rangle = 0}_{\text{Ensure LGI is CMF}}$$

– Solve for simultaneous null space

– Null vectors are center-of-mass free LGI

– Set of Null vectors are arbitrary

Apply unitary transformation to set of LGI (null vectors) to get Hamiltonian preferred LGIs

$$\left[\begin{array}{ccc}
\langle 0\sigma S||N^{(0,0)}_{\text{cm}}||0\sigma S\rangle & \cdots & \langle 0\sigma S||N^{(0,0)}_{\text{cm}}||\eta_{\max}\sigma S\rangle \\
\vdots & & \vdots \\
\langle \eta_{\max}\sigma S||N^{(0,0)}_{\text{cm}}||0\sigma S\rangle & \cdots & \langle \eta_{\max}\sigma S||N^{(0,0)}_{\text{cm}}||\eta_{\max}\sigma S\rangle \\
\hdashline
\langle 0\omega S||B^{(0,2)}_{\text{intr}}||0\sigma S\rangle & \cdots & \langle 0\omega S||B^{(0,2)}_{\text{intr}}||\eta_{\max}\sigma S\rangle \\
\langle 1\omega S||B^{(0,2)}_{\text{intr}}||0\sigma S\rangle & \cdots & \langle 1\omega S||B^{(0,2)}_{\text{intr}}||\eta_{\max}\sigma S\rangle \\
\vdots & & \vdots \\
\langle \eta'_{\max}\omega S||B^{(0,2)}_{\text{intr}}||0\sigma S\rangle & \cdots & \langle \eta'_{\max}\omega S||B^{(0,2)}_{\text{intr}}||\eta_{\max}\sigma S\rangle \\
\hdashline
\langle 0\omega' S||B^{(0,2)}_{\text{intr}}||0\sigma S\rangle & \cdots & \langle 0\omega' S||B^{(0,2)}_{\text{intr}}||\eta_{\max}\sigma S\rangle \\
\vdots & & \vdots
\end{array}\right]$$

Defining Hamiltonian preferred LGI

- Do low $N_{\max}$ calculation to get trial wavefunction
- Basis consists of sets states $|\gamma\sigma\upsilon\omega\kappa LSJ\rangle$ with the same symmetry labels σ and S but belonging to different irreps indexed by γ.
- For each σS, regroup into matrix where rows are index by γ and columns correspond to states in each irrep.
- Do SVD decomposition to get unitary transformation for LGI null vectors.

$$\begin{bmatrix} \\ \dots \\ \sigma S \\ \dots \\ \\ \end{bmatrix} \longrightarrow \underbrace{\begin{array}{cc} & \upsilon\omega\kappa L \\ \gamma & \begin{bmatrix} \quad & \quad \\ \quad & \quad \end{bmatrix} \end{array}}_{\sigma S}$$

Trucating by Sp(3,ℝ) irreps

Truncation by Sp(3,ℝ) **subspaces**: Accumulate wavefunction amplitudes over states with same Sp(3,ℝ) labels σS. (SA-NCSM, SpNCCI)

Keep all Sp(3,ℝ) *irreps with the same labels* σS.

Truncation by Sp(3,ℝ) irrep: Accumulate amplitudes over states belonging to a single Sp(3,ℝ) irrep (SpNCCI)

