Utilizing Symmetry Coupling Schemes in Ab Initio Nuclear Structure Calculations

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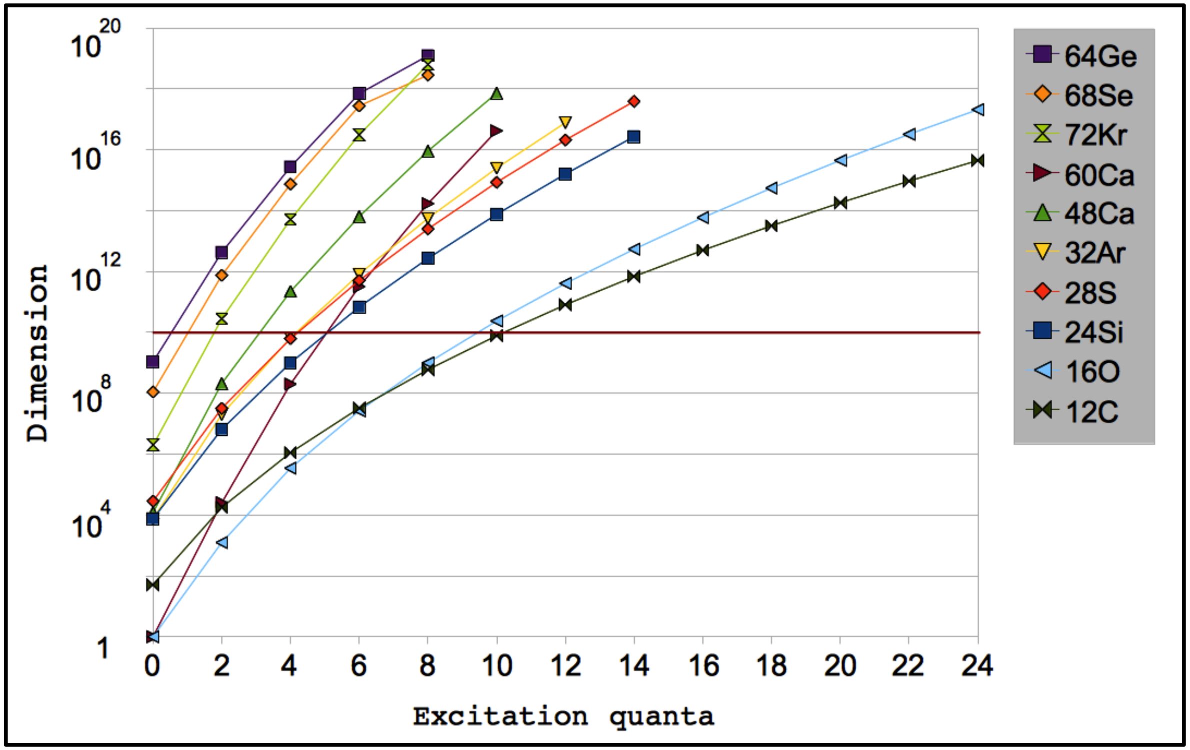
Symmetry-Guided Approach

Motivation

- nuclear collective modes span high $N\hbar\Omega$ spaces
- definition of model space based on many-body cutoff $N_{\max}$ may become computationally prohibitive

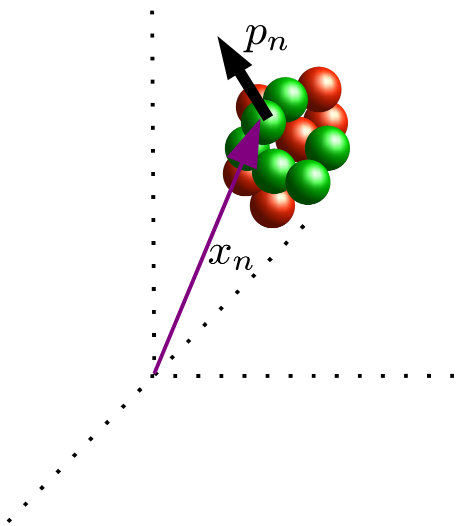


Utilizing symmetry-coupling schemes

- naturally "designed" for efficient desription of nuclear collective dynamics and geometry
- restrict high $N\hbar\Omega$ spaces to subspaces of physically relevant configurations
- preserve exact factorization of center-of-mass degrees of freedom

Nuclear Many-body Collective Dynamics

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



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

- Proof-of-principle: small number of Sp(3,R) basis states realize ~90% of 12C and 16O low-lying wave functions

Bottlenecks:

- Sp(3,R) coupling/recoupling coefficients unknown → Can not compute matrix elements of realistic interaction

- Each Sp(3,R) state is a linear combination of nearly all m-scheme configurations

Solution: utilize SU(3)-coupling scheme

- SU(3) is a subgroup of Sp(3,R)

SU(3) Symmetry-Adapted Basis

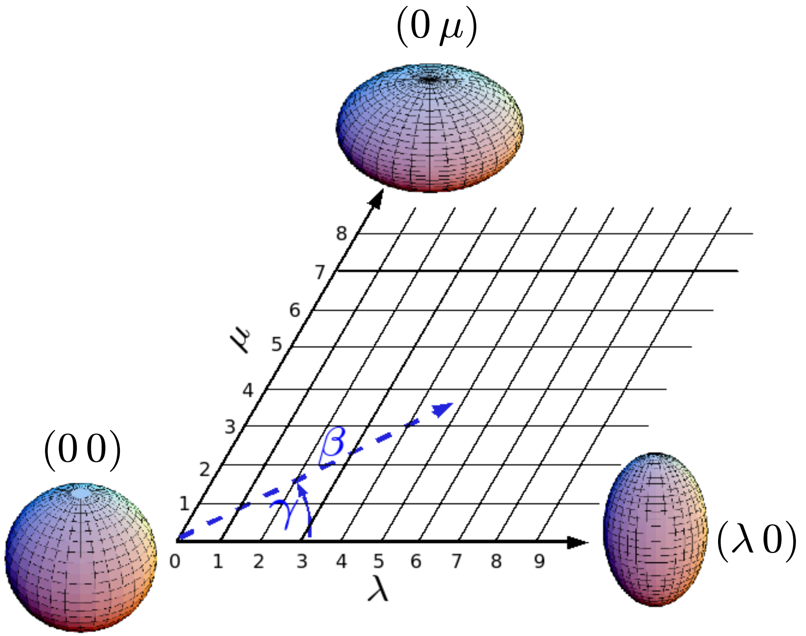
Physical SU(3) Basis:

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

$(\lambda\ \mu)$ → SU(3) quantum numbers

κ → multiplicity label

L → orbital angular momentum



- $(\lambda\ \mu)$ related to shape variables β and γ of the collective model
- Relevant for description of spatially deformed nuclei & nuclear collective motion

