Ab Initio No-Core Shell Model in SU(3)-Scheme Basis

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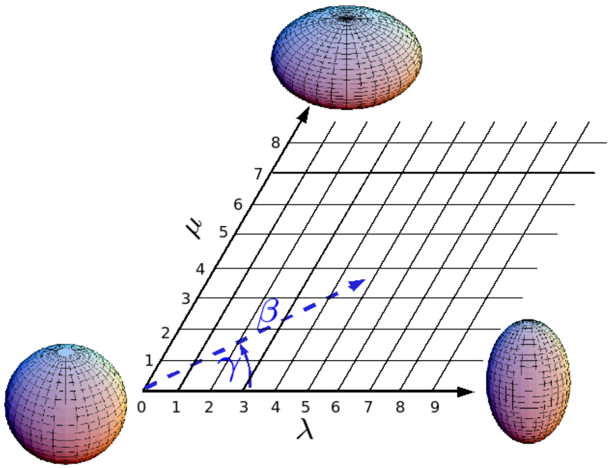
SU(3) symmetry-adapted approach

Motivation:

- identification of the important collective correlations ▶ model space truncation
- computational methods of the group theory in NCSM calculations

SU(3) symmetry



- relevant for description of spatially deformed nuclei
- $(\lambda\ \mu)$ related to shape variables β and γ of the collective model
- embedded in the symplectic model of the nuclear collective motion
- SU(3) contains rotational group SO(3) as a subgroup

SU(3) classification scheme

$$SU(3) \supset SO(3)$$

$$(\lambda\ \mu) \quad \kappa \quad L$$

- L: orbital angular momentum
- κ: multiplicity label – needed to distinguish multiple occurrence of L
- $(\lambda\ \mu)$: SU(3) quantum numbers

- Example: $(4\ 2)$

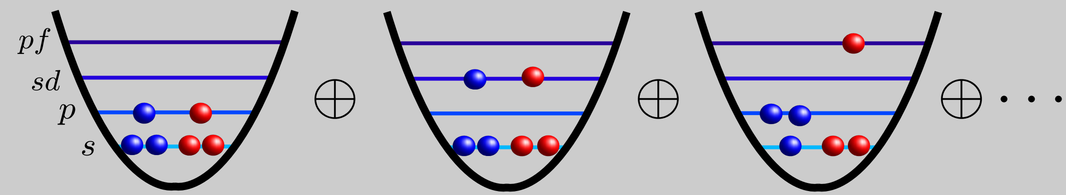
κ	L
0	0
0	2
1	2
0	3
0	4
1	4
0	5
0	6

Construction of SU(3) symmetry-adapted basis in NCSM

Step 1

- Generate distributions of nucleons over HO shells for a given Nmax model space

$N_{\max}$ =



Step 2

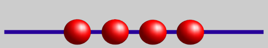
- for each set of nucleons in a HO shell determine antisymmetric representations of U(N)xU(2)

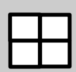
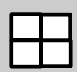
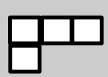
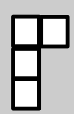
Step 3

- decompose each U(N) irrep into a complete set of SU(3) irreps

	U(2)	$\otimes$	U(10)	$\supset$	SU(3)
quantum labels:	S		[f]	α	$(\lambda\ \mu)$

- Example:
  4 nucleons in pf

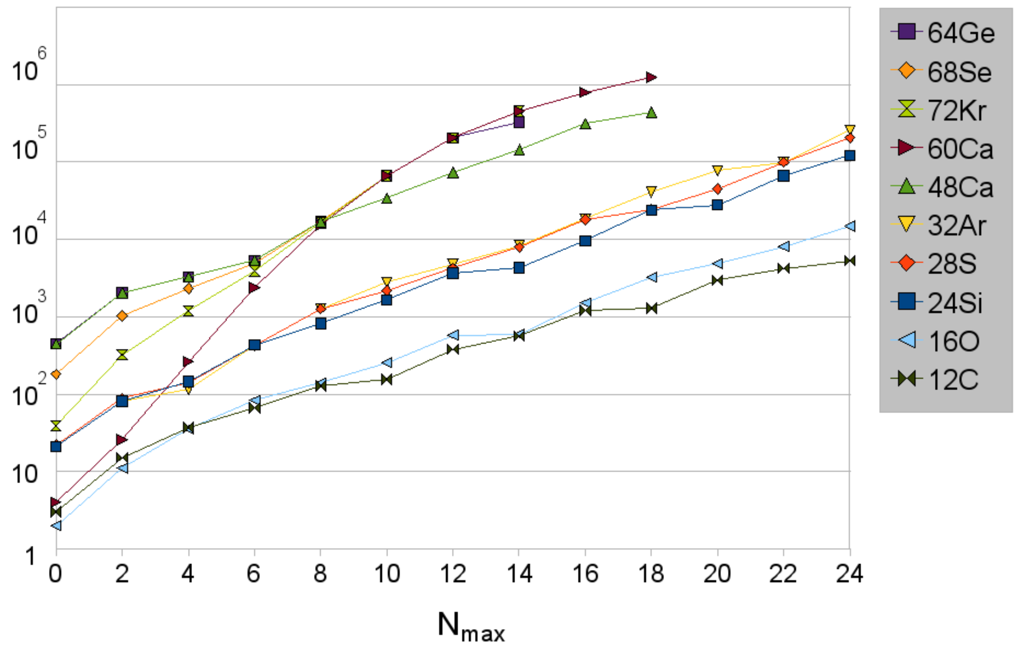


S	U(2)	U(10)		SU(3)
S=0			$\supset$	{ (8 2) (7 1) (4 4) (5 2) (0 6) (6 0) (3 3) (1 4) (4 1) (2 2) (1 1) (4 4) (2 2) }
S=1			$\supset$	{ (9 0) (6 3) (7 1) (4 4) (2 5) (5 2) (3 3) (1 4) (4 1) (2 2) (0 3) (3 0) (1 1) (5 2) (3 3) (1 4) (4 1) (3 0) }
S=2			$\supset$	{ (5 2) (0 6) (3 3) (2 2) (3 0) }

"seeds"

Construction of SU(3) symmetry-adapted basis in NCSM

Number of "seed" representations in NCSM model spaces



- just a single state from each "seed" needs to be constructed in order to calculate matrix elements of a realistic interaction in SU(3)-scheme

- Complete Nmax basis constructed by inter-shell coupling of "seeds"

Construction of SU(3) symmetry-adapted basis in NCSM

- SU(3) coupling $(\lambda_1\,\mu_1)\times(\lambda_2\,\mu_2)\to\{\rho^{\max}(\lambda\,\mu)\}$ ... similar to coupling of angular momenta but certain resulting irreps occur multiple times

$$(1\,1)\times(1\,1)\to\{(0\,0)\oplus(0\,3)\oplus(1\,1)\oplus(1\,1)\oplus(2\,2)\oplus(3\,0)\}$$

