Symmetry Adapted No-Core Shell Model Applications for Light Nuclei with QCD Inspired Interactions

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NSF Supported PetaApps Collaboration
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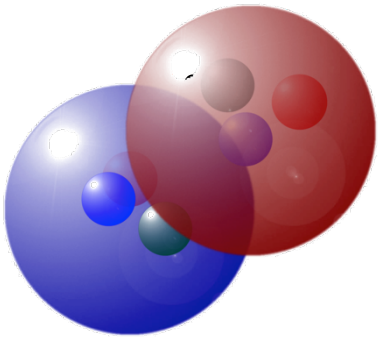
From Quarks and Gluons to Hadrons and Nuclei; Erice, Italy; September 16-24, 2011

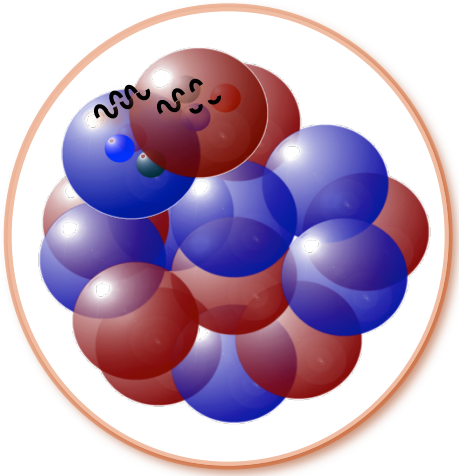
Louisiana State University
Baton Rouge, Louisiana

Ab Initio Vision

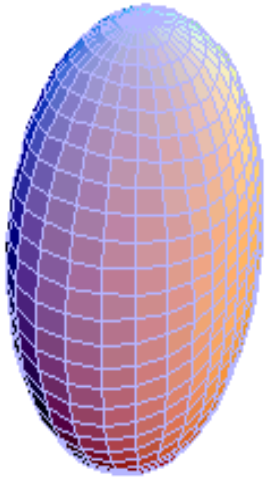
Fundamental Principles



Many-body Dynamics



Collective Properties



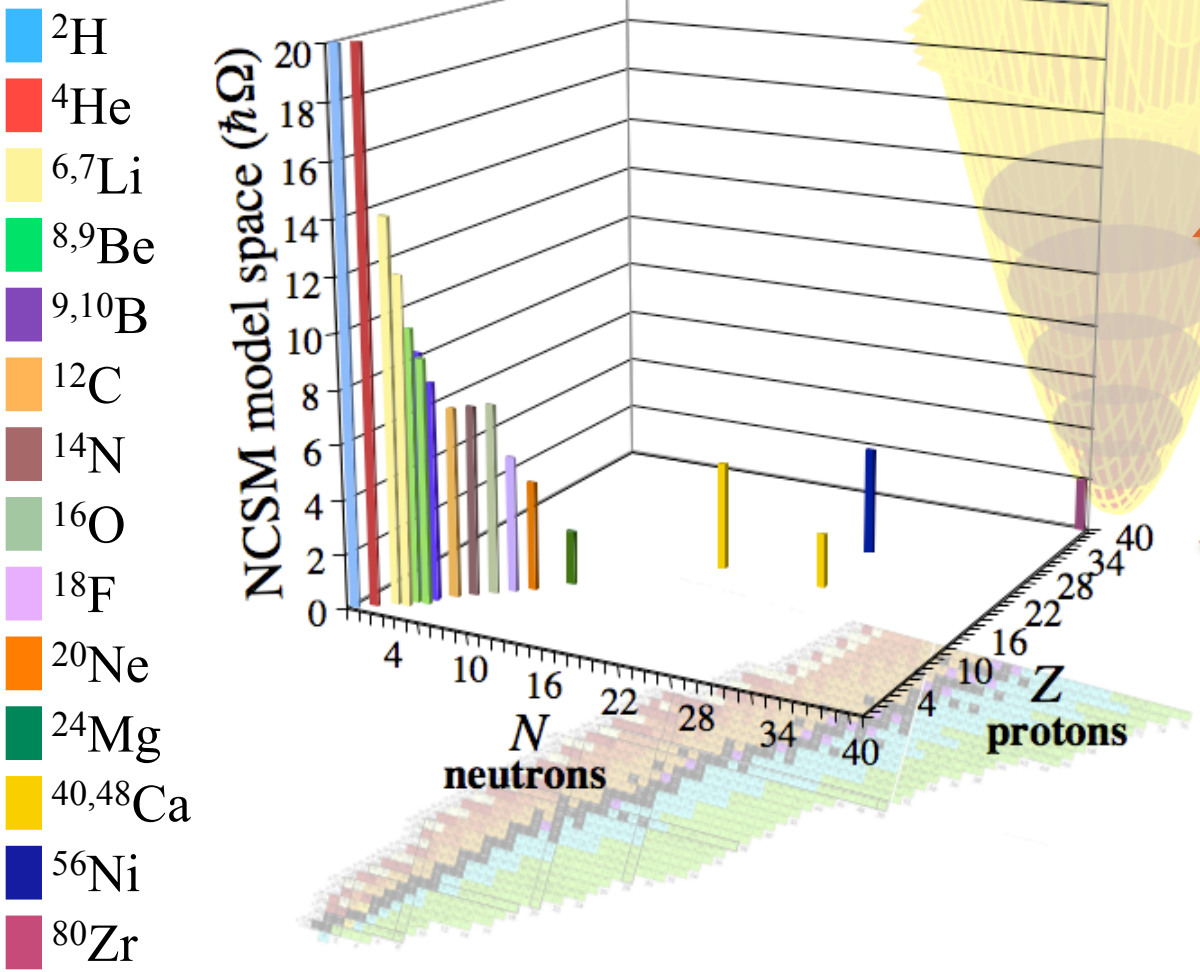
nucleon-nucleon interaction (NN, NNN, ...)

quarks/gluons

symmetry adapted NCSM

structure and reactions

Computational Limits of No Core Shell Model



Highly deformed modes, Cluster-like configurations, B(E2) w/o effective charges

'higher' spaces

'heavier' nuclei

… enables…

Symmetry Adapted NCSM

NCSM versus 'Symmetry Adapted' NCSM

NCSM*

(multi-$\hbar\omega$)

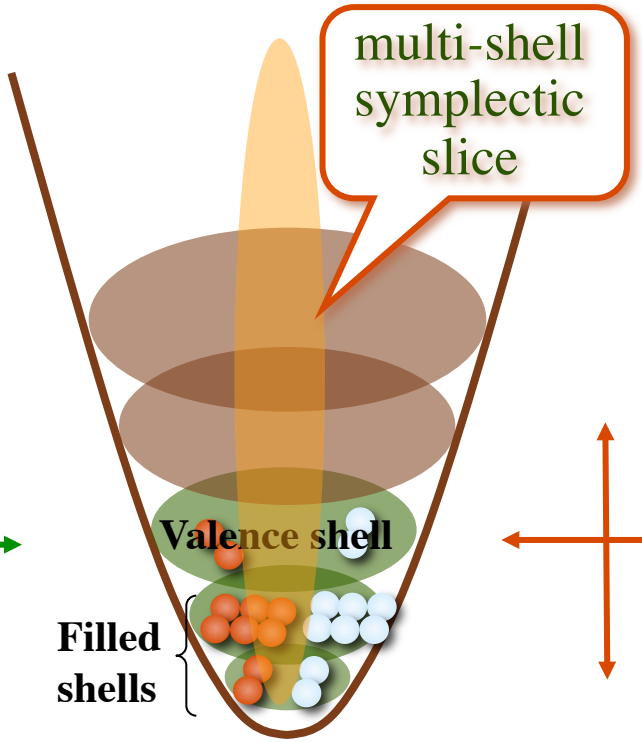
Horizontal discs

(all configurations)

N_{max}

$(0\hbar\omega)$ limit

*J. P. Vary, P. Navratil & B. R. Barrett ~2000



SA-NCSM*

(multi-$\hbar\omega$)

Vertical slices

(monopole & quadrupole collective excitations)

$0\hbar\omega$ SU(3) limit

*Complete (=NCSM) if all SU(3) reps included

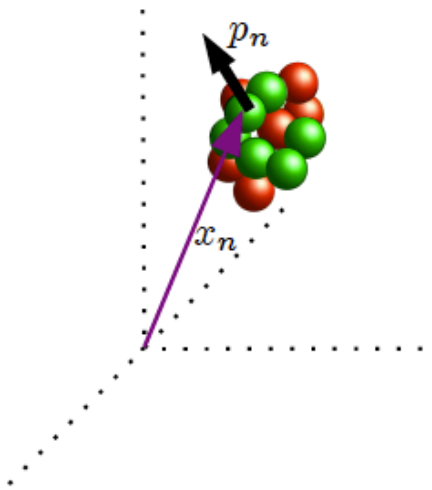
- Realistic interaction (local/ nonlocal; NN, NNN, …)
- In principle, exact solutions
- Reproduction of binding energies and spectral features of light nuclei

- Manage spurious center-of-mass motion
- Relation to the NCSM: fully microscopic!
- Reproduce rotational energy and E&M transition rates without effective charge
- Extensible: spaces; 3&4 body enabled, etc.