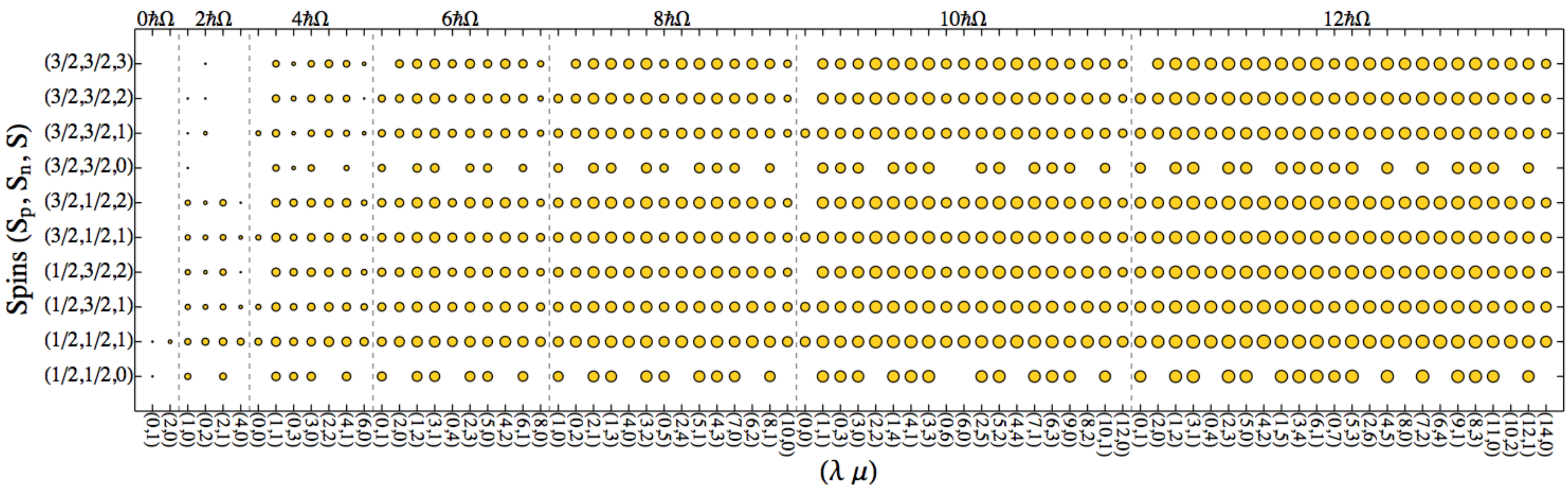
SU(3)-coupling scheme in NCSM

- multi-shell + proton-neutron + intrinsic spin degrees of freedom

$$|\ldots\ N\hbar\Omega\ \overbrace{S_p\, S_n S}^{\text{intrinsic spin part}}\ \overbrace{(\lambda\, \mu)\ \kappa\ L}^{\text{spatial part}}\ \ J\, M\rangle$$

Structure of NCSM Model Space in SU(3) Coupling Scheme

$^{6}\mathrm{Li}: \ N_{\mathrm{max}} = 12$



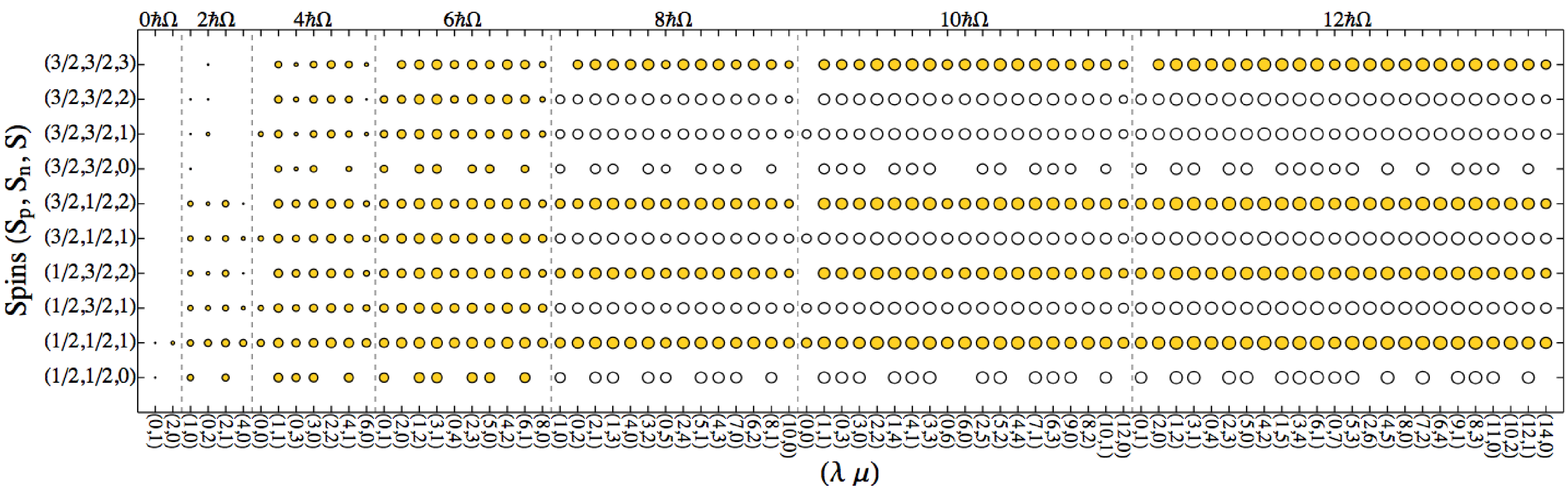
- Each disk represents a subspace of all states with quantum numbers: $N\hbar\Omega \ \ S_p S_n S \ \ (\lambda\,\mu)$

- Center-of-mass factorization exact within each subspace

$$N\hbar\Omega \ \ S_p S_n S \ \ (\lambda\,\mu) \quad \longrightarrow \quad \psi_{\mathrm{intr}} \otimes \psi_{\mathrm{c.m.}}^{(n\,0)}$$

Refining NCSM Model Space

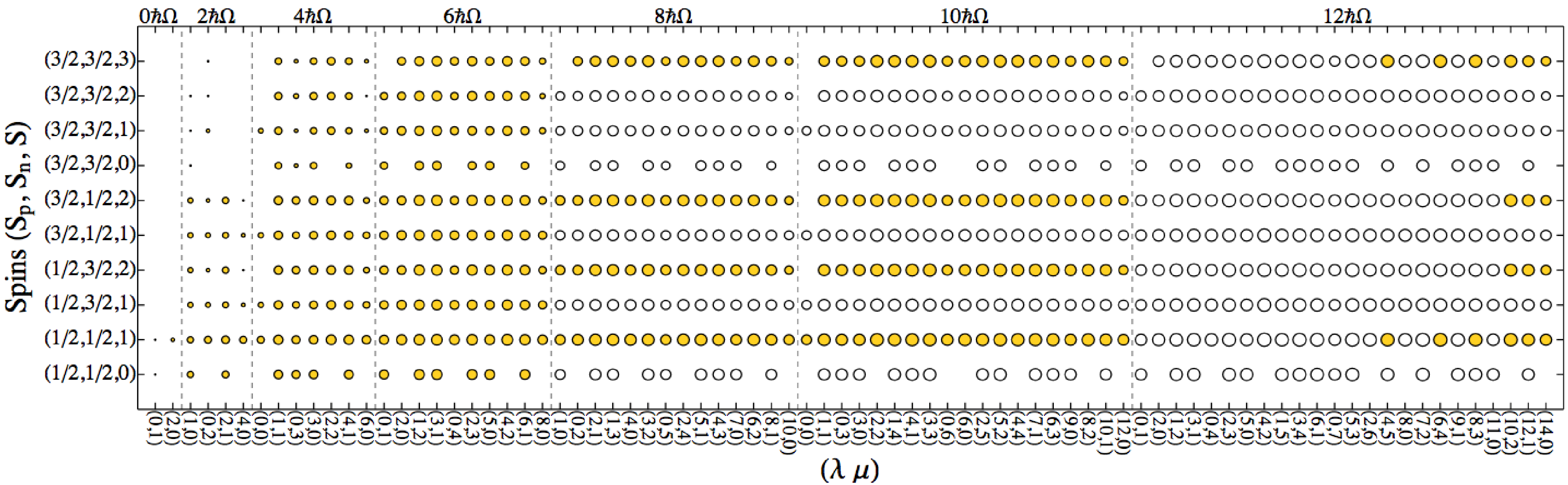
- Selecting basis states according to: **(1) intrinsic spins**



