Symplectic no-core configuration interaction framework for *ab initio* nuclear structure

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From Bound States to the Continuum
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Overview

Symplectic symmetry for *ab initio* calculations

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

D. J. Rowe, *Microscopic theory of the collective nuclear model*, Rep. Prog. Phys. **48**, 1419 (1985).

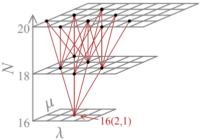
⇒ T. Dytrych, K. D. Sviratcheva, J. P. Draayer, C. Bahri, and J. P. Vary, J. Phys. G: Nucl. Part. Phys. **35**, 123101 (2008).

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

A. E. McCoy, Ph.D. thesis, University of Notre Dame (2018).
A. E. McCoy, M. A. Caprio, and T. Dytrych, Ann. Acad. Rom. Sci. Ser. Chem. Phys. Sci. **3**, 17 (2018), **arXiv:1605.04976**.
`https://github.com/nd-nuclear-theory/spncci`



Outline

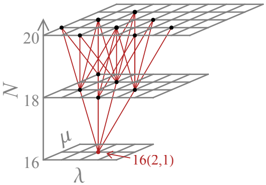
– Symplectic symmetry and the SpNCCI framework

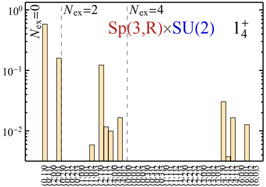
– A first look at symplectic structure of light nuclei

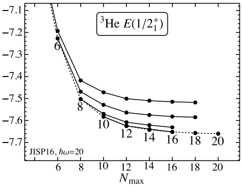
^{6}Li

– A simple example of convergence

^{3}He







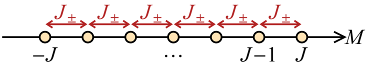
Working with symmetries

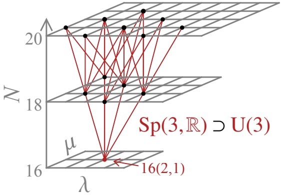
States are classified into "irreducible representations" (irreps)

Set of states connected by laddering action of generators

$J_\pm\,|JM\rangle \propto |J(M\pm1)\rangle$ *Ladder*

$J_0\,|JM\rangle = M\,|JM\rangle$ 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* $M_{\max} \equiv J$

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

J=0	0	0
0	J=2	0
0	0	J=4

Why 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 SU(3) tensors...

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

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

Kinetic energy is linear combination of generators

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

$$T = H^{(00)}_{00} - \sqrt{\tfrac{3}{2}} A^{(20)}_{00} - \sqrt{\tfrac{3}{2}} B^{(20)}_{00}$$

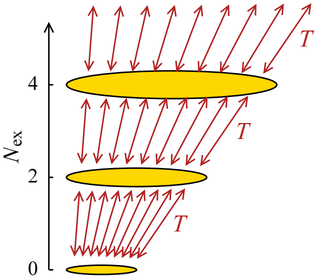
Symplectic reorganization of the many-body space

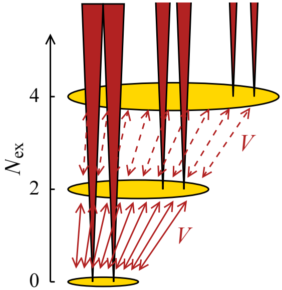
- *Recall:* Kinetic energy connects configurations with $N'_{\mathrm{ex}} = N_{\mathrm{ex}} \pm 2$
- But kinetic energy does not connect different $\mathrm{Sp}(3,\mathbb{R})$ irreps

$$T = H^{(00)}_{00} - \sqrt{\tfrac{3}{2}} A^{(20)}_{00} - \sqrt{\tfrac{3}{2}} B^{(20)}_{00}$$

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

By how much? How high in N_{ex} will irrep mixing be significant?





