Emergence of Simple Patterns in Complex Atomic Nuclei from First Principles

Tomáš Dytrych, Jerry P. Draayer, Kristina D. Launey

LOUISIANA STATE UNIVERSITY

Collaborators:

James P. Vary, Pieter Maris

Iowa State University

Mark Caprio

University of Notre Dame

Erik Saule, Umit Catalyurek

Ohio State University

Daniel Langr

Czech Technical University

Masha Sosonkina

Old Dominion University

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Outline

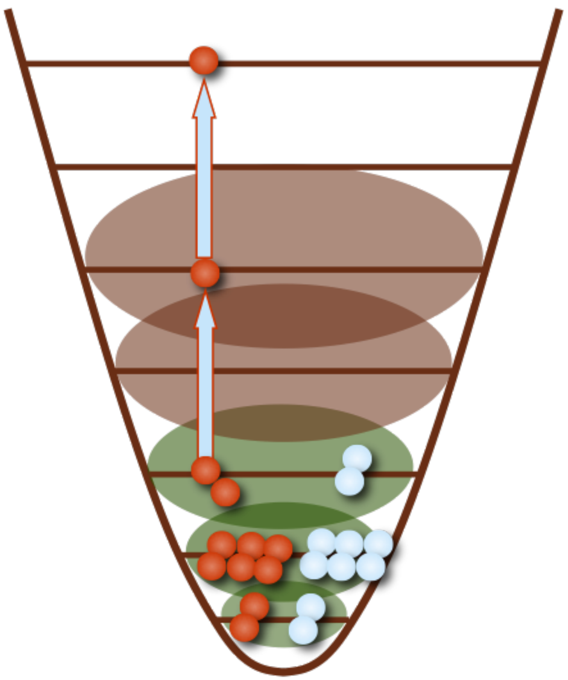
- Symmetry-Adapted No-Core Shell Model (SA-NCSM)
- SU(3)-coupled basis & model space truncation scheme
- Efficacy of SA-NCSM
- Emergence of symplectic Sp(3,R) symmetry
- Summary & outlook

Ab Initio No-Core Shell Model

- provides lowest eigenstates & energies of light nuclei (A≤16)

$$H|\psi\rangle = E|\psi\rangle$$

- solves matrix eigenvalue problem with nuclear Hamiltonian
- all nucleons active
- No restriction on interactions (NN, NNN, non-local, ...)



Standard basis of NCSM

Slater determinants: $\phi_i(\vec{r}_1, \ldots, \vec{r}_A) = \frac{1}{\sqrt{A}} \begin{vmatrix} \varphi_\alpha(\vec{r}_1) & \varphi_\alpha(\vec{r}_2) & \ldots & \varphi_\alpha(\vec{r}_A) \\ \varphi_\beta(\vec{r}_1) & \varphi_\beta(\vec{r}_2) & \ldots & \varphi_\beta(\vec{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_\gamma(\vec{r}_1) & \varphi_\gamma(\vec{r}_2) & \ldots & \varphi_\gamma(\vec{r}_A) \end{vmatrix}$