Refining NCSM Model Space

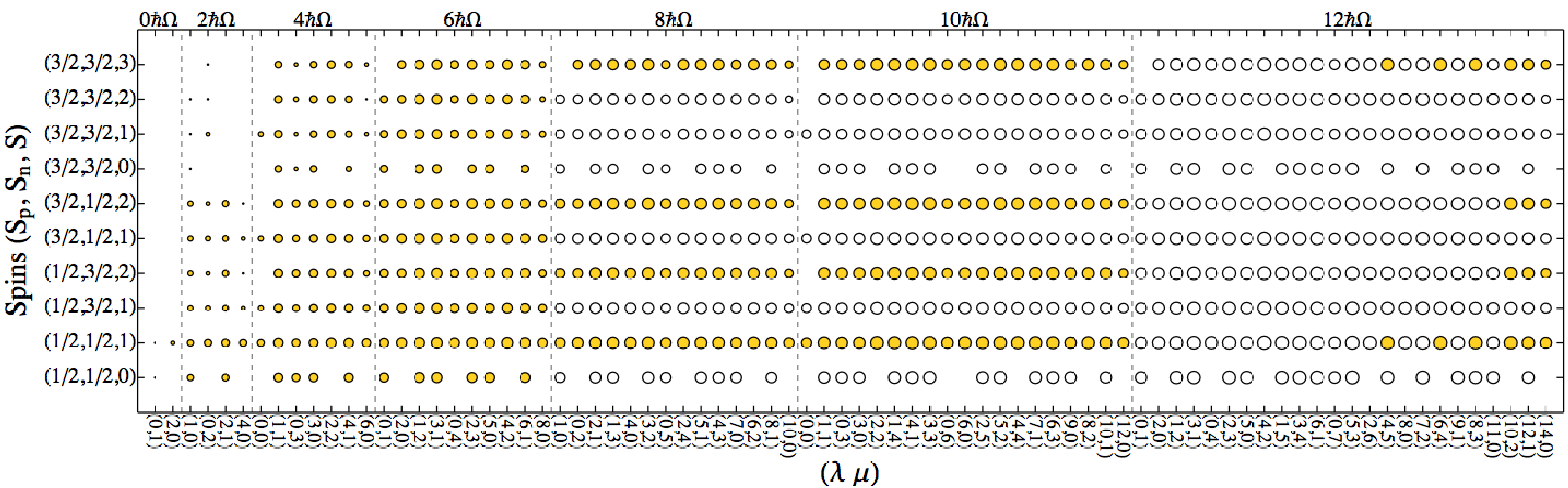
- Selecting basis states according to: (1) intrinsic spins

  (2) deformations



Refining NCSM Model Space

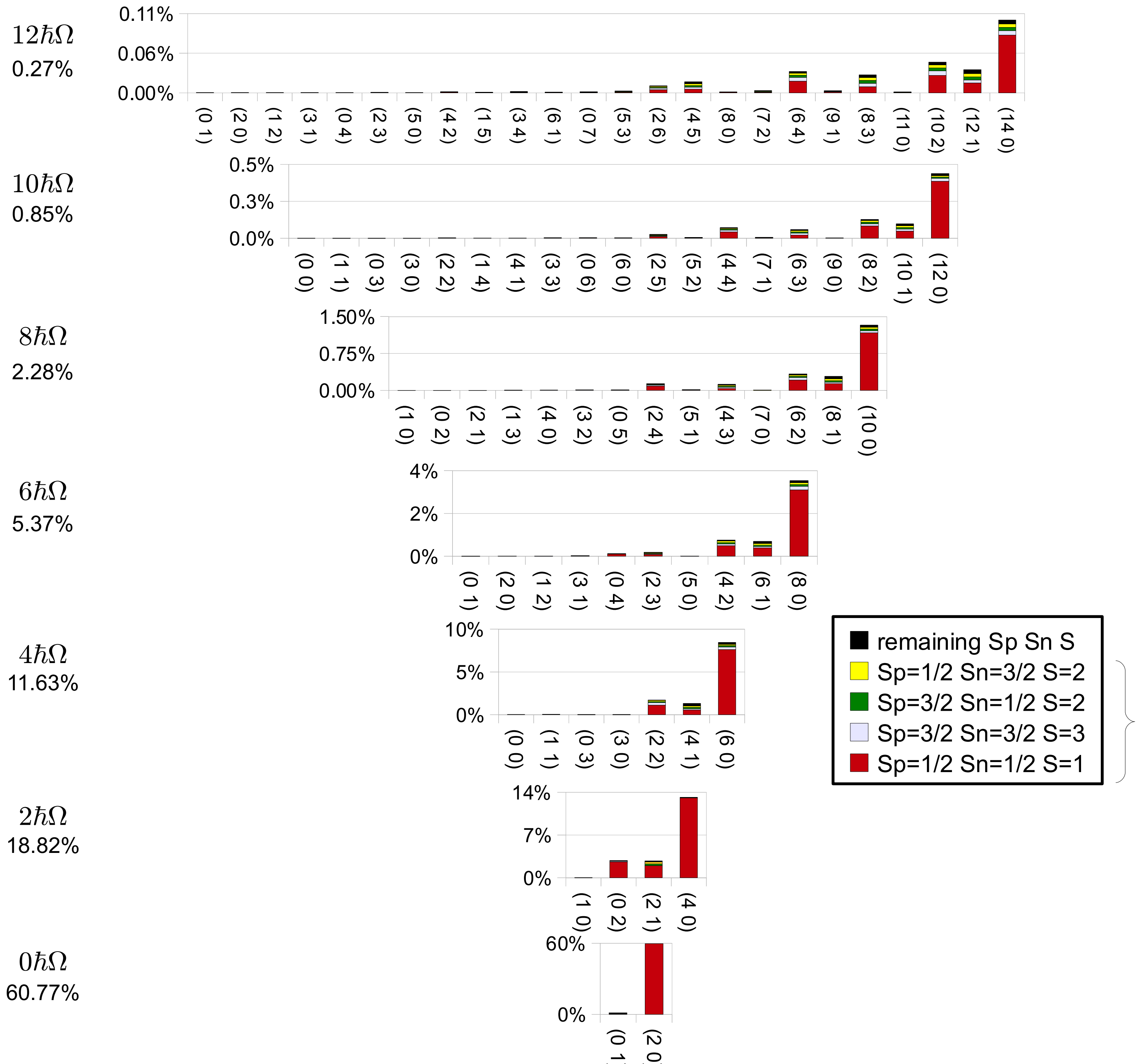
- Selecting basis states according to: (1) intrinsic spins
  (2) deformations



- Realistic interactions: enormous mixing of different $S_p S_n S$ $(\lambda\ \mu)$ subspaces

- Coherent mixing ?

