Symplectic no-core configuration interaction framework

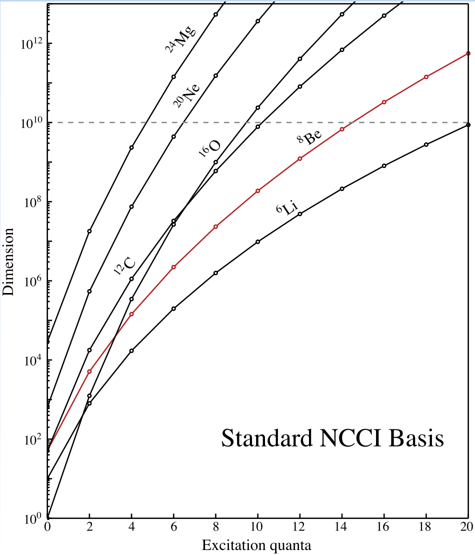
A. E. McCoy[1], M. A. Caprio[1], and T. Dytrych[2]

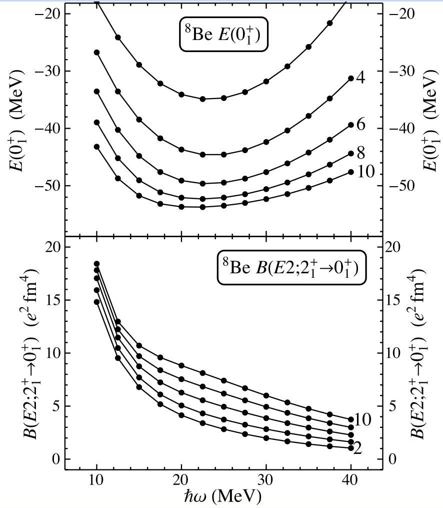
[1]University of Notre Dame

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

February 29, 2017

Dimension explosion for NCCI calculations





A. E. McCoy, M. A. Caprio, and T. Dytrych

Ab initio many-body calculations in a symplectic scheme

Outline

- How does the symplectic basis relate to the harmonic oscillator basis?
- Symplectic no-core configuration interaction (SpNCCI) framework
- Initial calculations

Acknowledgements

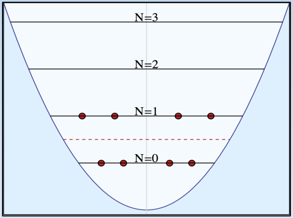
- David Rowe (University of Toronto)
- Pieter Maris (Iowa State University)
- Calvin Johnson (San Diego State University)
- Chao Yang (Lawrence Berkeley National Laboratory)
- Patrick Fasano (University of Notre Dame)

Harmonic oscillator basis

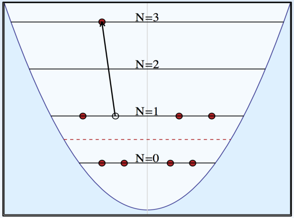
- States are configurations, i.e., distributions of particles over HO shells
- N_{ex}: total number of oscillator quanta above lowest Pauli allowed number.
- Wavefunctions are linear combinations of infinitely many HO configurations

$$|\Psi\rangle = c_0\phi_0 + c_1\phi_1 + c_2\phi_2 + ... + c_i\phi_i + ...$$

- Basis must be truncated
- How large must the basis be to contain states necessary for convergence?



