Ab initio multi-irrep symplectic no-core configuration interaction calculations

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Why the symplectic basis?

We want to reduce the size of the basis necessary for convergence

The nuclear potential only strongly couples low N_{ex} states, but the kinetic energy does strongly couple configurations at high N_{ex} to low N_{ex} states. To obtain converged results, the basis must include these high N_{ex} configurations.

- $\mathrm{Sp}(3,\mathbb{R})$ constains the kinetic energy operator. Selecting basis states by their symplectic irreps preselect these high N_{ex} states

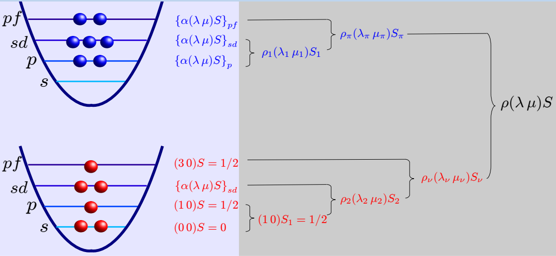
The nucleus is highly correlated, i.e., the wavefunctions are superpositions of many harmonic oscillator configurations.

- $\mathrm{Sp}(3,\mathbb{R})$ basis has naturally built-in correlations

SU(3)-NCSM basis

SU(3) generators

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



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

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

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.

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.

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

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

SU(3) generators

$$C^{(1,1)}_{LM} = Q_{2M}\delta_{L,2} + \sqrt{3}L_{1M}\delta_{L,1}$$

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

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

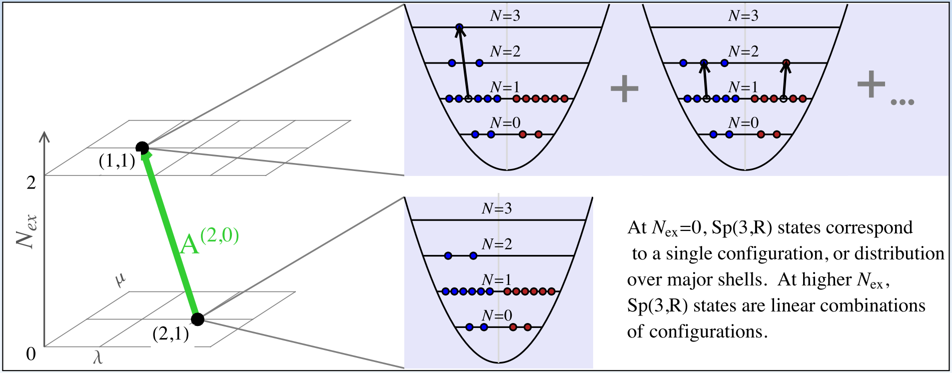
- σ Lowest grade U(3) irrep (LGI), labels the $\mathrm{Sp}(3,\mathbb{R})$ irrep
- υ $\mathrm{Sp}(3,\mathbb{R})$ to U(3) branching multiplicity
- ω U(3) symmetry of state in $\mathrm{Sp}(3,\mathbb{R})$ irrep
- κ U(3) to SO(3) branching multiplicity
- L Orbital angular momentum
- S Spin
- J Total angular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

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

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

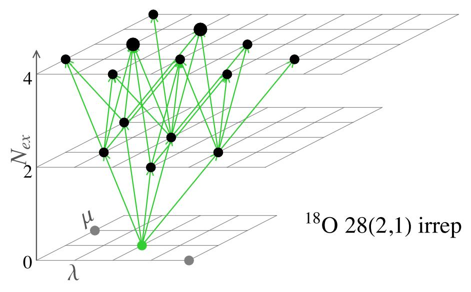


At N_{ex}=0, Sp(3,R) states correspond to a single configuration, or distribution over major shells. At higher N_{ex}, Sp(3,R) states are linear combinations of configurations.

Symplectic basis

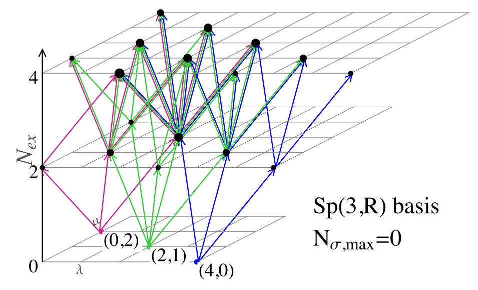
Symplectic irrep

- Start with lowest grade U(3) irrep (LGI)
- Repeatedly act on the LGI with the $\mathrm{Sp}(3,\mathbb{R})$ raising operator