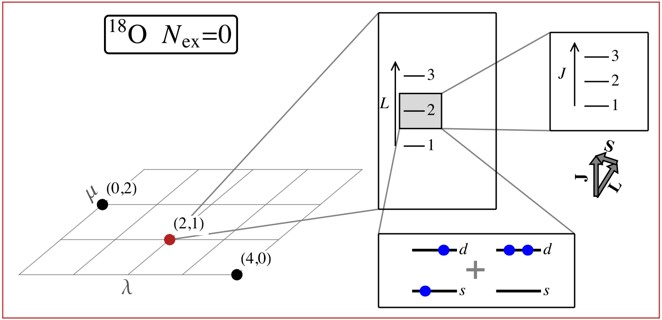
Elliott SU(3) symmetry

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

$$L_M^{(1)} \sim (b^\dagger \times \tilde{b})_M^{(1)} \qquad Q_M^{(2)} \sim (b^\dagger \times \tilde{b})_M^{(2)}$$

States classified into SU(3) irreps (λ,μ)

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



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) $\quad U(\nu) \supset U(3)$
- 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*

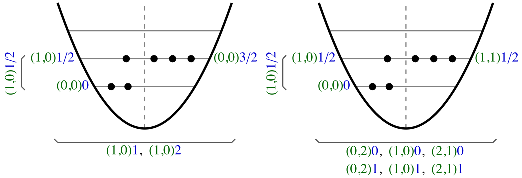
T. Dytrych *et al.*, Comput. Phys. Commun. **207**, 202 (2016).

T. Dytrych, computer code `LSU3shell`, `http://sourceforge.net/projects/lsu3shell`.

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

Center-of-mass: Factorizes within each $U(3) \times SU(2)$ subspace ωS $[= N(\lambda\mu)S]$

F.Q. Luo, M. A. Caprio, T. Dytrych, Nucl. Phys. A 897, 109 (2013).



Building an Sp(3, ℝ) irrep

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

$A^{(20)} \sim b^\dagger b^\dagger$	*"Raising"*	$\Delta N = +2$
$H^{(00)}, C^{(11)} \sim b^\dagger b$	U(3) *generators*	$\Delta N = 0$
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Start from single SU(3) irrep at lowest "grade" N

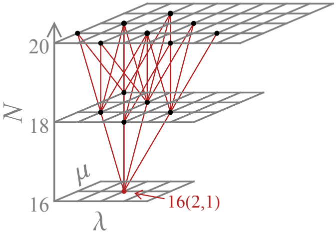
Lowest grade irrep (LGI)

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

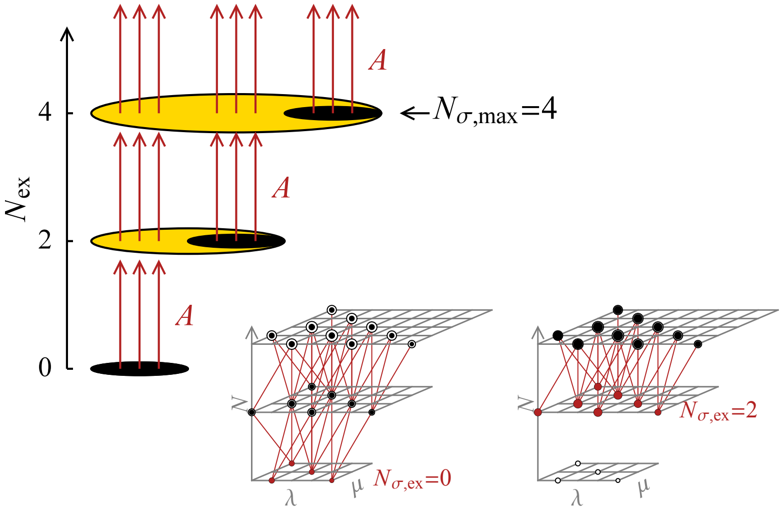
$$B^{(02)}|\sigma\rangle = 0$$

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

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



Building up the SpNCCI many-body space

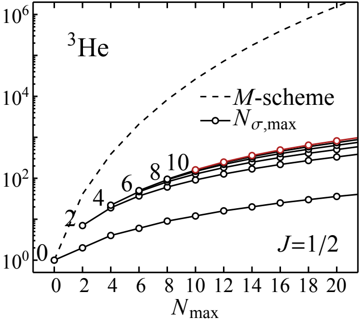


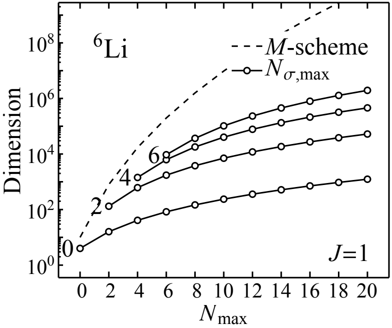
SpNCCI dimensions in $N_{\sigma,\max}$ truncation