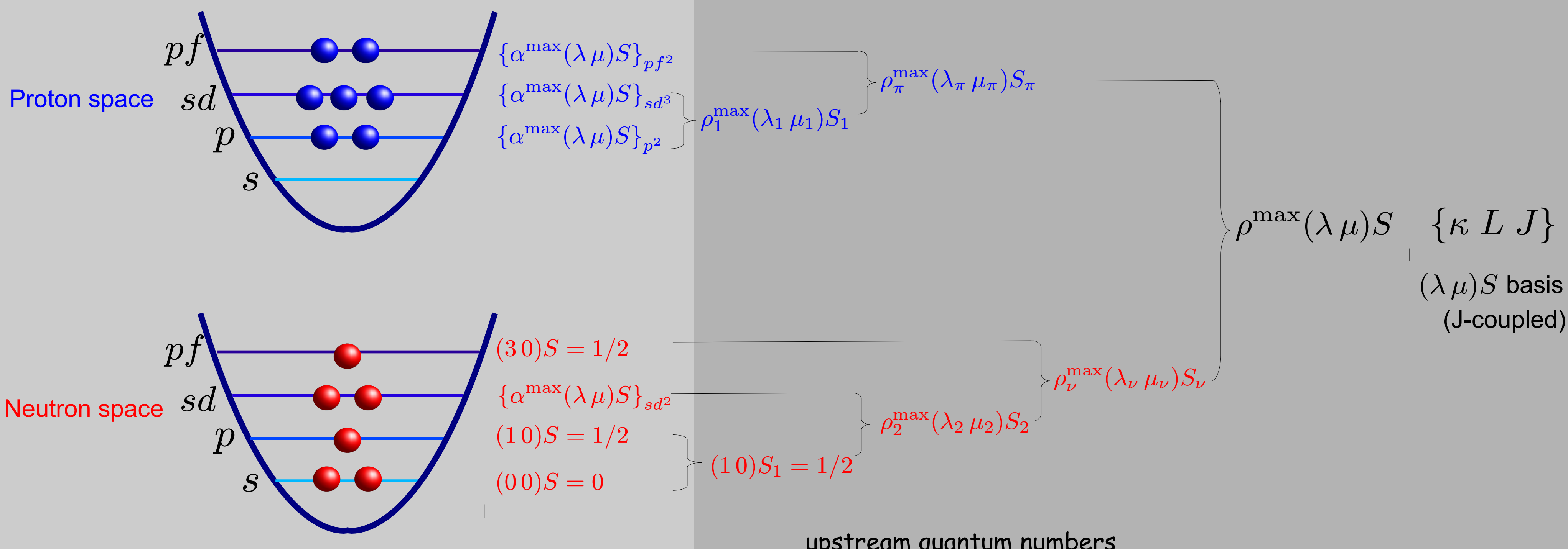
Complete NCSM basis constructed by SU(3) and spin couplings of the "seed" irreps

Step 1

- for a given distribution of protons/neutrons obtain "seed" irreps

Step 2

- perform SU(3)xSU(2) inter-shell coupling



- each combination of upstream quantum numbers is spanned by $(\Pi\alpha^{\max})(\Pi\rho^{\max})(\Pi\alpha^{\max})(\Pi\rho^{\max})\rho^{\max}\dim[\{\kappa\;L\;J\}]$ states

NCSM model space in SU(3) scheme

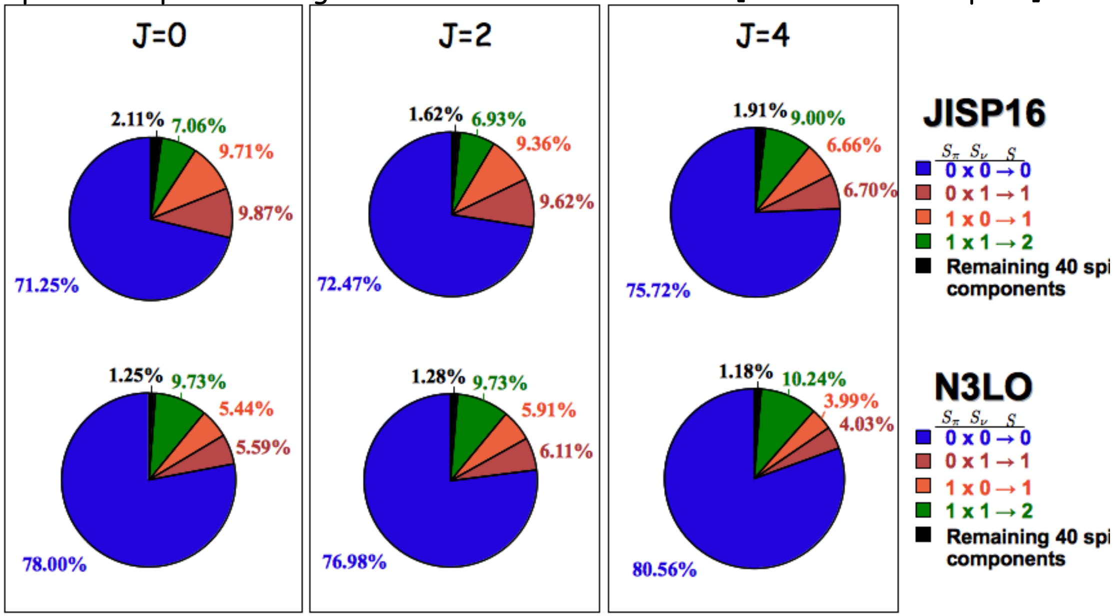
- SU(3)-scheme decomposes Nmax model space into subspaces of states labeled by S_π S_ν $(\lambda\ \mu)S$

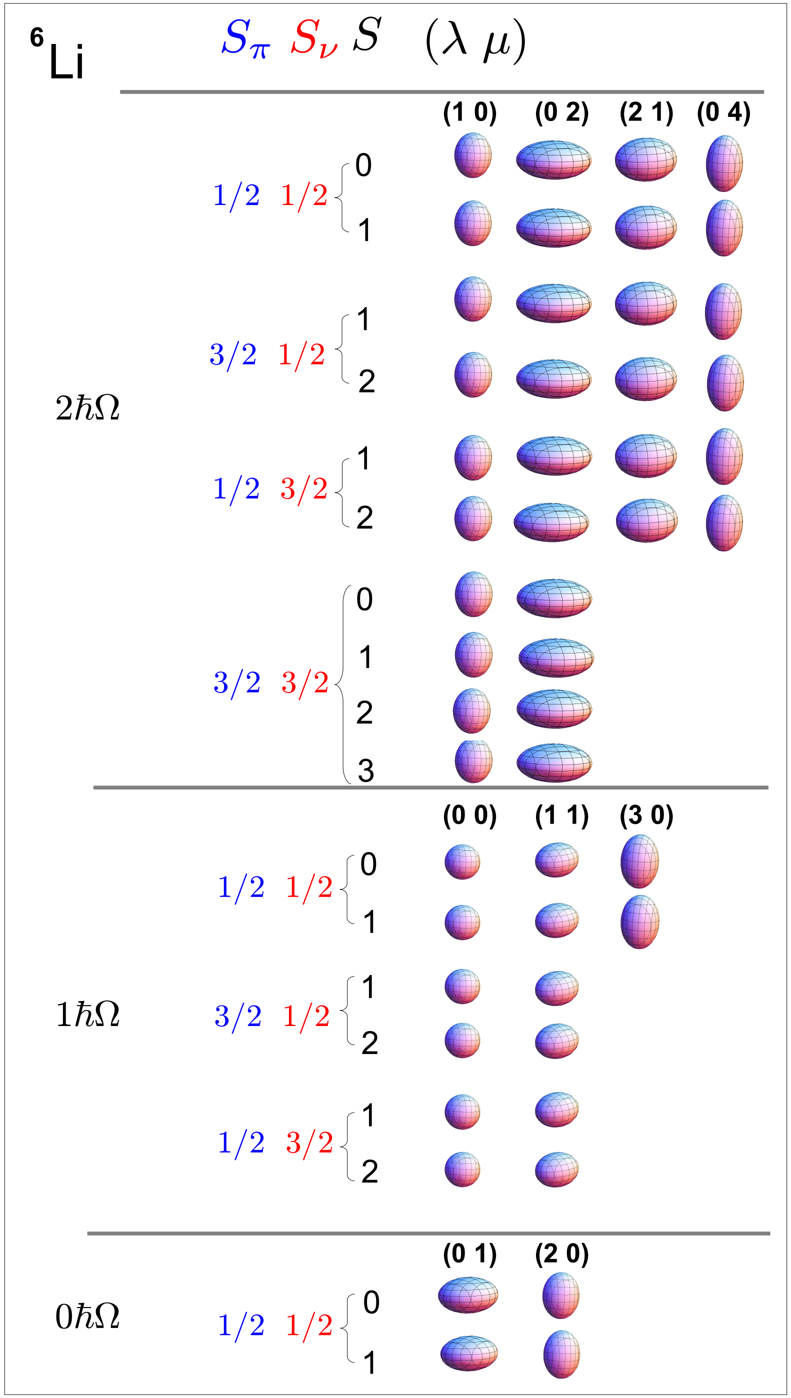
- the center-of-mass HO does not mix S_π S_ν $(\lambda\ \mu)S$