Sp(3,R) ⊃ SU(3) Structure

G. Rosensteel and D. J. Rowe ~1980

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



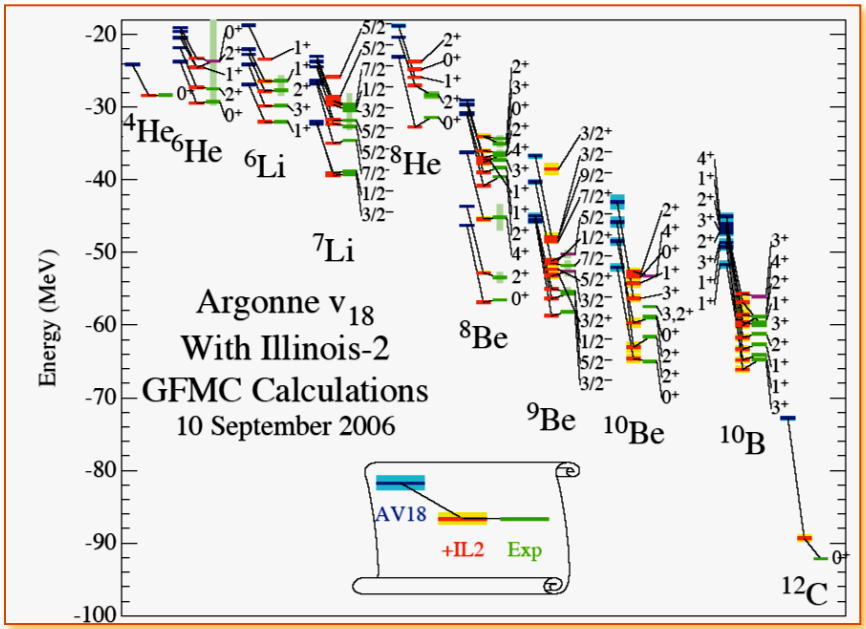
6	$\sum_n x_{ni}x_{nj}$	mass monopole and quadrupole moments
9	$\sum_n x_{ni}p_{nj} \pm x_{nj}p_{ni}$	(-) angular momentum (+) monopole and quadrupole deformations
6	$\sum_n p_{ni}p_{nj}$	quadrupole flow tensor (kinetic energy)
21	generators	

- 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 $S_\pi\ \ S_\nu\ \ S$

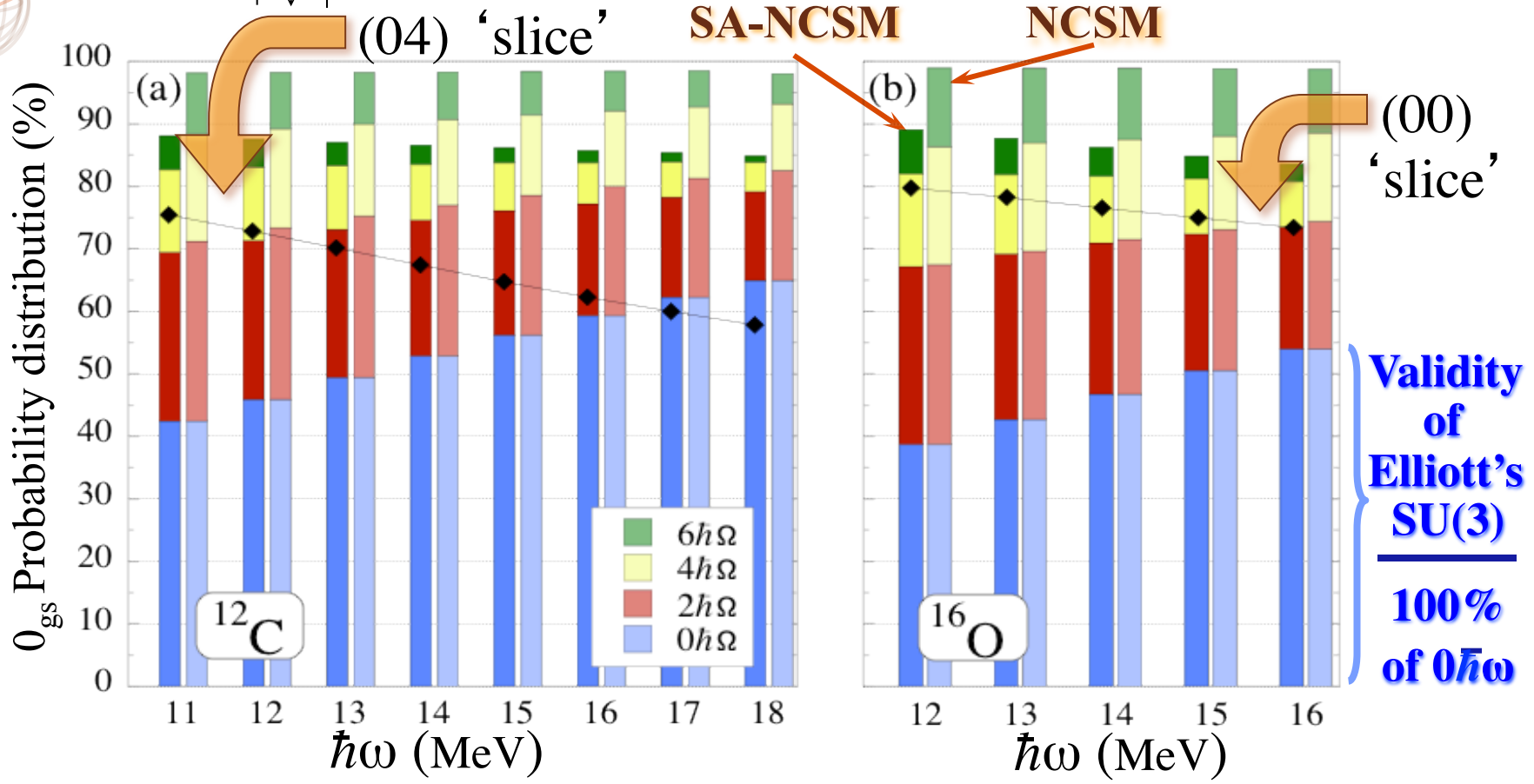
- Symplectic Sp(3,R) symmetry matches deformed geometry [SU(3)] with the various modes of the nuclear collective dynamics

… Risk / Benefit Analysis …



- Variational & Green's Function Monte Carlo (VMC/GFMC): A≤12, local interactions
- Coupled-cluster Theory (CCT): near closed-shell nuclei (^{4}He, ^{16}O, ^{40}Ca); model space truncation
- No-core Shell Model: A≤16, space truncation - binomial model space growth does you in
- Symmetry-adapted No-core Shell Model (first results, major investment time/effort required)

Probability Distribution: Ground States ^{12}C & ^{16}O



Validity of Elliott's SU(3)

100% of $0\hbar\omega$

Only **3** 0p-0h representations: ~85%

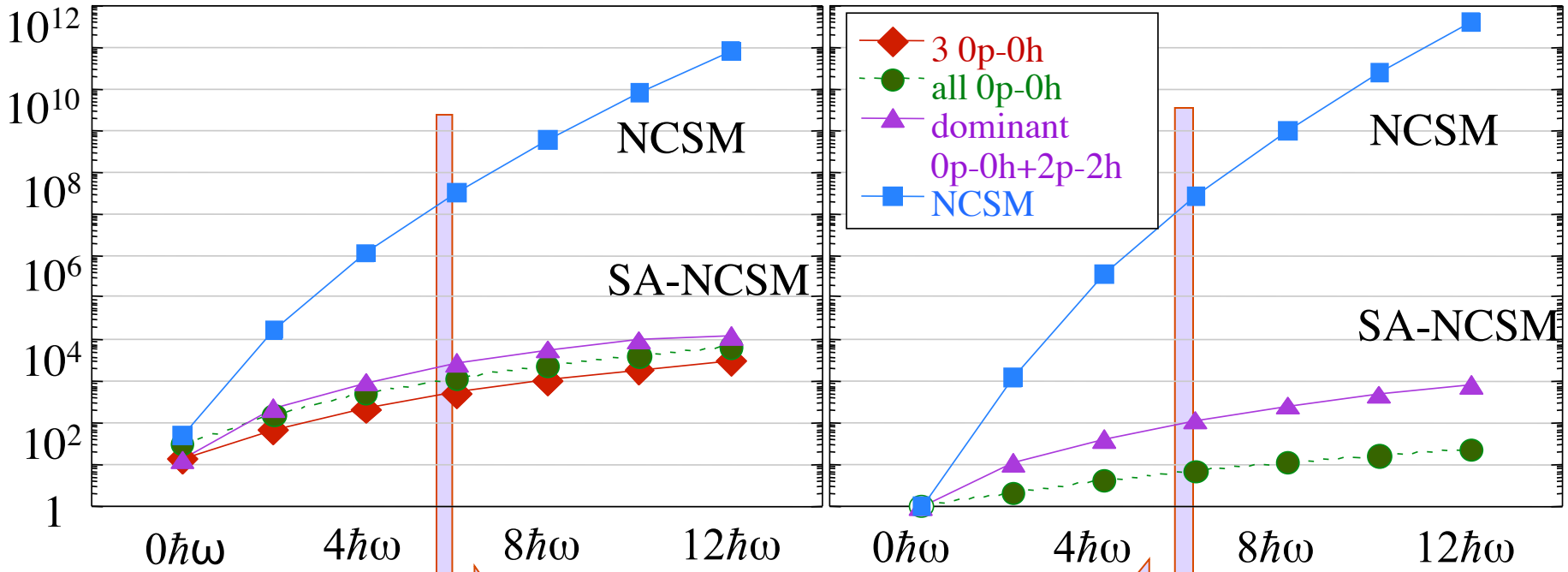
$N_\sigma(\lambda\mu)$
24.5(04) : most deformed
$24.5(12)^2$: spin one states

