Symplectic framework for *ab initio* nuclear structure.

II. Truncation schemes in a symplectic basis

Anna E. McCoy,[1,2] Mark A. Caprio,[1] Tomáš Dytrych[3]

[1]Department of Physics, University of Notre Dame, USA

[2]TRIUMF, Canada

[3]Nuclear Physics Institute, Academy of Sciences of the Czech Republic, Czechia

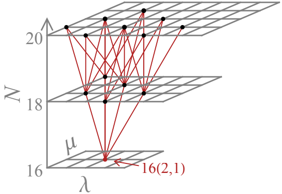
Progress in *Ab Initio* Techniques in Nuclear Physics, Vancouver, BC

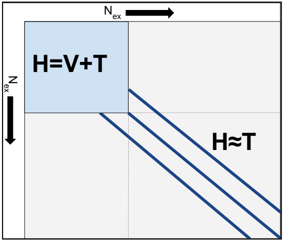
February 27, 2018 – March 2, 2018

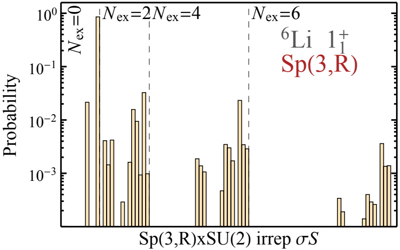
Outline

Truncation schemes

- $N_{\sigma,\max}$ truncation
- Truncation by $\mathrm{Sp}(3,\mathbb{R})$ subspaces
- Truncation by irrep

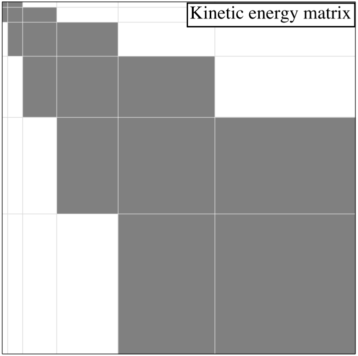




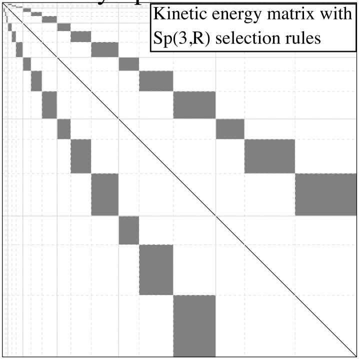


Kinetic energy

m-scheme basis



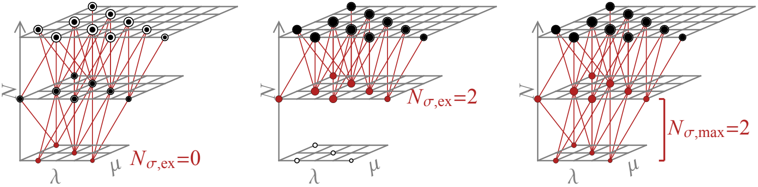
Symplectic basis



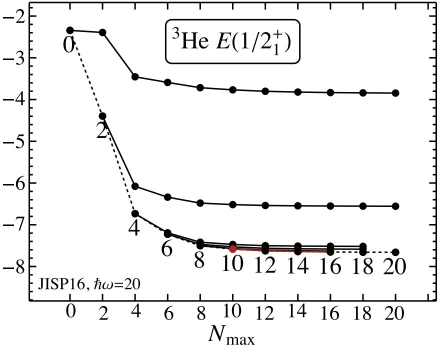
Symplectic basis

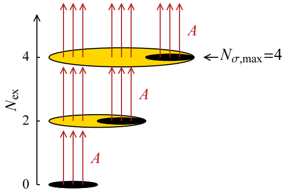
– Select a set of symplectic irreps, e.g., keep only irreps whose LGI have $N_{\text{ex}} \le N_{\sigma,\max}$ ($N_{\sigma,\max}$ **truncation**)

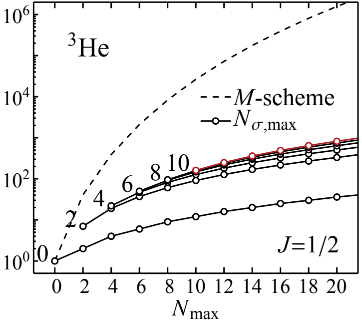
– Basis consists of states in chosen irreps with total number of excitation oscillator quanta $N_{\text{ex}} \le N_{\max}$.