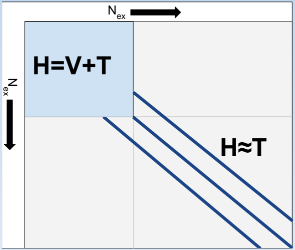
$N = 2n + \ell$

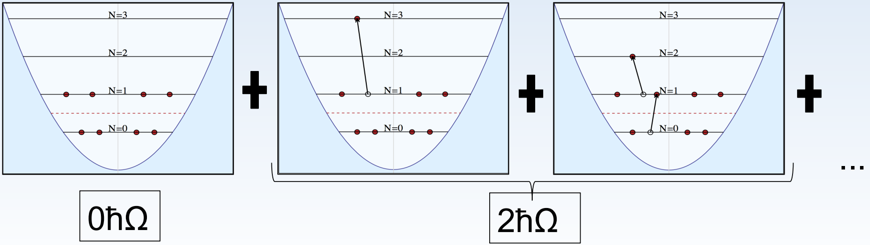


$N_{\mathrm{ex}} = 2$

N_{max} truncation

- Basis includes all configurations with $N_{\mathrm{ex}} \leq N_{\mathrm{max}}$
- Interaction strength expected to decrease with N
- Kinetic energy strongly couples configurations at low N_{ex} to those at high N_{ex}
- Basis must include these high N_{ex} configurations





Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-N_{ex} and high-N_{ex} configurations induced by kinetic energy.

Nuclear symmetries

Exact symmetries

- Spacial Translation (p)
- Time Translation (E)
- Rotation (J): SU(2)

Approximate symmetries

- Isospin (T)
- Elliot SU(3)
- Symplectic Sp(3,$\mathbb{R}$)

Why symplectic

Kinetic energy strongly connects states of different N_{ex} ($\Delta N_{\mathrm{ex}} = 2$)

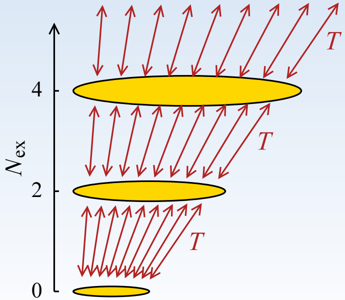
- Results in strong mixing of high N_{ex} configurations into many-body eigenstates

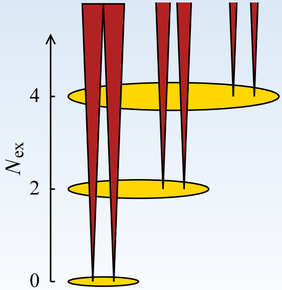
Kinetic energy conserves $\mathrm{Sp}(3,\mathbb{R})$ symmetry!

Symplectic reorganization of the many-body space

If we reorganize the many-body space by symplectic symmetry...

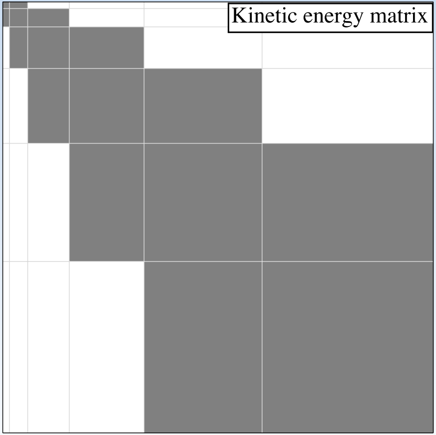
- Kinetic energy does not connect different symplectic irreducible representations (irrep)
- Resulting basis states are highly-correlated linear combinations of harmonic oscillator configurations



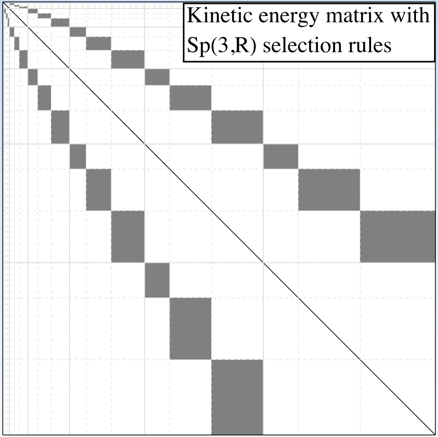


Kinetic energy

M-scheme basis



Symplectic basis



Exact symmetry under rotation: SU(2)