Truncate within σS *subspaces*

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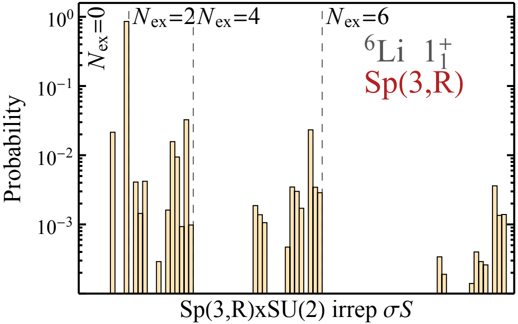
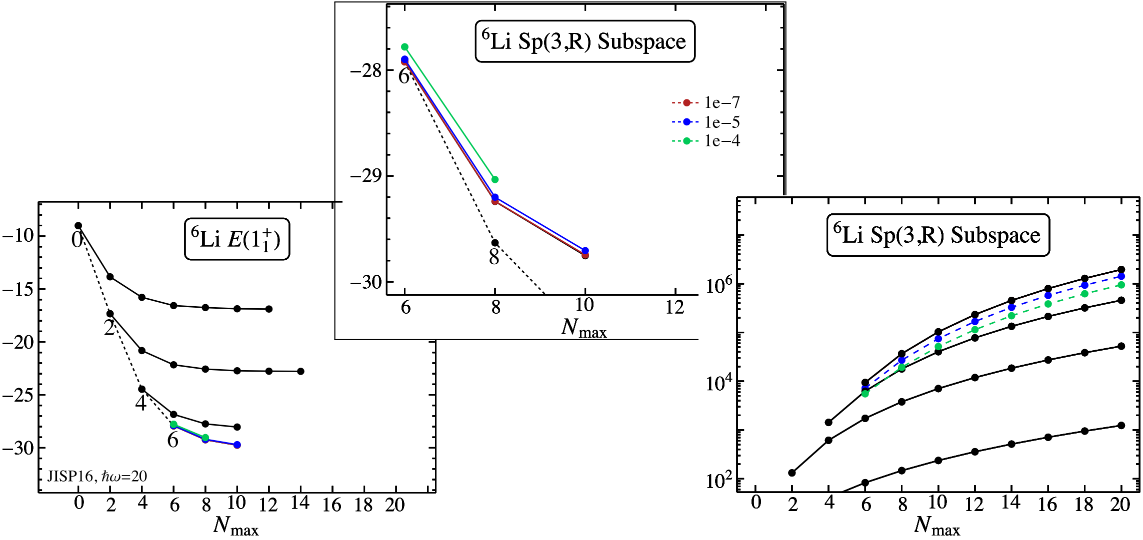
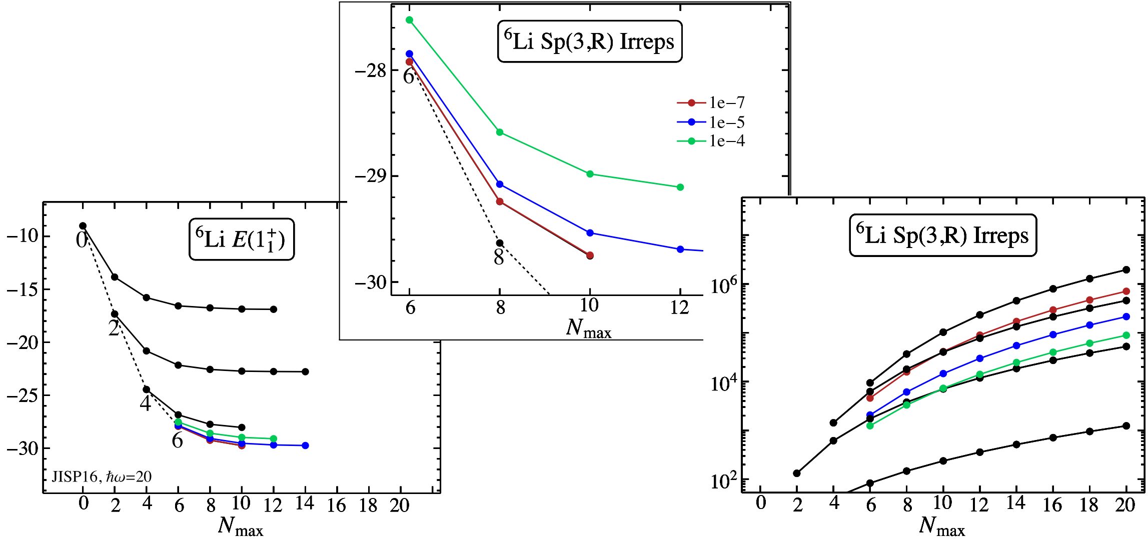


Truncations by Sp(3,ℝ) Subspaces



Truncations by Sp(3, ℝ) Irreps



Summary

- To obtain accurate binding energies (and other observables) it is necessary to include high $N_{\sigma,\text{ex}}$ irreps. ($N_{\sigma,\text{ex}} = 10, 12\ldots$)
- Not all $\text{Sp}(3,\mathbb{R})$ irreps at each $N_{\sigma,\text{ex}}$ significantly contribute
- Truncation by $\text{Sp}(3,\mathbb{R})$ irreps can significantly reduce the basis size

Going Forward...

- Develop systematic truncation methods *Importance truncation*
- Consider alternative methods for obtaining LGI unitary transformation
- MPI parallelize spncci
- Include three-body interactions

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