$2\hbar\omega$ 2p-2h irreps:
~ 4% (^{12}C)
~10% (^{16}O)

Major Reductions in Model Space

^{12}C ^{16}O

Dimension of Model Space



NCSM vs SA-NCSM

model space dimension

0.009% for ^{12}C

0.0004% for ^{16}O

T. Dytrych. K.D. Sviracheva, C. Bahri, J.P. Draayer, J.P. Vary, Phys. Rev. Lett. 98 (2007) 162503

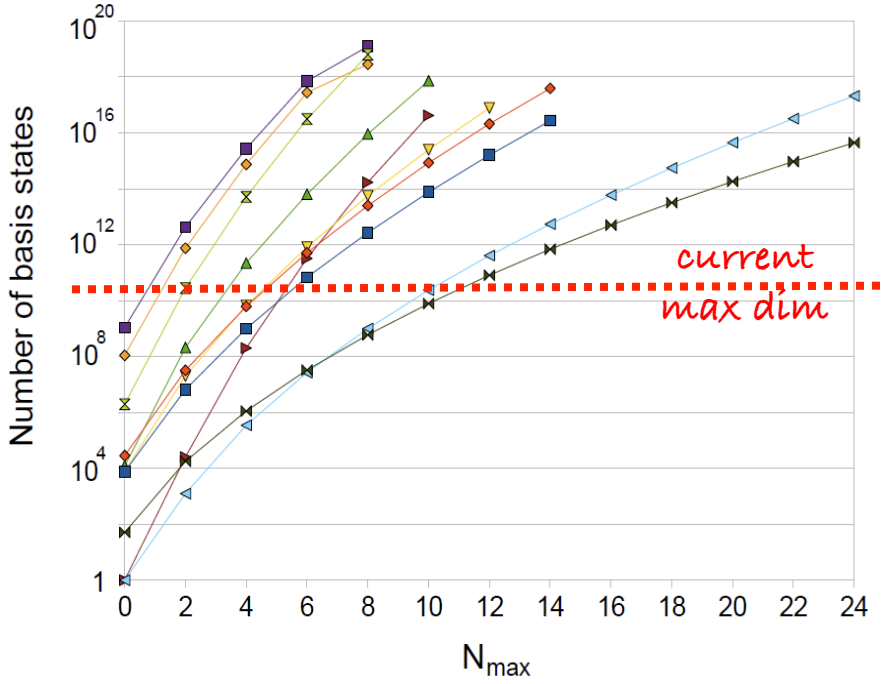
NCSM versus SA-NCSM

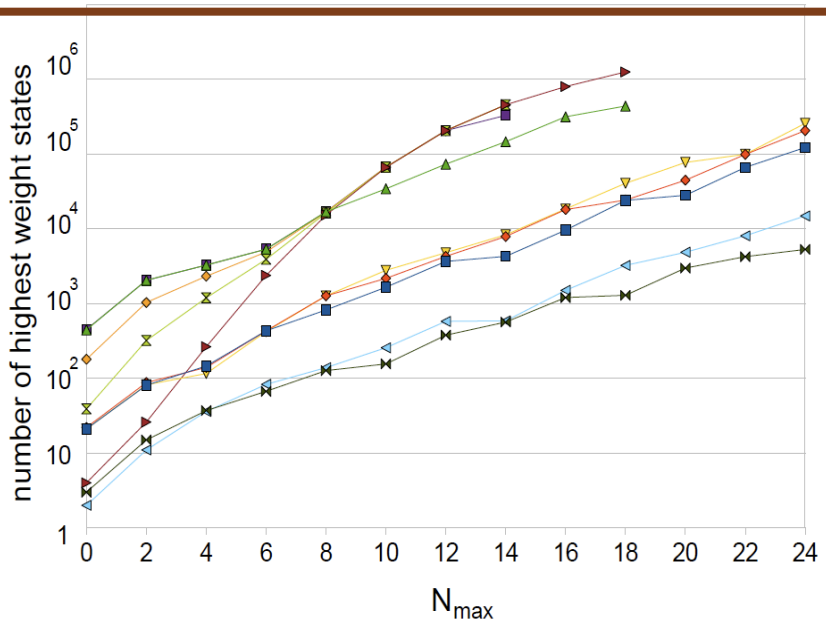
64Ge
68Se
72Kr
60Ca
48Ca
32Ar
28S
24Si
16O
12C

NCSM

Number of basis states

"Binominal Counting"





SA-NCSM

Number of 'seeds' required for complete calculation

"Cluster Bookkeeping"

Symmetry Adapted Theory

basis classification scheme

space *spin*

$U(N) \supset SU(3) \supset SO(3)$ $\quad U(2)$

$[f] \quad \alpha \; (\lambda,\mu) \quad \kappa \quad L \quad S$

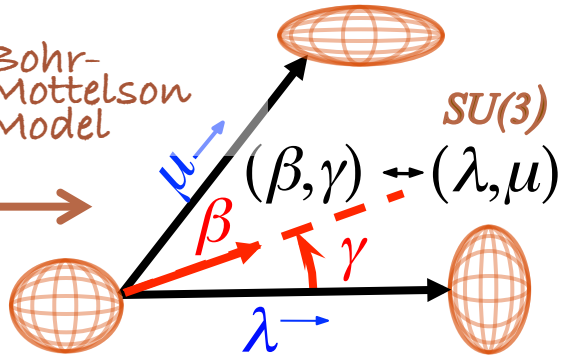
deformation *(LS) JM*

Elliott and Symplectic Model

Bohr-Mottelson Model

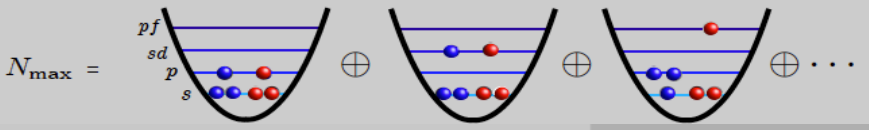
SU(3)

$(\beta,\gamma) \leftrightarrow (\lambda,\mu)$



Step 1

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



np coupling scheme

Step 2

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

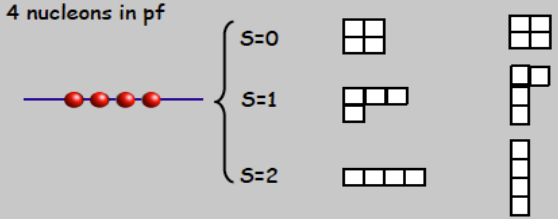
Step 3

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

'seed' configurations

	U(2)	⊗	U(10)	⊃	SU(3)
quantum labels:	S		[f]	α	(λ μ)

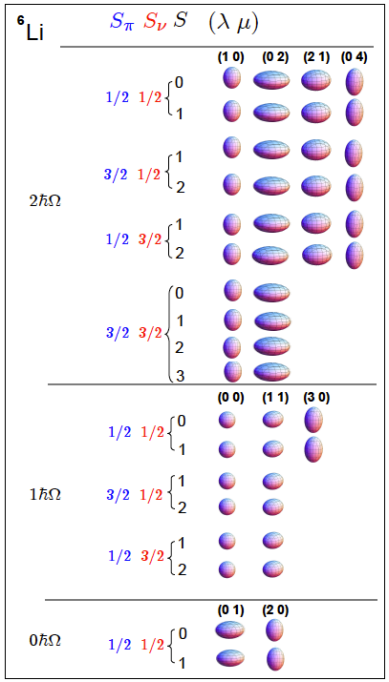
- Example: 4 nucleons in pf



$\supset \{(8\,2)\,(7\,1)\,(4\,4)\,(5\,2)\,(0\,6)\,(6\,0)\,(3\,3)\,(1\,4)\,(4\,1)\,(2\,2)\,(1\,1)\}$

$\supset \{(9\,0)\,(6\,3)\,(7\,1)\,(4\,4)\,(2\,5)\,(5\,2)\,(3\,3)\,(1\,4)\,(4\,1)\,(2\,2)\,(0\,3)\,(3\,0)\,(1\,1)\}$

