TRIUMF

Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

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

Anna E. McCoy

TRIUMF, Canada

APCTP-TRIUMF Joint Workshop
Pohang, South Korea
Sept. 18, 2018

Collaborators

Mark Caprio
University of Notre Dame

Tomáš Dytrych
Academy of Sciences of the Czech Republic,
Louisiana State University

Acknowledgements
David Rowe, University of Toronto
Chao Yang, LBNL
Pieter Maris, Iowa Stat University
Petr Navrátil, TRIUMF
Calvin Johnson, San Diego State University
Patrick Fasano, University of Notre Dame
Robert Power, University College Cork (REU)

Outline

- No-core configuration interaction (NCCI) frameworks
- Symplectic no-core configuration interaction (SpNCCI) framework
- Convergence in SpNCCI
- Symmetry decompositions of wavefunctions

Ab initio nuclear physics

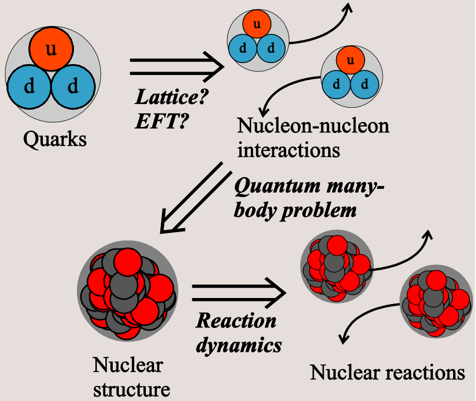
Goals:

Predict nuclear structure and reactions directly from QCD

Understanding the origins of simple patterns in complex nuclei

1. Realistic inter-nucleon interactions
   Chiral effective field theory
   Inverse scattering matrix
   Meson exchange currents

2. Method for solving the nuclear problem
   e.g., no-core configuration interaction (NCCI)
   also known as no-core shell model (NCSM)



Nuclear many-body problem

Solve many-body Schrodinger equation

$$\sum_{i}^{A} -\frac{\hbar^2}{2m_i}\nabla_i^2 \Psi + \frac{1}{2}\sum_{i,j=1}^{A} V(|r_i - r_j|)\Psi = E\Psi$$

Expanding wavefunctions in a basis

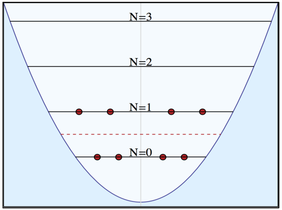
$$\Psi = \sum_{k=1}^{\infty} a_k \phi_k$$

Reduces to matrix eigenproblem

$$\begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

Harmonic oscillator basis

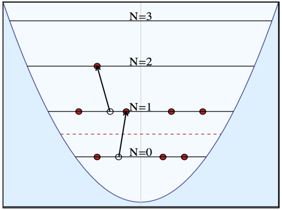
$$N = 2n + \ell$$

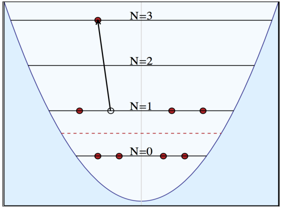


$N_{ex} = 0$

- Basis states are configurations, i.e., distributions of particles over harmonic oscillator shells (*nlj substates*)
- States organized by total number of oscillator quanta above lowest Pauli allowed number N_{ex}.
- Basis must by truncated, typically by restricting number of oscillator quanta to $N_{ex} \leq N_{max}$

How large must N_{max} be?





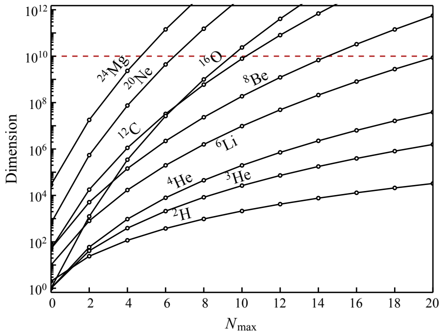
$N_{ex} = 2$

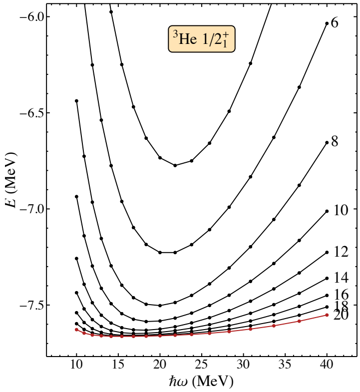
TRIUMF

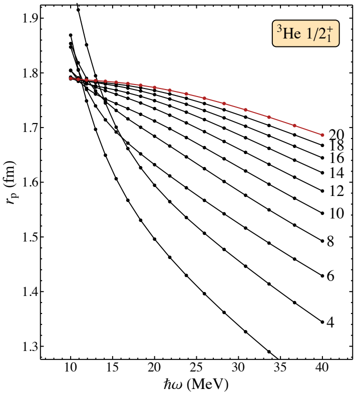
Convergence problem in NCCI frameworks

Results for calculations in a finite space depend upon:

- Many-body truncation $N_{\max}$
- Single-particle basis scale $\hbar\omega$



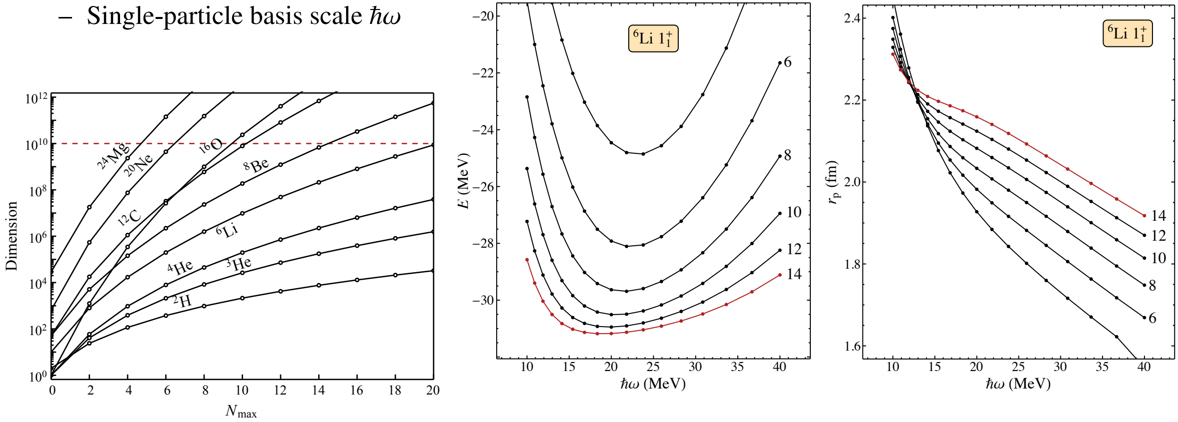




Convergence problem in NCCI frameworks

Results for calculations in a finite space depend upon:

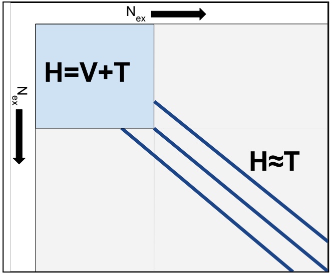
- Many-body truncation $N_{\max}$
- Single-particle basis scale $\hbar\omega$



Why must N_{max} be so large?