SU(2) generators

J_0	**Weight operator**
$J_\pm$	**Raising and lowering operator**

Action of the lowering operator

$$J_\pm \left|JM\right\rangle = \sqrt{(J \mp M)(J \pm M + 1)}\left|JM \pm 1\right\rangle$$

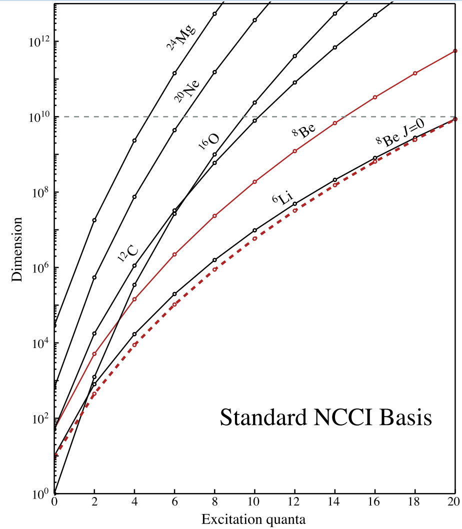
$$J_- \left|J -J\right\rangle = 0$$

Irreducible representation (irrep) J

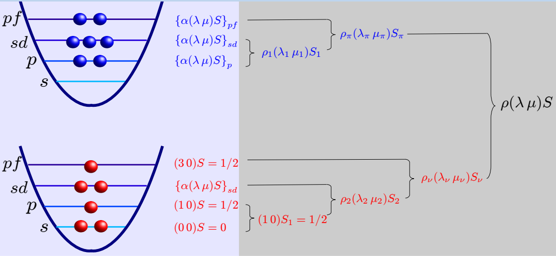
$$M = -J, \ldots, J$$

Hamiltonian matrix can be broken into J spaces (J-scheme)

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



SU(3)-NCSM basis



SU(3) generators

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

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

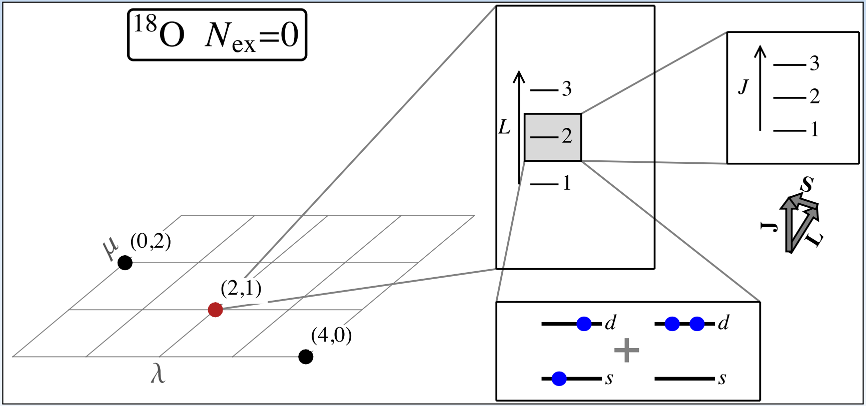
SU(3) symmetry of a nucleus is obtained by:

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

(λ,μ)	SU(3) irreducible representation (irrep)
κ	SU(3) to SO(3) branching multiplicity
L	Orbital angular momentum

References: J. P. Elliott, Proc. Roy. Soc. (London) A **245**, 562 (1958). M. Harvey, in *Advances in Nuclear Physics, Volume 1*, edited by M. Baranger and E. Vogt (1968), Annalen der Physik Vol. 1, p. 67.