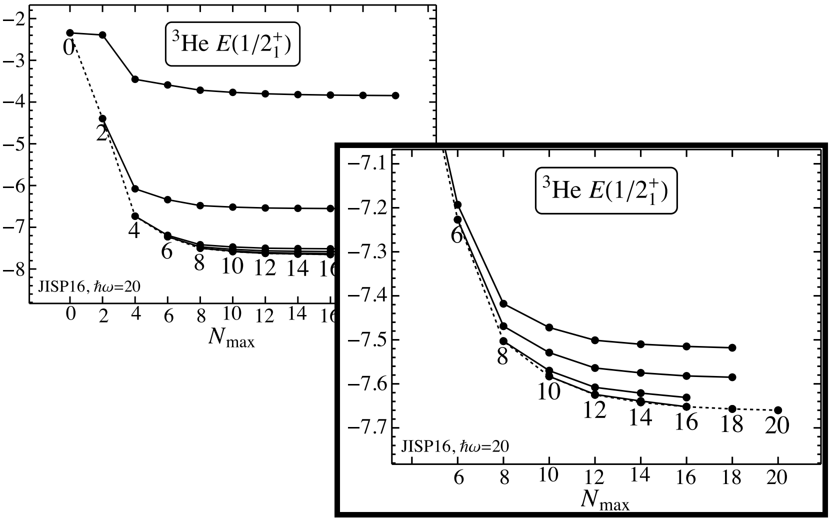
Convergence in the SpNCCI framework



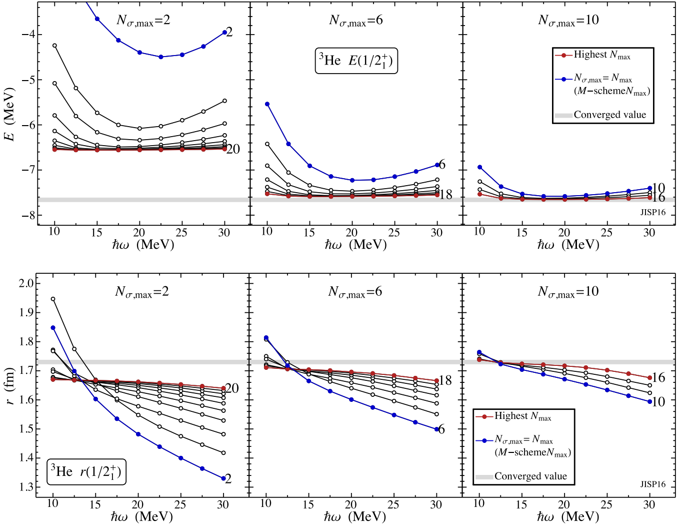




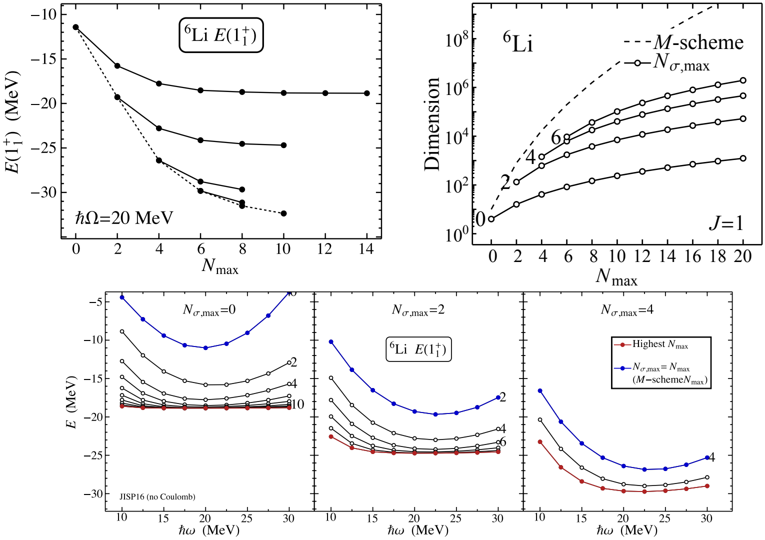
Convergence in the SpNCCI framework



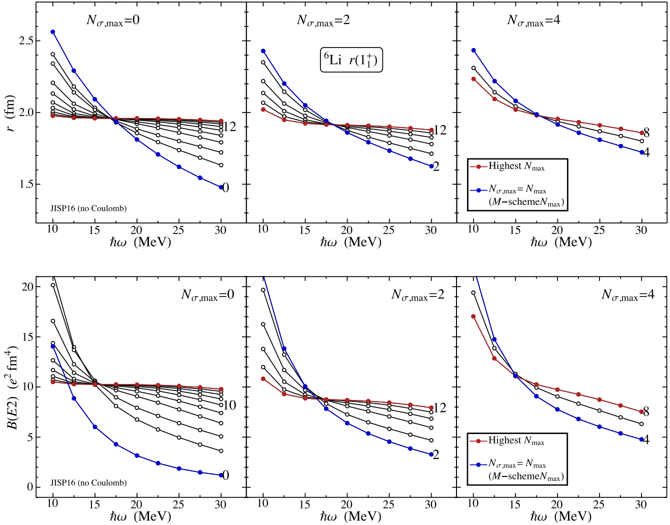
Convergence in the SpNCCI framework



Convergence in the SpNCCI framework



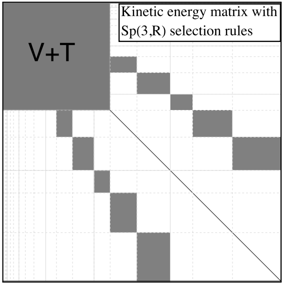
Convergence of observables



$N_{\sigma,\max}$ truncation

– Calculations converge with respect to $N_{\sigma,\max}$ at about $N_{\sigma,\max} = 10$