Emergence of Simple Patterns



~99% of the ground state

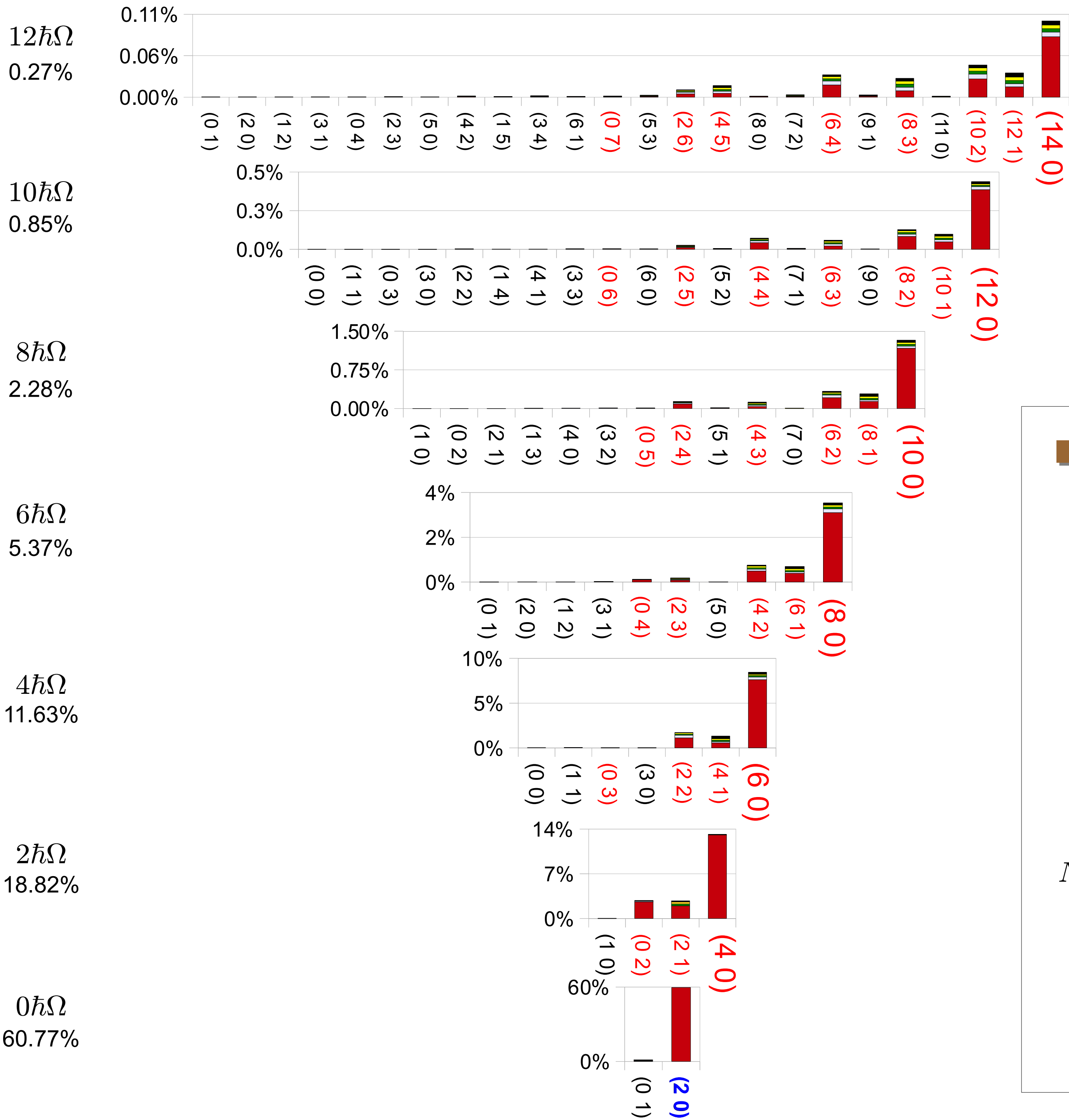
$^{6}\mathrm{Li} : 1^{+}_{\mathrm{gs}}$

$N_{\max} = 12$

JISP16 + Vcoul

$\hbar\Omega = 20$ MeV

Emergence of Simple Patterns



$^6\text{Li} : 1^+_{\text{gs}}$

$N_{\max} = 12$

JISP16 + Vcoul

$\hbar\Omega = 20$ MeV

Dominant shapes

- $N\hbar\Omega$ $(\lambda\,\mu)$ satisfying condition

$$\lambda + 2\mu = \lambda_0 + 2\mu_0 + N$$

the most deformed $0\hbar\Omega$ configuration $(\lambda_0\,\mu_0) = (2\,0)$

- Highest contribution

$N\hbar\Omega$ $(\lambda_0 + N \;\; \mu_0) = (2\,0)\;(4\,0)\;(6\,0)\ldots$

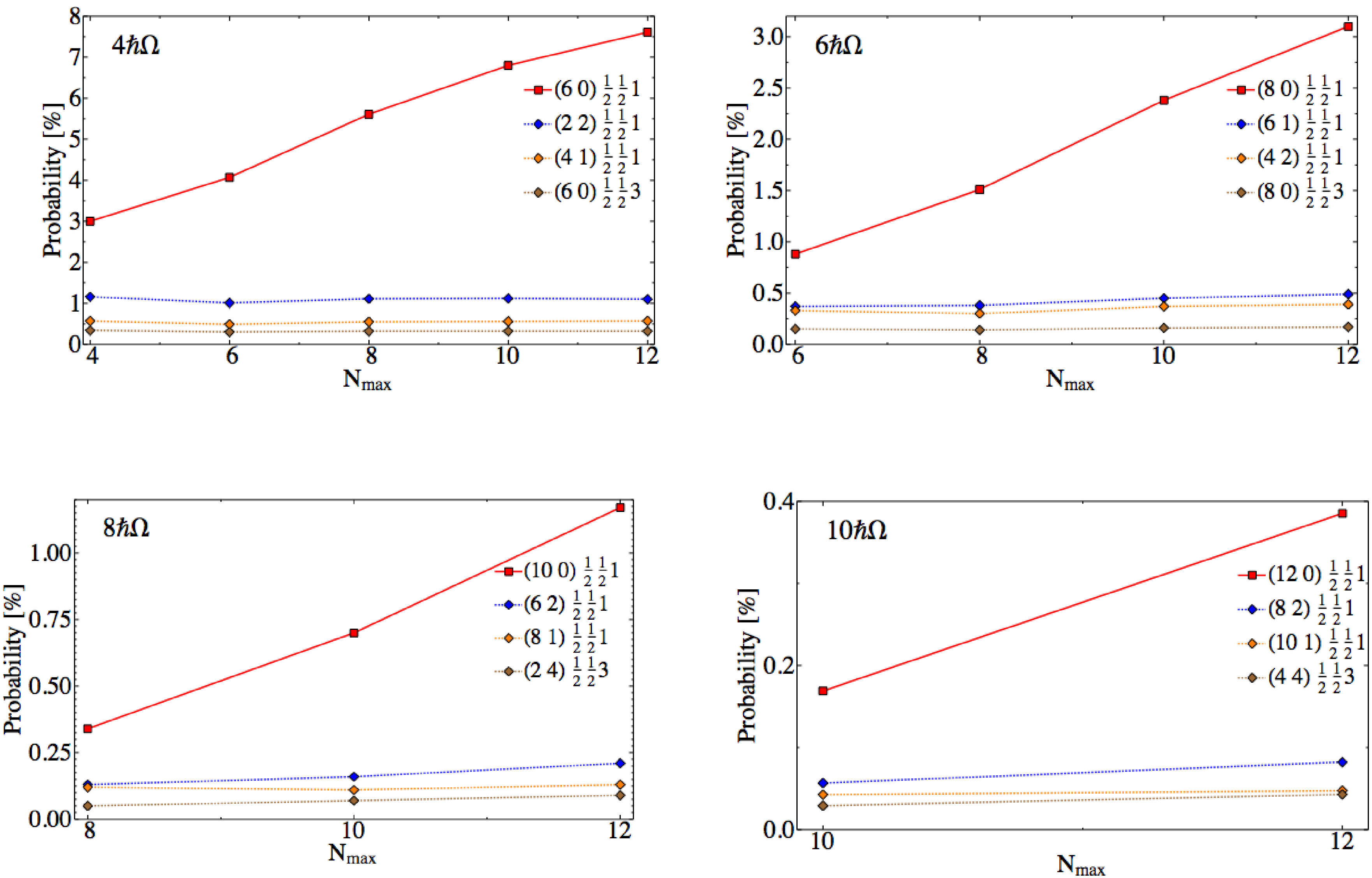
