Symplectic framework for *ab initio* nuclear structure. I. Symplectic symmetry

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Symplectic symmetry for *ab initio* nuclear theory?

T. Dytrych *et al.*, Phys. Rev. Lett. **98**, 162503 (2007).
T. Dytrych *et al.*, J. Phys. G: Nucl. Part. Phys. **35**, 123101 (2008).

[T]he symplectic group, $Sp(3,\mathbb{R})$, emerges as the appropriate dynamical group for a many-body theory of collective motion. The fact that the symplectic group is also a dynamical group for the harmonic oscillator, which plays a central role in the shell model, facilitates the construction of a remarkably powerful symplectic shell model formalism. . . The ultimate goal of diagonalising a realistic many-nucleon Hamiltonian in a $Sp(3,\mathbb{R}) \supset SU(3)$ shell model basis, to obtain a fully microscopic description of collective states from first principles, and then to use the $Sp(3,\mathbb{R})$ 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).

Overview

Symplectic no-core configuration interaction (SpNCCI) framework

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. (submitted), **arXiv:1605.04976**.
https://github.com/nd-nuclear-theory/spncci

Introduces correlated many-body basis for nuclear problem

Encodes an approximate $\mathrm{Sp}(3,\mathbb{R})$ *symmetry of the nucleus*

Our aims in pursuing symplectic many-body symmetry:

- To use symmetry to accelerate convergence of *ab initio* results
- To understand the symmetries underlying many-body correlations in nuclei

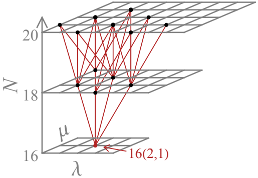
Outline

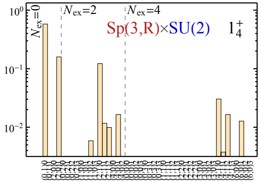
– Symplectic symmetry methods

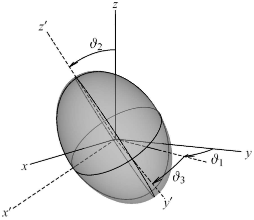
 ⇒ *Symplectic no-core configuration interaction framework*

– SU(3) and symplectic symmetry structure of ^{6}Li

– *Ab initio* rotation and symplectic symmetry in ^{7}Be







No-core configuration interaction (NCCI) approach

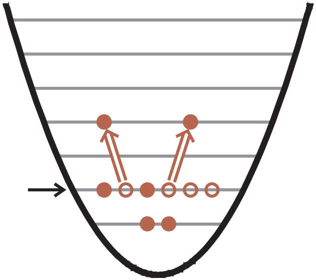
P. Navratil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).

- Begin with orthonormal single-particle basis: 3-dim harmonic oscillator
- Construct many-body basis from product states (Slater determinants)
- Basis state described by distribution of nucleons over oscillator shells
- Basis must be truncated: N_{max} truncation by oscillator excitations
- Results depend on truncation N_{max}

Convergence towards exact result with increasing N_{max}

$N_{\mathrm{tot}} = \sum_i N_i = N_0 + N_{\mathrm{ex}}$

$N_{\mathrm{ex}} \leq N_{\mathrm{max}}$ $\qquad N = 2n + l$



Structure of Hamiltonian in oscillator space

NCCI Hamiltonian $H = T_{\text{intr}} + V$

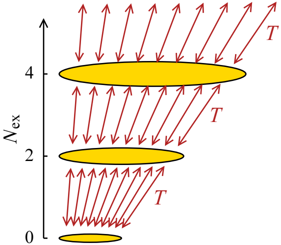
Interaction matrix elements fall off with N_{ex}

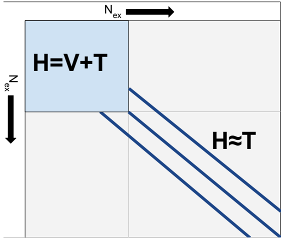
Kinetic energy has form $T \sim p^2 \sim b^\dagger b^\dagger + b^\dagger b + bb$

– Connects configurations with $N'_{\text{ex}} = N_{\text{ex}}, N_{\text{ex}} \pm 2$ *("tridiagonal")*

– Matrix elements *grow* $\propto N_{\text{ex}}$

Kinetic energy responsible for "mixing in" contributions from high-N_{ex} configurations





Symmetries in nuclei

Fundamental symmetries

- Rotation [SU(2)] & parity $\Rightarrow$ J, P

Approximate symmetries of the many-body problem

- Isospin [SU(2)] & Wigner spin-isospin [SU(4)]
- Pairing quasispin symmetries: SU(2), SO(5), …
- Phase space (or oscillator) symmetries: Elliott SU(3) & $\mathrm{Sp}(3,\mathbb{R})$

But symmetries are broken, so... Why symmetries?

- Identifying and characterizing emergent correlations

  E.g., isospin multiplets, Elliott rotation

- Symmetry as computational tool $H = H^{(0)}_{symm} + H'$

  "Right" basis for decomposing and truncating many-body space

$\mathrm{Sp}(3,\mathbb{R})$ conserved by kinetic energy!