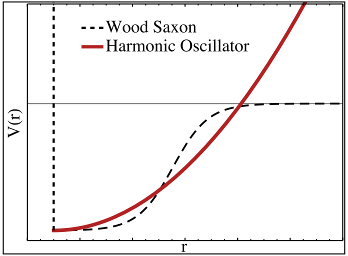
N_{max} truncation:

- Matrix elements of interaction decrease with N_{ex}
- Matrix elements of kinetic energy increase with N_{ex}
  Off diagonal matrix elements of kinetic energy lead to non-negligable amplitudes of high N_{ex} configurations in nuclear wavefunction



Mismatch between basis and wavefunctions

- Different asymptotic behavior
- Wavefunctions are linear combinations of many oscillator configurations *-highly correlated states*



Symmetries in physics

Fundamental symmetries

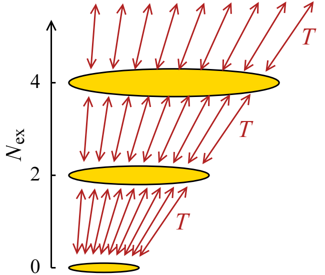
- Rotation [SU(2)] & parity $\Rightarrow$ J, P

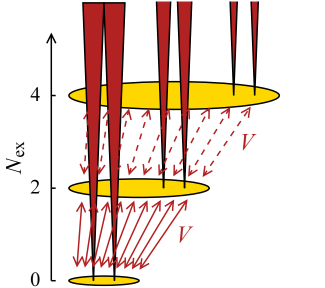
Approximate symmetries of the many-body problem

- Isospin [SU(2)] & Wigner spin-isospin [SU(4)]
- Phase space symmetries: Elliott SU(3) & Sp(3,$\mathbb{R}$)

Kinetic energy conserves Sp(3,$\mathbb{R}$)

- Sp(3,$\mathbb{R}$) can be used to identify important high-lying configurations
- Reduce the necessary size of the many-body basis





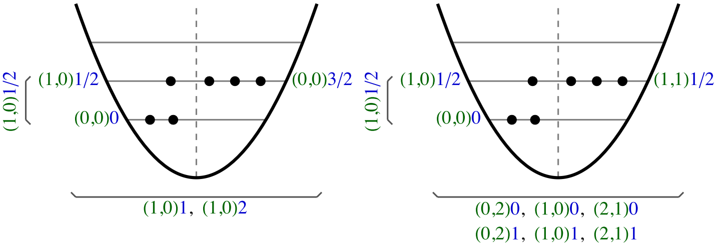
SU(3)-NCSM

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



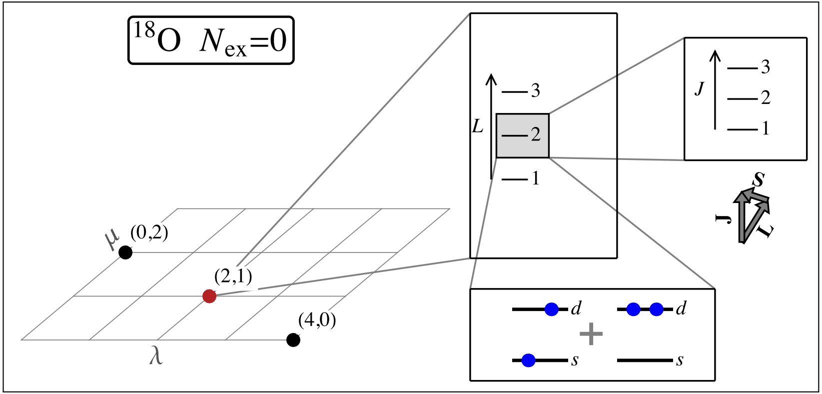
SU(3) symmetry of a configuration

- 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

SU(3)-NCSM

SU(3)-coupled configurations are correlated:

Configurations are linear combinations of distributions of particles over original (nlj) orbitals



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

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

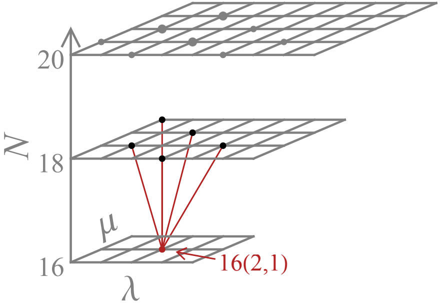
Lowest grade irrep (LGI)

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

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

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

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



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

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

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

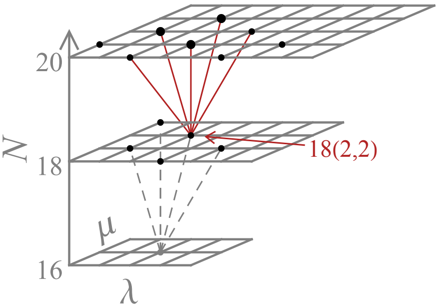
Start from a single U(3) irrep at lowest "grade" N

Lowest grade irrep (LGI)

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

$$B^{(02)}\,|\sigma\rangle = 0$$
$$|\psi^\omega\rangle \sim [A^{(20)}A^{(20)}\cdots A^{(20)}\,|\sigma\rangle]^\omega$$

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



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

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

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

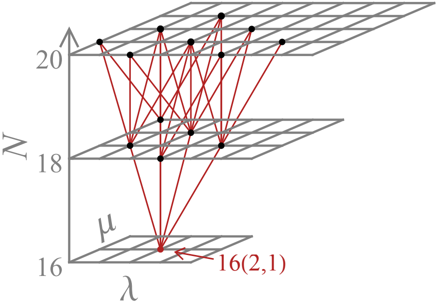
Start from a single U(3) irrep at lowest "grade" N