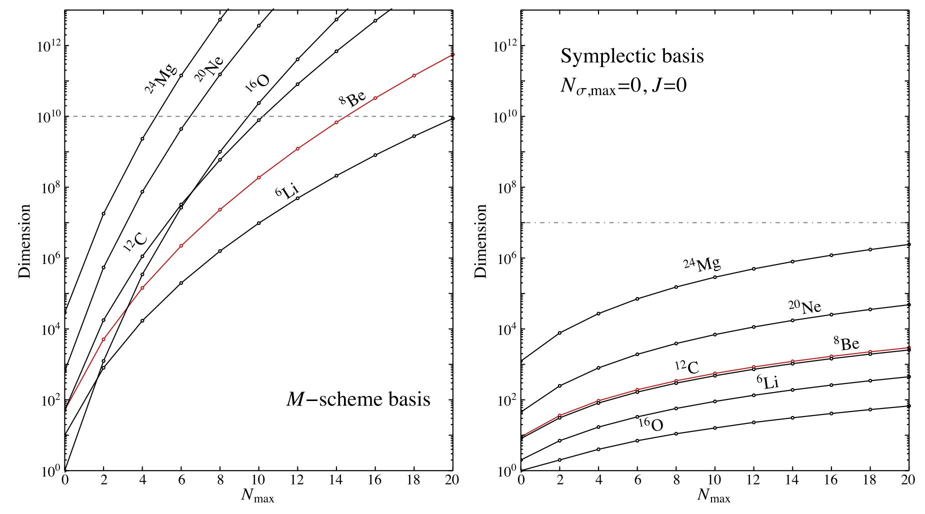


Symplectic basis

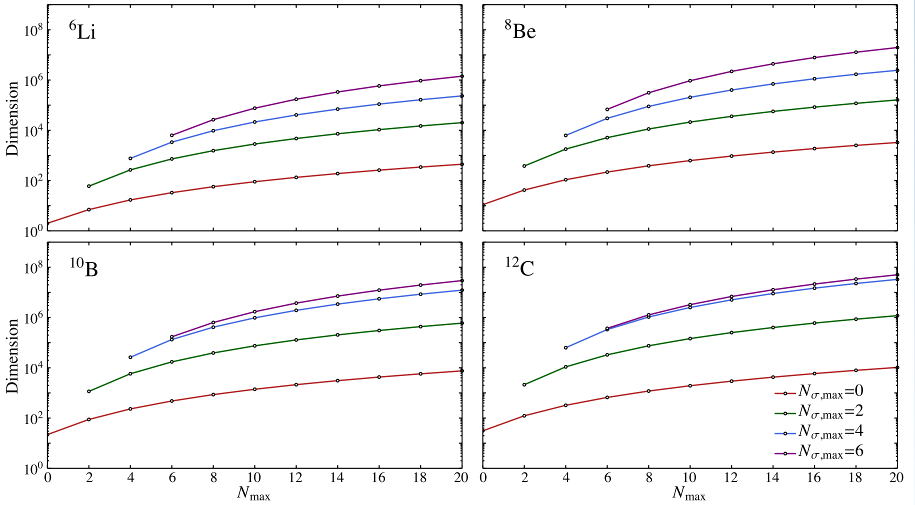
- Select a set of LGI's and their allowed spins S by, e.g., taking all LGI's with oscillator excitations N_{ex} less than some $N_{\sigma,\mathrm{max}}$
- Truncate each $\mathrm{Sp}(3,\mathbb{R})$ irrep by total number of oscillator excitations N_{max}



Basis dimension comparison



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



Constructing the Hamiltonian matrix

Inputs:

- Relative matrix elements of the potential (JISP16, chiral, etc.)

Calculating matrix elements:

- Generated indexed list of state labels $|\sigma\upsilon\omega\kappa LSJ\rangle$
- Expand the LGI's in the SU(3)-NCSM basis
- Calculate SU(3) reduced matrix elements of small set of "unit tensor" operators between LGI's
- Recursively calculate the matrix elements between all other basis states, starting from these unit tensor reduced matrix elements

Conclusions

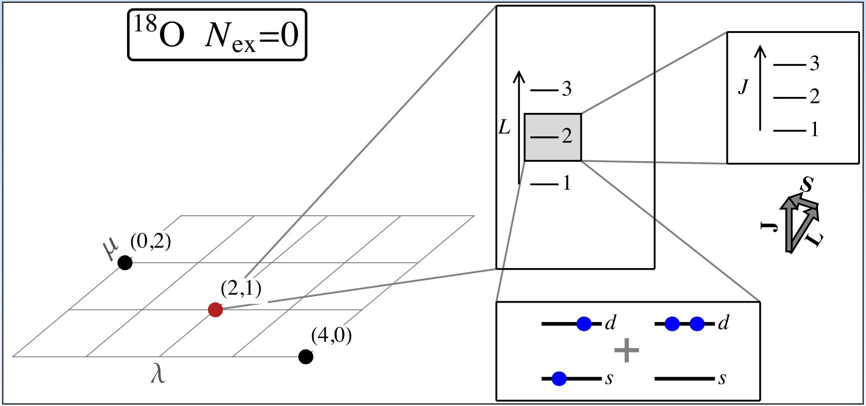
Current status:

- Interfacing symplectic code with LSU3shell code for LGI matrix elements

Major questions:

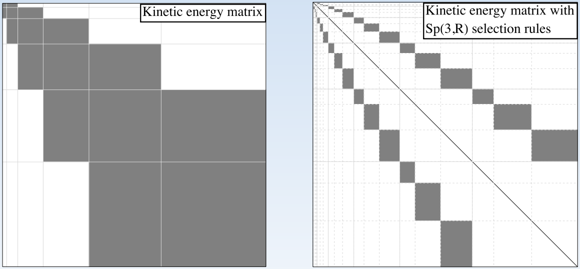
- What truncation of the basis will bring us closest to converged results?
  - Truncating by $N_{\sigma,\mathrm{max}}$ and N_{max}
  - Importance truncation to identify dominant $\mathrm{Sp}(3,\mathbb{R})$ irreps
- How is convergence related to interaction?
- What can identifying dominant $\mathrm{Sp}(3,\mathbb{R})$ symmetries tell us about collective behavior?
  - $\mathrm{Sp}(3,\mathbb{R})$ contains generators of monopole and quadrupole moments and deformations, orbital angular momentum and quadrupole flow dynamics
  - Related to rotor-model and giant quadrupole resonance in the large oscillator quanta limit
  - Overlap between clusters and symplectic symmetry (A. Dreyfuss)

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



Advantages of a group theoretical basis

- **Reduce redundancy in calculations by using, e.g., the Wigner-Eckhart theorem**
- **Identify non-zero matrix elements using selection rules before computation**



- **Reduce complexity of calculations**