– Take all $\mathrm{Sp}(3,\mathbb{R})$ irreps with $\mathrm{U}(3)\times\mathrm{SU}(2)$ LGIs through $N_{\sigma,\max}$

– Truncate each of these irreps at $N_{\max}$ excitation quanta

– For $N_{\sigma,\max} = N_{\max}$: Maps to the center-of-mass free subspace of the traditional NCCI $N_{\max}$ space *Benchmark!*





Construction of LGIs for SpNCCI $\mathrm{Sp}(3,\mathbb{R})$ irreps

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

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

    E.g., $\mathrm{Sp}(3,\mathbb{R})$ *importance truncation?*

Recursive scheme for SpNCCI matrix elements

Expand Hamiltonian in terms of fundamental SU(3) "unit tensor" operators $\mathcal{U}^{N_0(\lambda_0,\mu_0)}(a,b)$

Analogous to second-quantized expansion of two-body operators in terms of two-body matrix elements: $H \propto \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|H|\gamma\delta\rangle\, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$

$$H = \sum \langle a\|H^{N_0(\lambda_0,\mu_0)}\|b\rangle\, \mathcal{U}^{N_0(\lambda_0,\mu_0)}(a,b)$$

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

Compute matrix elements of $\mathcal{U}$ between LGIs using SU(3)-NCSM

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

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

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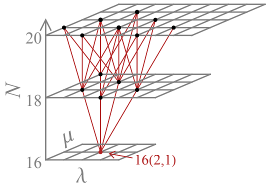
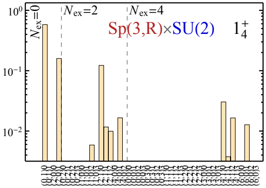
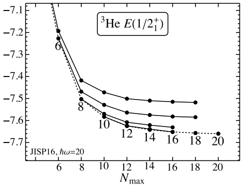
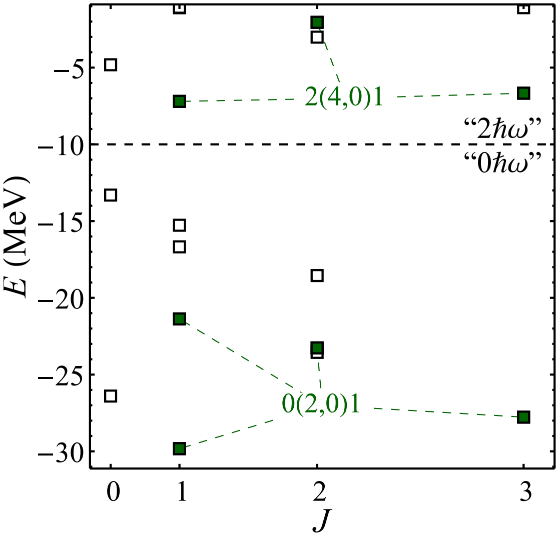






Structure of the NCCI spectrum of ^{6}Li



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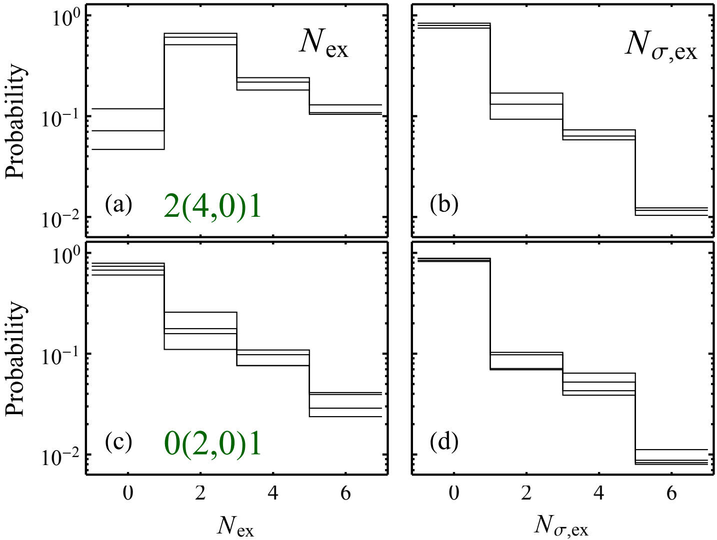
JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\mathrm{MeV}$