$\supset \{(5\,2)\,(0\,6)\,(3\,3)\,(2\,2)\,(3\,0)\}$



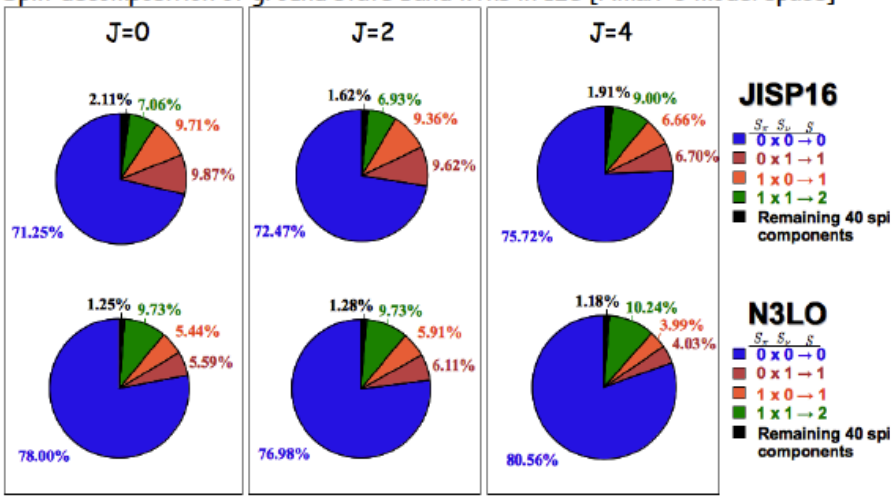
Low Spin and High Deformation Dominance

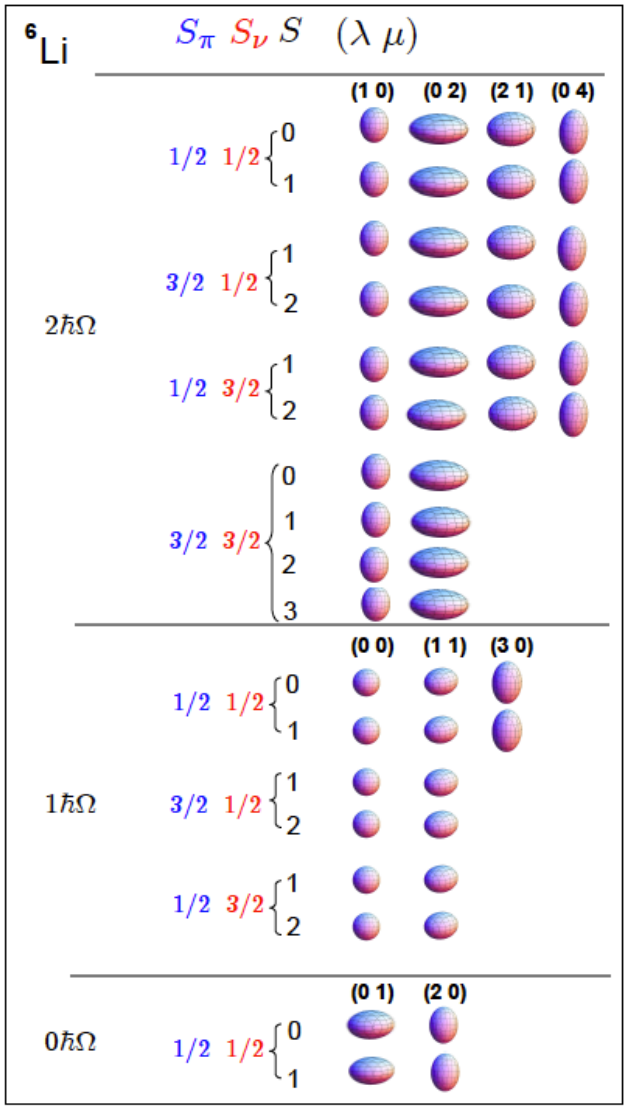
- SU(3)-scheme decomposes Nmax model space into subspaces of states labeled by $S_\pi \;\; S_\nu \;\; (\lambda\,\mu)S$
- the center-of-mass HO does not mix $S_\pi \;\; S_\nu \;\; (\lambda\,\mu)S$

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

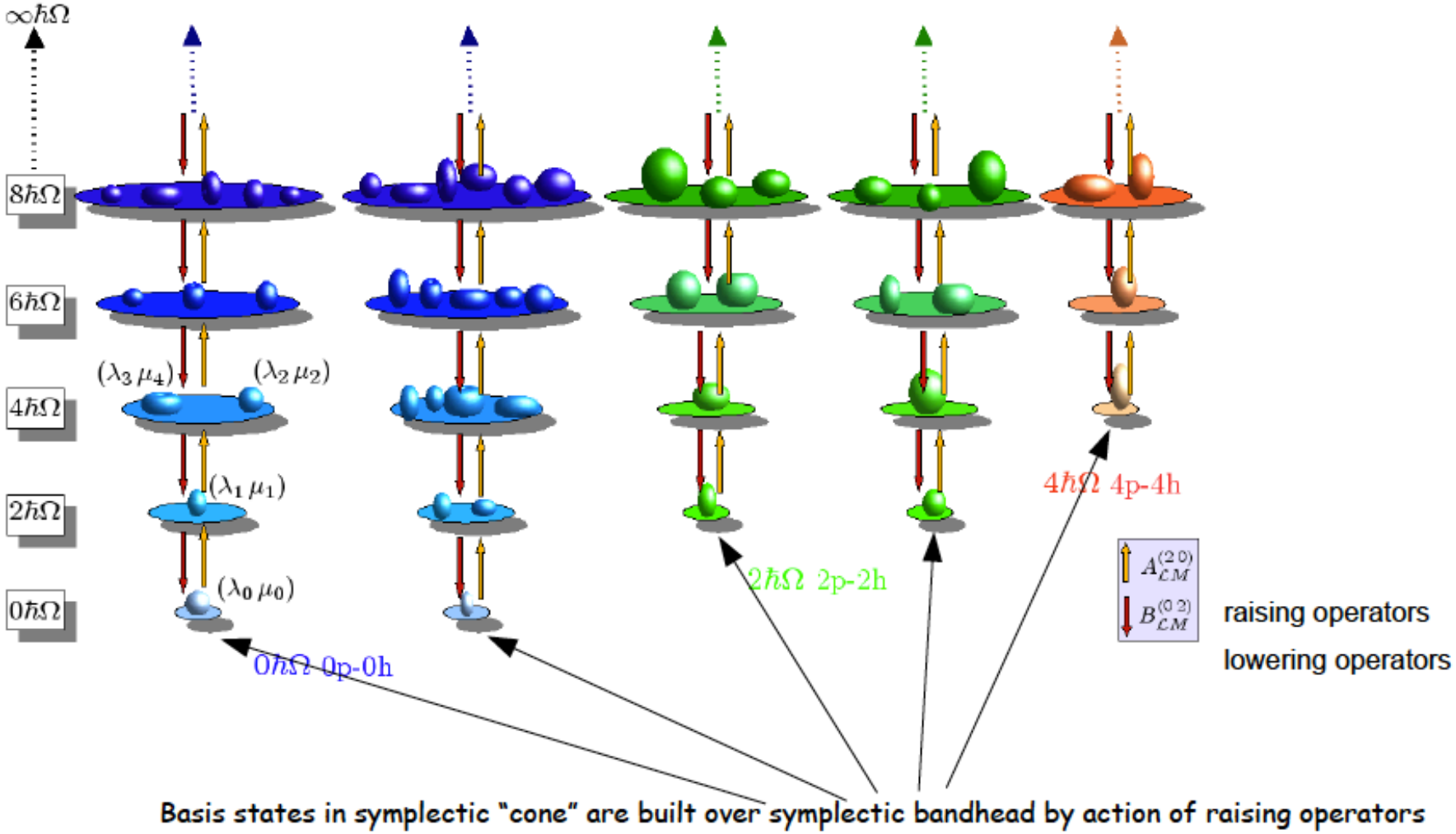
- truncation according to intrinsic spin $S_\pi \;\; S_\nu \;\; S$