c.m. spurious states can be removed from each subspace exactly

- truncation according to intrinsic spin S_π S_ν S

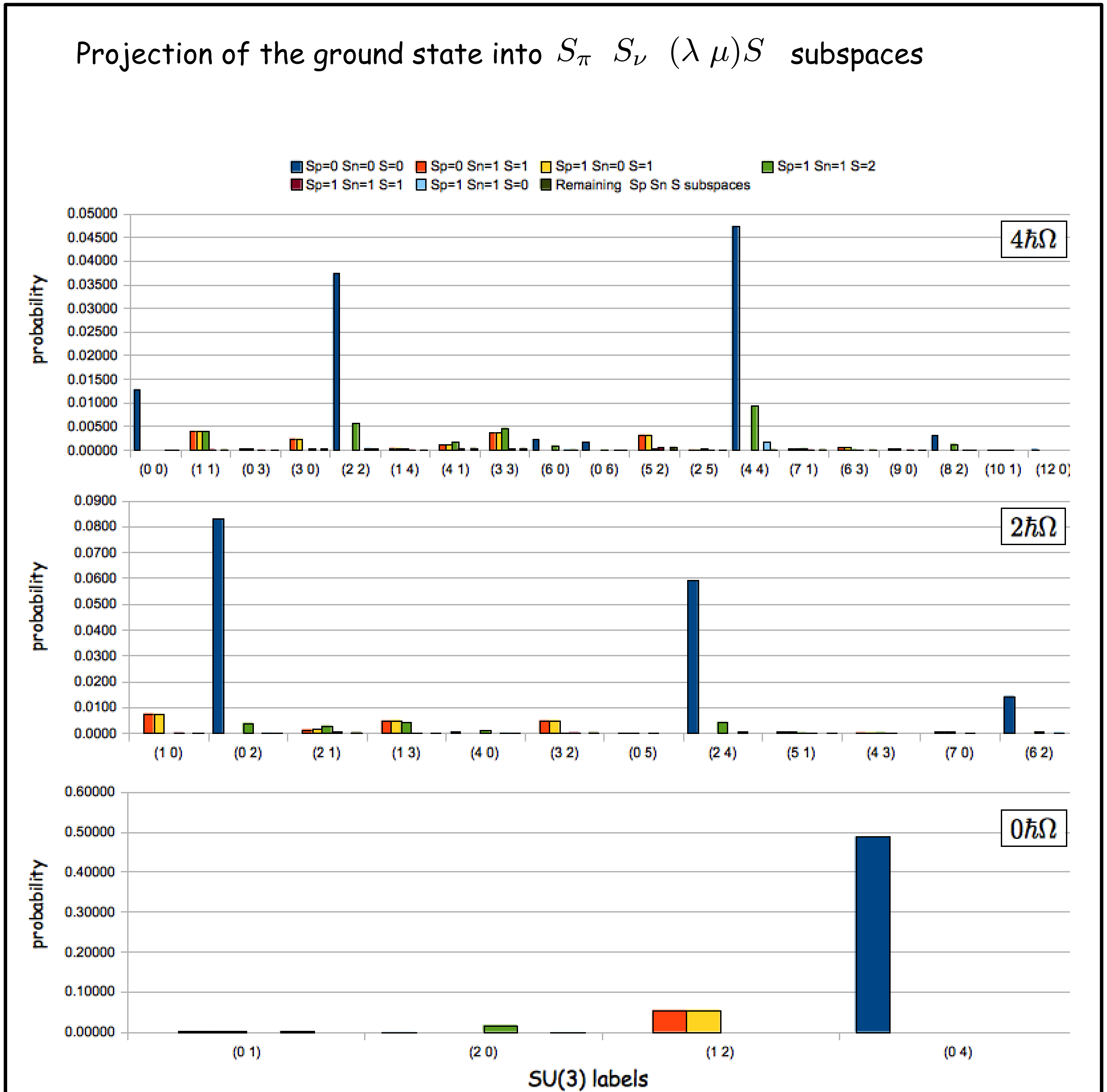
Spin-decomposition of ground state band wfns in 12C [Nmax=6 model space]





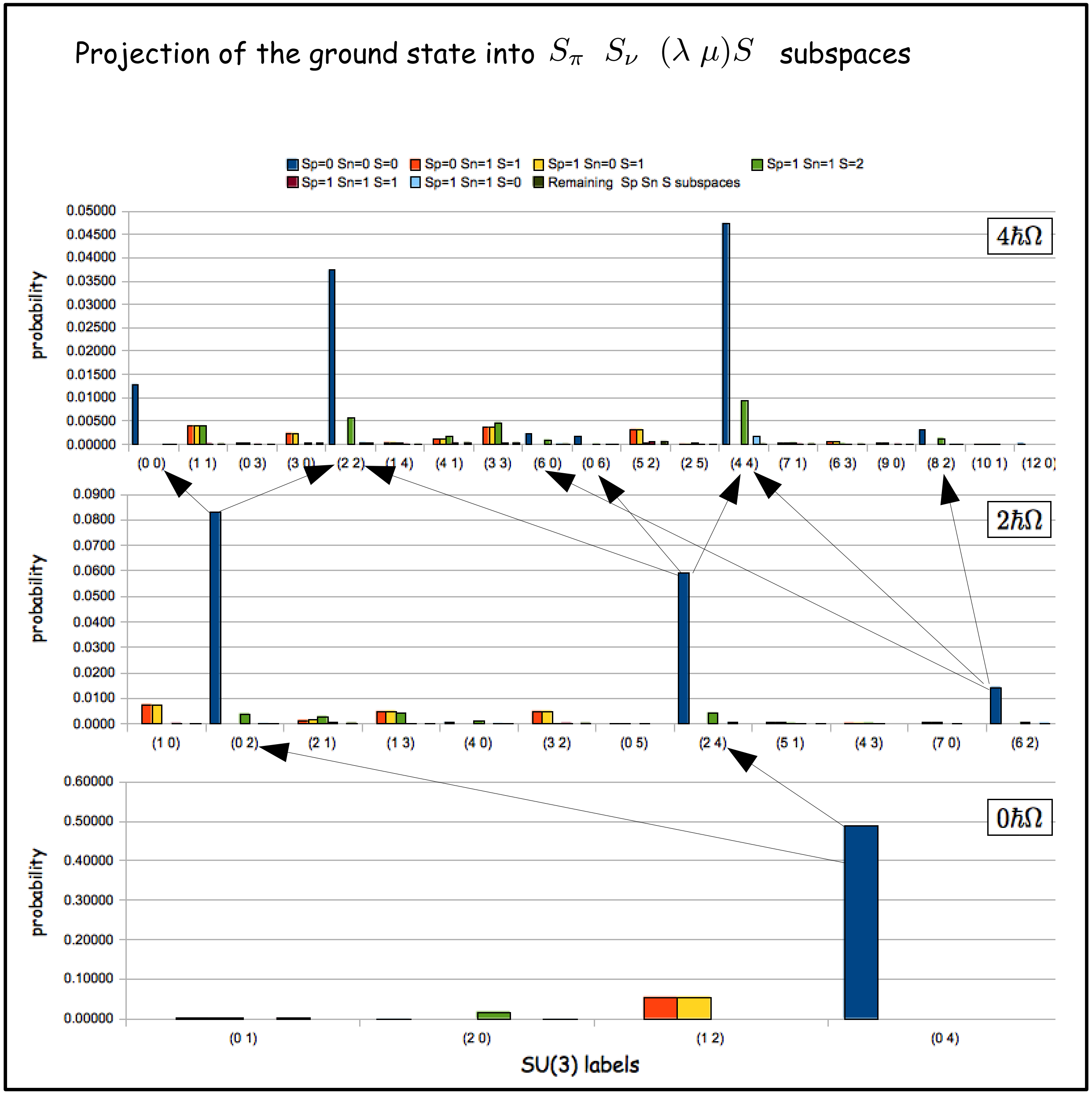
12C J=0 ground state

- Low spin components dominate
- And there is a certain pattern in dominant SU(3) quantum labels $(\lambda\ \mu)$