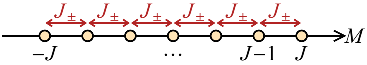
Working with symmetries

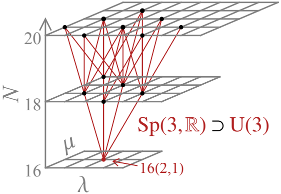
States are classified into "irreducible representations" (irreps)

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-Eckhart theorem *Clebsch-Gordan*
- Commutators ⇒ Recurrence relations

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

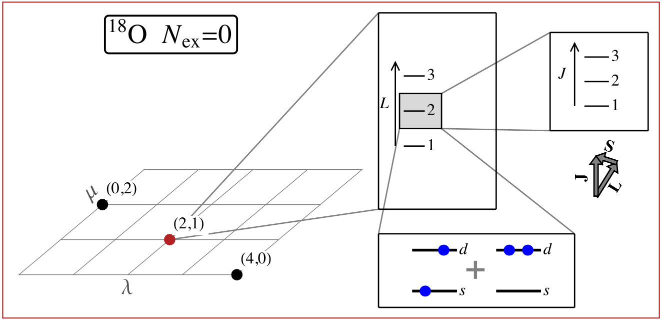
Elliott SU(3) symmetry

Generators of SU(3) ⊃ SO(3)

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

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

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



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...

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

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

Kinetic energy is linear combination of generators

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

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

Symplectic reorganization of the many-body space

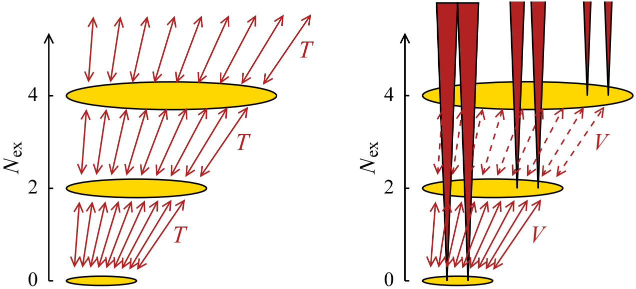
– *Recall:* Kinetic energy connects configurations with $N'_{\mathrm{ex}} = N_{\mathrm{ex}} \pm 2$

– 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?



Building an Sp(3,ℝ) irrep

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

$A^{(20)}$	$\sim b^\dagger b^\dagger$	*"Ladder"*	*Raises N*
$H^{(00)}, C^{(11)}$	$\sim b^\dagger b$	*"Weight"*	U(3) *generators* ($\Delta N = 0$)
$B^{(02)}$	$\sim bb$	*"Ladder"*	*Lowers N*

Start from single SU(3) irrep at lowest "grade" N

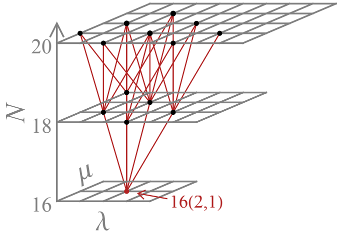
Lowest grade irrep (LGI)

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

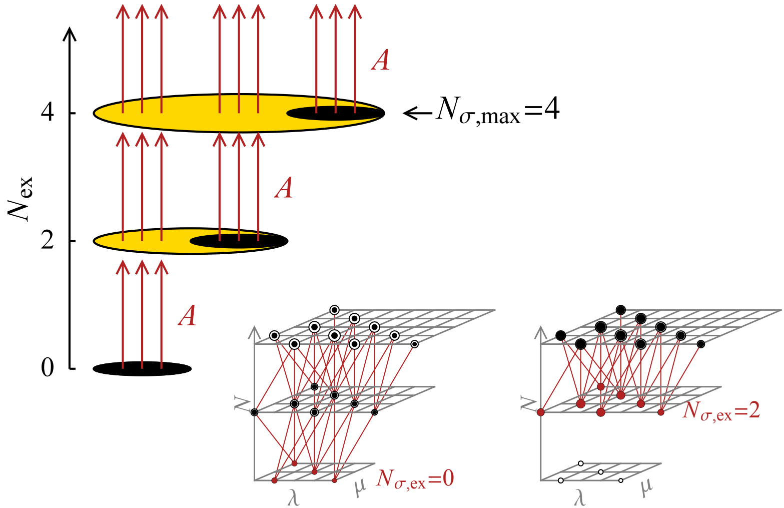
$$B^{(02)}|\sigma\rangle = 0$$

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

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



Building up the SpNCCI many-body space



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 and $c_a^\dagger c_b^\dagger c_c c_d$

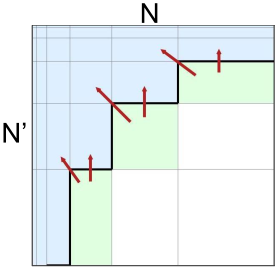
$$H = \sum \langle a\|H^{N_0(\lambda_0,\mu_0)}\|b\rangle\, \mathcal{U}^{N_0(\lambda_0,\mu_0)}(a,b)$$