- Consistent with symplectic model

$Sp(3,R) \supset Sp(2,R) \supset Sp(1,R)$

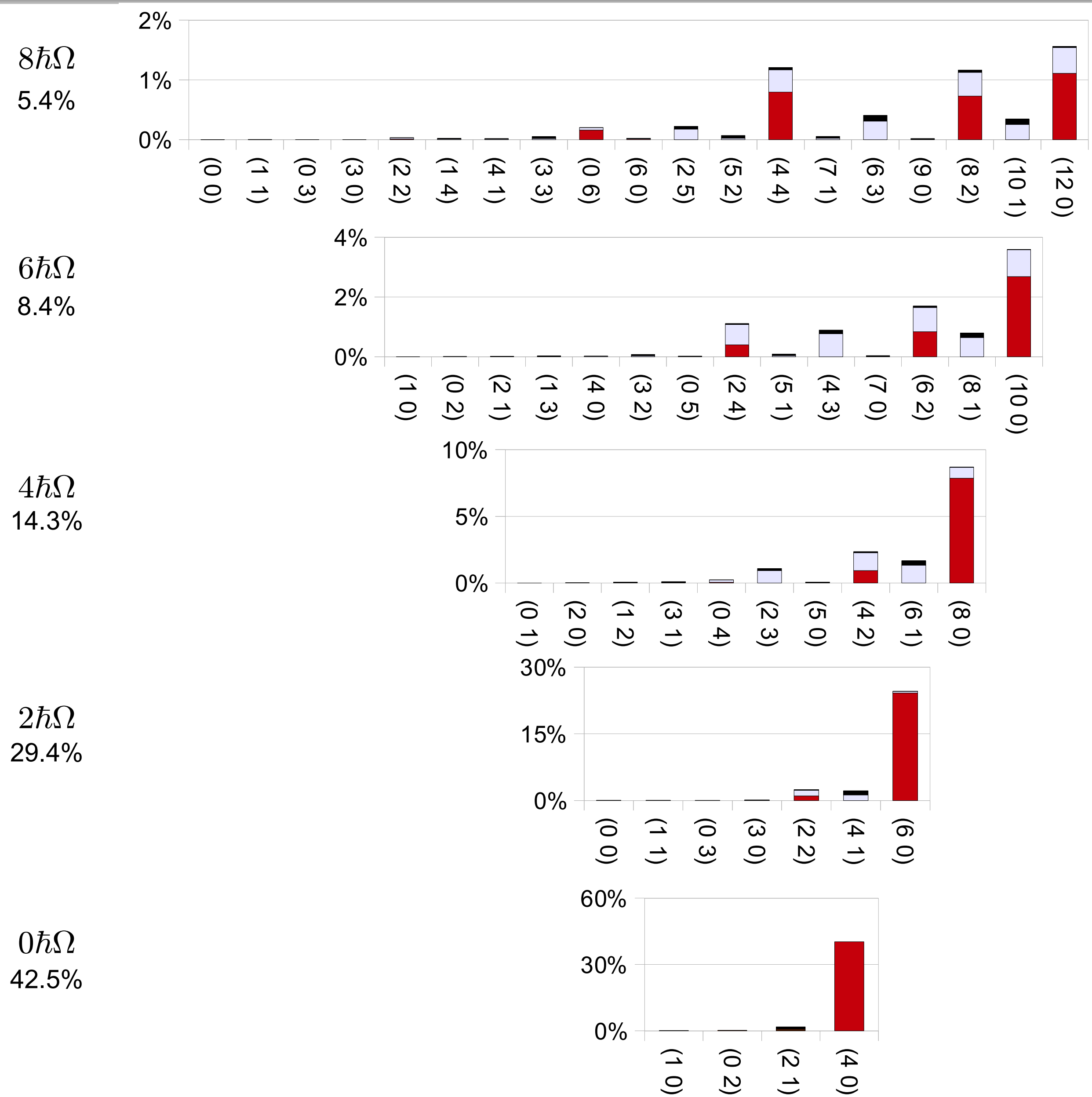
Role of Model Space Truncation

Effects of higher N_{max}

- intrinsic spin mixing decreasing
- Contribution of the most deformed configurations $N\hbar\Omega$ $(2{+}N\,0)$ rapidly increasing



Chiral N3LO Interaction



$^{8}\text{Be} : 0^{+}_{gs}$

$N_{\max} = 8$

N3LO + Vcoul

$\hbar\Omega = 25$ MeV

- remaining Sp Sn S
- Sp=1 Sn=1 S=2
- Sp=0 Sn=0 S=0

~98% of the ground state

Dominant shapes

- $N\hbar\Omega\ (\lambda\,\mu)$ satisfying condition

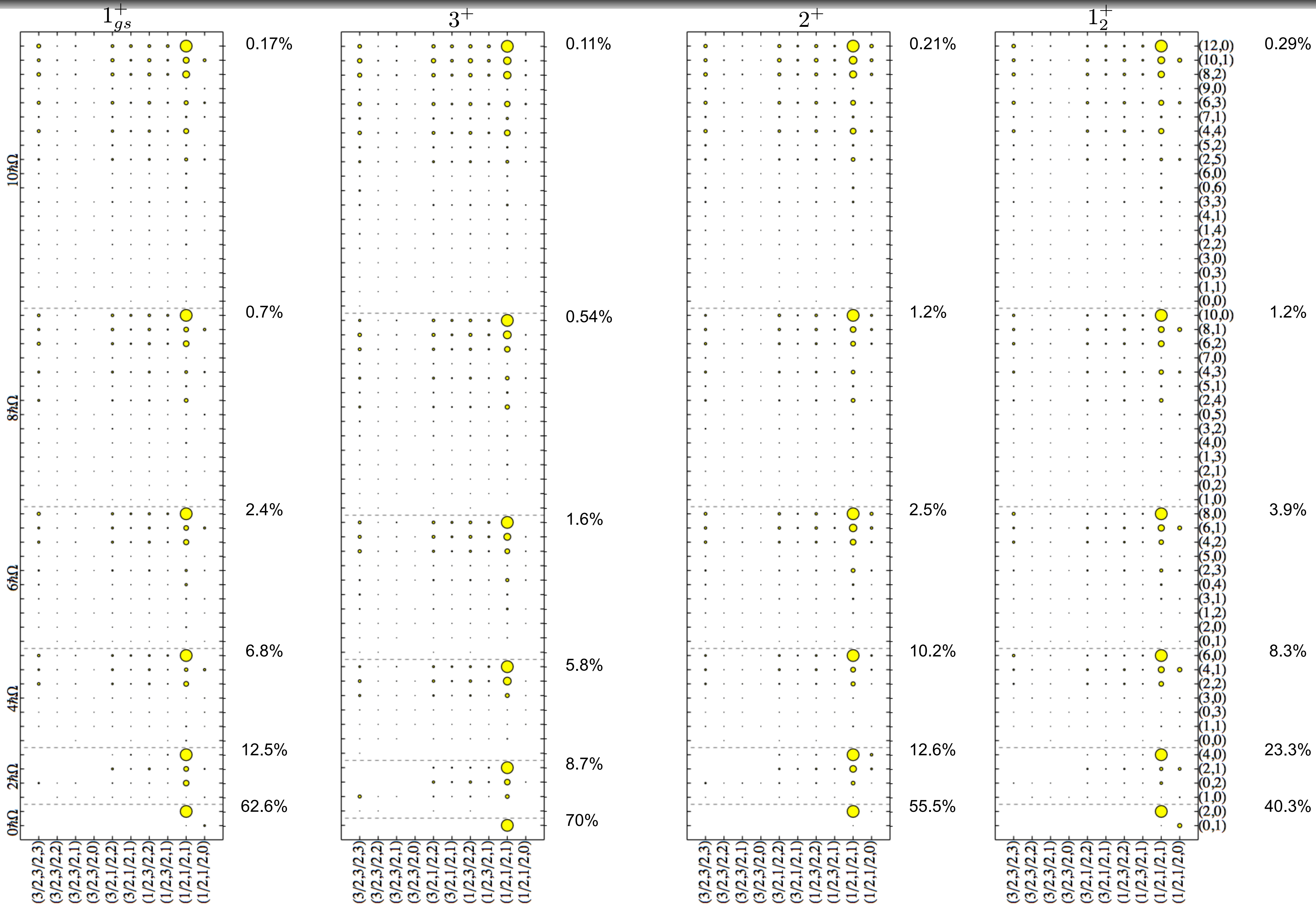
$$\lambda + 2\mu = \lambda_0 + 2\mu_0 + N$$