– Interaction terms stop strongly mixing $\mathrm{Sp}(3,\mathbb{R})$ irreps

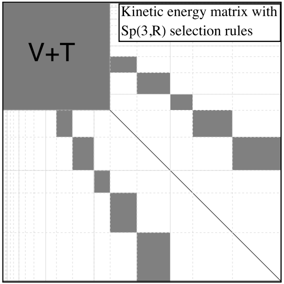


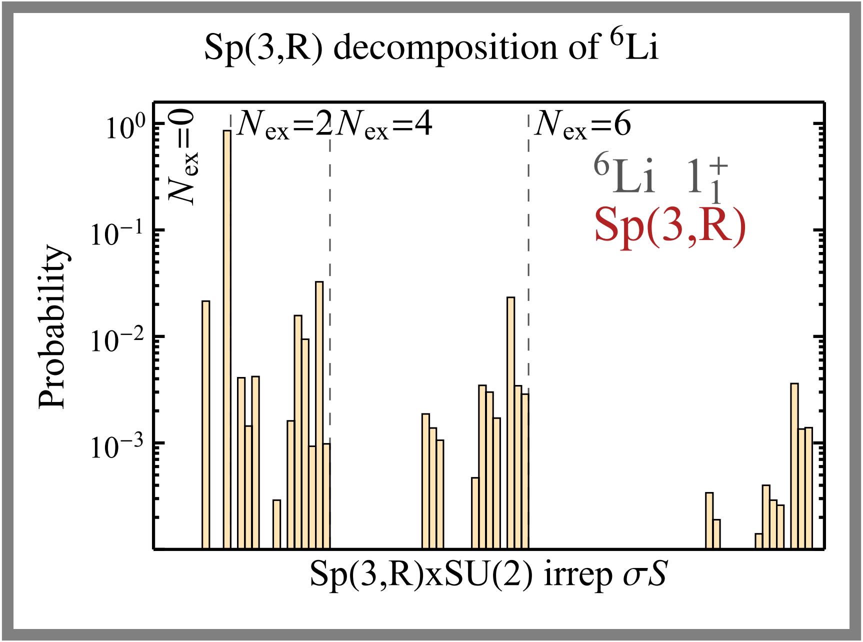
$N_{\sigma,\max}$ truncation

– Calculations converge with respect to $N_{\sigma,\max}$ at about $N_{\sigma,\max} = 10$

– Interaction terms stop strongly mixing $\mathrm{Sp}(3,\mathbb{R})$ irreps

$N_{\sigma,\max} = 10$ is too large for heavier nuclei





Sp(3,R) decomposition of ^{6}Li
$N_{\rm ex}$=0
$N_{\rm ex}$=2
$N_{\rm ex}$=4
$N_{\rm ex}$=6
^{6}Li 1_1^+
Sp(3,R)
10^0
10^{-1}
10^{-2}
10^{-3}
Probability
Sp(3,R)xSU(2) irrep σS

Truncation by $\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspaces

- Decompose wave functions by $\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspaces

  SpNCCI arXiv:1802.01771 [nucl-th]

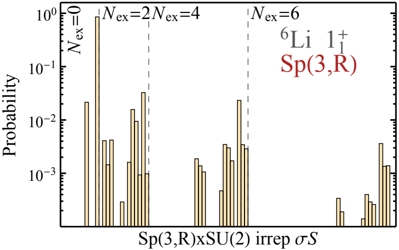
  BIGSTICK arXiv:1801.08432 [physics.comp-ph]

- Truncate basis to include only $\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspaces that contribute to wave function with probabilities that lie above some threshold

What threshold do we use?

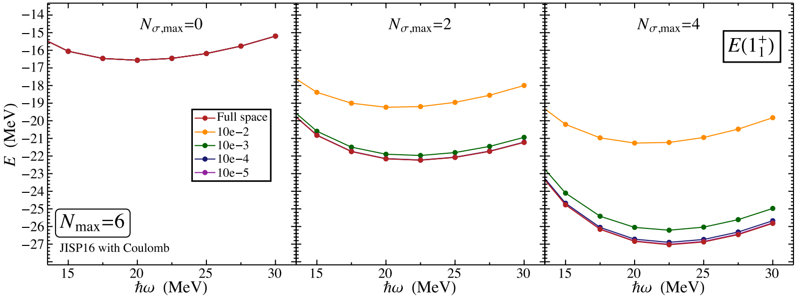
Does desired threshold depend on N_{ex}?

Effect on observables?



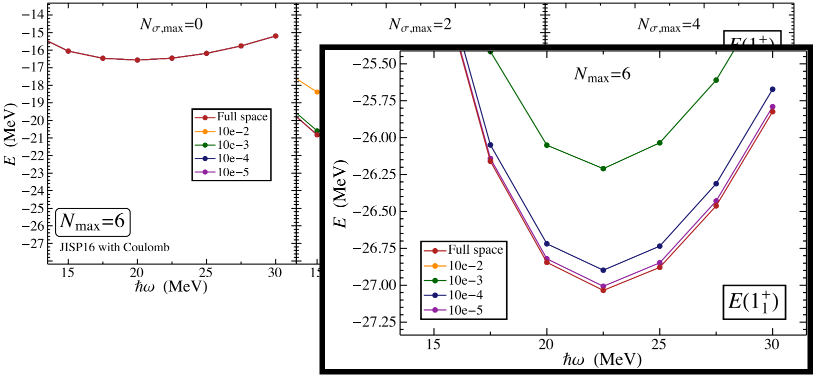
$Sp(3,\mathbb{R})\times SU(2)$ subspace truncations of ^{6}Li