SU(3)-NCSM basis: ^{18}O

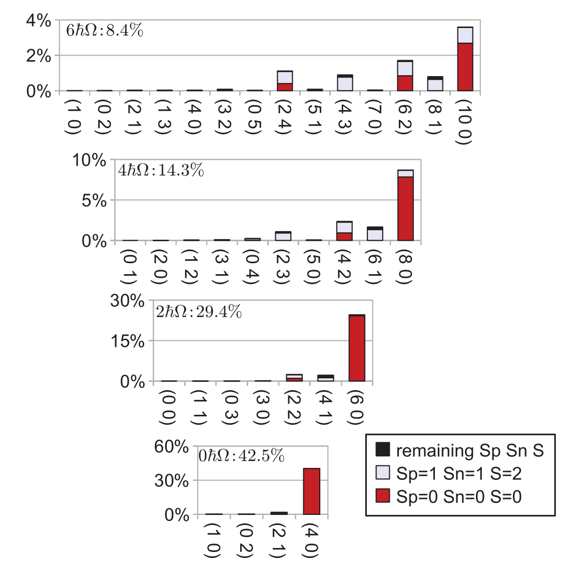


SU(3) has built-in correlations

SU(3) decomposition

- Ground state wavefunction dominated by a few SU(3) irreps
- SU(3) irreps consistent with Sp(3,R) symmetry

SU(3) decomposition of $^{8}\mathrm{Be}\ 0^{+}_{gs}$
Nmax=10
$\hbar\Omega = 20$ MeV
Chiral $N^{3}LO$



T. Dytrych *et al.*, Phys. Rev. Lett. **111** (2013) 252501.

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

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

$A^{(20)}_{LM} = \frac{1}{\sqrt{2}} \sum_i (b_i^\dagger \times b_i^\dagger)^{(20)}_{LM}$	$\mathrm{Sp}(3,\mathbb{R})$ raising
$B^{(02)}_{LM} = \frac{1}{\sqrt{2}} \sum_i (b_i \times b_i)^{(02)}_{LM}$	$\mathrm{Sp}(3,\mathbb{R})$ lowering
$C^{(11)}_{LM} = \sqrt{2} \sum_i (b_i^\dagger \times b_i)^{(11)}_{LM}$	**SU(3) generators**
$H^{(00)}_{00} = \sqrt{3} \sum_i (b_i^\dagger \times b_i)^{(00)}_{00}$	**HO Hamiltonian**

The kinetic energy

$$T_{00} = \frac{1}{2}(2H^{(0,0)}_{00} - \sqrt{6}A^{(2,0)}_{00} - \sqrt{6}B^{(0,2)}_{00})$$

$\mathrm{Sp}(3,\mathbb{R})$ states with spin: $|\sigma\upsilon\omega\kappa LSJM\rangle$

$$\begin{array}{ccccccc} \mathrm{Sp}(3,\mathbb{R}) & \supset & \mathrm{U}(3) & \supset & \mathrm{SO}(3) & & \\ \sigma & \upsilon & \omega & \kappa & L & & \\ & & & & \otimes & \supset & \mathrm{SU}(2) \\ & & & & \mathrm{SU}(2) & & J \\ & & & & S & & \end{array}$$

- σ Lowest grade U(3) irrep (LGI), labels the $\mathrm{Sp}(3,\mathbb{R})$ irrep
- υ $\mathrm{Sp}(3,\mathbb{R})$ to U(3) branching multiplicity
- ω U(3) symmetry of state in $\mathrm{Sp}(3,\mathbb{R})$ irrep
- κ U(3) to SO(3) branching multiplicity
- L Orbital angular momentum
- S Spin
- J Total angular momentum

$\mathrm{U}(3) = \mathrm{U}(1) \otimes \mathrm{SU}(3)$

$\sigma = N_\sigma(\lambda_\sigma, \mu_\sigma)$

$\omega = N_\omega(\lambda_\omega, \mu_\omega)$

References: D. J. Rowe, Rep. Prog. Phys. **48**, 1419 (1985). Y. Suzuki and K. T. Hecht, Nuc. Phys. A **455**, 315 (1986).