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





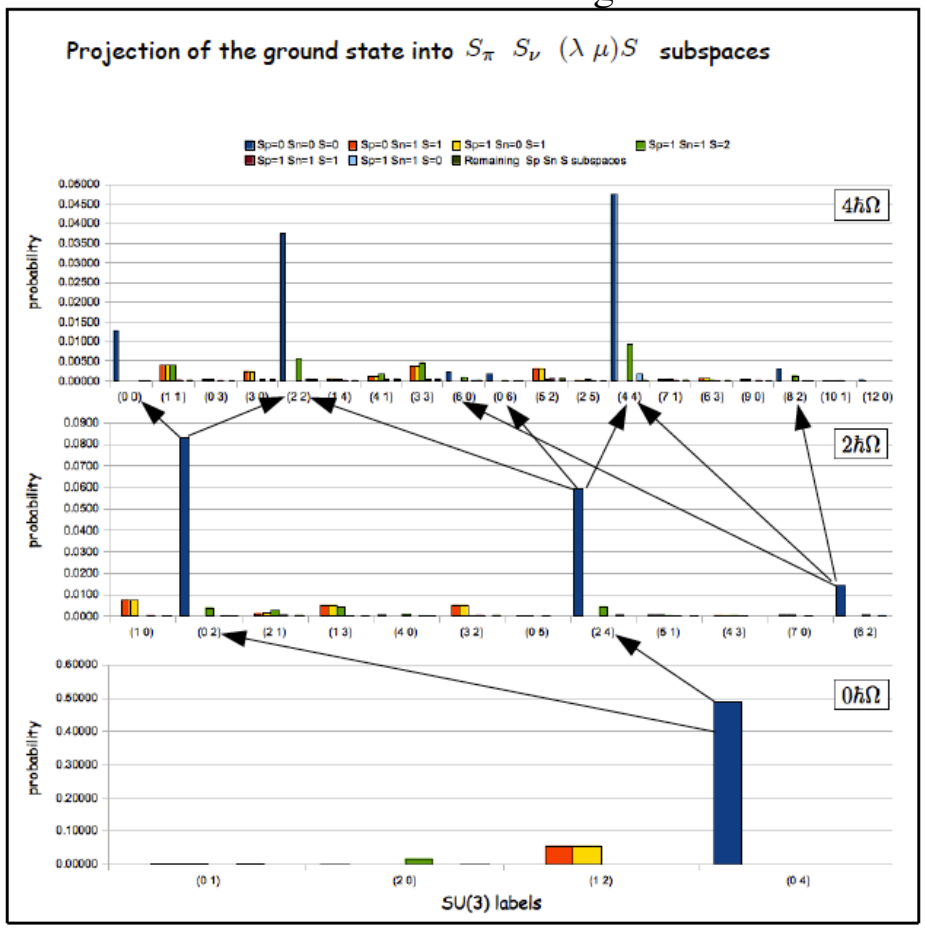
Physical / Algebraic Structure



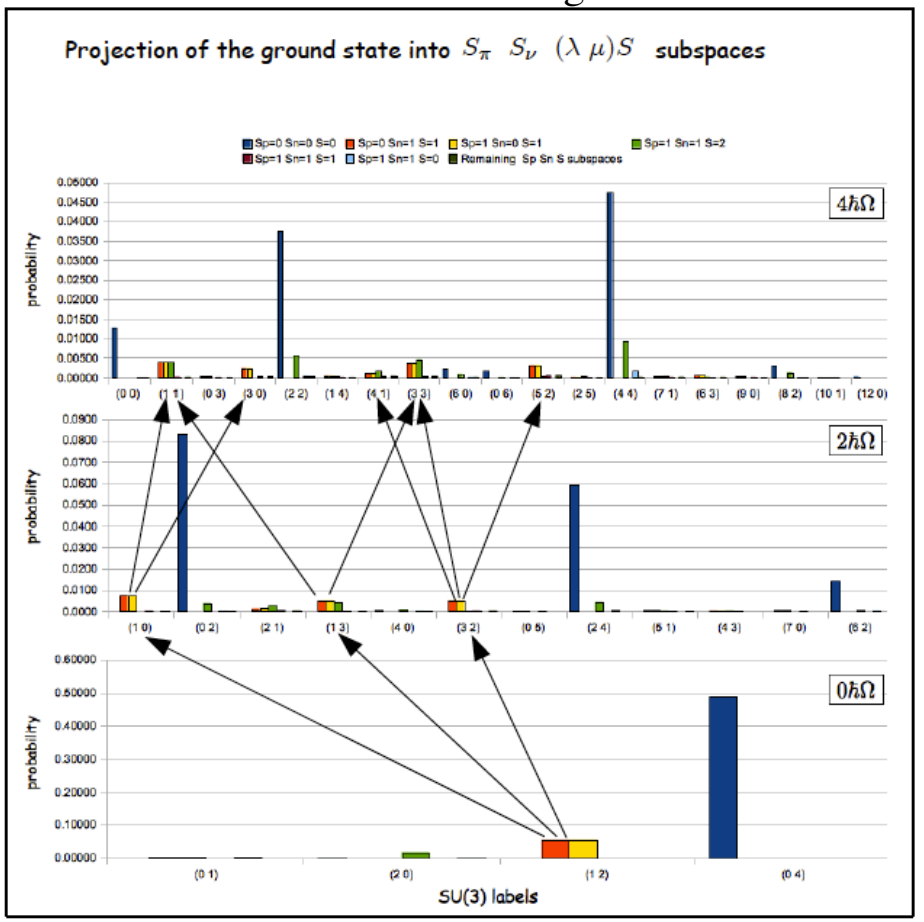
Symplectic (1p-1h, $2\hbar\omega$) Raising Operator

Action of raising operator that has (2,0) SU(3) tensor character (symplectic generator) →

^{12}C (L=0, S=0, $J_{gs} = 0^+$)



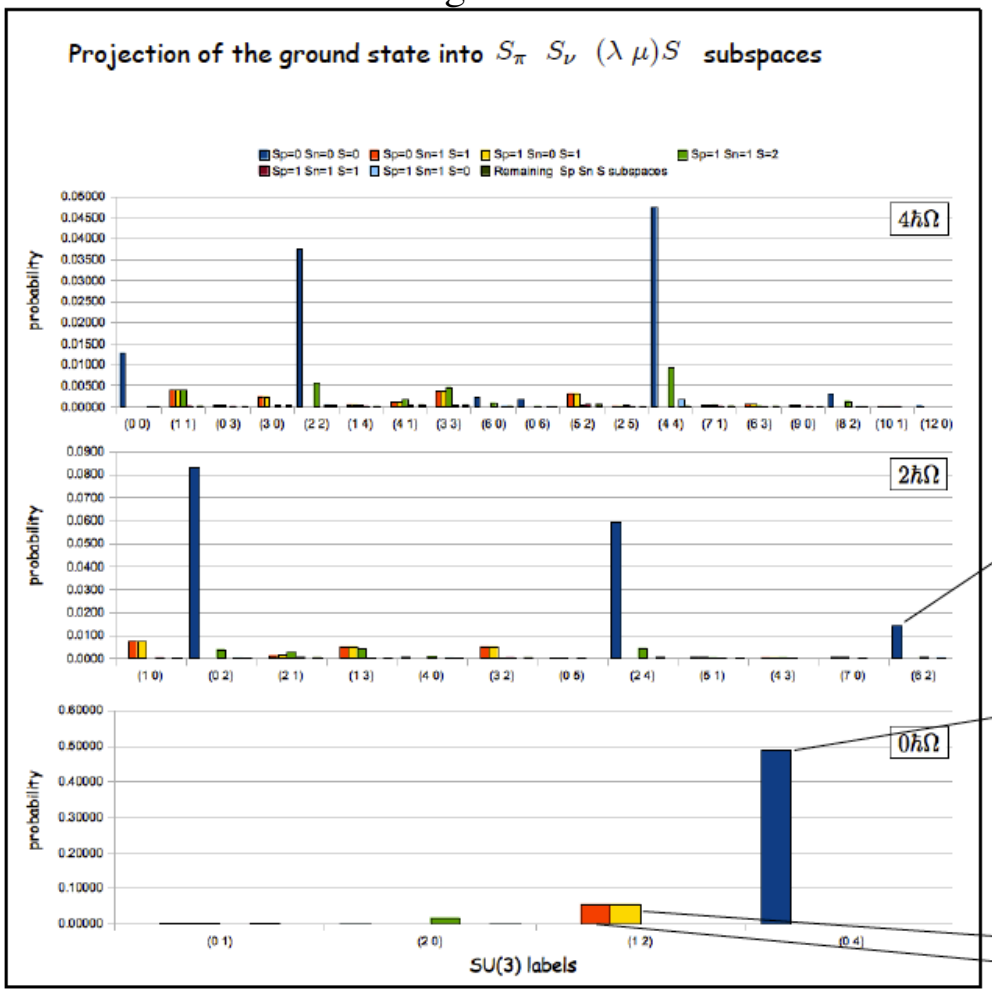
^{12}C (L=1, S=1, $J_{gs} = 0^+$)

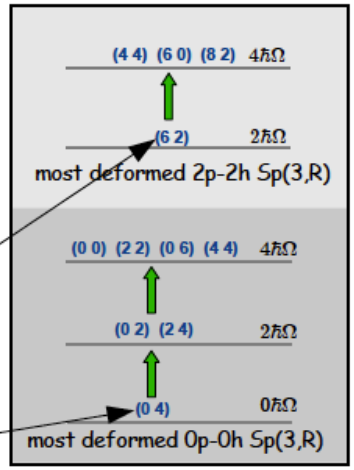


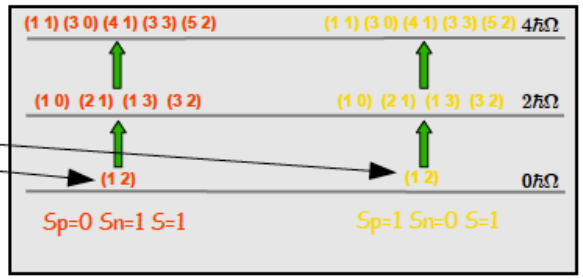
Dominate Modes - (1p-1h, 2ħω & 2p-2h, 2ħω)

