Ab initio symplectic no-core configuration interaction calculations (SpNCCI)

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Challenges in *Ab Initio* Calculations

- Nuclear wavefunction is highly correlated
- Lowest energy wavefunction contain highly excited configurations
- Harmonic oscillator basis grows very rapidly with increasing N_{max}

Construct physically adapted basis with built-in correlations:

symplectic basis

Why the symplectic basis?

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.

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

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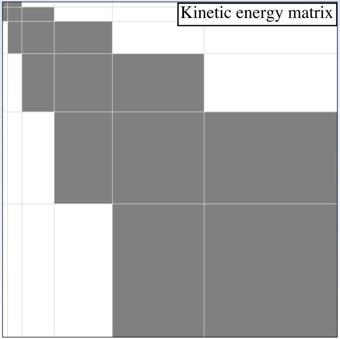

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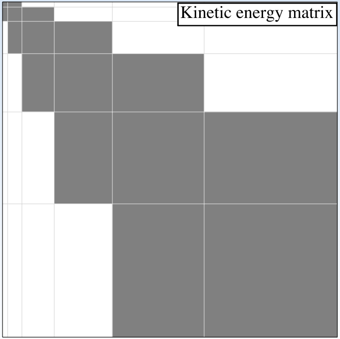
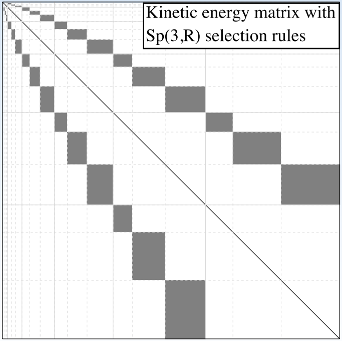
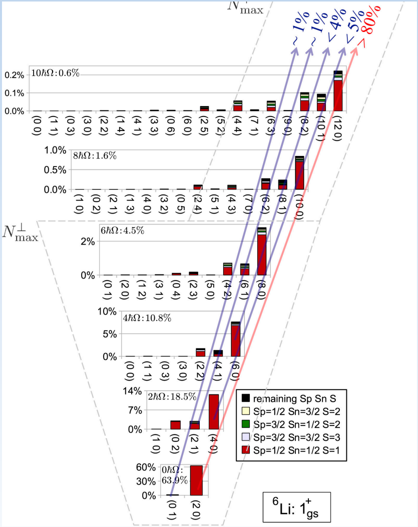




Why the symplectic basis?

The nucleus is highly correlated

- $Sp(3, \mathbb{R})$ basis has naturally built-in correlations
- Do these correlations better match physical wavefunction?



R. B Baker, Ab initio symplectic-model results for light and medium-mass nuclei, Progress in ab initio techniques in nuclear physics, Vancouver, 2016.

Outline

Build in correlations using symmetries

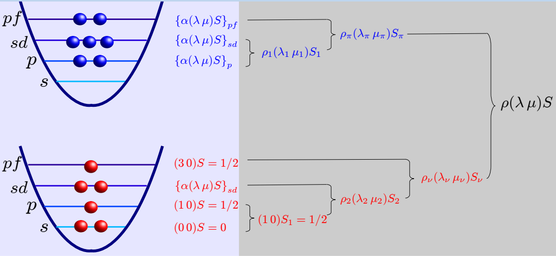
- SU(3): Linear combination of states with same particle distribution over major shells
- Sp(3,R): Linear combination of states with different major shell configurations