Restrict basis to $Sp(3,\mathbb{R})\times SU(2)$ subspaces which contribute to a chosen reference wave function above a threshold value

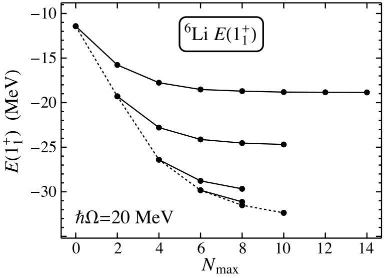


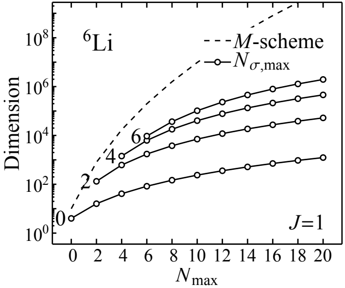
$Sp(3,\mathbb{R})\times SU(2)$ subspace truncations of ^{6}Li

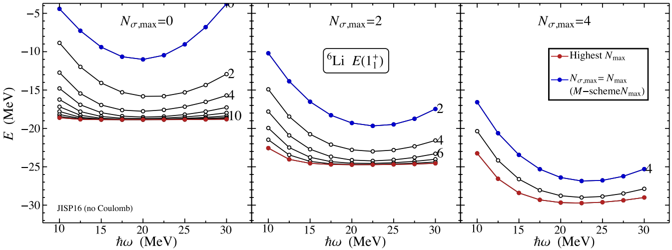
Restrict basis to $Sp(3,\mathbb{R})\times SU(2)$ subspaces which contribute to a chosen reference wave function above a threshold value



Convergence in the SpNCCI framework





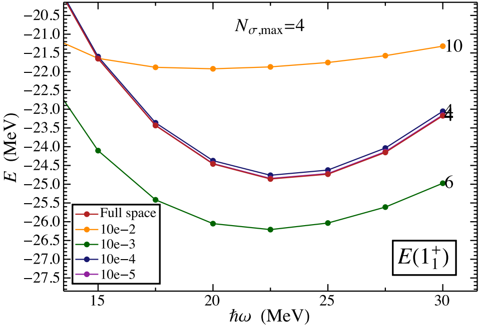


$\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspace truncations of ^{6}Li

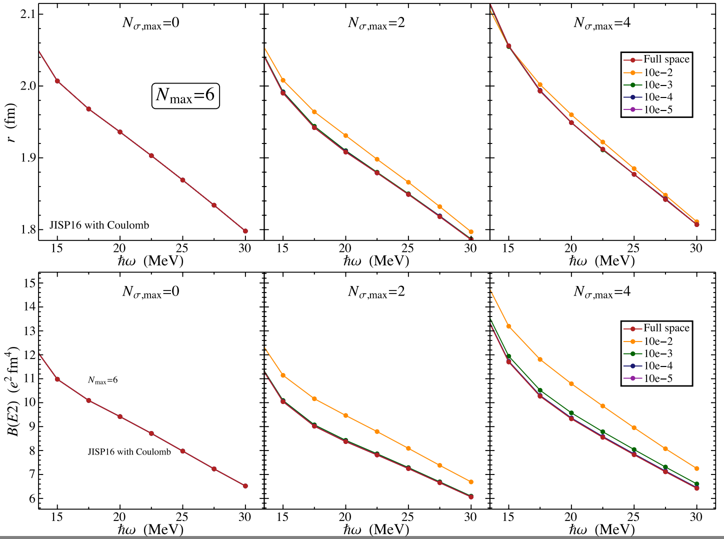
- Need to include higher $N_{\sigma,\mathrm{ex}}$ irreps
- Need to include higher $N_{\max}$ states within irreps
- Limit on basis size