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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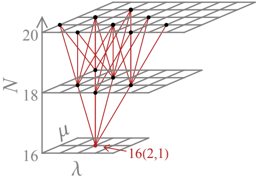
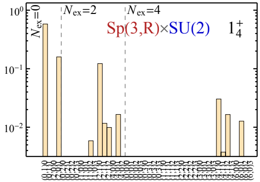
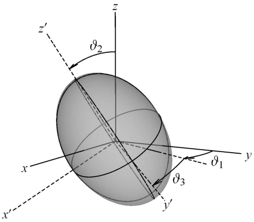
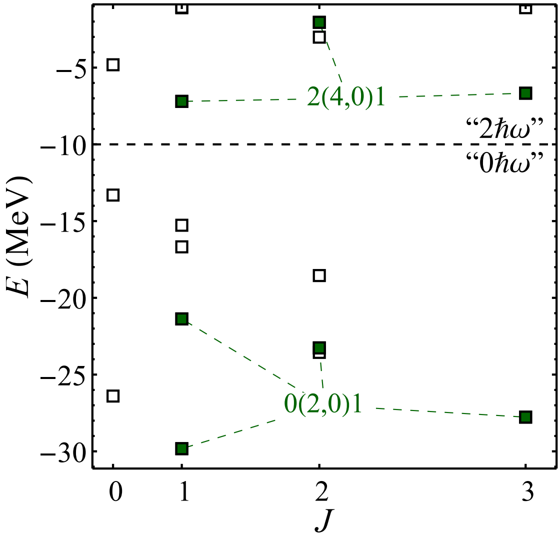






Structure of the NCCI spectrum of ^{6}Li



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

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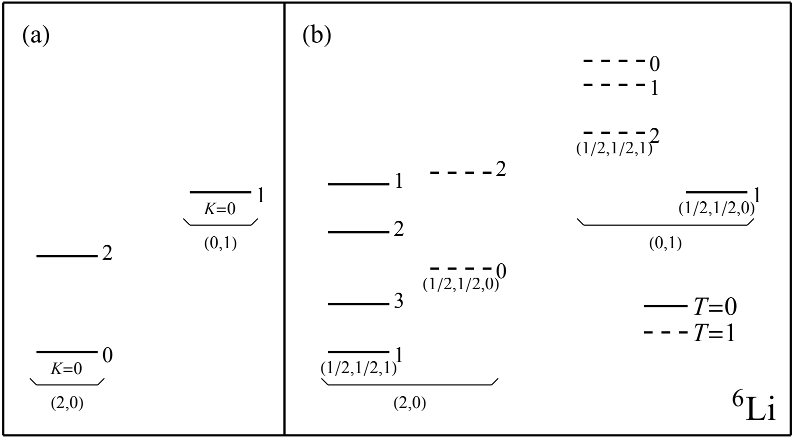
What we might expect for ^{6}Li from Elliott SU(3)



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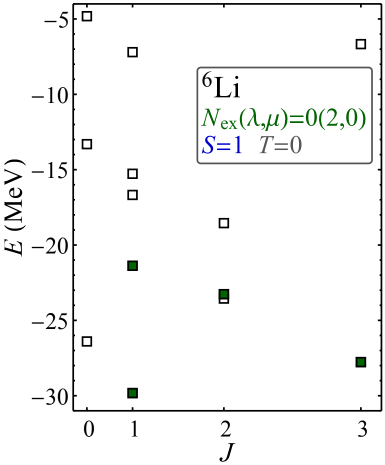
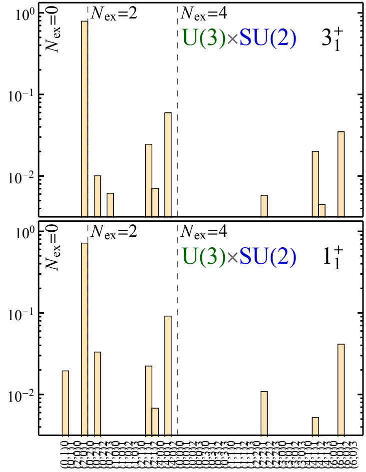
Schematic Hamiltonian $E = \alpha_1 Q \cdot Q + \alpha_2 L \cdot S + \alpha_3 \delta_{T=1}$, fit to experiment

Decomposition by U(3) content

Expected "valence space" U(3) families are indeed found ($N_{\mathrm{ex}} = 0$)





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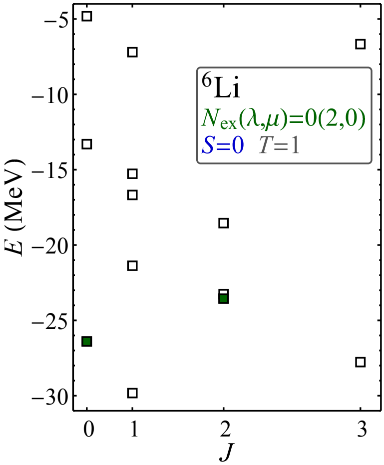

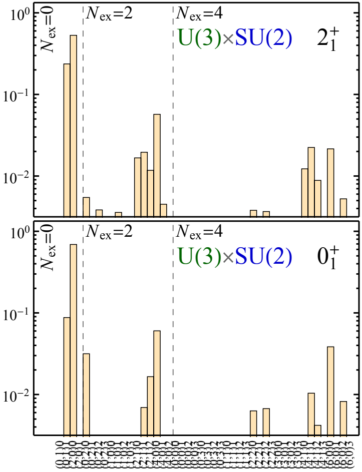

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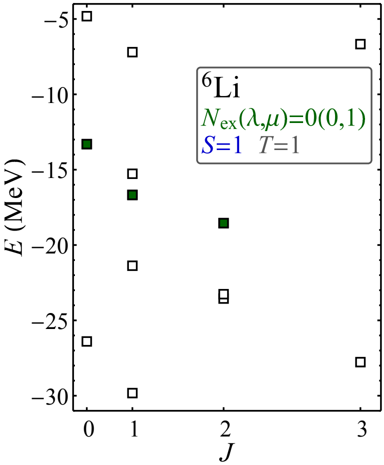