Decomposition of ^{6}Li states by N_{ex} and $N_{\sigma,ex}$



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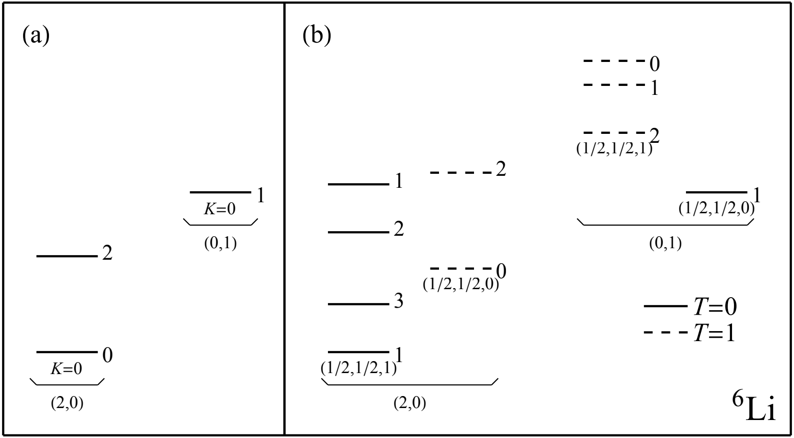
What we might expect for ^{6}Li from Elliott SU(3)



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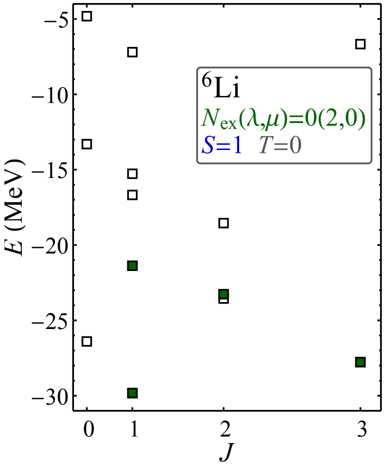
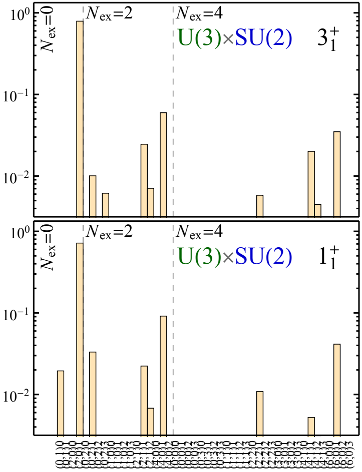
Schematic Hamiltonian $E = \alpha_1 Q \cdot Q + \alpha_2 L \cdot S + \alpha_3 \delta_{T=1}$, fit to experiment

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





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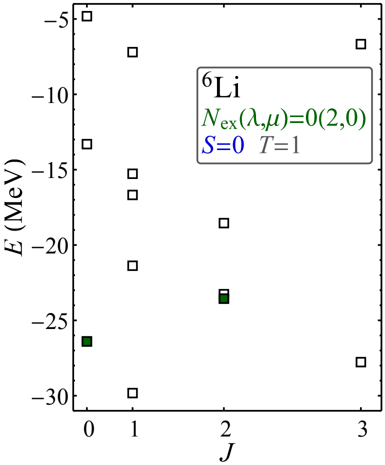

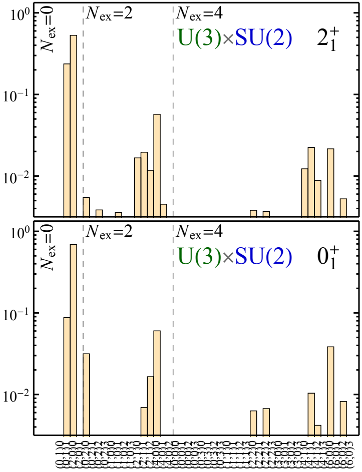

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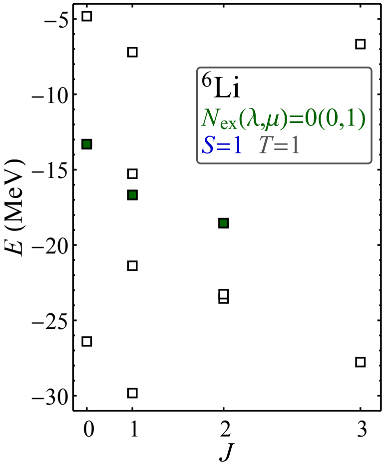