Carrying out calculations in SpNCCI framework

SU(3)-NCSM basis

SU(3) generators

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



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

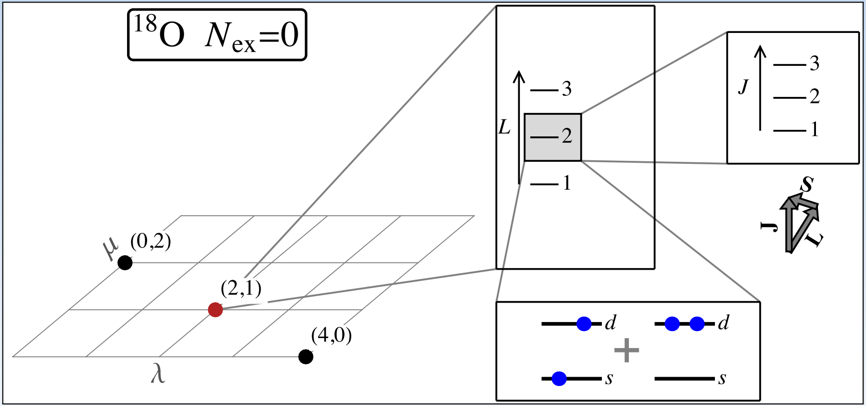
SU(3) symmetry of a nucleus is obtained by:

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



$N_{\text{ex}} = \sum_i (2n_i + l_i) - N_0$

Elliot SU(3) rotations

SU(3) subgroup of $Sp(3,\mathbb{R})$

$$C_{2M} \propto Q_{2M} \quad C_{1M} \propto L_{1M}$$

– SU(3) symmetry labeled by (λ,μ)

– Each particle has symmetry $(\eta,0)$

– Couple particles to get total symmetry

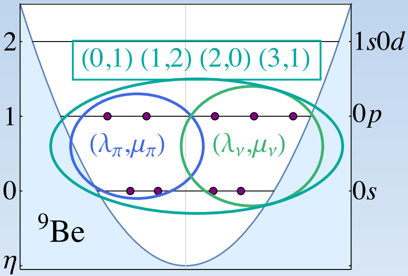
$$(\eta_1,0)\times(\eta_2,0)\times(\eta_3,0)\times\ldots\rightarrow(\lambda,\mu)$$

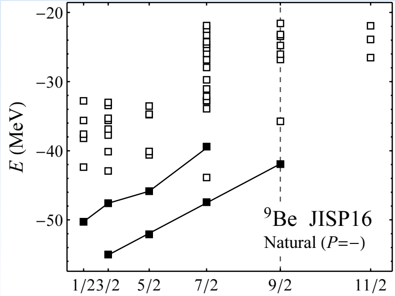
SU(3) rotations

$$(\lambda,\mu)\times S\rightarrow\{L_1,L_2,L_3,\ldots\}\times S\rightarrow\{J_1,J_2,J_3\ldots\}$$

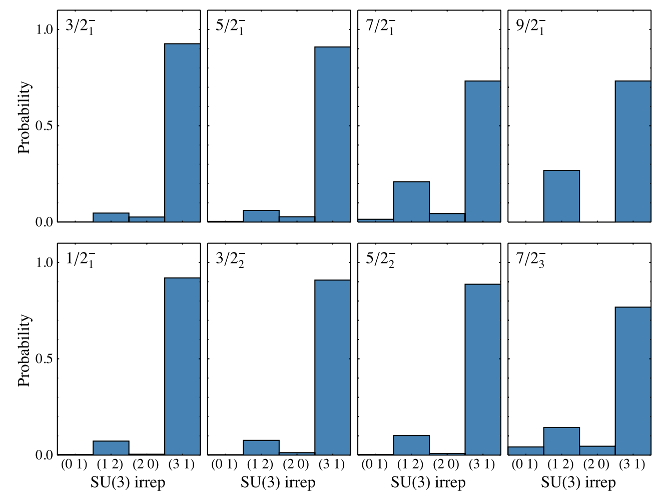
$S=1/2$, $(3,1)$:

L	Aligned	Anti-aligned
1	3/2	1/2
2	5/2	3/2
3	7/2	5/2
4	9/2	7/2





SU(3) decomposition of NCCI rotation band members



Calculated with LSU3shell
$N_{\max} = 6$, JISP16

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

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

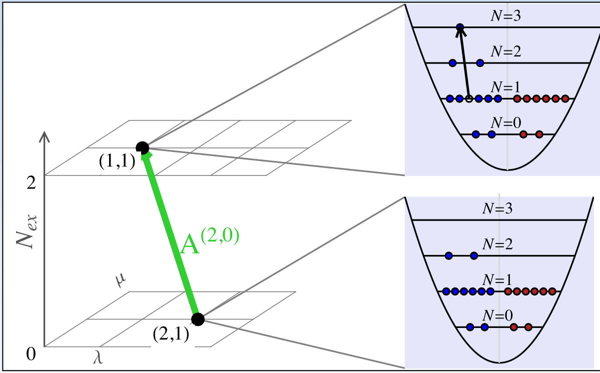
- σ Lowest grade U(3) irrep (LGI), labels the $\mathrm{Sp}(3,\mathbb{R})$ irrep
- υ $\mathrm{Sp}(3,\mathbb{R})$ to U(3) branching multiplicity
- ω U(3) symmetry of state in $\mathrm{Sp}(3,\mathbb{R})$ irrep
- κ U(3) to SO(3) branching multiplicity
- L Orbital angular momentum
- S Spin
- J Total angular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

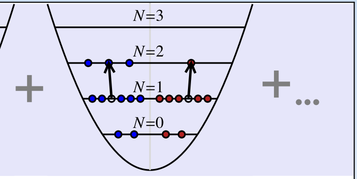
$$\mathrm{U}(3) = \mathrm{U}(1) \otimes \mathrm{SU}(3)$$
$$\sigma = N_\sigma(\lambda_\sigma, \mu_\sigma)$$
$$\omega = N_\omega(\lambda_\omega, \mu_\omega)$$

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

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

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



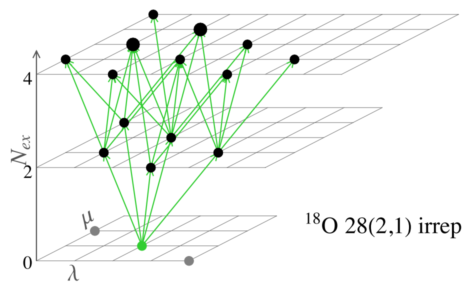


At N_{ex}=0, Sp(3,R) states correspond to a single configuration, or distribution over major shells. At higher N_{ex}, Sp(3,R) states are linear combinations of configurations.