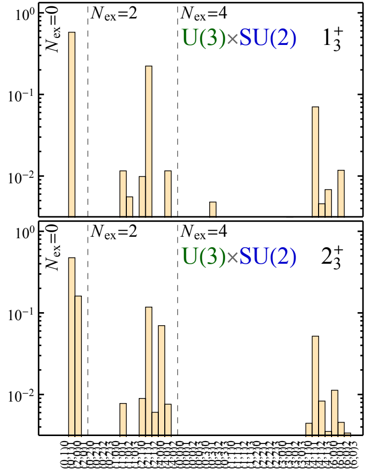

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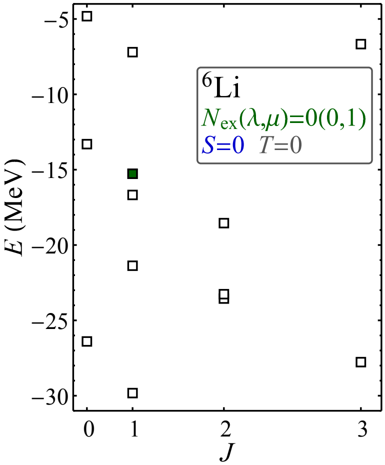
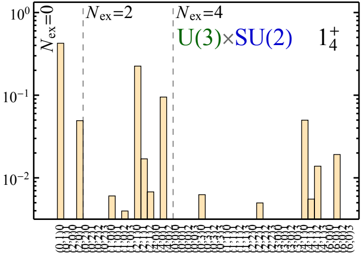
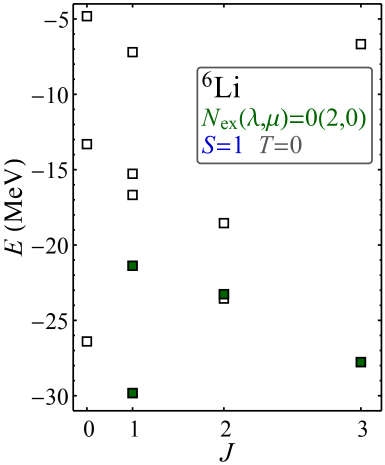


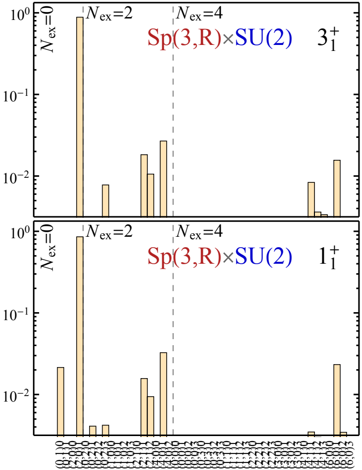


JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\text{MeV}$

Decomposition by Sp(3,ℝ) content

These are "dressed" with $N_{\mathrm{ex}} = 2, 4, \ldots$ excitations,
but excitations are primarily within same Sp(3,ℝ) irrep