the most deformed $0\hbar\Omega$ configuration $(\lambda_0\,\mu_0) = (4\,0)$

- Highest contribution

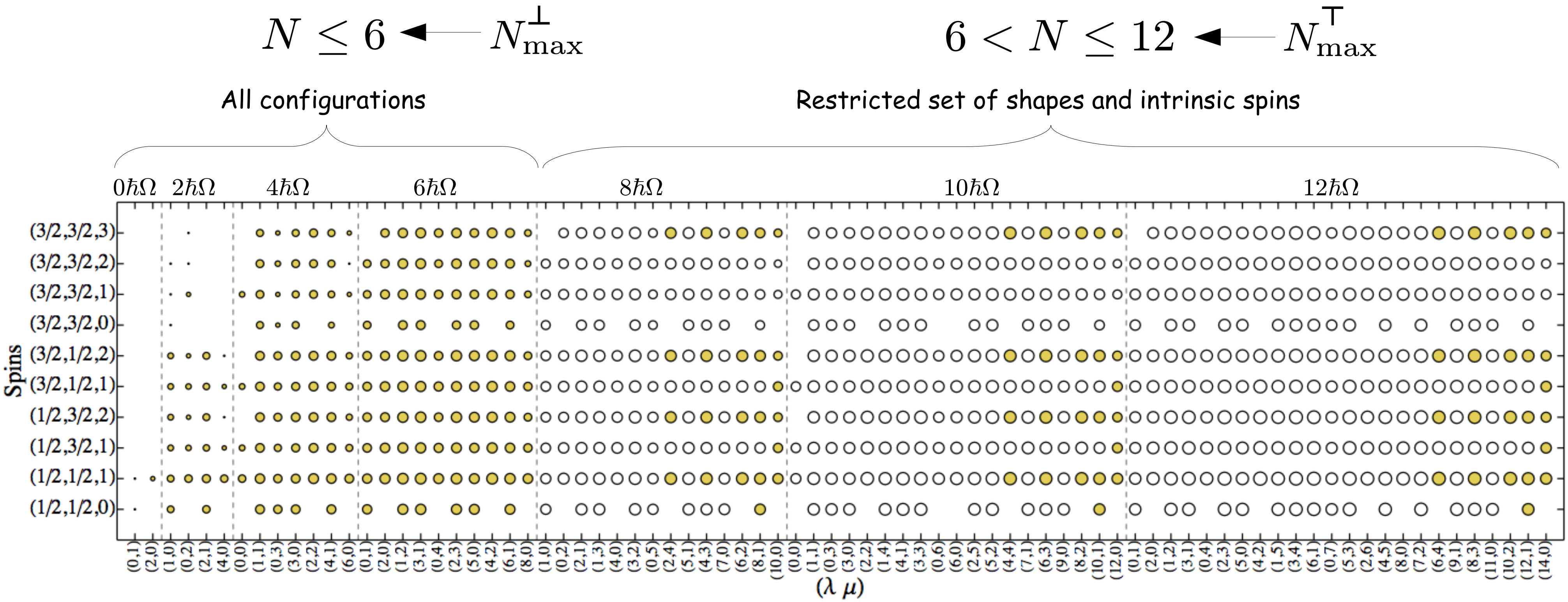
$N\hbar\Omega\ (\lambda_0 + N\ \ \mu_0) = (4\,0)\ (6\,0)\ (8\,0)\ldots$

^{6}Li - structure of T=0 states



Symmetry-Guided Selection of Model Space

- Model Space in SU(3)-scheme: $N_{\max}^{\top} \langle N_{\max}^{\perp} \rangle$

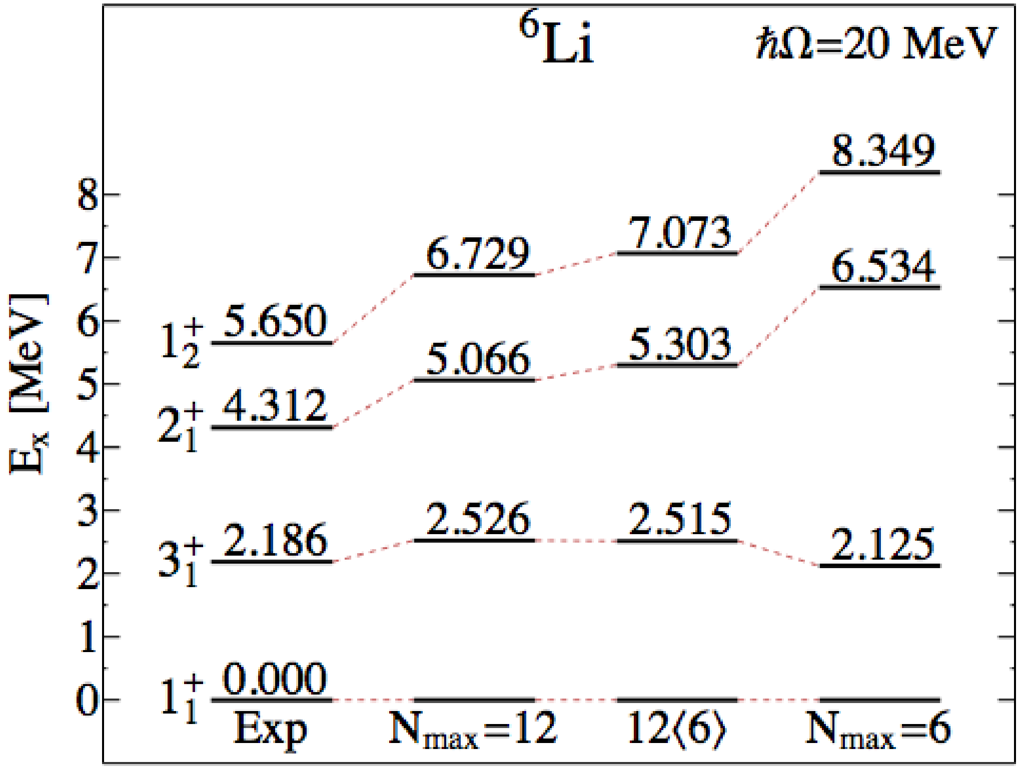


$$^{6}\text{Li} : 12\langle 6 \rangle$$

Spectroscopic Properties in 12<6> Model Space

- Interaction: JISP16 + Vcoul
  $17.5 \leq \hbar\Omega \leq 25$ MeV

- Excitation Energies



- Binding energy: 98% - 99% of complete space result

Physical Observables in 12<6> Model Space

- Magnetic dipole moments: agreement within 0.3% for odd-J and 5% for J=2

$\hbar\Omega = 20$ MeV

Magnetic dipole moments $[\mu_N]$

	1^+_{gs}	3^+	2^+	1^+_2
$N_{\max} = 12$	0.838	1.866	0.970	0.338
$12\langle 6\rangle$	0.839	1.866	1.014	0.338

- point-particle rms matter radii: agreement within 1%

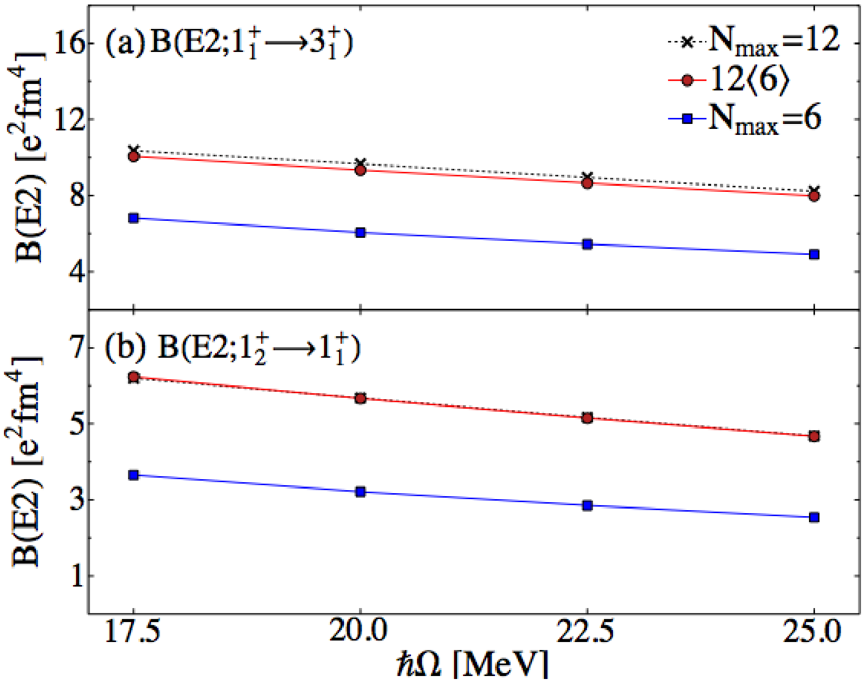
$\hbar\Omega = 20$ MeV

Matter rms radii [fm]