Lowest grade irrep (LGI)

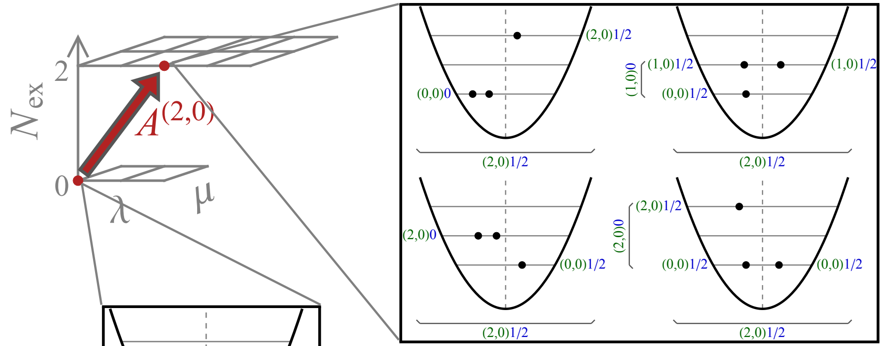
Ladder upward in N using $A^{(20)}$ *No limit!*

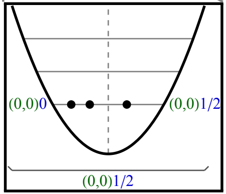
$$B^{(02)}\,|\sigma\rangle = 0$$
$$|\psi^\omega\rangle \sim [A^{(20)}A^{(20)}\cdots A^{(20)}\,|\sigma\rangle]^\omega$$

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



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

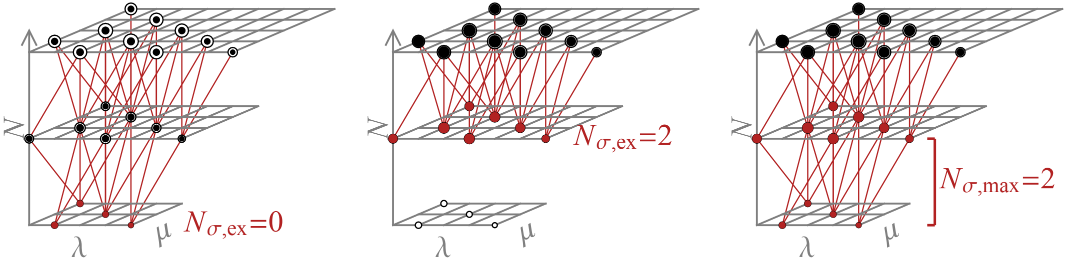
– Reorganize many-body basis into $\mathrm{Sp}(3,\mathbb{R})$ irreps

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

  T. Dytrych et al., J. Phys. G: Nucl. Part. Phys. **35** (2008) 123101.
  T. Dytrych et al., Phys. Rev. Lett.**111** (2013) 252501.

  - Diagonalize $Sp(3,\mathbb{R})$ Casimir operator in SU(3)-coupled basis

    T. Dytrych, symmetry adapted no-core shell model

  - 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

  Y. Suzuki and K. T. Hecht, Nuc. Phys. A **455** (1986) 315.

  - Reduce calculation to sum over coefficients and LGI matrix elements

    Y. Suzuki and K. T. Hecht, Nuc. Phys. A **455** (1986) 315.

  - 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 $\mathcal{U}(a,b)$

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

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*

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

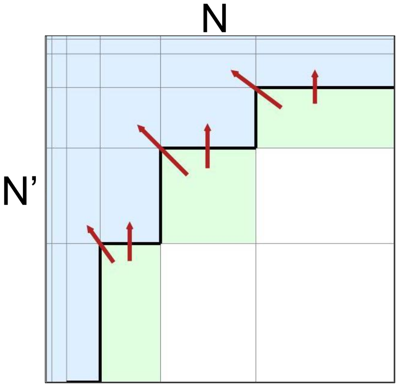
SpNCCI framework

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

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

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

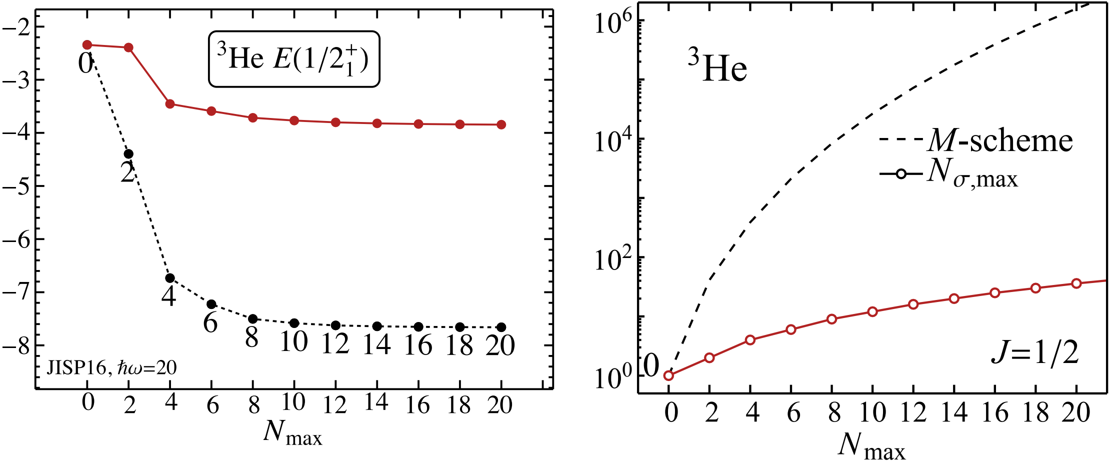
2. Compute the matrix elements of the unit tensors $\mathcal{U}(a,b)$ in the symplectic many-body basis