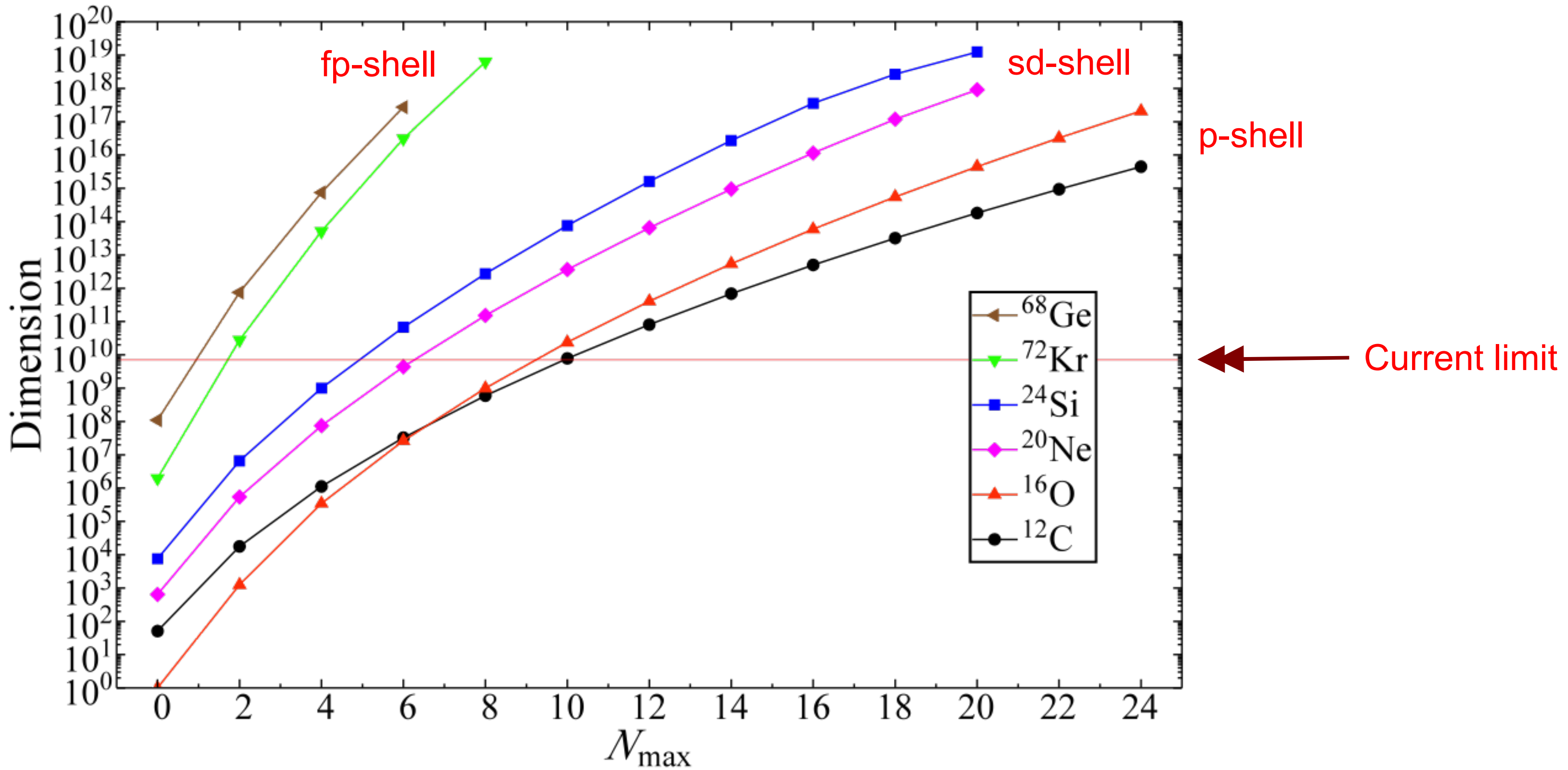
single particle states of harmonic oscilator

- Model space defined by Nmax

The Good

- Fast computation of matrix elements
- Hamiltonian matrix is sparse
- Exact separation between intrinsic and center-of-mass motion

Scale explosion



- higher configurations needed
  - improve convergence of the spectrum
  - reproduce experimental observables
  - describe collective and cluster states