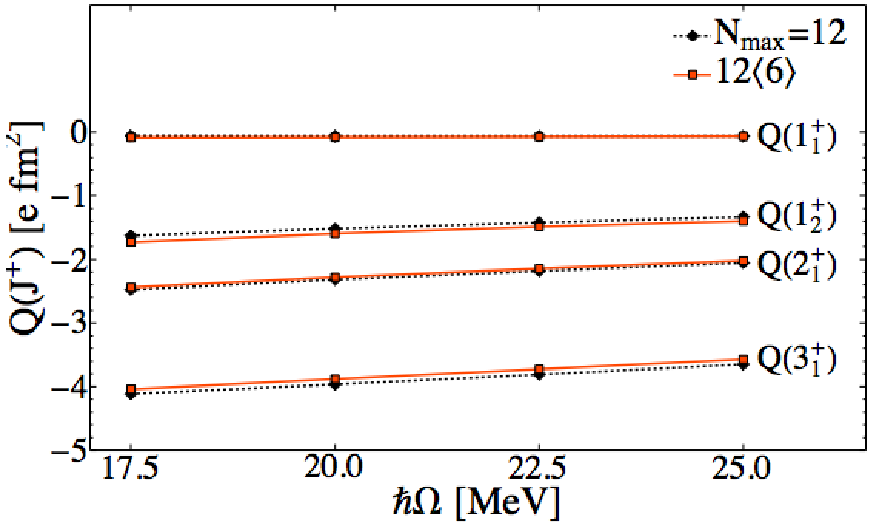
	1^+_{gs}	3^+	2^+	1^+_2
$N_{\max} = 12$	2.119	2.063	2.204	2.313
$12\langle 6\rangle$	2.106	2.044	2.180	2.290

Physical Observables in 12<6> Model Space

- BE2 transitions

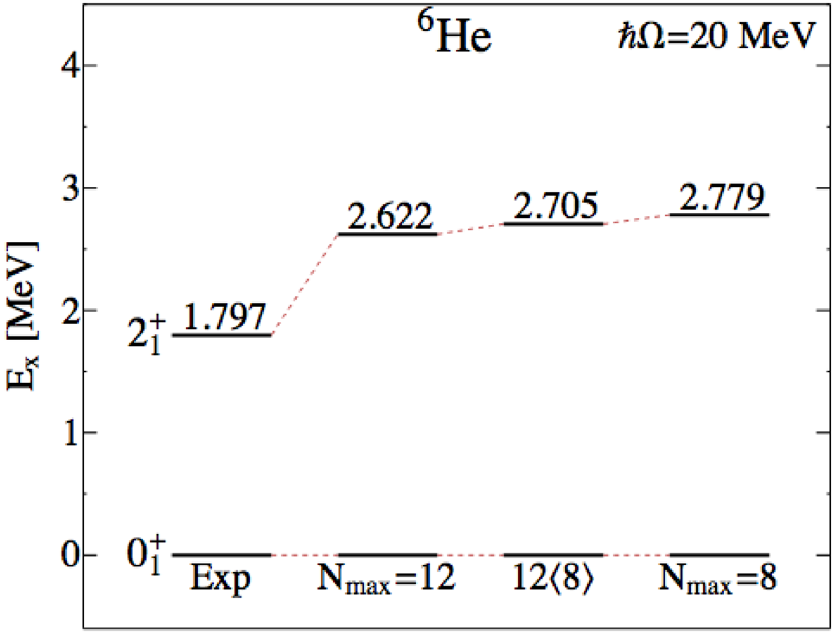


- E2 moments



^{6}He in Symmetry-Guided Model Space

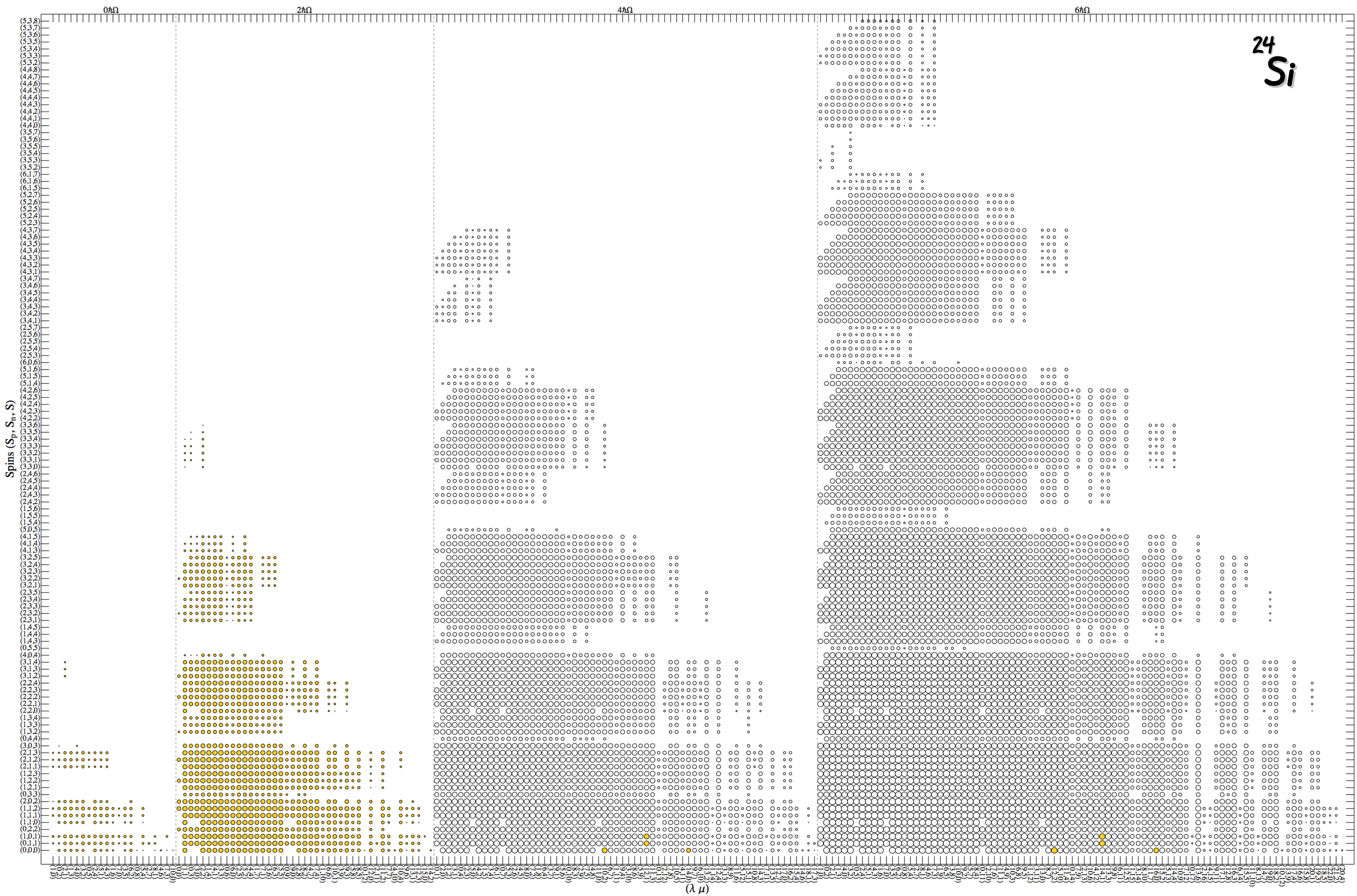
- Rotational band dominated by $(\lambda_0\,\mu_0) = (2\,0)$ → same set of important shapes