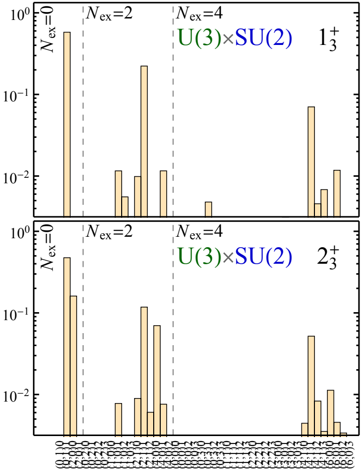

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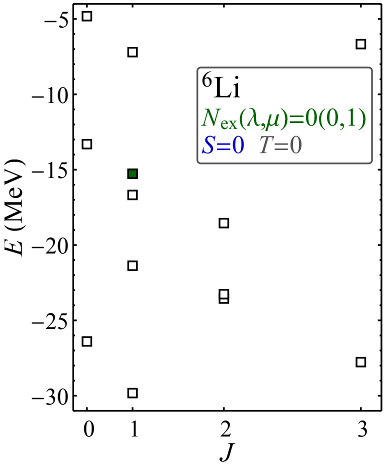

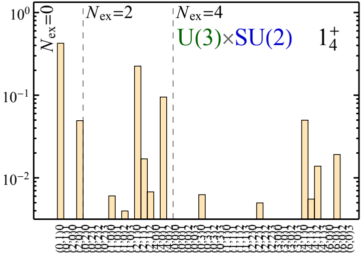

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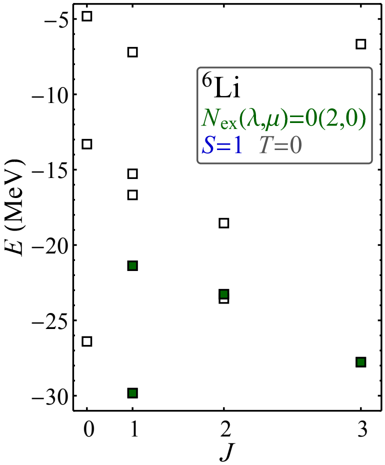
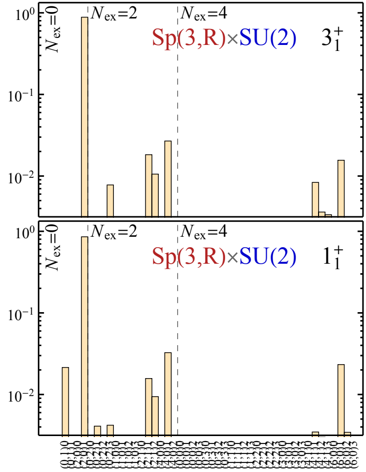
Decomposition by Sp(3,ℝ) content

But excited contributions primarily from same Sp(3,ℝ) irrep





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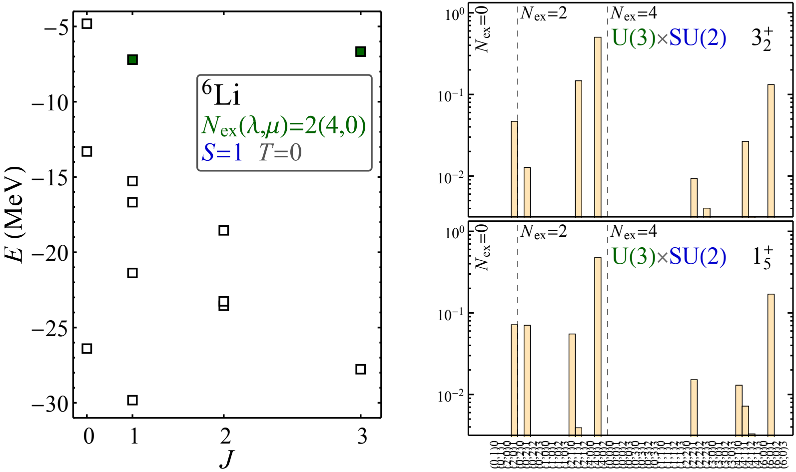
Decomposition by U(3) content