"Best" results for each truncation in basis $\leq 3\times 10^3$

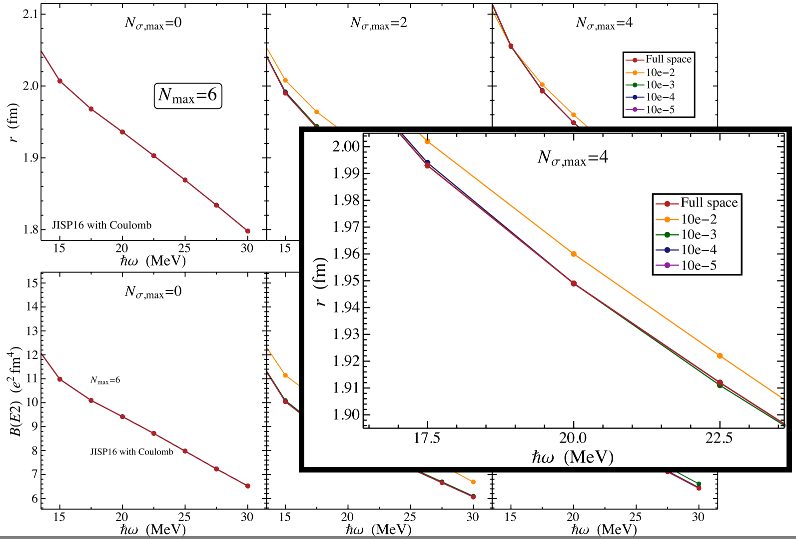
Challenge is to eliminate enough subspaces to include higher $N_{\sigma,\max}$ and $N_{\max}$ irreps while still including enough of each $N_{\sigma,\mathrm{ex}}$ subspace to get accurate predictions.



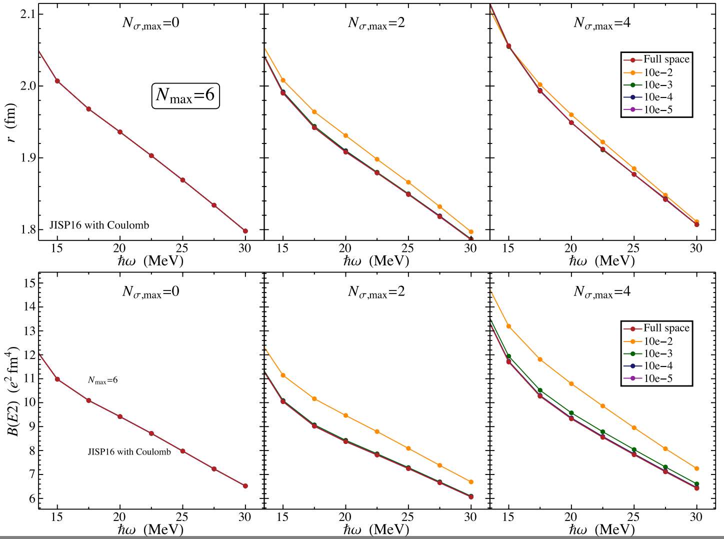
$Sp(3,\mathbb{R}) \times SU(2)$ subspace truncations of ^{6}Li



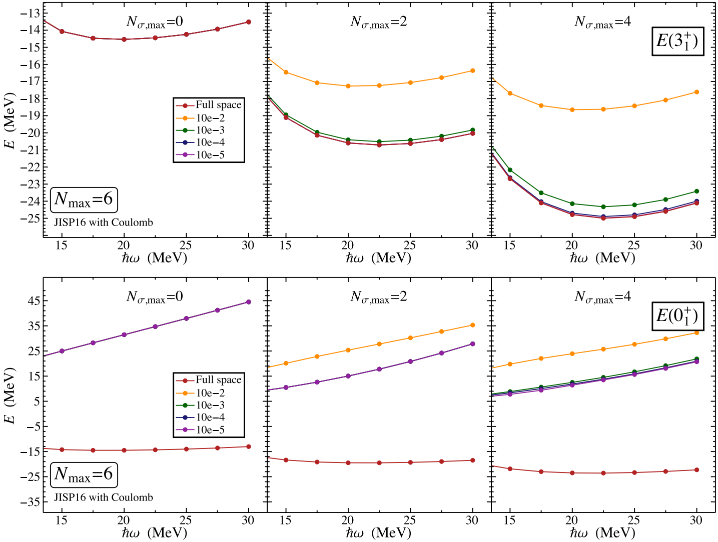
$\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ subspace truncations of ^{6}Li