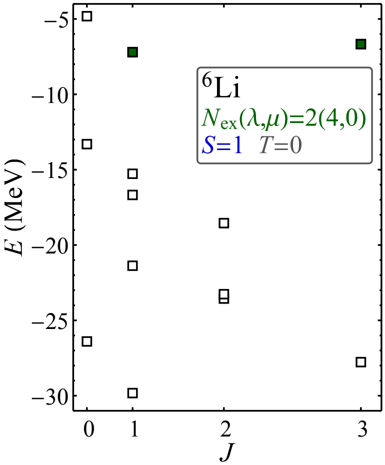


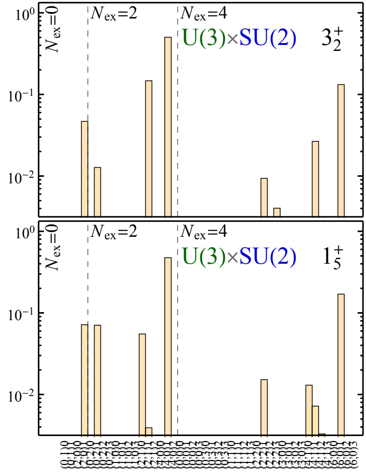


JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\mathrm{MeV}$

Decomposition by U(3) content

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

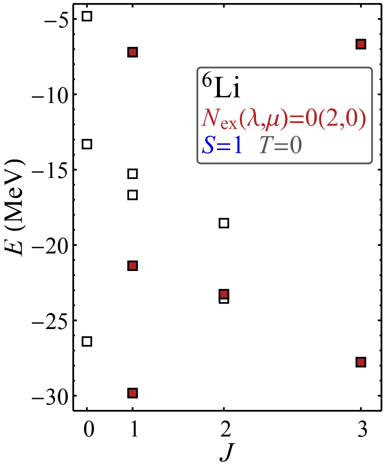


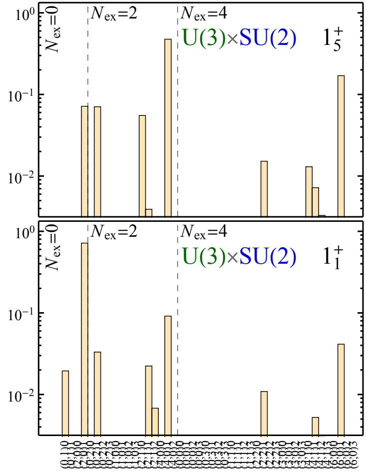


JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\text{MeV}$

Decomposition by U(3) content

The U(3) content is quite different…





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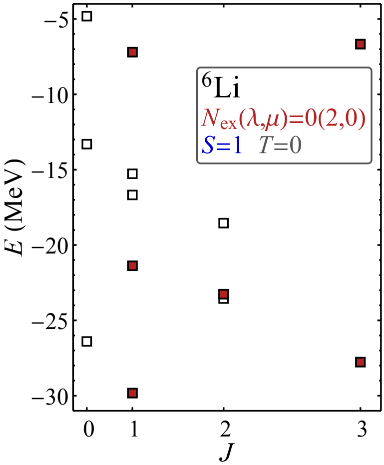
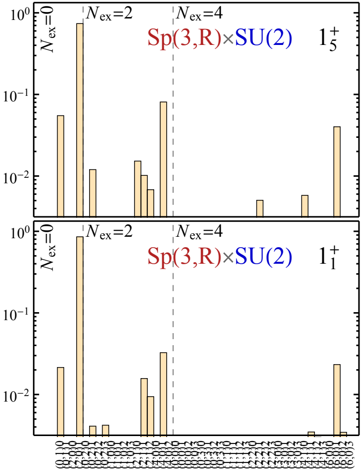
Decomposition by Sp(3, ℝ) content

The U(3) content is quite different…

But these excited states lie within ground state's Sp(3, ℝ) irrep





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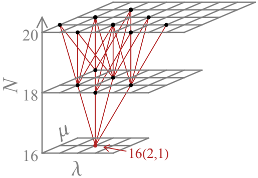
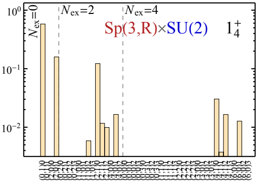
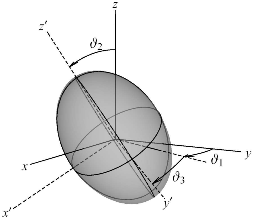






Rotational features emerge in *ab initio* calculations

M. A. Caprio, P. Maris, J. P. Vary, and R. Smith, Int. J. Mod. Phys. E **24**, 1541002 (2015), arXiv:1509.00102.

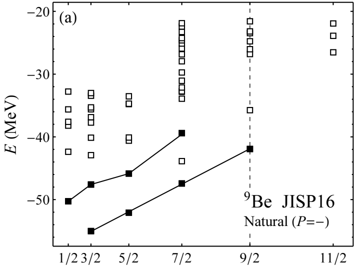
Cluster rotation?

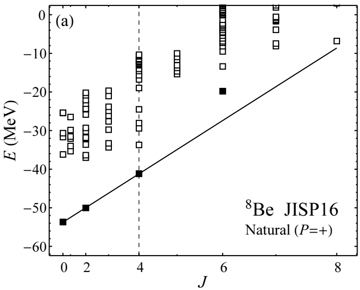
Valence shell structure?

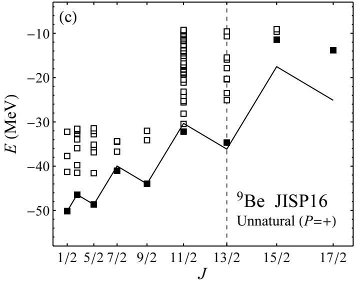
Elliott SU(3)

Multishell dynamics?

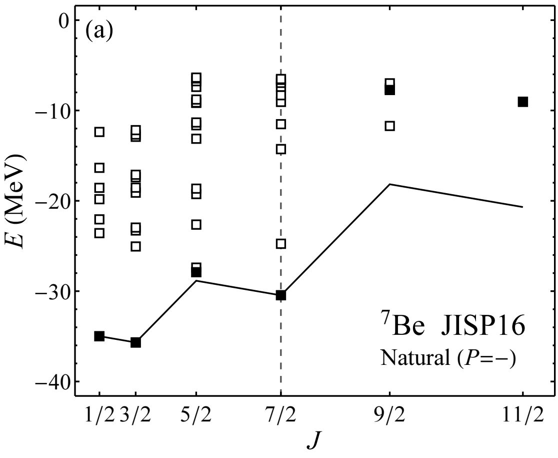
Symplectic Sp(3, ℝ)?







Yrast $K = 1/2$ rotational band in ^{7}Be



JISP16 + Coulomb, $N_{\max} = 10$, $\hbar\omega = 20\,\text{MeV}$. [IJMPE **24**, 1541002 (2015).]