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

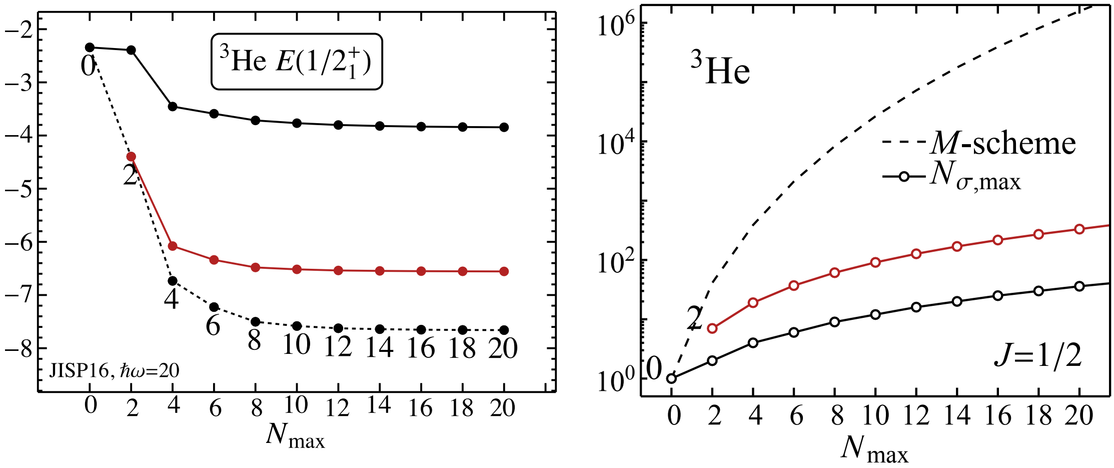
3. Construct the Hamiltonian matrix by combing the decomposition of the Hamiltonian in terms of unit tensor with matrix elements of relative unit tensors.