Next excitations recognizably form "$2\hbar\omega$" U(3) families ($N_{\mathrm{ex}} = 0$)



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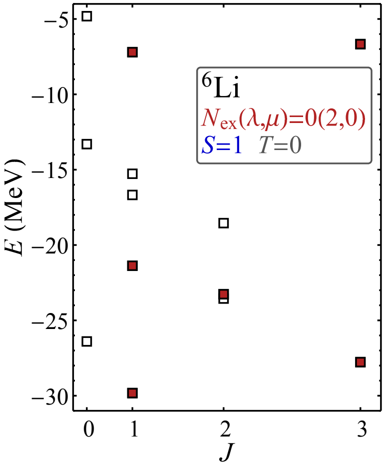
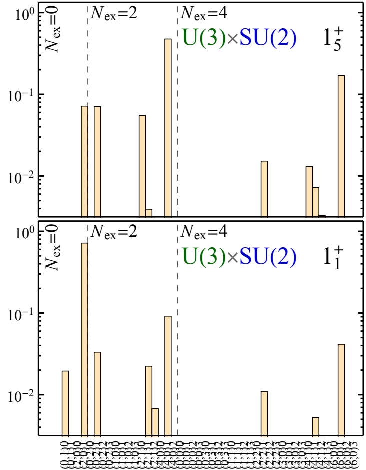
Decomposition by U(3) content

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





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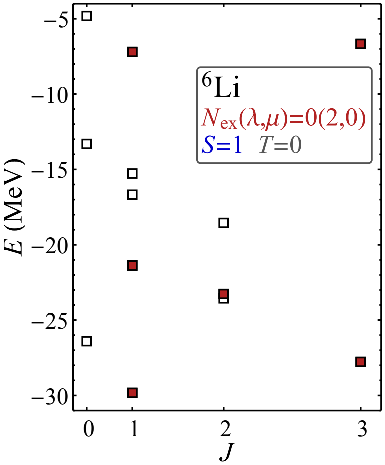
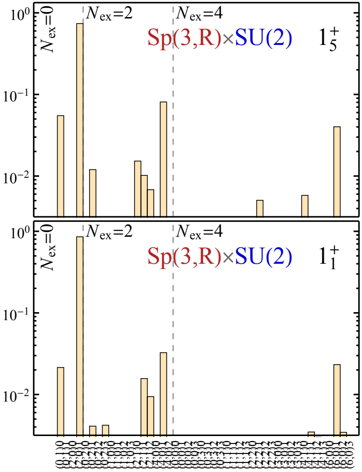
Decomposition by $Sp(3,\mathbb{R})$ content

The 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 $Sp(3,\mathbb{R})$ irrep





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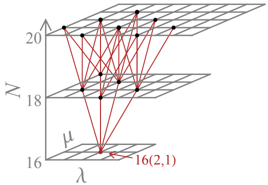
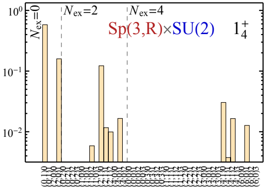
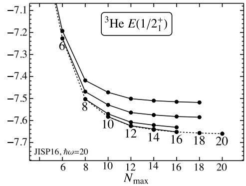
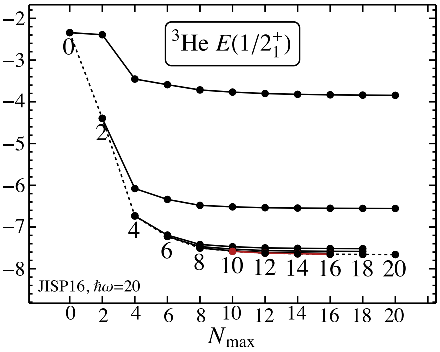
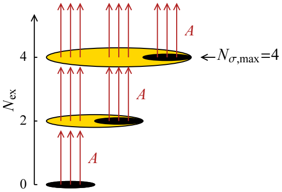