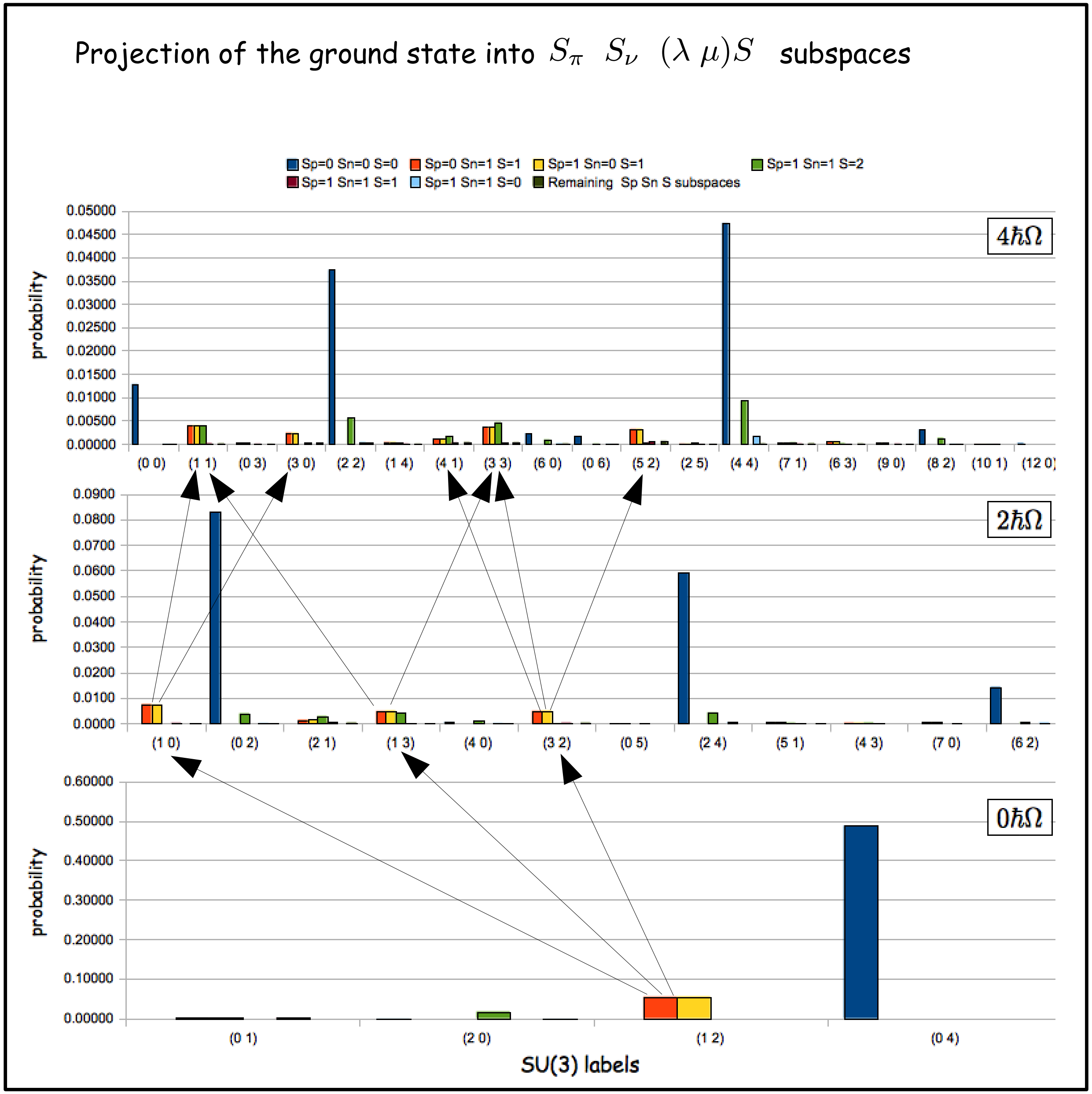
12C J=0 ground state

Action of a raising operator that has (2 0) SU(3) tensorial character



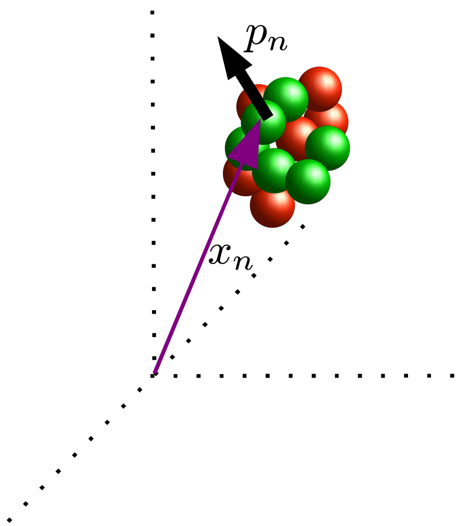
12C J=0 ground state

Action of a raising operator that has (2 0) SU(3) tensorial character



Symmetry of the many-body collective dynamics

- Sp(3,R): symmetry of the nuclear collective dynamics



6 → $\sum_n x_{ni} x_{nj}$ mass monopole and quadrupole moments

9 → $\sum_n x_{ni} p_{nj} \pm x_{nj} p_{ni}$ (-) angular momentum
(+) monopole and quadrupole deformations