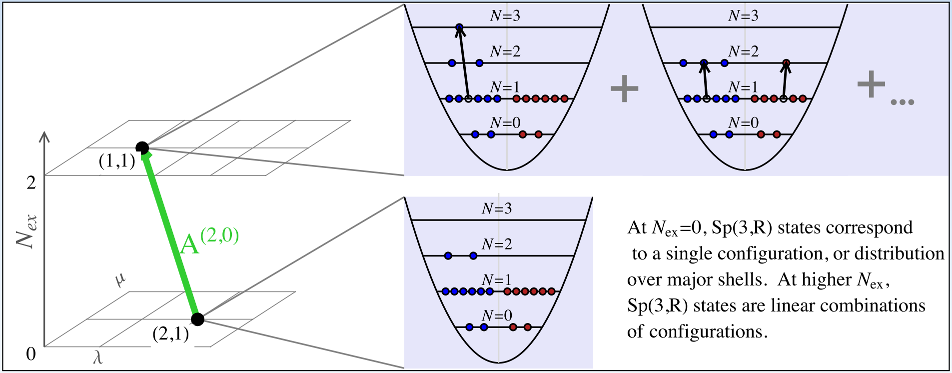
Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-N_{ex} and high-N_{ex} configurations induced by kinetic energy.
- SpNCCI basis states incorporate $\mathrm{Sp}(3,\mathbb{R})$, SU(3) and $\mathrm{SU}(2)$ symmetries.

Sp(3, $\mathbb{R}$) raising operator

$$A^{(20)}_{LM} = \frac{1}{\sqrt{2}} \sum_i (b_i^\dagger \times b_i^\dagger)^{(20)}_{LM}$$

Sp(3, $\mathbb{R}$) raising operator relates states with different number of oscillator excitation quanta N_{ex}.



At N_{ex}=0, Sp(3,R) states correspond to a single configuration, or distribution over major shells. At higher N_{ex}, Sp(3,R) states are linear combinations of configurations.

- Symplectic states have built in correlations across distributions of particles over major oscillator shells.

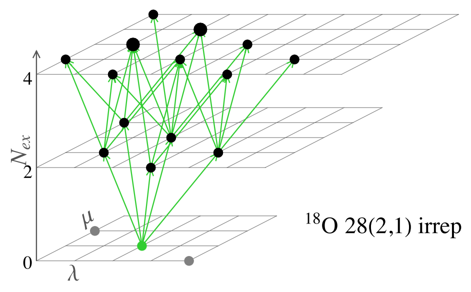
Symplectic basis

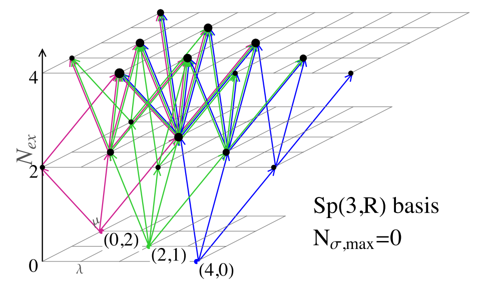
Symplectic irrep

- Start from lowest N_{ex} U(3) irrep: **lowest grade irrep (LGI)**
- Repeatedly act on the LGI with the $\mathrm{Sp}(3,\mathbb{R})$ raising operator
$$|\psi\rangle = AA\cdots A\,|\mathrm{LGI}\rangle$$
- Truncate each $\mathrm{Sp}(3,\mathbb{R})$ irrep by total number of oscillator excitations N_{max}