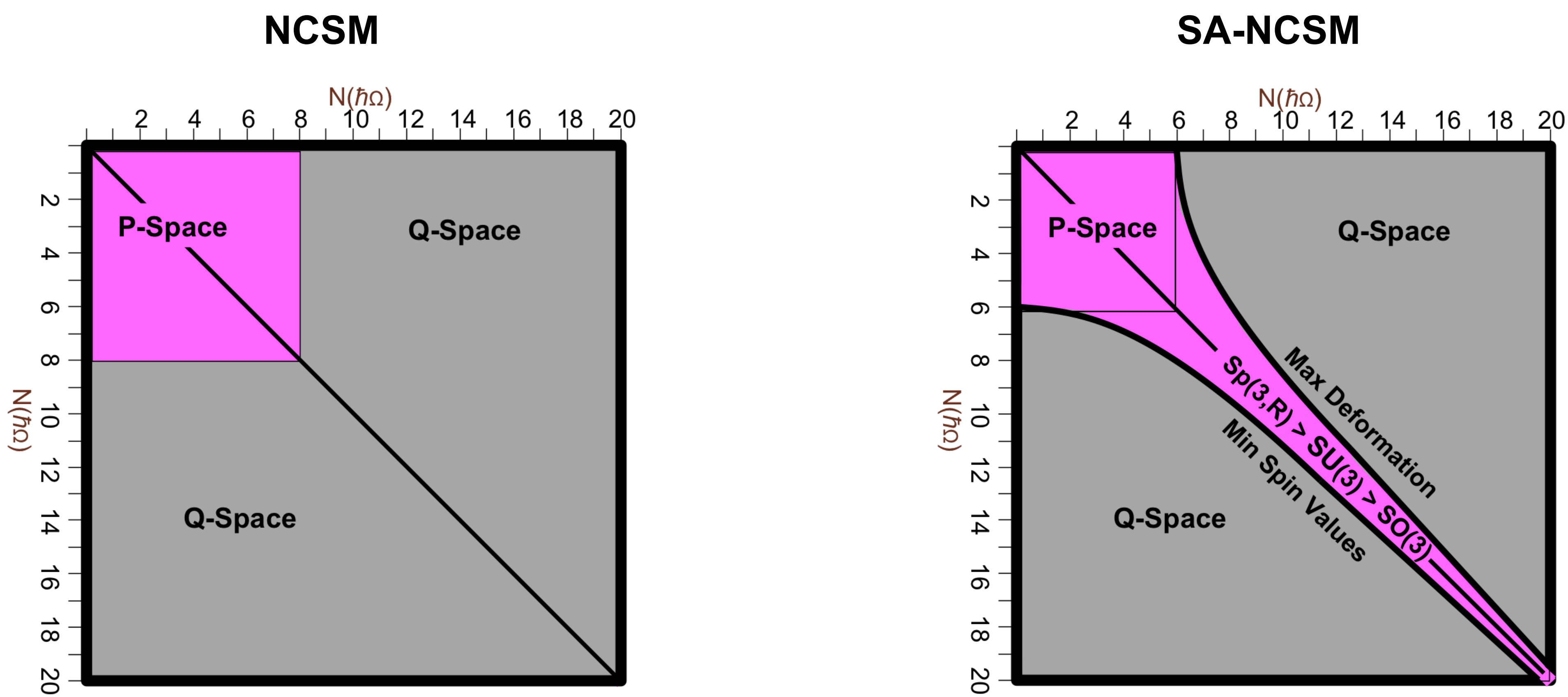
- NCSM extensions
  - NCSM with core
  - Monte-Carlo NCSM
  - Importance Truncated NCSM
  - **Symmetry-adapted NCSM**

Symmetry-Adapted Approach

Key Features

- Use basis "designed" for desription of nuclear collective dynamics and nuclear deformation