6 → $\sum_n p_{ni} p_{nj}$ quadrupole flow tensor

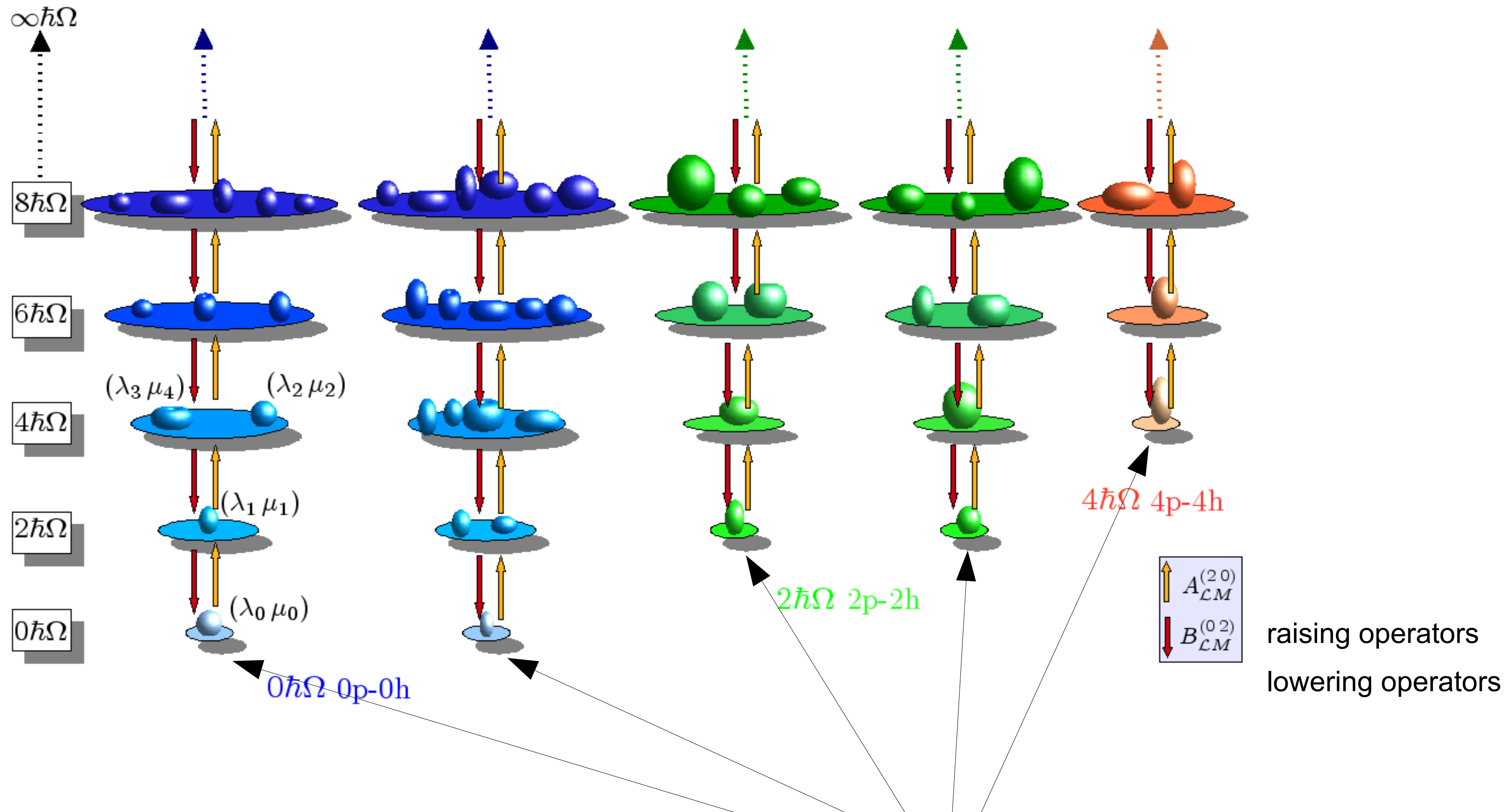
21 generators

- quadrupole and monopole vibrations and deformations
- rotational dynamics from rigid rotor to irrotational flow

- SU(3) is a subgroup of Sp(3,R) → Symplectic basis states are labeled by $(\lambda\ \mu)$ and also by $S_\pi\ \ S_\nu\ \ S$

- Symplectic Sp(3,R) symmetry matches deformed geometry [SU(3)] with the various modes of the nuclear collective dynamics

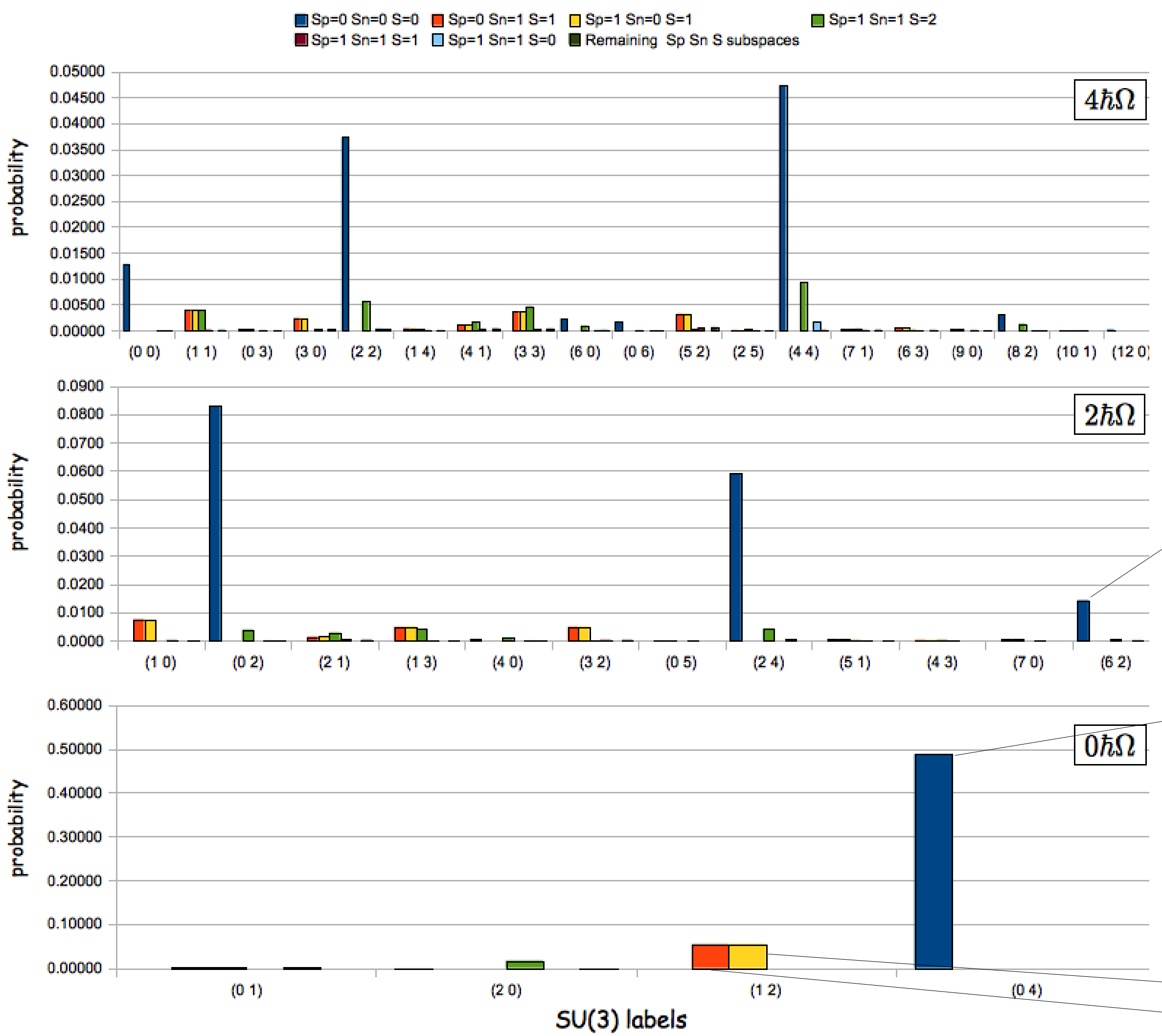
Symmetry of the many-body collective dynamics



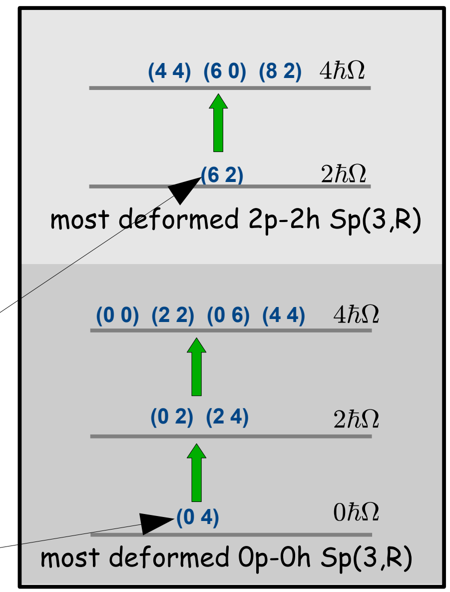
Basis states in symplectic "cone" are built over symplectic bandhead by action of raising operators

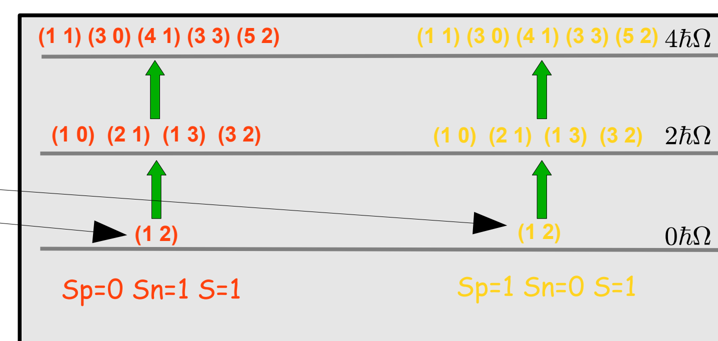
12C J=0 ground state

Projection of the ground state into $S_\pi \; S_\nu \; (\lambda\,\mu)S$ subspaces