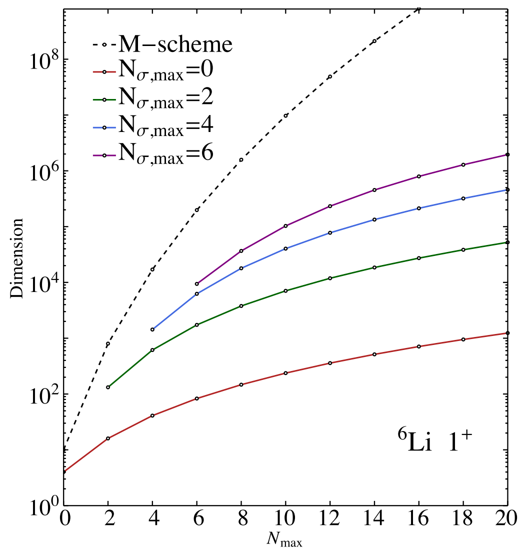
Defining SpNCCI basis

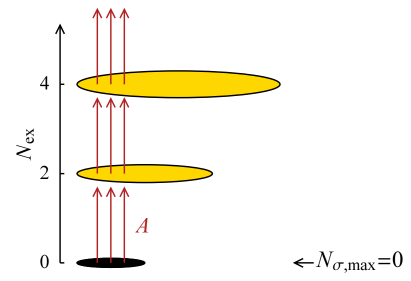
- Select a set of symplectic irreps
- *E.g.*, select only irreps whose LGI have $N_{\mathrm{ex}} \leq N_{\sigma,\mathrm{max}}$



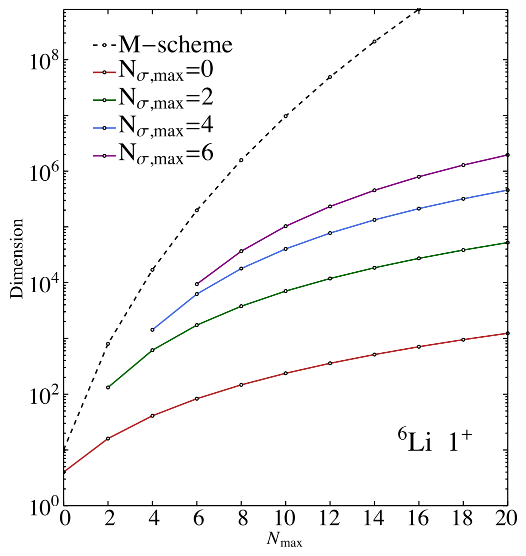


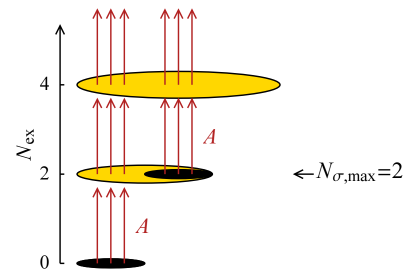
Basis dimensions with increasing $N_{\sigma,\max}$



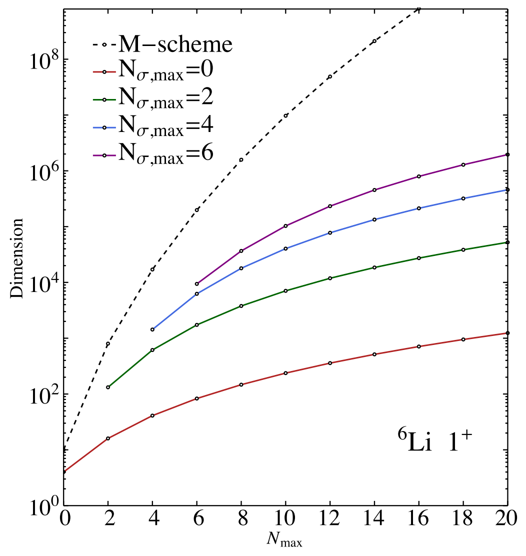


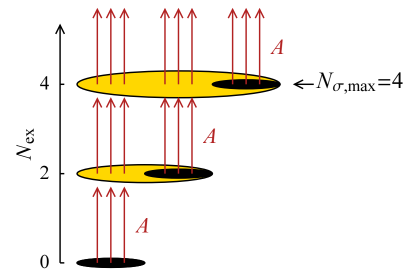
Basis dimensions with increasing $N_{\sigma,\max}$