^{12}C ($J_{gs} = 0^+$)

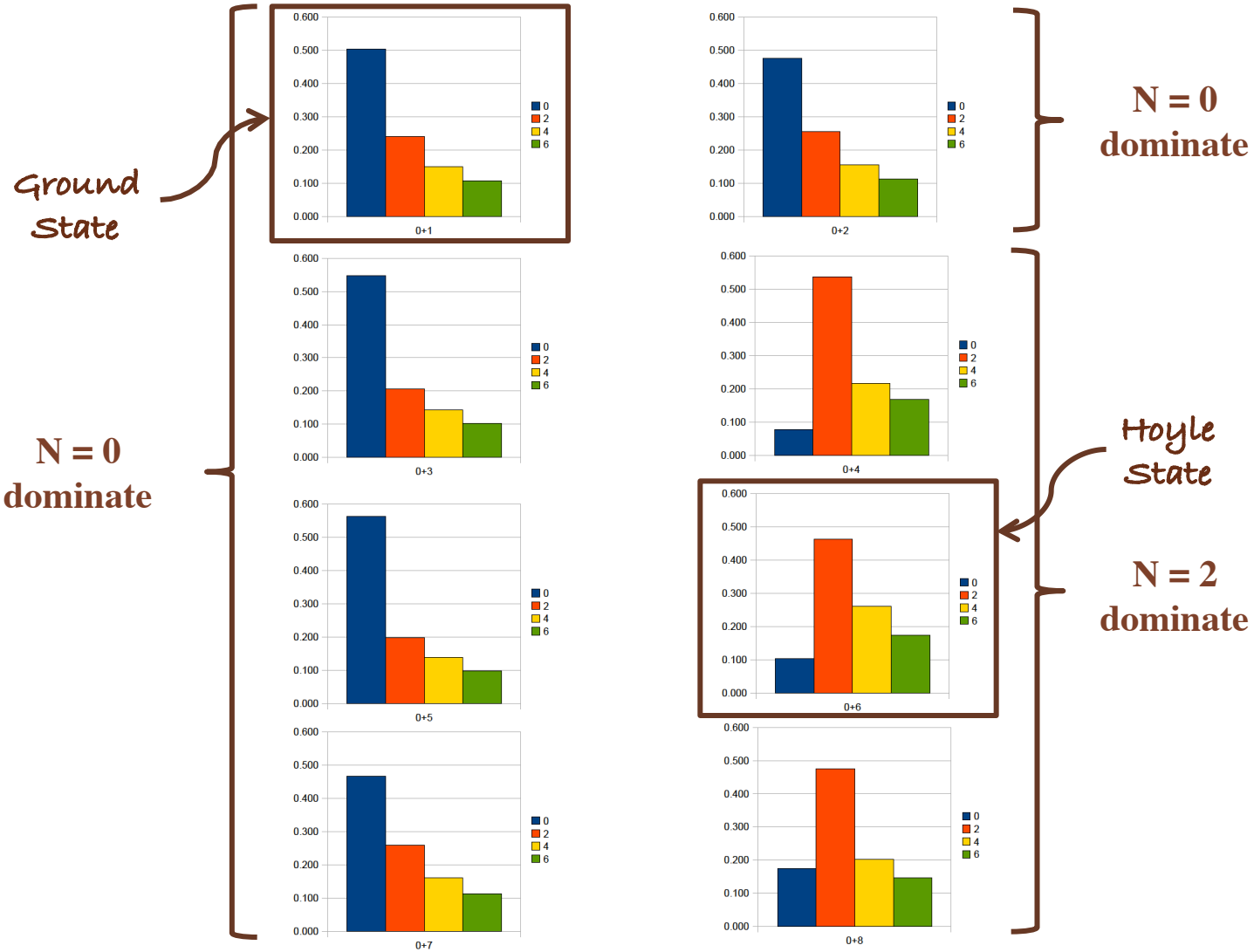
- most important subspaces contain states of the three leading Sp(3,R) irrep
- Significant contribution from the most deformed 2p-2h Sp(3,R) irrep