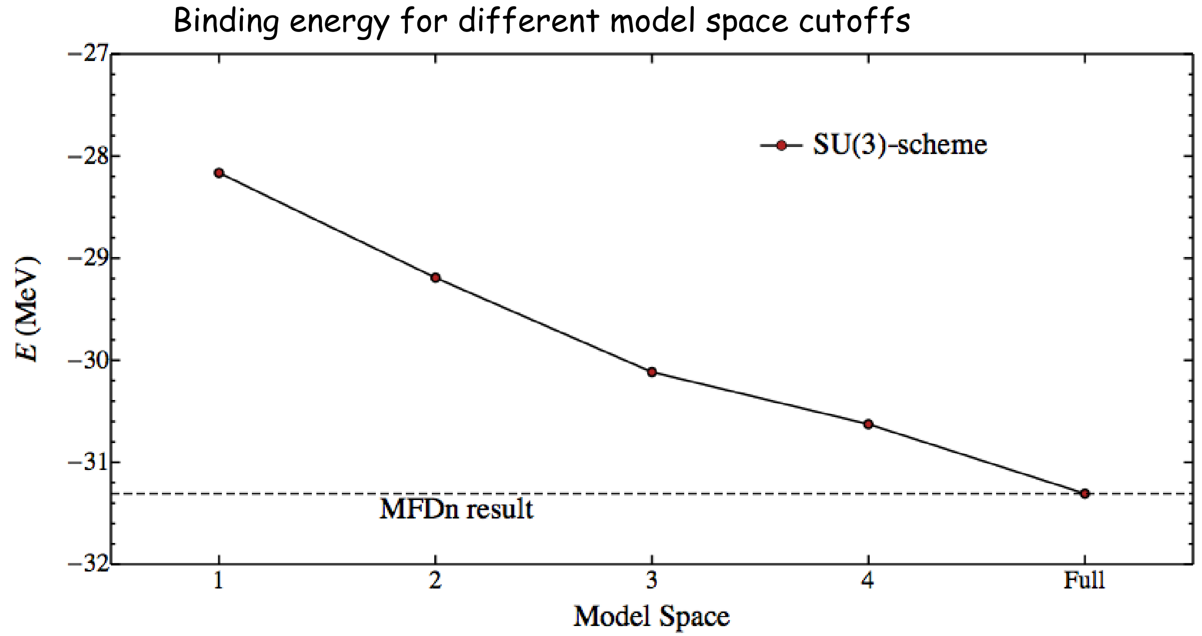


- most important subspaces contain states of the three leading Sp(3,R) irrep
- Significant contribution from the most deformed 2p-2h Sp(3,R) irrep





12C ground state – binding energy in SU(3)-scheme



- Definition of model space:

$0\hbar\Omega$
$2\hbar\Omega$ } full space
$\oplus$
$4\hbar\Omega$ restricted set of $S_\pi\ S_\nu S\ (\lambda\,\mu)$

S_π S_ν S	1		2		3		4
0 0 0	(4 4) (2 2) (0 0)				(8 2) (6 0)		(0 6)
1 1 2	(4 4) (2 2) (3 3)		(1 1)				(4 1) (8 2) (6 0)
1 0 1		$\oplus$	(1 1) (3 3)	$\oplus$	(5 2) (3 0)	$\oplus$	(4 1)
0 1 1			(1 1) (3 3)		(5 2) (3 0)		(4 1)
1 1 0							(4 4)

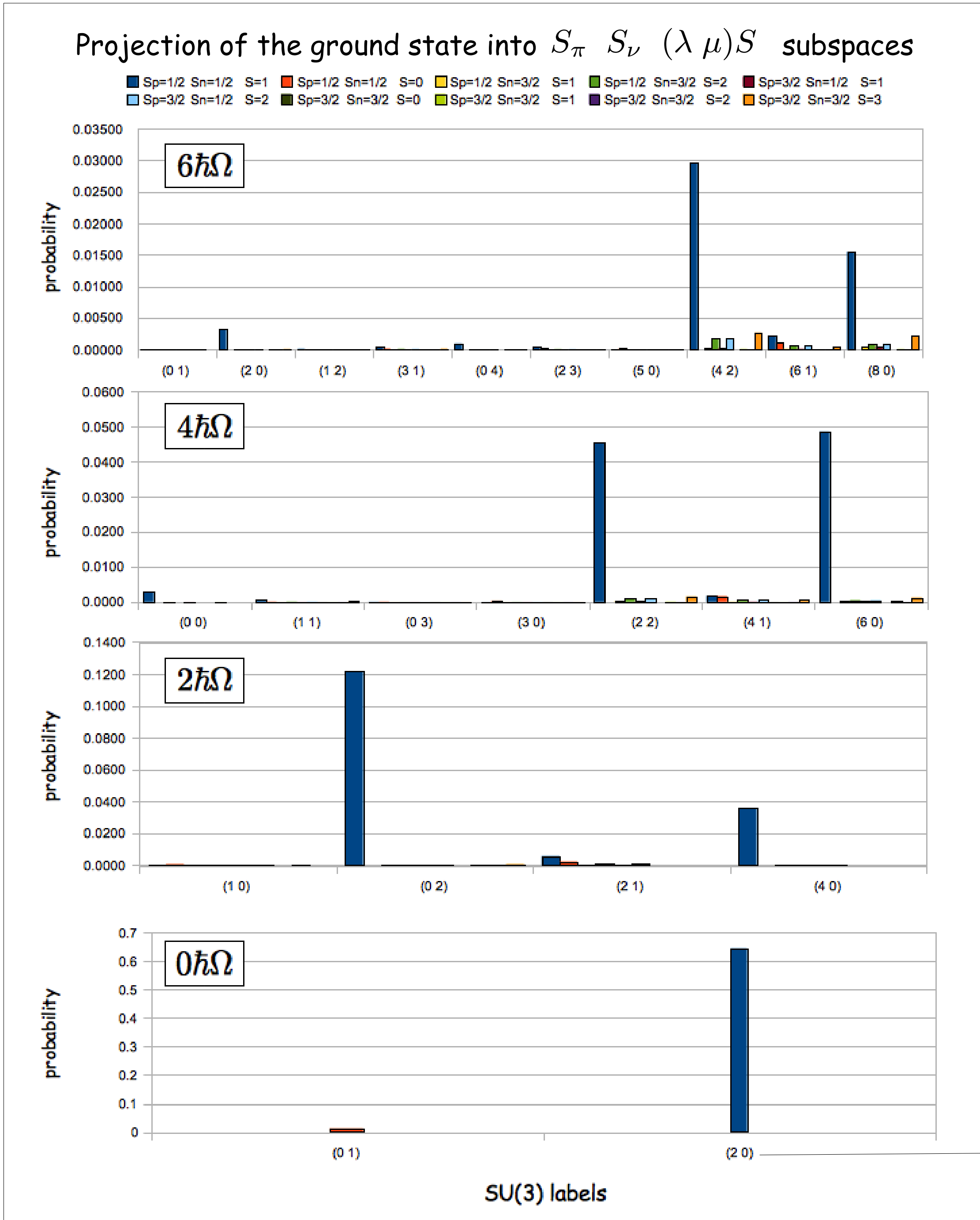
- 98.8% overlap with the ground state
98.1% binding energy

$(\lambda\ \mu)$ - subspaces included in the model space 4   full $4\hbar\Omega$ model space