Symplectic basis

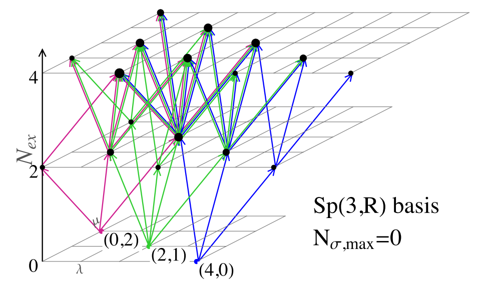
Symplectic irrep

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

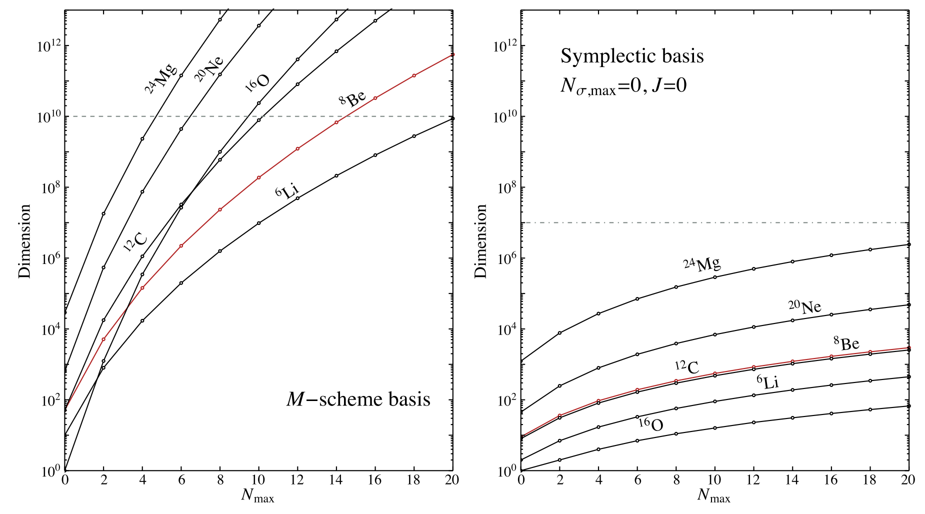


Symplectic basis

- 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}

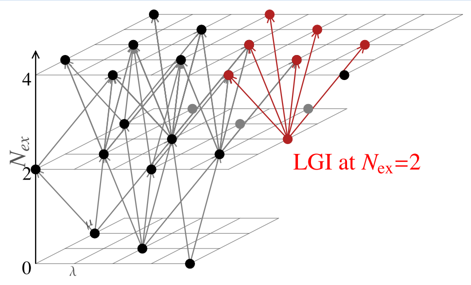


Basis dimension comparison



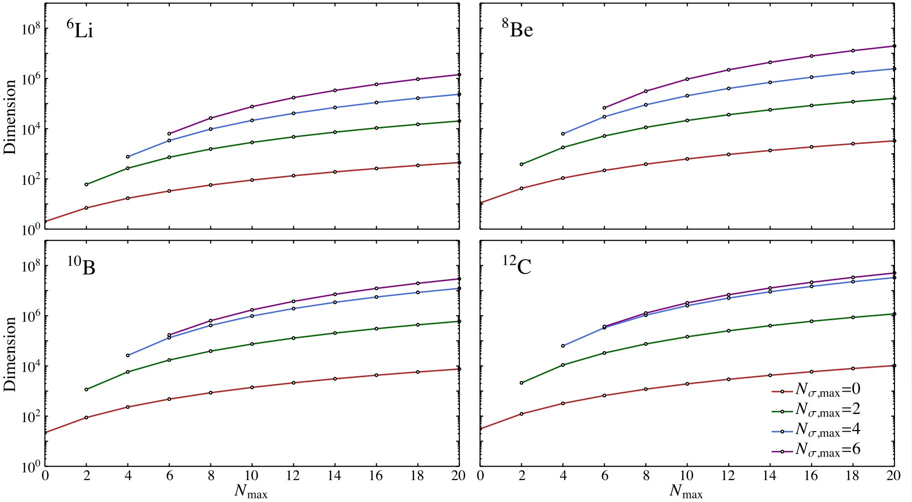
LGI's with $N_{\sigma,\max} > 0$

- Not all states with $N_{\text{ex}} = 2$ are not contained in $N_{\sigma,\max} = 0$ irreps
- These states are $N_{\sigma,\max} = 2$ LGI
- LGI with $N_{\sigma} > 0$ may have center of mass excitation
- Very straightforward to identify and eliminate center of mass excitation



- The dimension of the symplectic basis is equal to the dimension of the *m*-scheme basis only if the symplectic basis includes all LGI up to $N_{\sigma,\max} = N_{\max}$.

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



Calculating Hamiltonian matrix elements

In the *m*-scheme basis:

$$H_{ij} = (-1)^P \delta_{i_1,j_1} ... \delta_{i_{A-2},j_{A-2}} \langle ab|H|cd\rangle$$

Calculating Hamiltonian matrix elements

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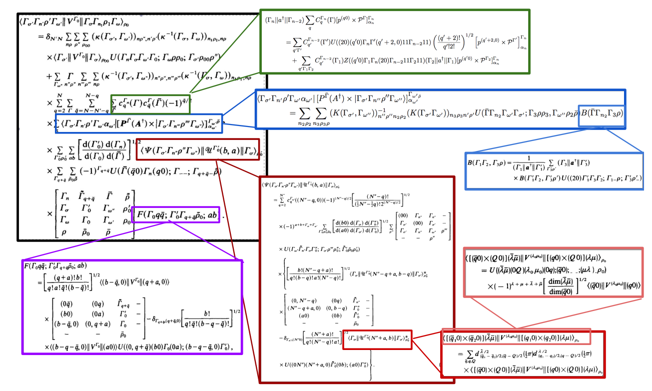
In the $\mathrm{Sp}(3,\mathbb{R})$ basis:



Calculating Hamiltonian matrix elements

- Expand operators in terms of SU(3) unit tensors

$$H^{\omega_0\kappa_0 S_0} = \sum_{\substack{\bar{N}\bar{S}\\ \bar{N}'\bar{S}'}} \underbrace{\langle(\bar{N}',0)\bar{S}'|||H^{\omega_0\xi_0 S_0}|||(\bar{N},0)\bar{S}\rangle}_{\text{Relative matrix element in HO basis}} \mathcal{U}^{\omega_0 S_0}(\bar{N}'\bar{S}',\bar{N}\bar{S})$$