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

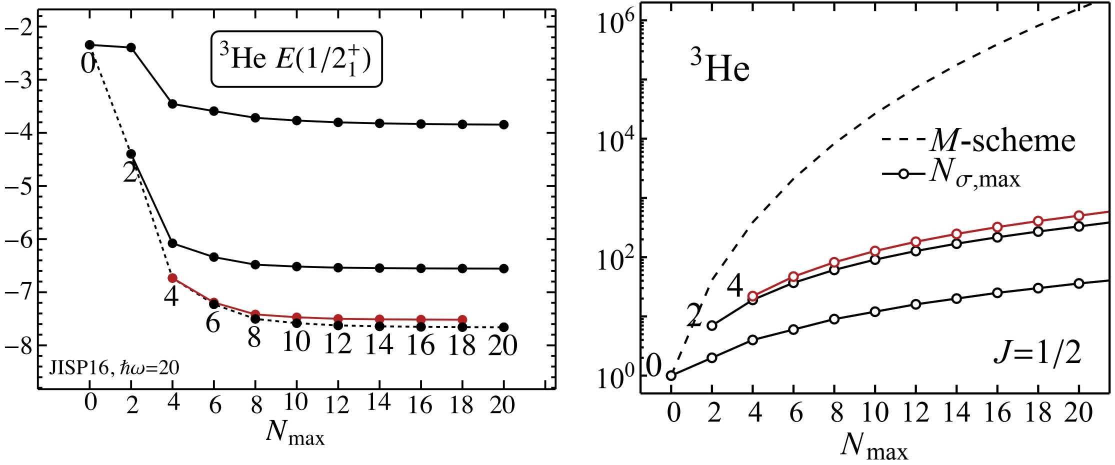
Convergence in the SpNCCI framework



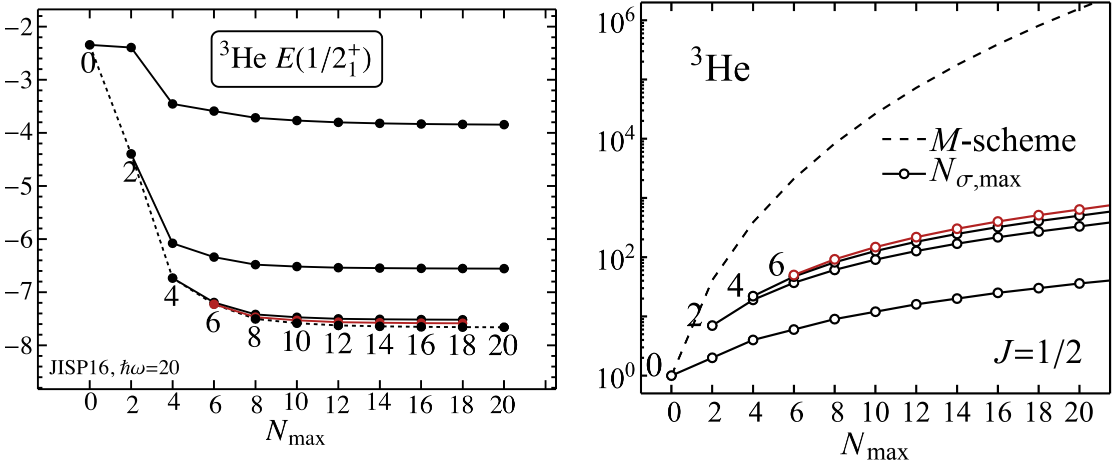
Convergence in the SpNCCI framework



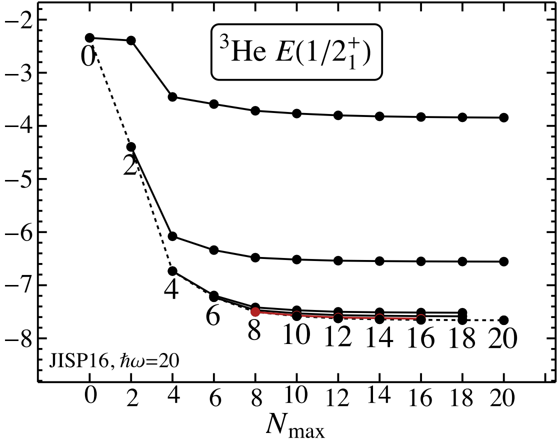
Convergence in the SpNCCI framework

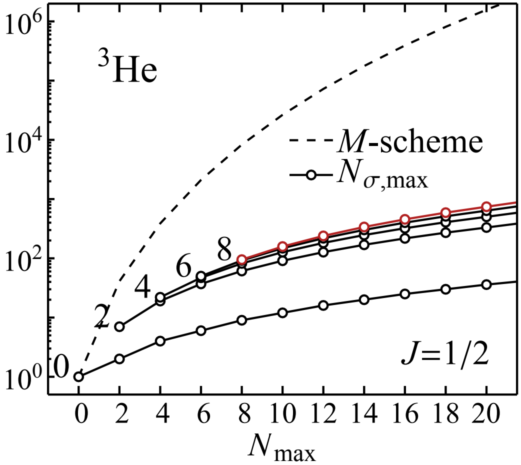


Convergence in the SpNCCI framework

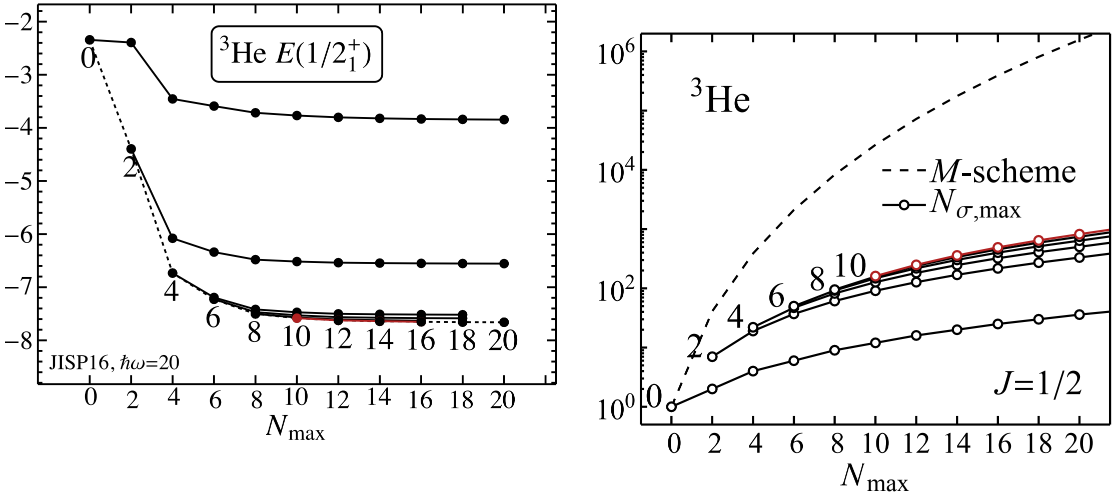


Convergence in the SpNCCI framework

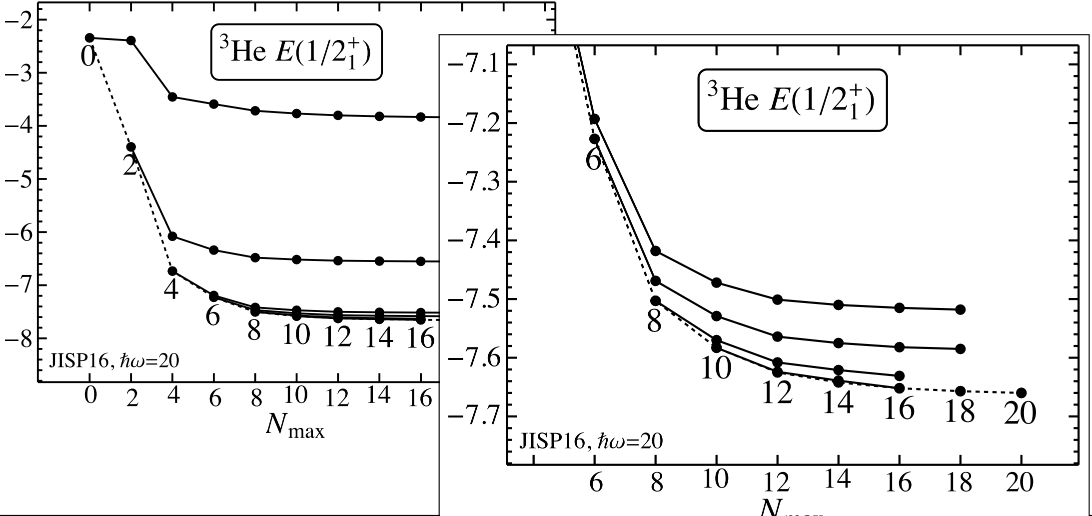




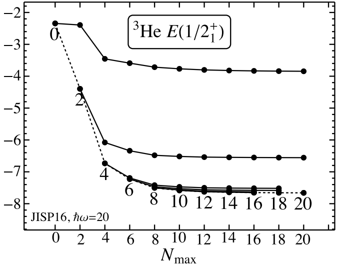
Convergence in the SpNCCI framework

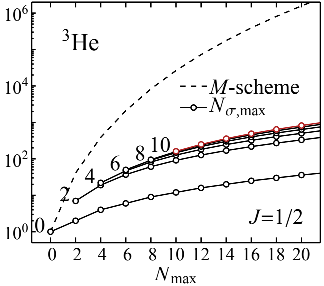


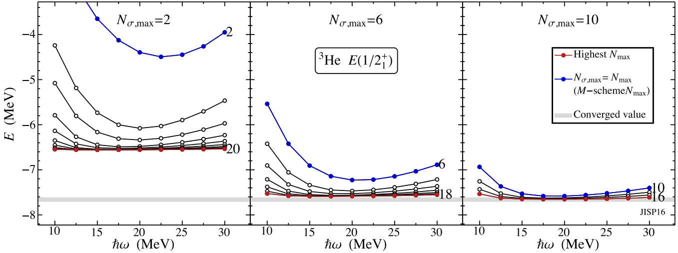
Convergence in the SpNCCI framework

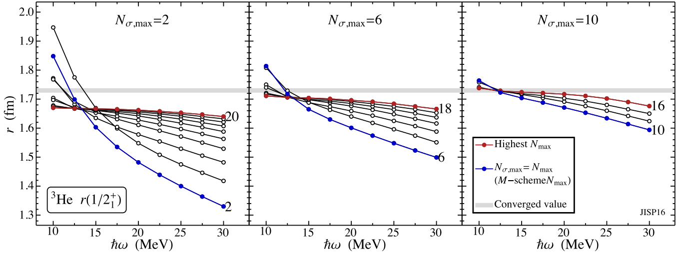


Convergence in the SpNCCI framework

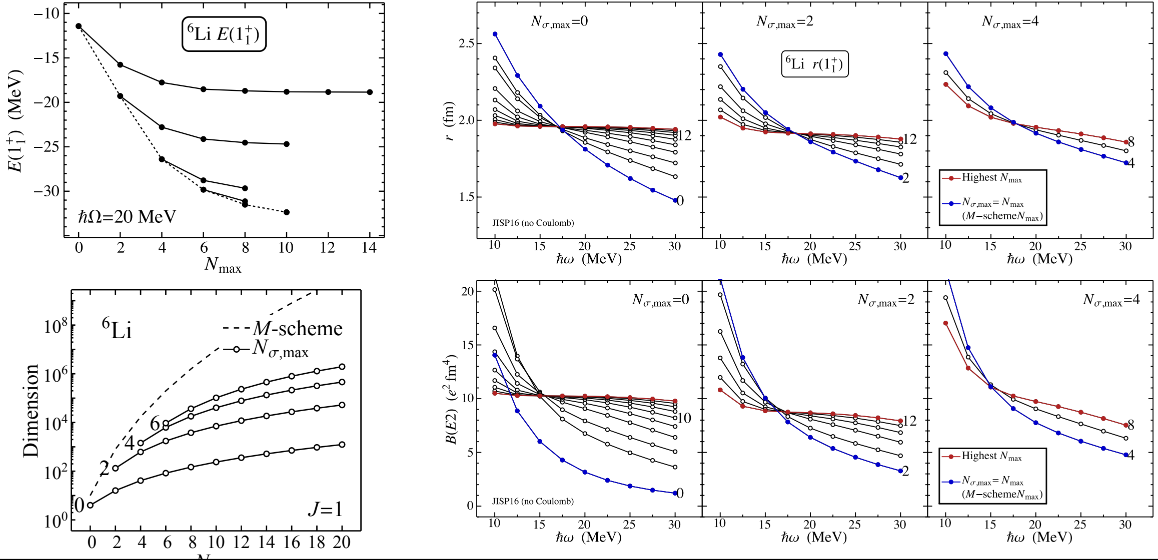








Convergence in the SpNCCI framework



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

- Need convergence with respect to symplectic parameter $N_{\sigma,\max}$

- Convergence with respect to $N_{\sigma,\max}$ achieved when results do not change as more irreps are included

Convergence in the SpNCCI framework