- restrict model space to physically most relevant configurations



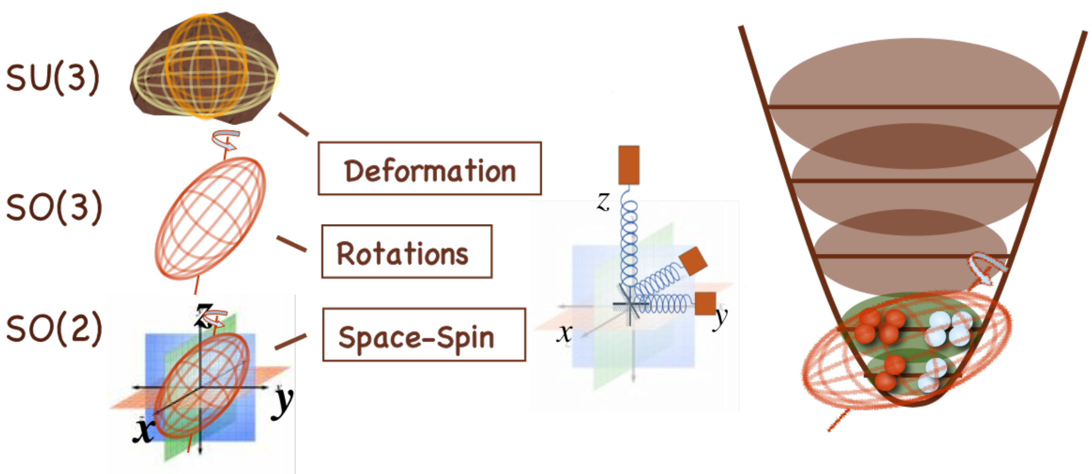
- preserve exact factorization of center-of-mass degrees of freedom

Symmetries of Nuclear Collective Motion

Microscopic models of nuclear collective motion

$\mathrm{SU}(3)$

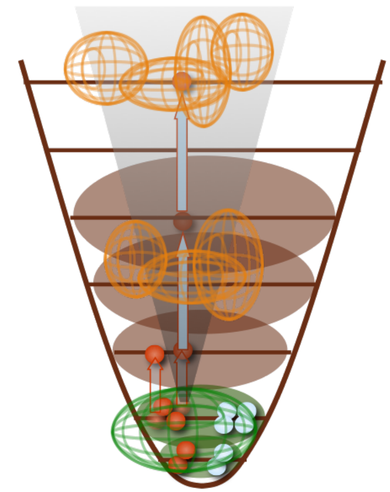
Elliott's model (1958)



- nuclear deformations and rotations in a valence shell

$\mathrm{Sp}(3,\mathrm{R}) \supset \mathrm{SU}(3)$

Symplectic model (1976)