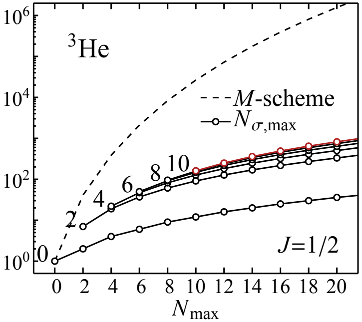




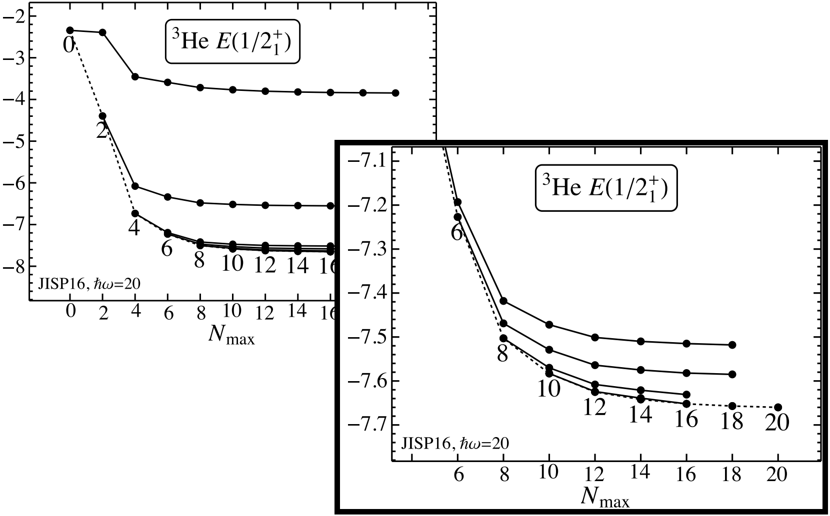
Convergence in the SpNCCI framework



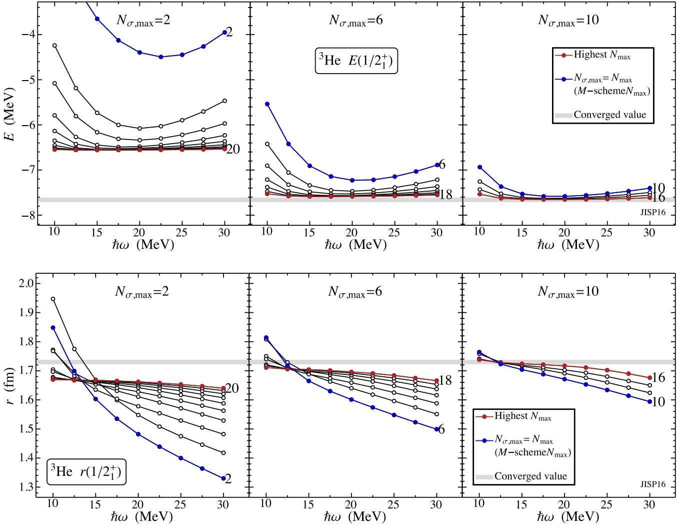




Convergence in the SpNCCI framework



Convergence in the SpNCCI framework

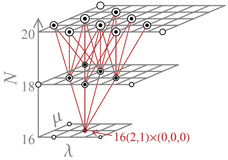


Symplectic symmetry: Summary and outlook

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

- Identify lowest-grade U(3) irreps (LGIs) in SU(3)-NCSM space
- SU(3)-NCSM gives "seed" matrix elements for LGIs *At low* N_{ex}
- Use commutator structure to recursively calculate matrix elements

A. E. McCoy, Ph.D. thesis, University of Notre Dame (2018).
`https://github.com/nd-nuclear-theory/spncci`



Some very preliminary observations in light nuclei

- Confirm $\mathrm{Sp}(3,\mathbb{R})$ as approximate symmetry

  Mixing of a few dominant irreps

- Families of states with similar $\mathrm{Sp}(3,\mathbb{R})$ structure

A. E. McCoy, M. A. Caprio, and T. Dytrych, Ann. Acad. Rom. Sci. Ser. Chem. Phys. Sci. **3**, 17 (2018), **arXiv:1605.04976**.

Computational scheme to be explored and developed

- How high must we go in $N_{\sigma,\mathrm{ex}}$ for $\mathrm{Sp}(3,\mathbb{R})$ irreps?
- Importance truncation of basis by $\mathrm{Sp}(3,\mathbb{R})$ irrep?

I.e., going beyond first baseline implementation, to take full advantage of the approximate symmetry