Basis dimensions with increasing $N_{\sigma,\max}$





Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-N_{ex} and high-N_{ex} configurations induced by kinetic energy.
- SpNCCI basis states incorporate $\mathrm{Sp}(3,\mathbb{R})$, SU(3) and $\mathrm{SU}(2)$ symmetries.
- A symplectic irrep is generated by starting with the lowest N_{ex} configuration and repeatedly acting with the symplectic raising operator A.

$$A\,|N\rangle \rightarrow |N+2\rangle$$

Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-N_{ex} and high-N_{ex} configurations induced by kinetic energy.
- SpNCCI basis states incorporate $\mathrm{Sp}(3,\mathbb{R})$, SU(3) and $\mathrm{SU}(2)$ symmetries.
- A symplectic irrep is generated by starting with the lowest N_{ex} configuration and repeatedly acting with the symplectic raising operator A.

$$A\,|N\rangle \rightarrow |N+2\rangle$$

- Truncation by symplectic irrep allows us to include relevant high N_{ex} configurations in basis without needing to include full N_{ex} subspace.

Calculations in a symplectic basis

T. Dytrych *et al.*, J. Phys. G: Nucl. Part. Phys. **35** (2008) 123101.

T. Dytrych *et al.*, Phys. Rev. Lett. **111** (2013) 252501.

- Expand $\mathrm{Sp}(3,\mathbb{R})$ states in terms of SU(3)-NCSM states
  - Diagonalize $\mathrm{Sp}(3,\mathbb{R})$ Casimir operator in SU(3)-coupled basis
    R. B. Baker, *Ab initio symplectic-model results for light and medium-mass nuclei*, Progress in *Ab Initio* Techniques in Nuclear Physics, Vancouver, BC, 2016.
  - Obtain expansion of LGIs in SU(3)-coupled basis, then repeatedly apply symplectic raising operator to LGIs
    F. Q. Luo, Ph.D. thesis, University of Notre Dame (2014).
- Expand matrix elements in terms of LGI matrix elements using operator commutators (Suzuki and Hecht approach)
  Y. Suzuki and K. T. Hecht, Nuc. Phys. A **455** (1986) 315.
  J. Escher and J. P. Draayer, J. Math. Phys. **39** (1998) 51223.

SpNCCI recurrence scheme

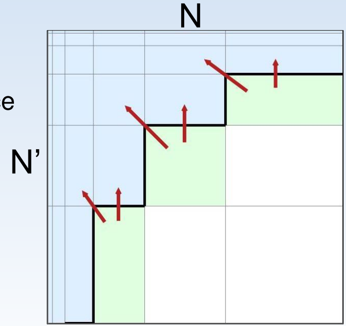
- Expand Hamiltonian in terms of fundamental "unit tensor" operators $\mathcal{U}(a,b)$ (analogous to TBME expansion of two-body operators in terms of $c_a^\dagger c_b^\dagger c_c c_d$)

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

- Expand only LGIs in SU(3)-NCSM basis
- Compute seed matrix elements (`LSU3shell`)

  T. Dytrych *et al.*, Compt. Phys. Commun. **207** (2016) 202.
- Compute matrix elements of $\mathcal{U}(a,b)$ via recurrence

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



Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-N_{ex} and high-N_{ex} configurations induced by kinetic energy.
- SpNCCI basis states incorporate $\mathrm{Sp}(3,\mathbb{R})$, SU(3) and $\mathrm{SU}(2)$ symmetries.
- A symplectic irrep is generated by starting with the lowest N_{ex} configuration and repeatedly acting with the symplectic raising operator A.

$$A\,|N\rangle \rightarrow |N+2\rangle$$

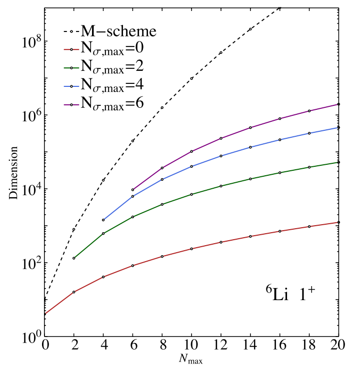
- Truncation by symplectic irrep allows us to include relevant high N_{ex} configurations in basis without needing to include full N_{ex} subspace.
- Matrix elements are computed recursively and so explicit construction of full basis is not necessary.