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

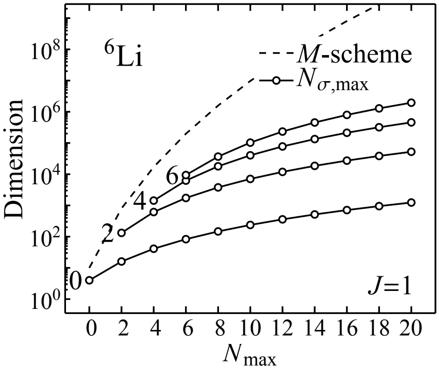
– Need convergence with respect to symplectic parameter $N_{\sigma,\mathrm{max}}$

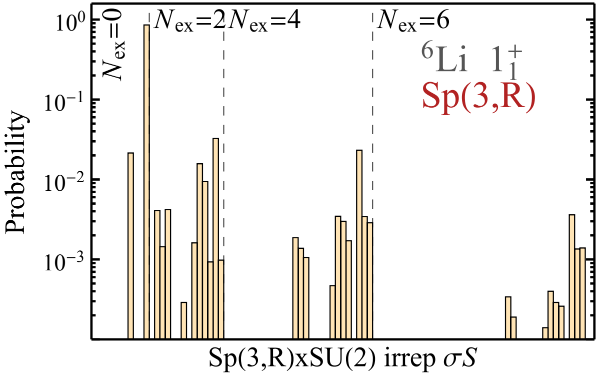
– Convergence with respect to $N_{\sigma,\mathrm{max}}$ achieved when results do not change as more irreps are included

But do we need all of the irreps at each $N_{\sigma,\mathrm{max}}$?

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

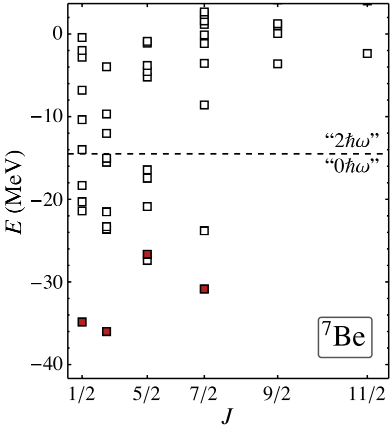
- The ^{6}Li ground state is dominantly a single irrep $Sp(3,\mathbb{R})$ ($\approx 86\%$)
- Only a subset of the $Sp(3,\mathbb{R})$ irreps contribute at more than 0.01%
- SpNCCI basis can be further truncated by specific irreps

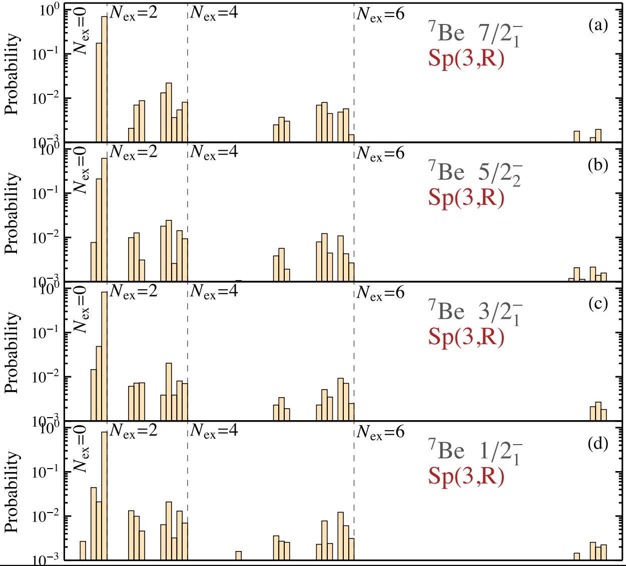




Sp(3, ℝ) decomposition ^{7}Be

Families of states emerge with very similar Sp(3, ℝ) decompositions





TRIUMF

Nuclear rotations

Intrinsic state $|\phi_K\rangle$ rotating the the lab frame

$$|\psi_{JKM}\rangle \propto \int d\theta \left(\mathcal{D}^J_{MK}(\theta)\,|\phi_k;\theta\rangle + (-1)^{J+K}\mathcal{D}^J_{M-K}(\theta)\,|\phi_{\bar{K}};\theta\rangle \right)$$