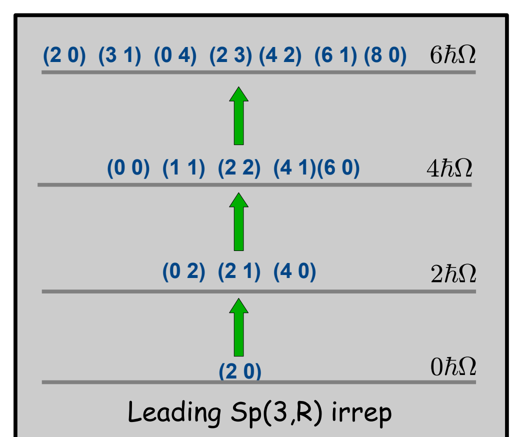
Sp=0 Sn=0 S=0	**(0 0)**(1 1)(0 3)(3 0)**(2 2)**(1 4)(4 1)(3 3)**(0 6)(6 0)**(2 5)(5 2)**(4 4)**(7 1)(6 3)(9 0)**(8 2)**(10 1)(12 0)
Sp=1 Sn=1 S=2	(0 0)**(1 1)**(0 3)(3 0)**(2 2)**(1 4)**(4 1)(3 3)**(0 6)**(6 0)**(2 5)(5 2)**(4 4)**(7 1)(6 3)(9 0)**(8 2)**(10 1)
Sp=0 Sn=1 S=1	(0 0)**(1 1)**(0 3)**(3 0)**(2 2)(1 4)**(4 1)(3 3)**(0 6)(6 0)(2 5)**(5 2)**(4 4)(7 1)(6 3)(9 0)(8 2)(10 1)
Sp=1 Sn=0 S=1	(0 0)**(1 1)**(0 3)**(3 0)**(2 2)(1 4)**(4 1)(3 3)**(0 6)(6 0)(2 5)**(5 2)**(4 4)(7 1)(6 3)(9 0)(8 2)(10 1)
Sp=1 Sn=1 S=0	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2) **(4 4)**(7 1)(6 3)(9 0)(8 2)(10 1)
Sp=1 Sn=1 S=1	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)(10 1)
Sp=0 Sn=2 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=1 Sn=2 S=1	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=1 Sn=2 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=1 Sn=2 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=2 Sn=0 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=2 Sn=1 S=1	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=2 Sn=1 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=2 Sn=1 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)(6 3)(9 0)(8 2)
Sp=2 Sn=2 S=0	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)
Sp=2 Sn=2 S=1	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)
Sp=2 Sn=2 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)
Sp=2 Sn=2 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)
Sp=2 Sn=2 S=4	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(2 5)(5 2)(4 4)(7 1)

Sp=0 Sn=3 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(5 2)
Sp=3 Sn=0 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(0 6)(6 0)(5 2)
Sp=3 Sn=1 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)
Sp=3 Sn=1 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)
Sp=3 Sn=1 S=4	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)
Sp=1 Sn=3 S=2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)
Sp=1 Sn=3 S=3	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)
Sp=1 Sn=3 S=4	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)
Sp=2 Sn=3 S=1	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=2 Sn=3 S=2	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=2 Sn=3 S=3	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=2 Sn=3 S=4	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=2 Sn=3 S=5	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=3 Sn=2 S=1	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=3 Sn=2 S=2	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=3 Sn=2 S=3	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=3 Sn=2 S=4	(1 1)(0 3)(3 0)(2 2) (4 1)
Sp=3 Sn=2 S=5	(1 1)(0 3)(3 0)(2 2) (4 1)

6Li J=1 ground state Nmax=6

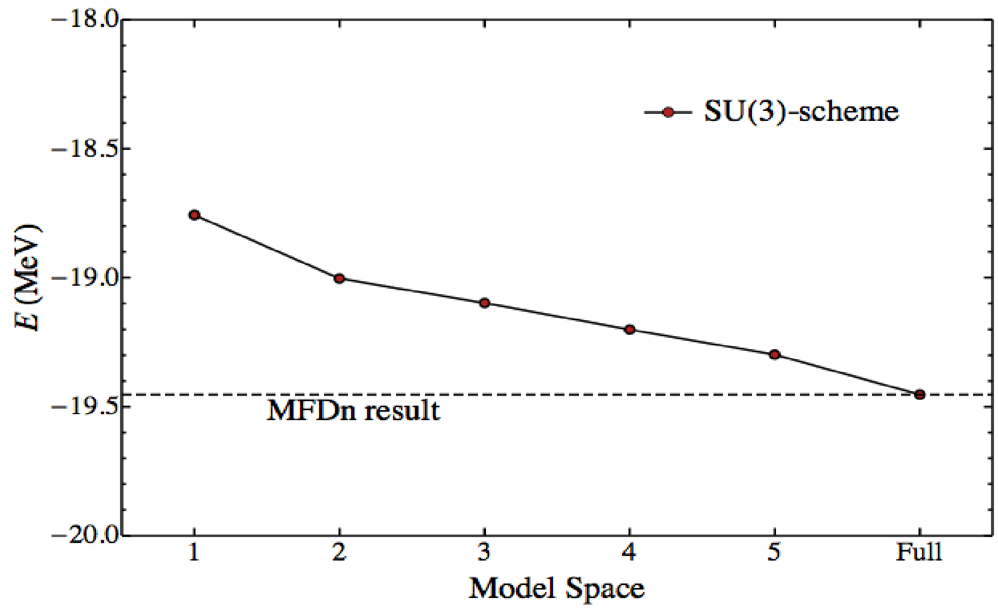


- most important subspaces contain states of the leading Sp(3,R) irrep



6Li ground state – binding energy in SU(3)-scheme

Binding energy for different model space cutoffs



Definition of model space:

$0\hbar\Omega$, $2\hbar\Omega$, $4\hbar\Omega$ } full space

$\oplus$

$6\hbar\Omega$ restricted set of $S_\pi \; S_\nu S \; (\lambda\,\mu)$

S_π	S_ν	S	1		2		3		4		5
1/2	1/2	1	(2 0) (4 2) (6 1) (8 0)		(0 4)						
3/2	1/2	2	(4 2)		(8 0)		(6 1)				
1/2	3/2	2	(4 2)		(8 0)		(6 1)				
3/2	3/2	3	(4 2) (8 0)	$\oplus$		$\oplus$		$\oplus$	(6 1)	$\oplus$	
1/2	1/2	0			(6 1)						
3/2	1/2	1							(8 0)		(4 2)
1/2	3/2	1							(8 0)		(4 2)

S_π S_ν S $(\lambda\,\mu)$

99.6% overlap with the ground state
98.7% binding energy

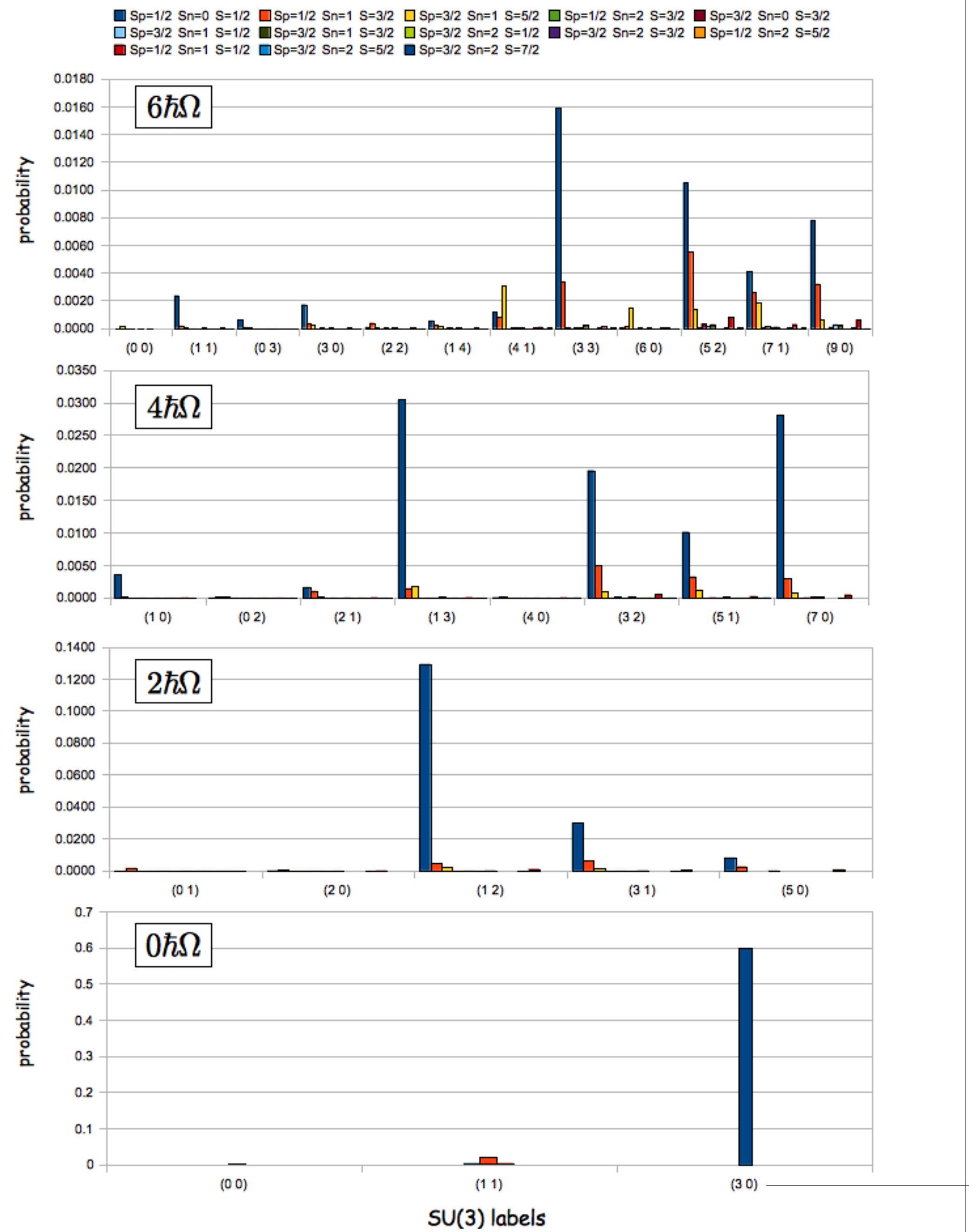
$(\lambda\,\mu)$ - subspaces included in the model space 5