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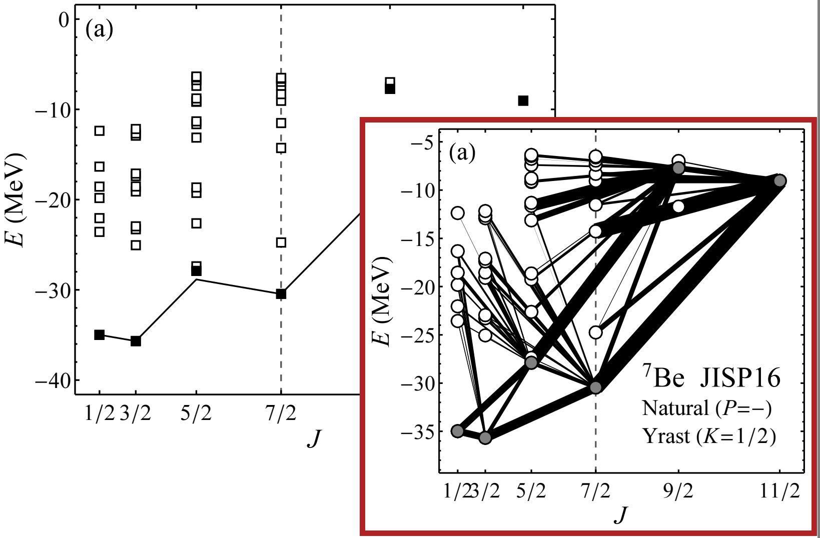
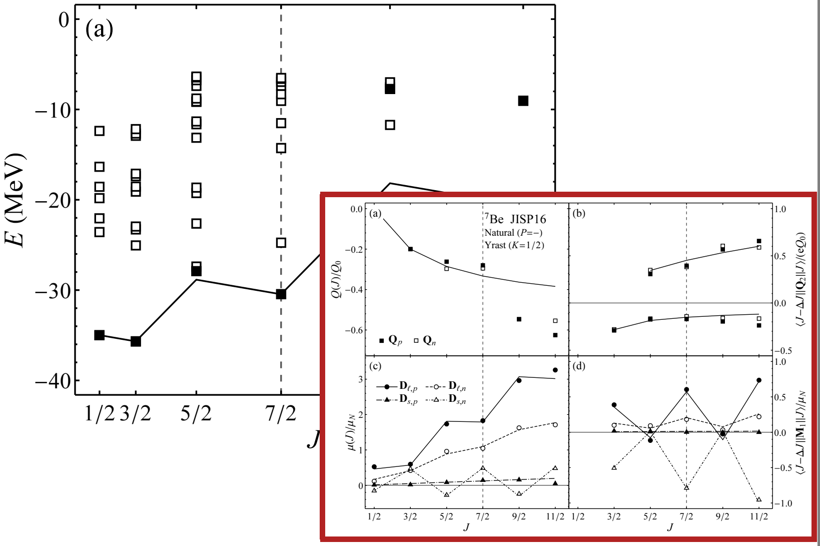


JISP16 + Coulomb, $N_{\mathrm{max}} = 10$, $\hbar\omega = 20\,\mathrm{MeV}$. [IJMPE **24**, 1541002 (2015).]

Yrast $K = 1/2$ rotational band in ^{7}Be



JISP16 + Coulomb, $N_{\max} = 10$, $\hbar\omega = 20$ MeV. [IJMPE **24**, 1541002 (2015).]

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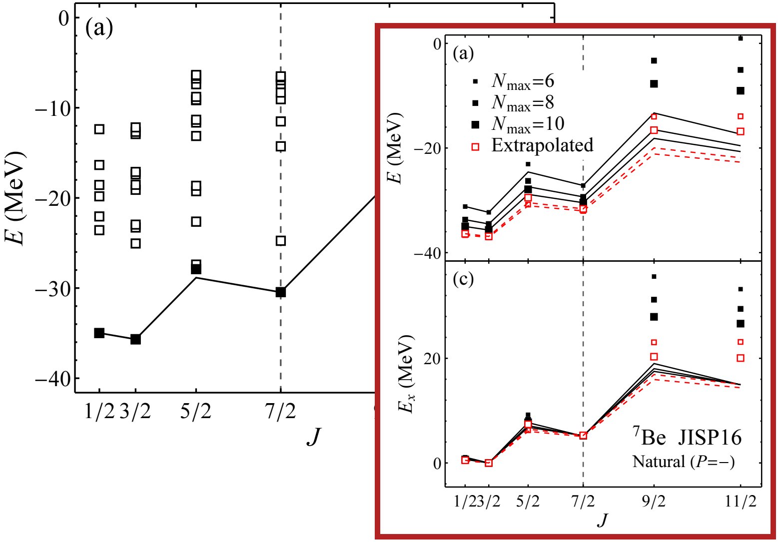


JISP16 + Coulomb, $N_{max} = 10$, $\hbar\omega = 20$ MeV. [IJMPE **24**, 1541002 (2015).]