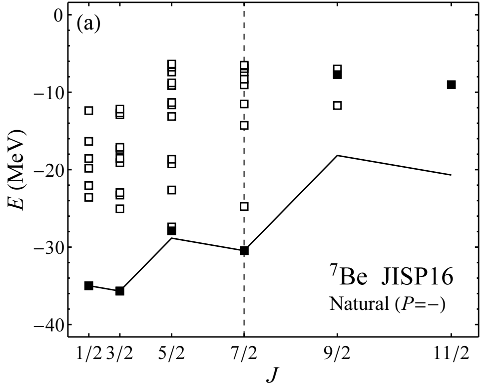
$$E(J) = E_0 + A[J(J+1) + a(-1)^{J+1/2}(J+1/2)]$$

Electric Quadrupole (E2) transitions

$$B(E2; J_f K \to J_i K) = \frac{|\langle J_f\|Q_2\|j_i\rangle|^2}{2J_i+1}$$

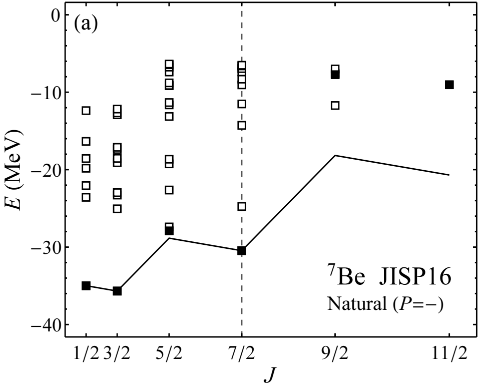
$$\langle J_f\|Q_2\|J_i\rangle \propto (2J_i+1)^{1/2}(J_i K 2 0|J_f K)(eQ_0)$$

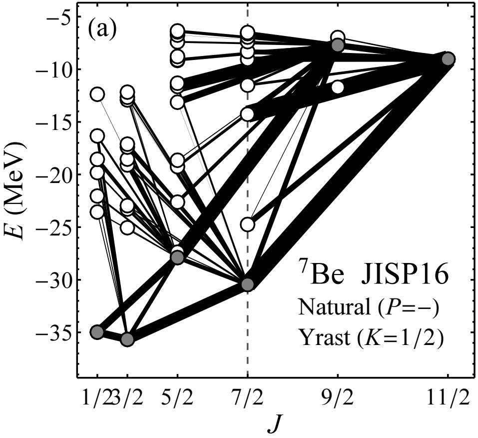
$$(eQ_0) \equiv (16\pi/5)^{1/2}\langle\phi_K|Q_{2,0}|\phi_K\rangle$$



M. A. Caprio, P. Maris and J.P. Vary, Phys. Lett. B **719** (2013) 179

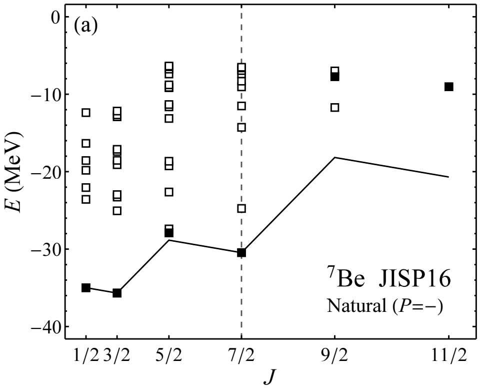
Yrast $K = 1/2$ rotational band in ^{7}Be

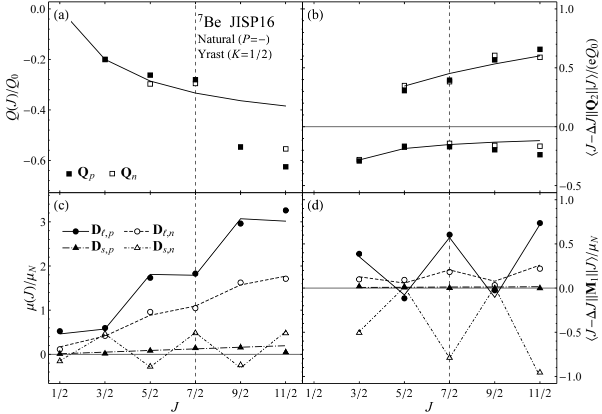




M. A. Caprio, P. Maris and J.P. Vary, Phys. Lett. B **719** (2013) 179

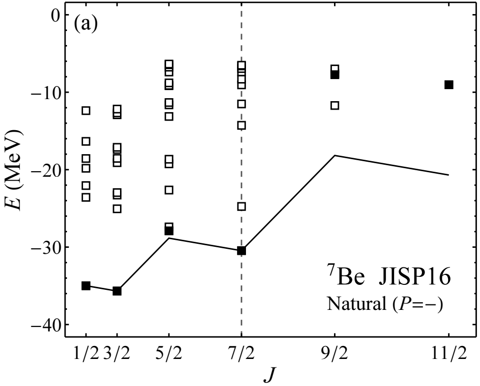
Yrast $K = 1/2$ rotational band in ^{7}Be