- Binding energy: over 99% of complete space result

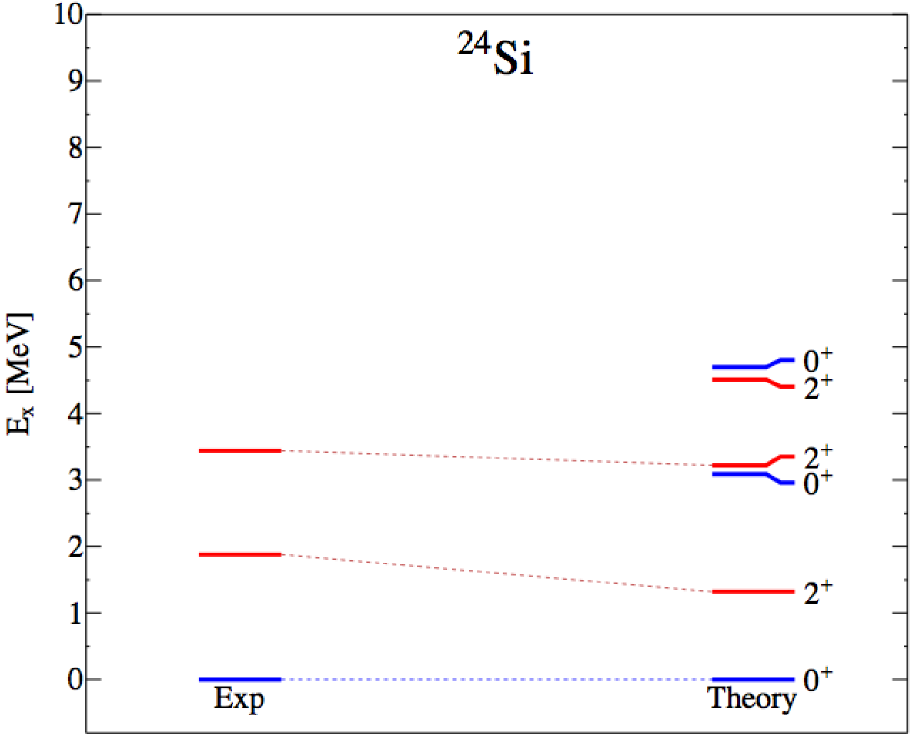
	$N_{\max} = 12$	$12\langle 8\rangle$
$B(E2; 2_1^+ \to 0_1^+)[e^2\text{fm}^4]$	0.181	0.184
$Q(2_1^+)[e\text{fm}^2]$	-0.690	-0.711
$\mu(2_1^+)[\mu_N]$	-0.873	-0.817
$r_m(2_1^+)[\text{fm}]$	2.153	2.141
$r_m(0_1^+)[\text{fm}]$	2.113	2.110

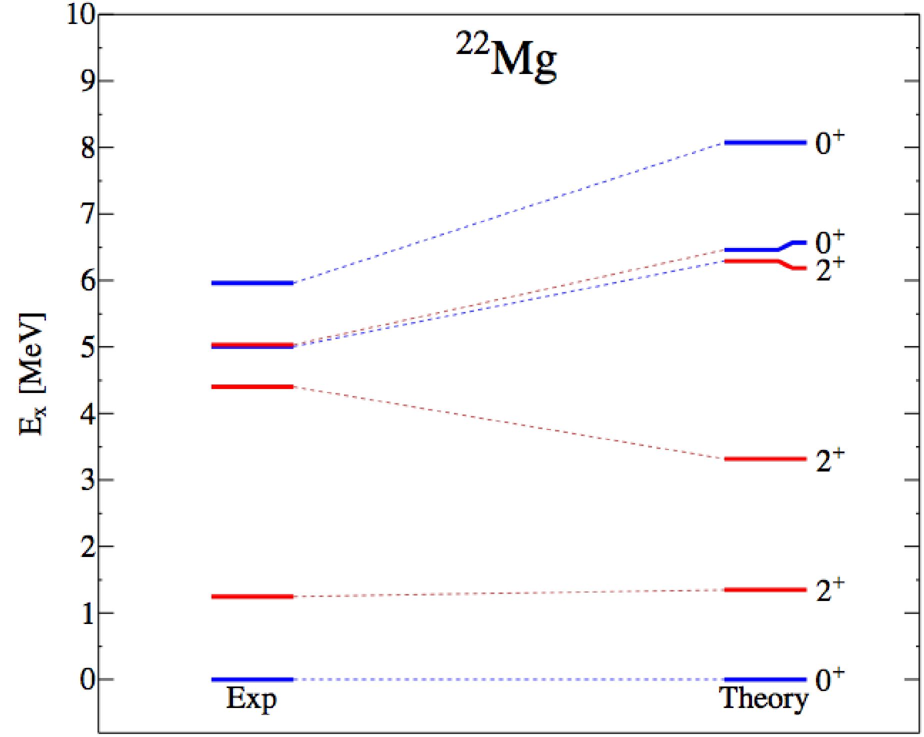
Outlook: Towards ds-shell Nuclei



Outlook: Towards ds-shell Nuclei

- SRG-N3LO $\lambda = 2.0\ \mathrm{fm}^{-1}$ $\hbar\Omega = 15\ \mathrm{MeV}$





Outlook: Utilizing Sp(3,R) States

- Expansion of Sp(3,R)-scheme states in SU(3) basis

Sp(3,R) generators

$$\hat{A}_{ij} = \sum_n b^\dagger_{ni} b^\dagger_{nj} \qquad \hat{B}_{ij} = \sum_n b_{ni} b_{nj} \quad \Longrightarrow \quad \hat{T}^{(0\,0)} := -\left[\hat{A} \times \hat{B}\right]^{(0\,0)} + \lambda \hat{N}_{\mathrm{cm}}$$

HO laddering operators

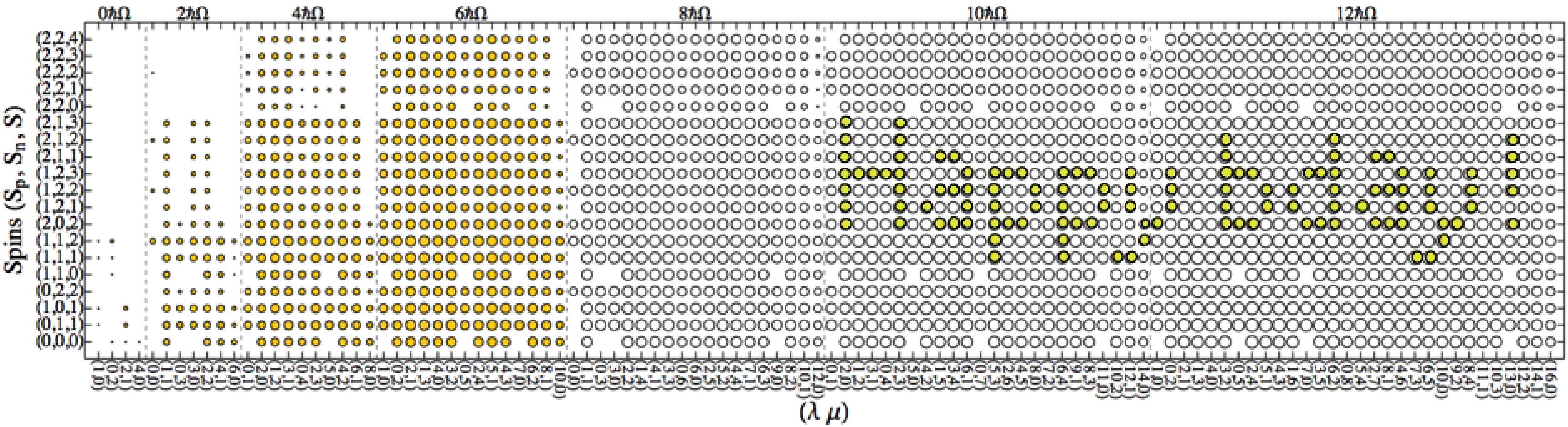
- $\hat{T}^{(0\,0)}$
  - Block diagonal in SU(3)-basis $N\hbar\Omega \; S_p S_n S \; (\lambda\,\mu)$
  - Eigenvalues are analytical - function of Sp(3,R) quantum labels
  - Eigenvector have good Sp(3,R) symmetry

- Computations combining SU(3) & Sp(3,R) basis are the next goal

Summary

- We have combined SU(3)-coupling basis with ab initio NCSM framework
  - Unveiled simple patterns that favor strong quadrupole deformation and low intrinsic spins in light p-shell nuclei
  - Patterns seem not to depend on particular NN forces and support model space truncation scheme
  - Expansion of Sp(3,R) states in terms of SU(3)-basis implemented

- Outlook
  - Move towards ds-shell nuclei
  - Combine SU(3) & Sp(3,R) basis
  - Inclusion of NNN forces



0ħΩ
2ħΩ
4ħΩ
6ħΩ
8ħΩ
10ħΩ
12ħΩ
Spins (Sp, Sn, S)
(2,2,4)
(2,2,3)
(2,2,2)
(2,2,1)
(2,2,0)
(2,1,3)
(2,1,2)
(2,1,1)
(1,2,3)
(1,2,2)
(1,2,1)
(2,0,2)
(1,1,2)
(1,1,1)
(1,1,0)
(0,2,2)
(1,0,1)
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(λ μ)