- Matrix element of *H* in symplectic basis is given by

$$\langle\sigma'\upsilon'\omega'S'|||H^{\omega_0\kappa_0 S_0}|||\sigma\upsilon\omega S\rangle_{\rho_0} = \sum_{\substack{\bar{N}\bar{N}'\\ \bar{S}'\bar{S}}} \langle(\bar{N}',0)\bar{S}'|||H^{\omega_0\xi_0 S_0}|||(\bar{N},0)\bar{S}\rangle \, \langle\sigma'\upsilon'\omega'S'|||\mathcal{U}^{\omega_0\kappa_0 S_0}(\bar{N}'\bar{S}',\bar{N}\bar{S})|||\sigma\upsilon\omega S\rangle_{\rho_0}$$

- Matrix elements of unit tensors in symplectic basis computed recursively

$$\begin{aligned}
&\langle\sigma'\upsilon'\omega'S'||\mathcal{U}^{\omega_0 S_0}(\bar{r}'\bar{S},\bar{r}\bar{S})||\sigma\upsilon\omega S\rangle_{\rho_0} \\
&\quad = \sum_{\substack{n\rho n_1\omega_0'\rho_0'\\ \omega_1\rho_1\upsilon_1}} (K_\sigma^\omega)^{-1}_{\upsilon,(n\rho)}(n||a^{\dagger(2,0)}||n_1)U((2,0)n_1\omega\sigma;n_{-}\rho;\omega_1\rho_{1-})(K_\sigma^{\omega_1})_{(n_1\rho_1)\upsilon_1}U(\omega_0(2,0)\omega'\omega_1;\omega'_{0}\text{-}\rho'_0;\omega_{-}\rho_0) \\
&\qquad \times \sum_{q\omega_0''q'\bar{\omega}_0} (-1)^{\omega_0''-\omega_0'+\frac{q'}{2}} U(\omega_0(q,0)\omega_0'(2-q,0);\omega_0'';(2,0))U((2-q-q',0)(q',0)\omega_0'\omega_0'';(2-q,0);\bar{\omega}_0) \\
&\qquad \times \left[\frac{(\bar{r})!}{q!(\bar{r}-q)!}\right]^{1/2} \left[\frac{(q'+\bar{r}')!}{q'!\bar{r}'!}\right]^{1/2} \left[\frac{d(\bar{\omega}_0)d(\bar{r},0)d(\bar{r}',0)}{d(\omega_0)d(\bar{r}-q,0)(d(q'+\bar{r}',0)}\right]^{1/2} \\
&\qquad \times U((\bar{r}',0)(0,\bar{r})\omega_0''(q,0);\omega_0;(0,\bar{r}-q))U((q',0)(\bar{r}',0)\bar{\omega}_0(0,\bar{r}-\bar{q})(q'+\bar{r}',0)\omega_0'') \\
&\qquad \times \sum_{\omega''\nu''\rho_0''} U((2-q-q',0)\bar{\omega}_0\omega'\omega_1;\omega'_{0}\text{ -}\rho_0';\omega''\rho''_{0}\text{ -})\langle\sigma'\upsilon'\omega'S'||P^{(2-q-q',0)}||\sigma'\nu''\omega''S'\rangle \\
&\qquad\qquad \times \langle\sigma'\nu''\omega''S'||\mathcal{U}^{\bar{\omega}_0 S_0}(\bar{r}'+q'\bar{S}',\bar{r}-q\bar{S})||\sigma\upsilon_1\omega_1 S\rangle_{\rho_0''}
\end{aligned}$$

Constructing the Hamiltonian matrix

Calculating matrix elements:

- 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
- Generated indexed list of state labels $|\sigma\upsilon\omega\kappa LSJ\rangle$
- Recursively calculate the matrix elements between all other basis states, starting from these unit tensor reduced matrix elements

Inputs:

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

Conclusions

Current status:

- Interfacing SpNCCI 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}
  - Truncate by 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