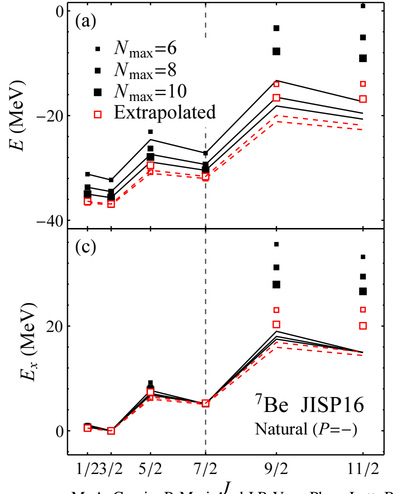




M. A. Caprio, P. Maris and J.P. Vary, Phys. Lett. B **719** (2013) 179

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

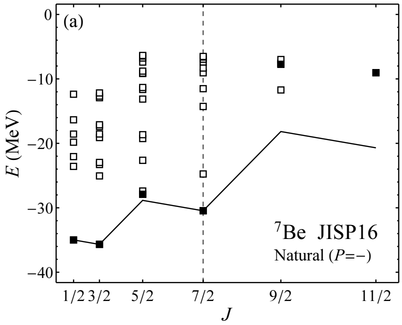


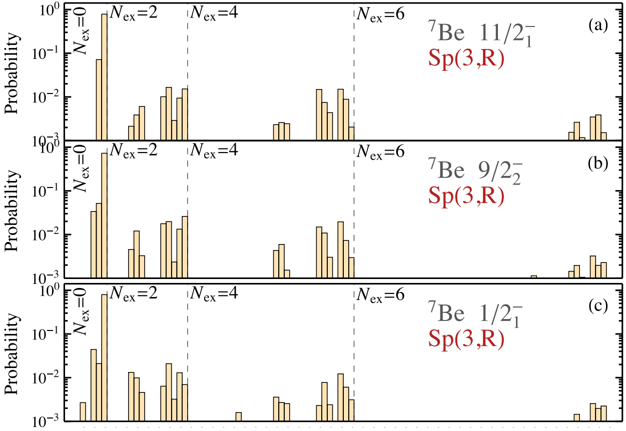


M. A. Caprio, P. Maris and J.P. Vary, Phys. Lett. B **719** (2013) 179

Sp(3, ℝ) decomposition ^{7}Be

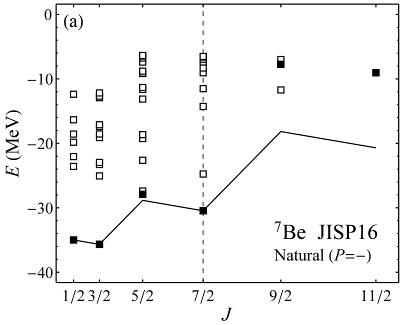
Excited states with same Sp(3, ℝ) content

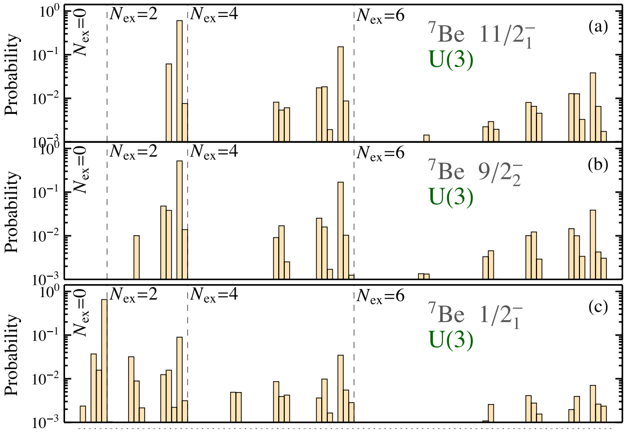




Sp(3, ℝ) decomposition ^{7}Be

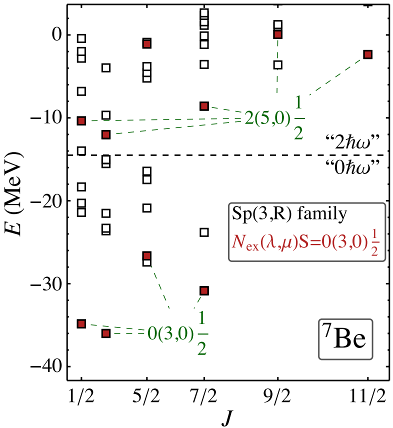
Excited states with same Sp(3, ℝ) content but different SU(3) content

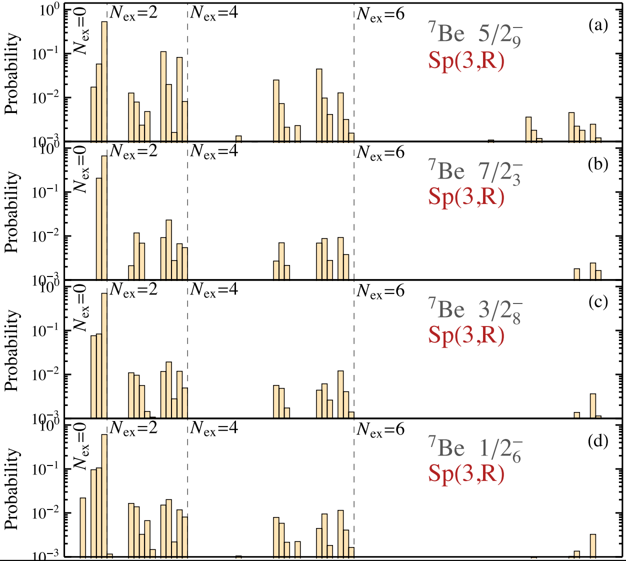




Sp(3, ℝ) decomposition ^{7}Be

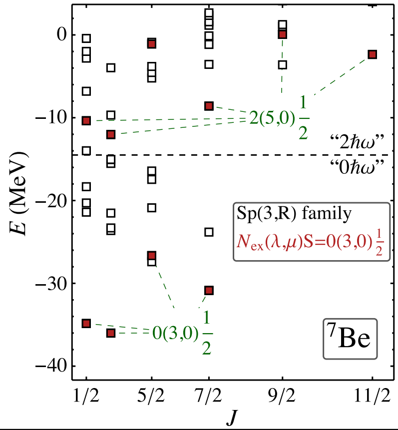
Excited states with same Sp(3, ℝ) content but different SU(3) content

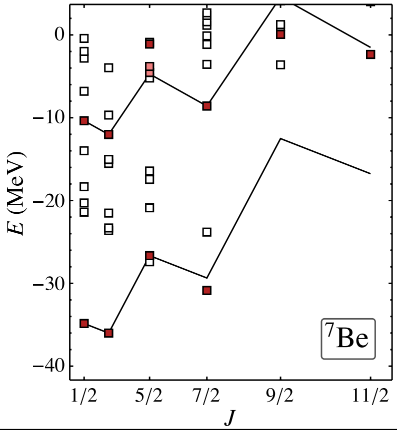




Sp(3, ℝ) decomposition ^{7}Be

Excited states with same Sp(3, ℝ) content but different SU(3) content





Summary

In $N_{\sigma,\max}$ truncation scheme…

- Calculations converge with respect to $N_{\sigma,\max}$ at about $N_{\sigma,\max} = 10$
- Interaction terms stop mixing $Sp(3,\mathbb{R})$ irreps
- Observables converge rapidly within an $N_{\sigma,\max}$ space
- Only a fraction of the full $N_{\sigma,\max}$ space dominantly contributes

Families of states emerge with same $Sp(3,\mathbb{R})$ content

TRIUMF

Canada’s national laboratory
for particle and nuclear physics
and accelerator-based science

TRIUMF: Alberta | British Columbia | Calgary | Carleton | Guelph | Manitoba | McGill | McMaster | Montréal | Northern British Columbia | Queen’s | Regina | Saint Mary’s | Simon Fraser | Toronto | Victoria | Western | Winnipeg | York

Thank you!
Merci!

Follow us at TRIUMFLab