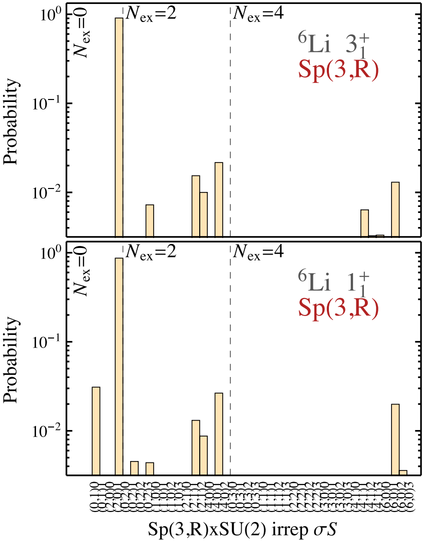
$\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspace truncations of ^{6}Li



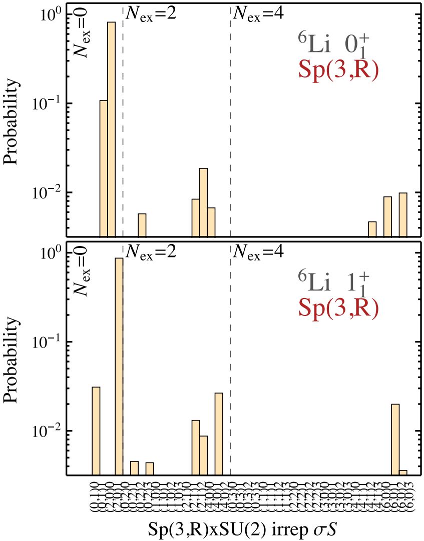
$Sp(3,\mathbb{R}) \times SU(2)$ subspace truncations of ^{6}Li



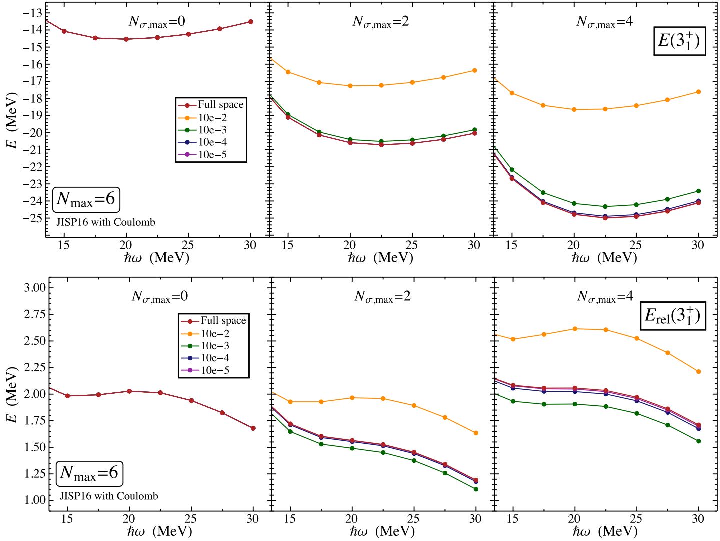
$\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ subspace truncations of $^6\mathrm{Li}$



$Sp(3,\mathbb{R}) \times SU(2)$ subspace truncations of ^{6}Li



$Sp(3,\mathbb{R}) \times SU(2)$ subspace truncations of ^{6}Li



$\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspace truncations of $^6\mathrm{Li}$

- Accuracy of binding energies depends on small $(10^{-4}-10^{-5})$ contributions from higher $N_{\sigma,\max}$ irreps
- Observables do not depend on these low threshold irreps