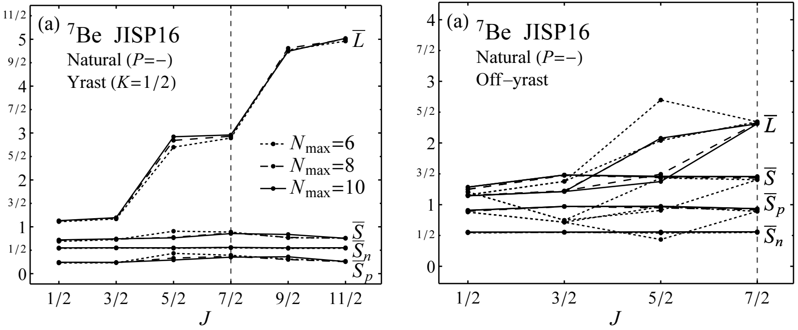
Angular momentum (LS) structure

Effective angular momenta $\bar{L}$, $\bar{S}_p$, $\bar{S}_n$, and $\bar{S}$ *"Root mean square"*

$$\bar{L}(\bar{L}+1) \equiv \langle \mathbf{L}\cdot\mathbf{L} \rangle \quad \bar{S}(\bar{S}+1) \equiv \langle \mathbf{S}\cdot\mathbf{S} \rangle$$

Yrast band: $L = 1, 3, 5, \ldots$ spin doublets, $S = 1/2$ from neutron

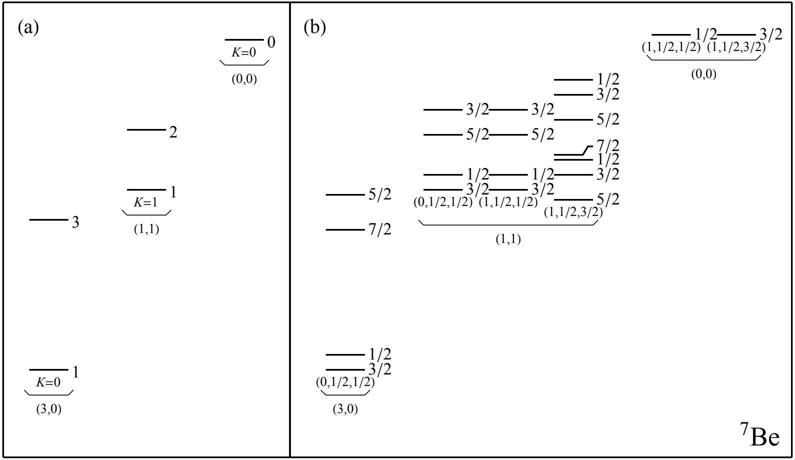
Off-yrast states: $S_p \approx 1$, so α cluster must be broken



JISP16 + Coulomb, $N_{\text{max}} = 10$, $\hbar\omega = 20\,\text{MeV}$. With P. Maris and J. P. Vary.

M. A. Caprio, University of Notre Dame

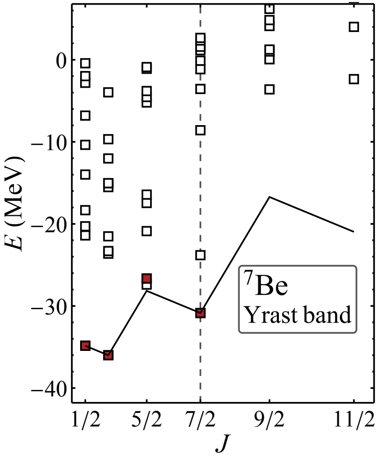
What we might expect for ^{7}Be from Elliott SU(3)

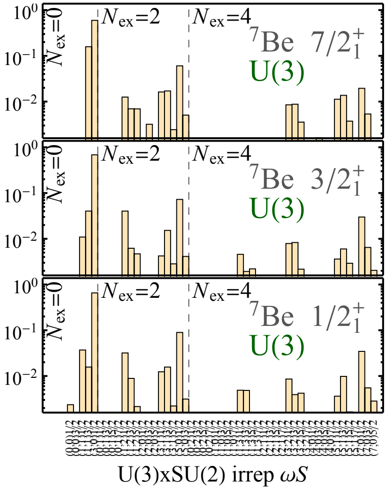


Decomposition by U(3) content

Yrast band up to maximal "valence" angular momentum has U(3)

$N_{\text{ex}}(\lambda,\mu) = 0(3,0)$ $S = 1/2$



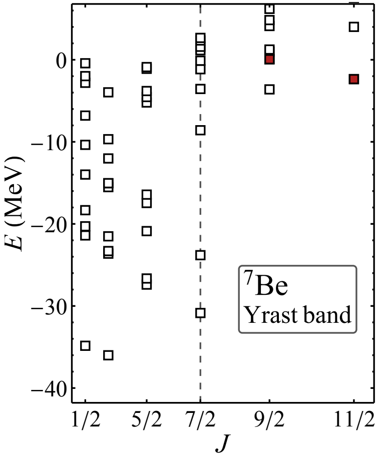


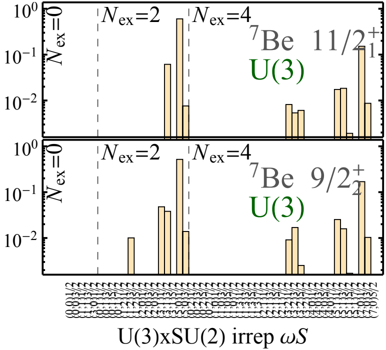
JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\text{MeV}$