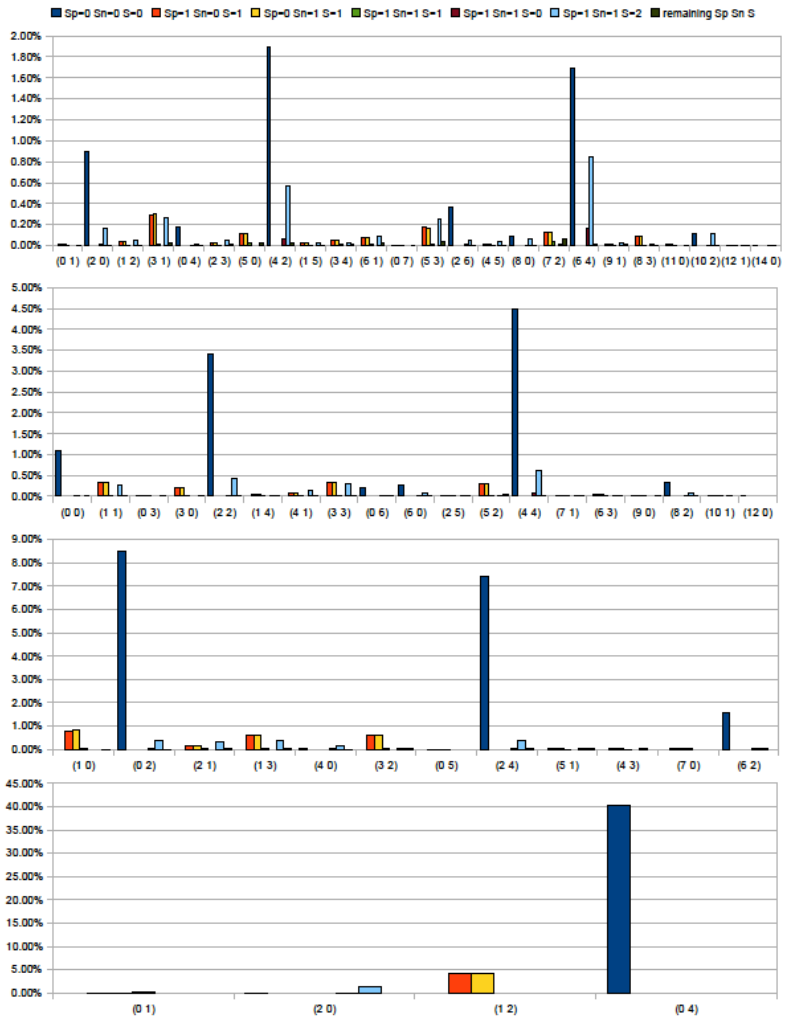


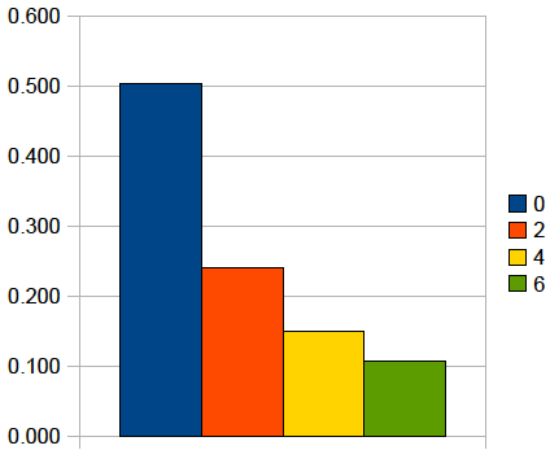


… low-lying 0^+ states in ^{12}C ($N_{max}=6$) …

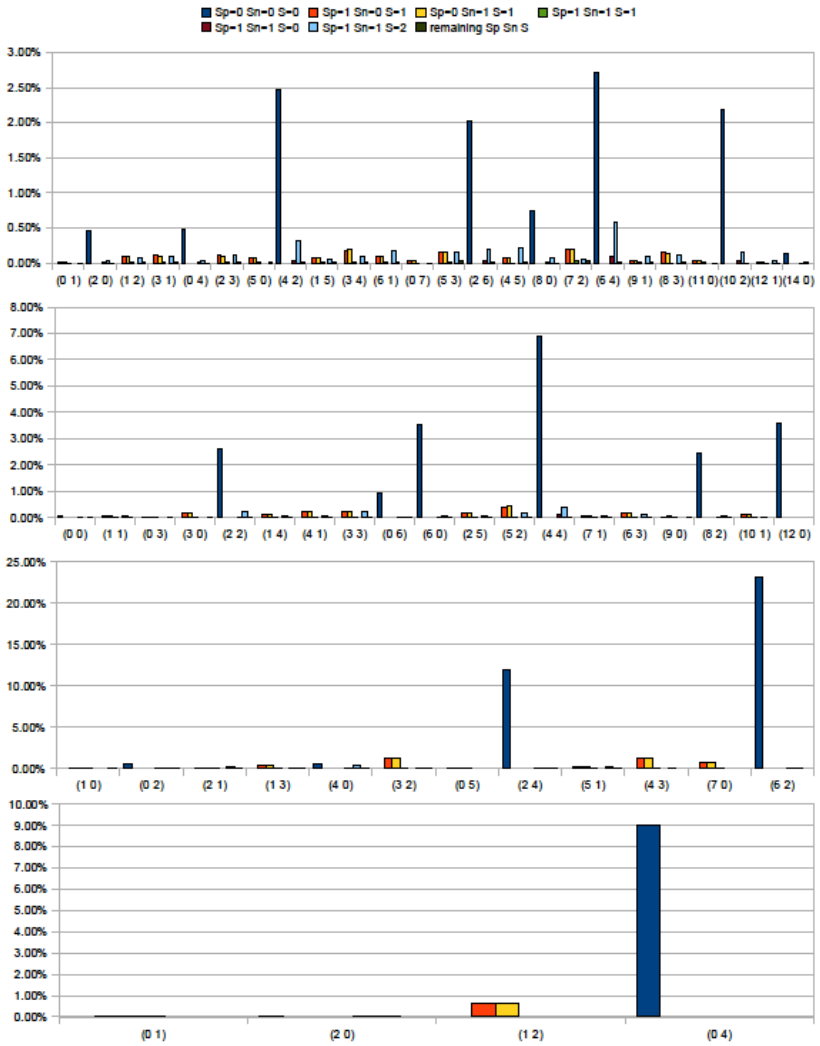


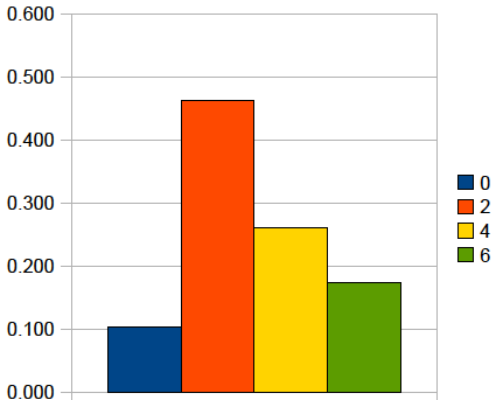
… Structure of 1^{st} 0^+ in ^{12}C …



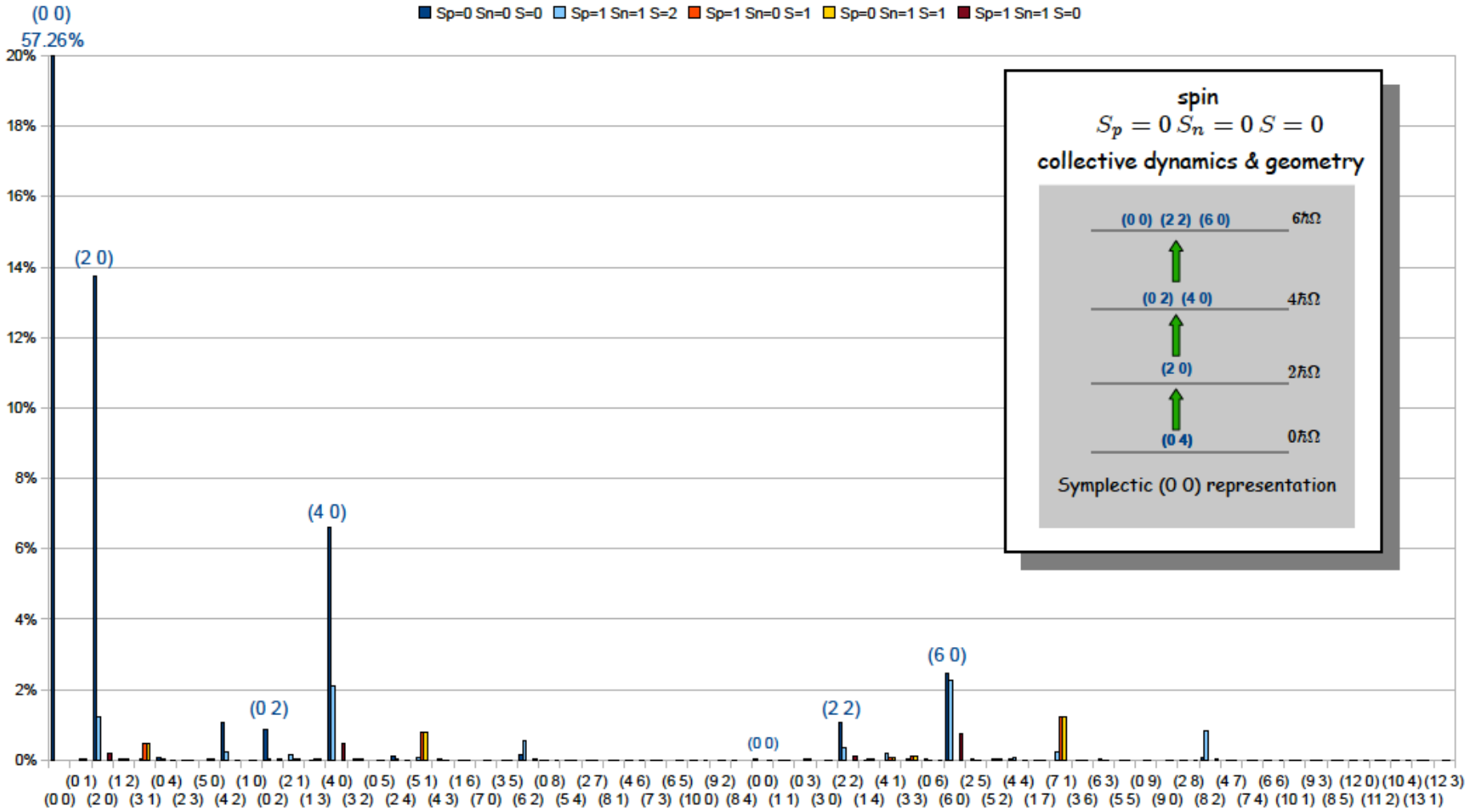


… Structure of 7th 0+ in 12C …

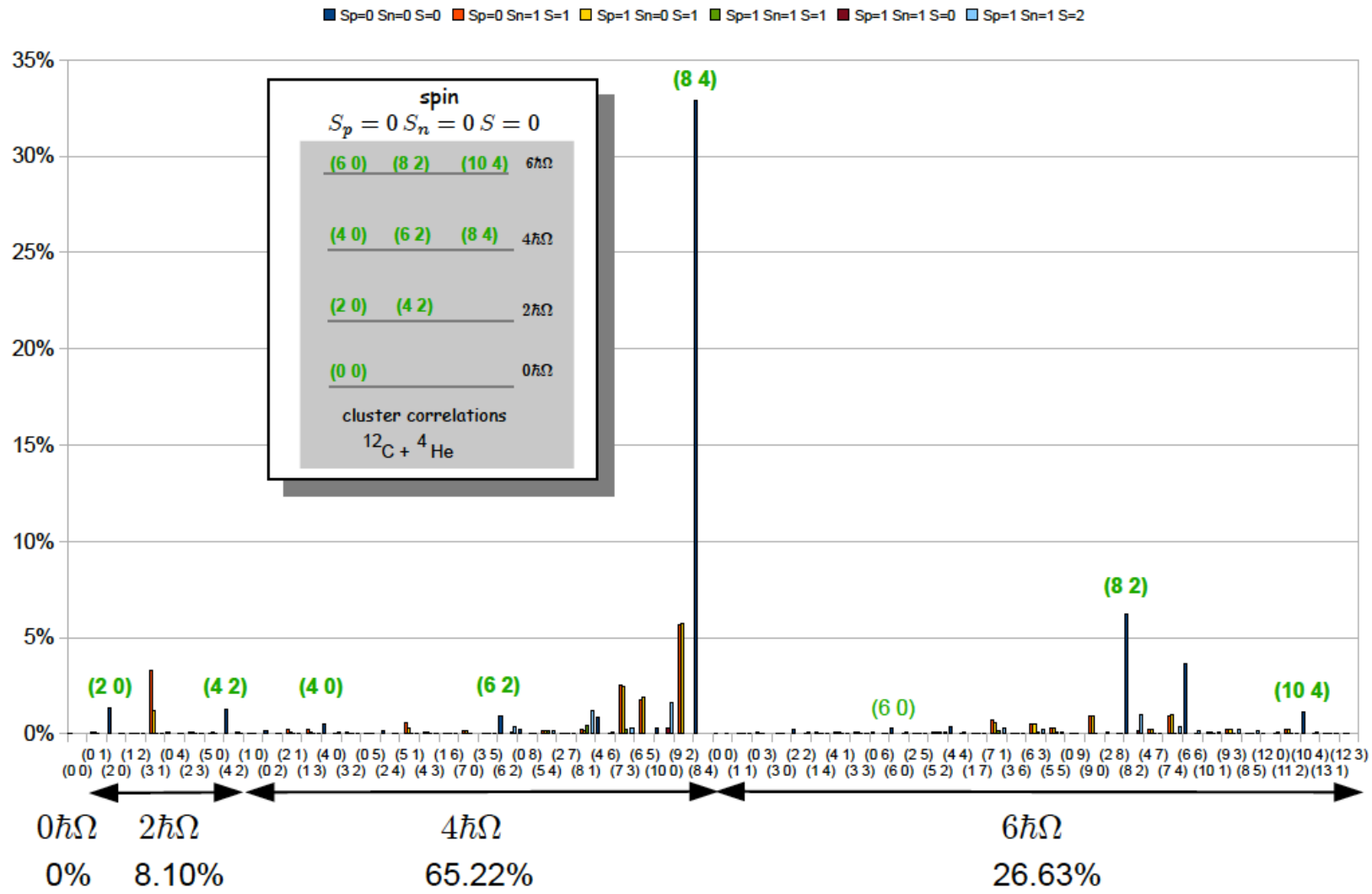




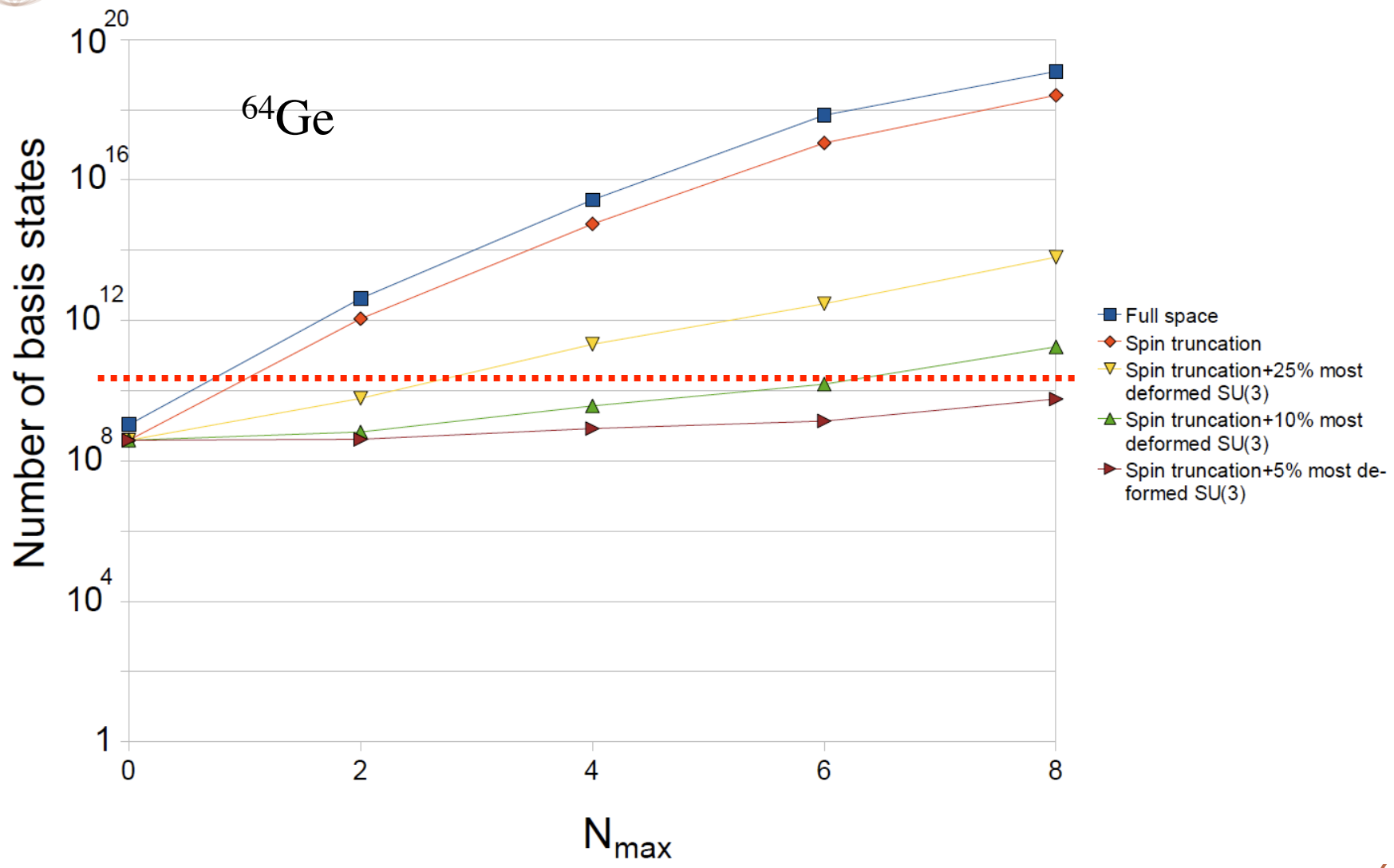
… Structure of 1^{st} 0^+ (Ground State) of ^{16}O …



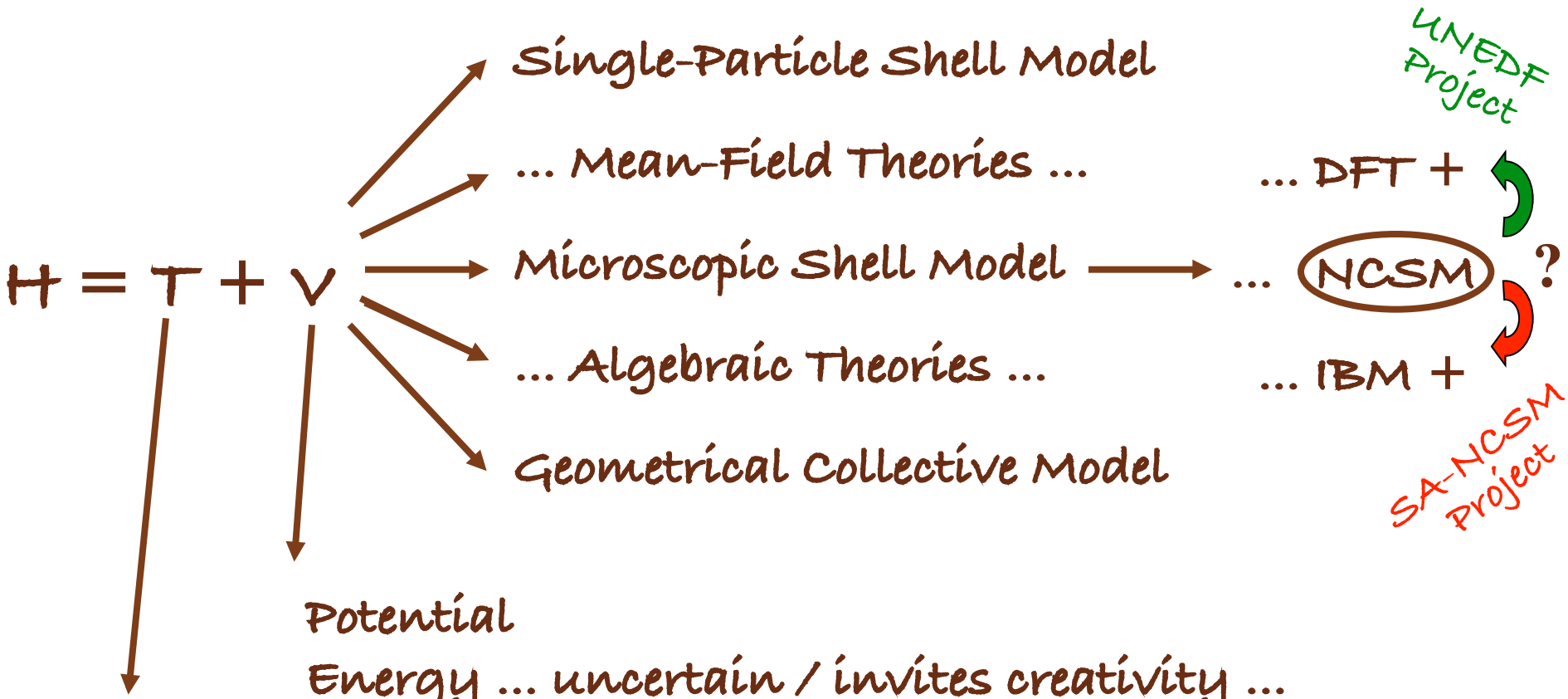
… Structure of 14^{th} 0^+ of ^{16}O …



Reaching Higher / Symmetry Winnowing



… Emerging 'Shell Model' Philosophy …



Looking Forward – 2nd Decade of 21st Century

- Stand alone SA-NCSM code tested/available
  (…balance utilization of computer resources…)

- Designed to handle up to 4-body interactions
  (…importance of alpha-particle correlations…)

- Continued development/targeted applications
  (^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg …an extensible theory…)

… Stay Tuned …