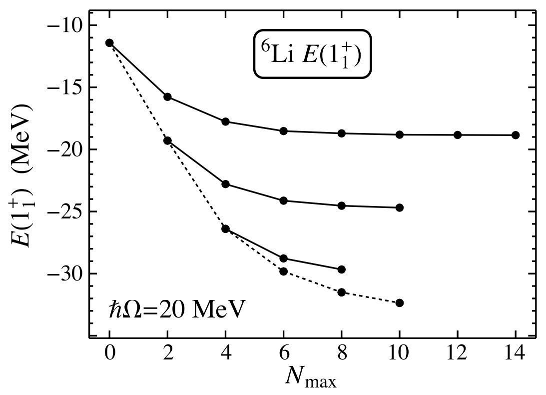
Initial results

^{6}Li, JISP16 (no Coulomb)

- Examine convergence with $N_{\sigma,\max}$
- Need to include all irreps strongly connected by interaction

  At what $N_{\max}$ does the interaction fade away and the kinetic energy dominate?



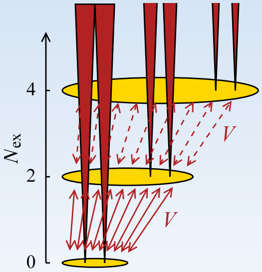


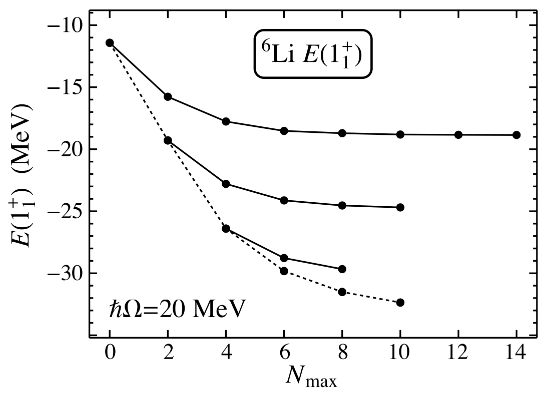
Initial results

^{6}Li, JISP16 (no Coulomb)

- Examine convergence with $N_{\sigma,\max}$
- Need to include all irreps strongly connected by interaction

  At what $N_{\max}$ does the interaction fade away and the kinetic energy dominate?





Recap

- *Ab initio* NCCI calculations are computationally bound by the large basis size necessary for convergence — which arises, in large part, because of strong connections between low-N_{ex} and high-N_{ex} configurations induced by kinetic energy.
- SpNCCI basis states incorporate $\mathrm{Sp}(3,\mathbb{R})$, SU(3) and $\mathrm{SU}(2)$ symmetries.
- A symplectic irrep is generated by starting with the lowest N_{ex} configuration and repeatedly acting with the symplectic raising operator A.

$$A\,|N\rangle \rightarrow |N+2\rangle$$

- Truncation by symplectic irrep allows us to include relevant high N_{ex} configurations in basis without needing to include full N_{ex} subspace.
- Matrix elements are computed recursively and so explicit construction of full basis is not necessary.
- We have initial results as of 5 days, 5 hours and 43 minutes ago.

Going forward

- Significant improvement can be made to SpNCCI code (memory usage and parallelization) to extend calculations to higher $N_{\sigma,\max}$ and $N_{\max}$ (and heavier nuclei).
- Exploration of basis truncations: restrict basis to physically preferred LGI's
  - Extract physically preferred transformed LGI set from wave functions in low $N_{\max}$ reference calculation
  - Determine preferred LGI set from self consistency approach
    D. J. Rowe, Phys. Rev. Lett. **97** (2006) 202501.
  - ...