Decomposition by U(3) content

Yrast band *beyond* maximal "valence" angular momentum has U(3)

$N_{\text{ex}}(\lambda,\mu) = 2(5,0)$ $S = 1/2$





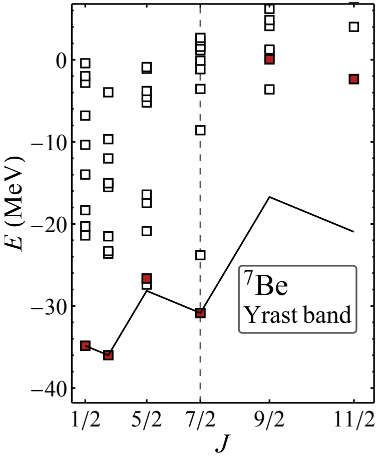
JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\text{MeV}$

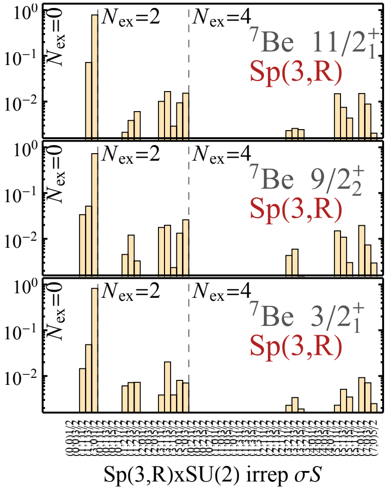
M. A. Caprio, University of Notre Dame

Decomposition by Sp(3, ℝ) content

But… Extended yrast band lies within single Sp(3, ℝ) irrep

$N_{\mathrm{ex}}(\lambda,\mu) = 0(3,0)$ $S = 1/2$

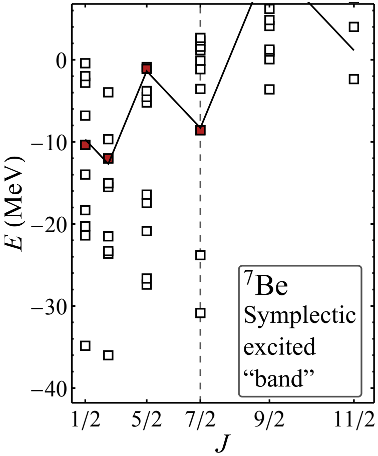


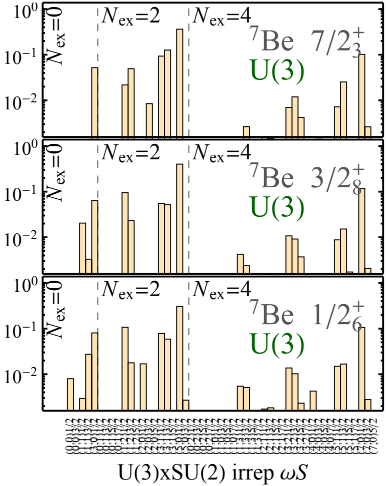


Decomposition by U(3) content

Excited states connected to yrast band are dominantly U(3)

$N_{\mathrm{ex}}(\lambda,\mu) = 2(5,0)$ $S = 1/2$



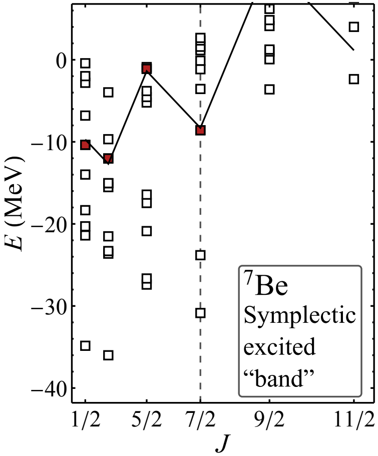


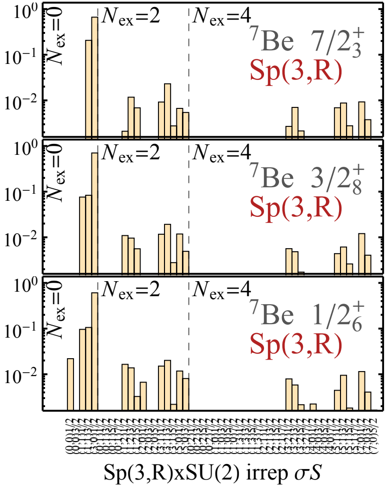
JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\mathrm{MeV}$

Decomposition by Sp(3, ℝ) content

But… These excited states lie within yrast band's Sp(3, ℝ) irrep

$N_{ex}(\lambda,\mu) = 0(3,0)$ $S = 1/2$





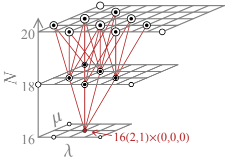
JISP16 (no Coulomb), SpNCCI, $N_{\sigma,\max} = N_{\max} = 6$, $\hbar\omega = 20\,\text{MeV}$

Summary and outlook

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

  Mixing of a few dominant irreps
- Families of states with similar $Sp(3,\mathbb{R})$ structure

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

Computational scheme to be explored and developed

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

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