  In $N_{\max}=6$, $N_{\sigma,\max}=4$ *basis truncated by threshold value* 10^{-3}
  - 1^+_{gs} *energy almost* $1\,\mathrm{MeV}$ *larger than in the full space*
  - *RMS radius is within* $10^{-3}\,\mathrm{fm}$
- Truncations based on single wave function provide reasonable truncation for other members of the same irrep family, but not all states
- Need to adjust truncations to accommodate angular momentum selection rules

$\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ subspace truncations of ^{6}Li

- Accuracy of binding energies depends on small ($10^{-4} - 10^{-5}$) contributions from higher $N_{\sigma,\max}$ irreps
- Observables do not depend on these low threshold irreps

  In $N_{\max} = 6$, $N_{\sigma,\max} = 4$ *basis truncated by threshold value* 10^{-3}

  - 1^+_{gs} *energy almost* $1\,\mathrm{MeV}$ *larger than in the full space*
  - *RMS radius is within* $10^{-3}\,\mathrm{fm}$

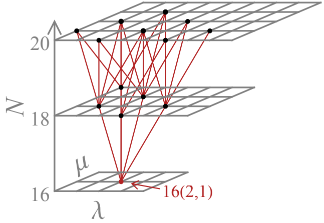
- Truncations based on single wave function provide reasonable truncation for other members of the same irrep family, but not all states
- Need to adjust truncations to accommodate angular momentum selection rules

Truncation by $\mathrm{Sp}(3,\mathbb{R})$ *subspace limited by size of subspace (~ 10 or ~100 irreps per subspace)*

Truncations by irreps

- Within each $\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ subspace only a few irreps may actually dominantly contribute

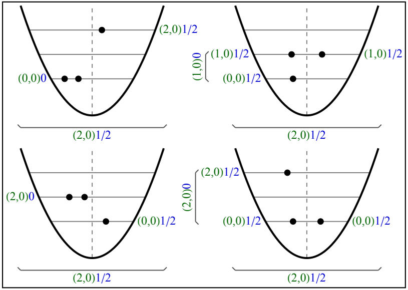
- Want to identify dominantly contributing irreps in each subspace (linear combinations of original irreps)



Truncations by irrep

At $N_{\mathrm{ex}} = 2$, ^{3}He LGIs are linear combinations of configurations with the same final SU(3)×SU(2) symmetry

Irreps starting from LGIs, which are different linear combinations of these configurations, make up the $\mathrm{Sp}(3,\mathbb{R})\times\mathrm{SU}(2)$ subspace (2,0)1/2



Truncations by irrep

How do we identify linear combinations of configurations which form LGI?

- LGIs are annihilated by $\mathrm{Sp}(3,\mathbb{R})$ lowering operator $B^{(0,2)}$
- Linear combinations span the null space of $B^{(0,2)}$ in SU(3) coupled configuration basis
- The linear combinations obtained using null solver are *arbitrary*
- Is there a particular linear combination that dominantly contributes to the wave function?

  "Hamiltonian preferred" linear combination

Summary

In $\mathrm{N}_{\sigma,\max}$ truncation scheme…

- Calculations converge with respect to $N_{\sigma,\max}$ at about $N_{\sigma,\max} = 10$

$\mathrm{Sp}(3,\mathbb{R}) \times \mathrm{SU}(2)$ subspace truncation…

- Details of binding energies depend on contributions from irreps around the 10^{-5} threshold
- Observables appear to depend less on low threshold irreps
- Truncations based on single wave function provide reasonable truncation for other members of the same irrep family

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

- Need to identify "Hamiltonian preferred LGI"

  Projecting wave functions onto LGI subspaces

Outlook

Truncation scheme to be explored and developed…

- Extending truncation by $Sp(3,\mathbb{R}) \times SU(2)$ subspaces
- Truncation by irrep
- Other truncations …

Computational scheme to be explored and developed…

- Restructure code for efficient massively parallel calculations
  `https://github.com/nd-nuclear-theory/spncci`
- Extend framework for 3-body interactions
  Petr Navratil