full model space

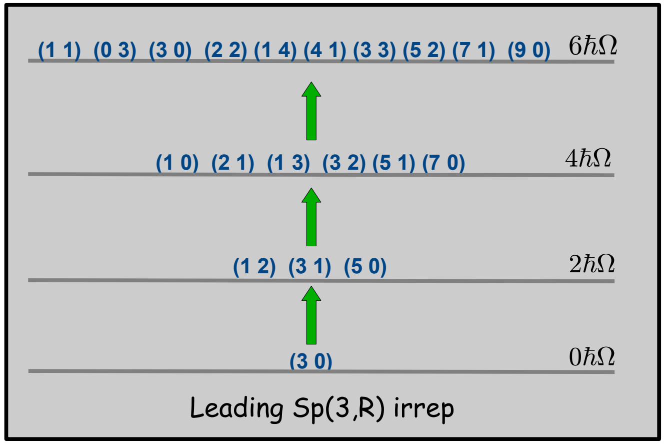
Sp=1/2	Sn=1/2	S=0	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) (4 2) **(6 1)** (8 0)
Sp=1/2	Sn=1/2	S=1	(0 1) **(2 0)** (1 2) (3 1) **(0 4)** (2 3) (5 0) **(4 2)** **(6 1)** **(8 0)**
Sp=1/2	Sn=3/2	S=1	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) **(4 2)** (6 1) **(8 0)**
Sp=1/2	Sn=3/2	S=2	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) **(4 2)** **(6 1)** **(8 0)**
Sp=3/2	Sn=1/2	S=1	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) **(4 2)** (6 1) **(8 0)**
Sp=3/2	Sn=1/2	S=2	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) **(4 2)** **(6 1)** **(8 0)**
Sp=3/2	Sn=3/2	S=0	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) (4 2) (6 1) (8 0)
Sp=3/2	Sn=3/2	S=1	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) (4 2) (6 1) (8 0)
Sp=3/2	Sn=3/2	S=2	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) (4 2) (6 1) (8 0)
Sp=3/2	Sn=3/2	S=3	(0 1) (2 0) (1 2) (3 1) (0 4) (2 3) (5 0) **(4 2)** **(6 1)** **(8 0)**

7Li J=3/2 ground state

Projection of the ground state into $S_\pi \; S_\nu \; (\lambda\;\mu)S$ subspaces

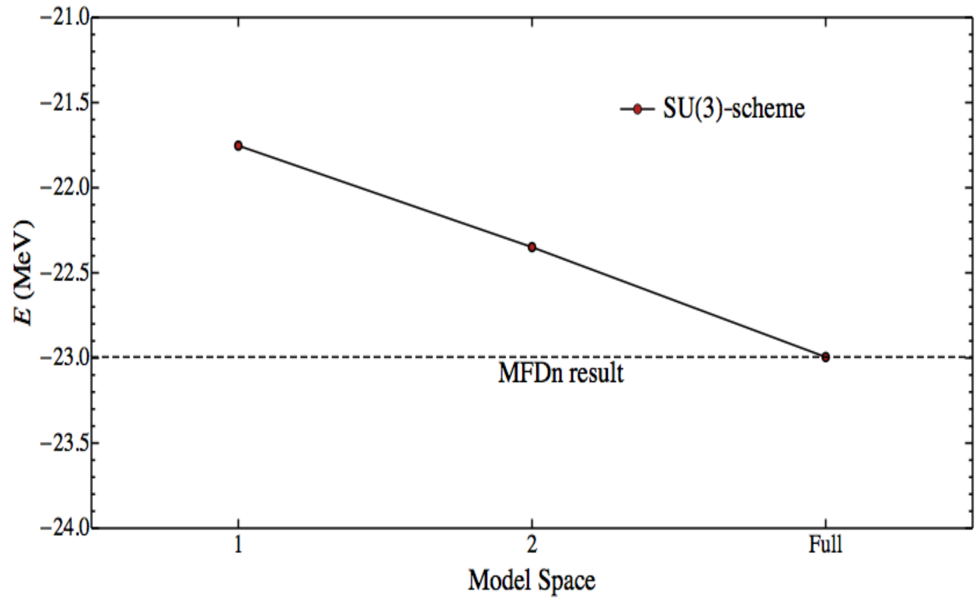


- most important subspaces contain states of the leading Sp(3,R) irrep
- most important spin components have similar deformations



7Li J=3/2 ground state

Binding energy for different model space cutoffs



Definition of model space:

$$\left.\begin{array}{l} 0\hbar\Omega \\ 2\hbar\Omega \\ 4\hbar\Omega \end{array}\right\} \text{full space}$$

$$\oplus$$

$6\hbar\Omega$ restricted set of $S_\pi\ S_\nu S\ (\lambda\,\mu)$

S_π	S_ν	S	1		2
1/2	0	1/2	(1 1)(3 3)(5 2)(9 0)(7 1)		(3 0)(4 1)
1/2	1	3/2	(3 3)(5 2)(9 0)(7 1)	$\oplus$	
3/2	1	5/2	(3 3)		(5 2)(7 1)(9 0)

99.1% overlap with the ground state
97.2% binding energy

$(\lambda\ \mu)$ - subspaces included in the model space 2

full model space	
Sp=1/2 Sn=0 S=1/2	(0 0)**(1 1)**(0 3)**(3 0)**(2 2)(1 4)**(4 1)(3 3)**(6 0)**(5 2)(7 1)(9 0)**
Sp=1/2 Sn=1 S=3/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)**(3 3)**(6 0)**(5 2)(7 1)(9 0)**
Sp=1/2 Sn=1 S=1/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)**(3 3)**(6 0)**(5 2)(7 1)(9 0)**
Sp=1/2 Sn=2 S=3/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=1/2 Sn=2 S=5/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=0 S=3/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=1 S=1/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=1 S=3/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=1 S=5/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=2 S=1/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=2 S=3/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=2 S=5/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)
Sp=3/2 Sn=2 S=7/2	(0 0)(1 1)(0 3)(3 0)(2 2)(1 4)(4 1)(3 3)(6 0)(5 2)(7 1)(9 0)

Conclusion & Outlook

- methods for evaluation of a realistic NN interaction in SU(3)-scheme developed and validated
- we have tested SU(3) and spin based truncation scheme which keeps ability to decouple the center-of-mass exactly
- Our results reaffirm the importance of the symplectic symmetry
- **Outlook:**
  - Implement evaluation of three-body interactions in SU(3)-scheme
  - Effective interactions for SU(3)-scheme model space
  - Inclusion of the symplectic configurations for large model spaces