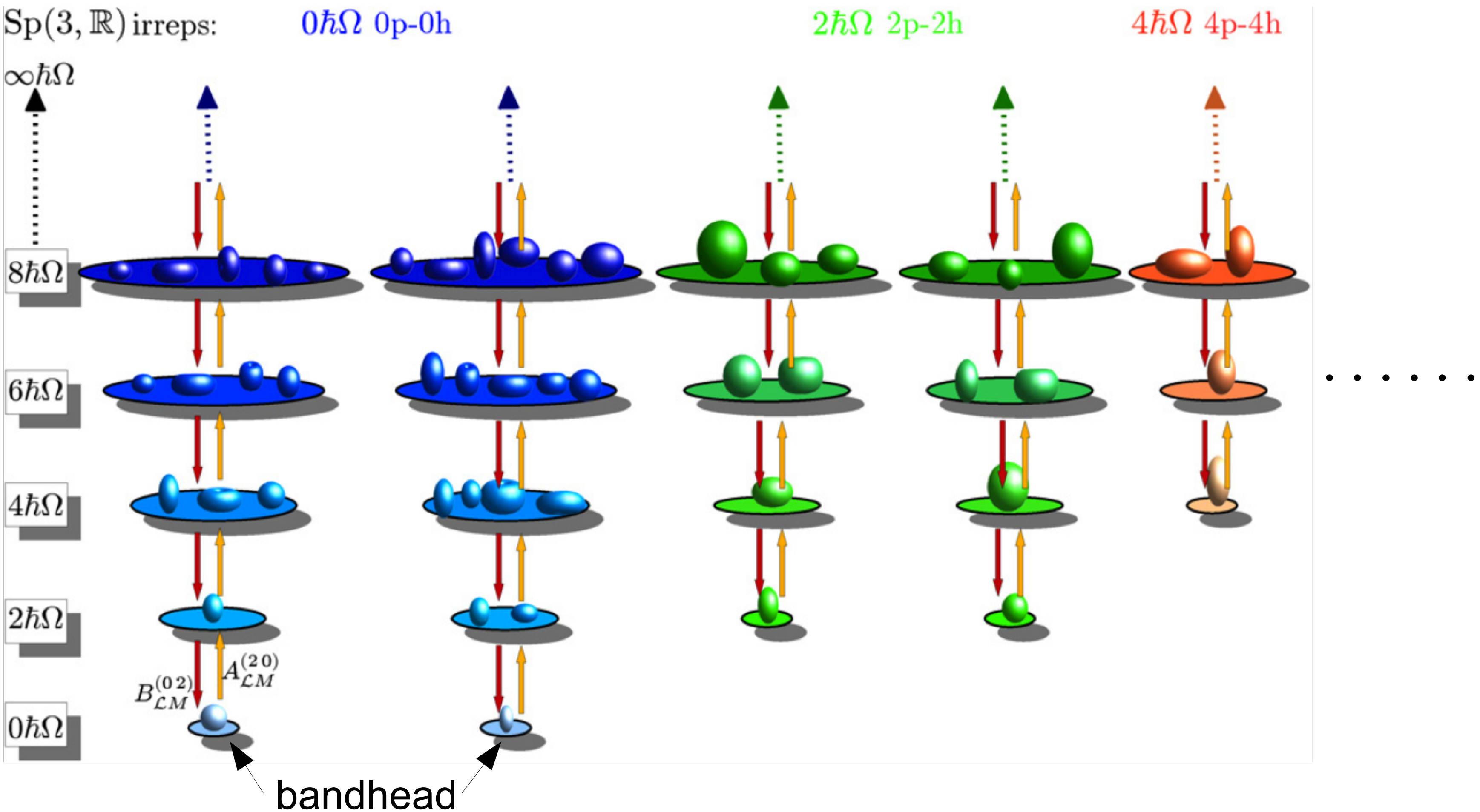


- Multi-shell extension of Elliott's model
- Microscopic realization of Bohr-Mottelson model

Kinetic energy
Harmonic oscillator potential
Orbital angular momentum
Monopole & Quadrupole momentum

- Both models provide complete basis of nuclear Hilbert space

Model Space in Symplectic Basis



- Proof-of-principle: small number of symplectic slices realize ~90% of 12C and 16O low-lying wave functions

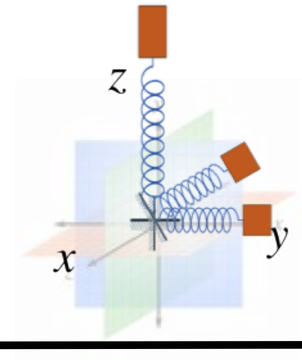
Showstopper:

- 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

SU(3)-coupled Basis

- Quantum labels

number of HO excitations



N

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total proton, total neutron and total intrinsic spins $S_p \, S_n S$

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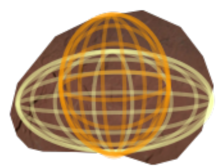
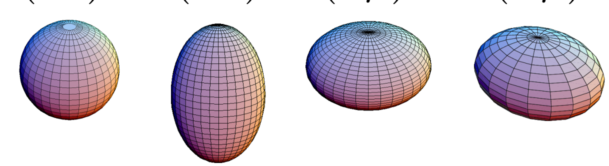
deformation SU(3)



$(\lambda \, \mu)$

$(0 \, 0)$ $(\lambda \, 0)$ $(0 \, \mu)$ $(\lambda \, \mu)$



rotation SO(3)

L

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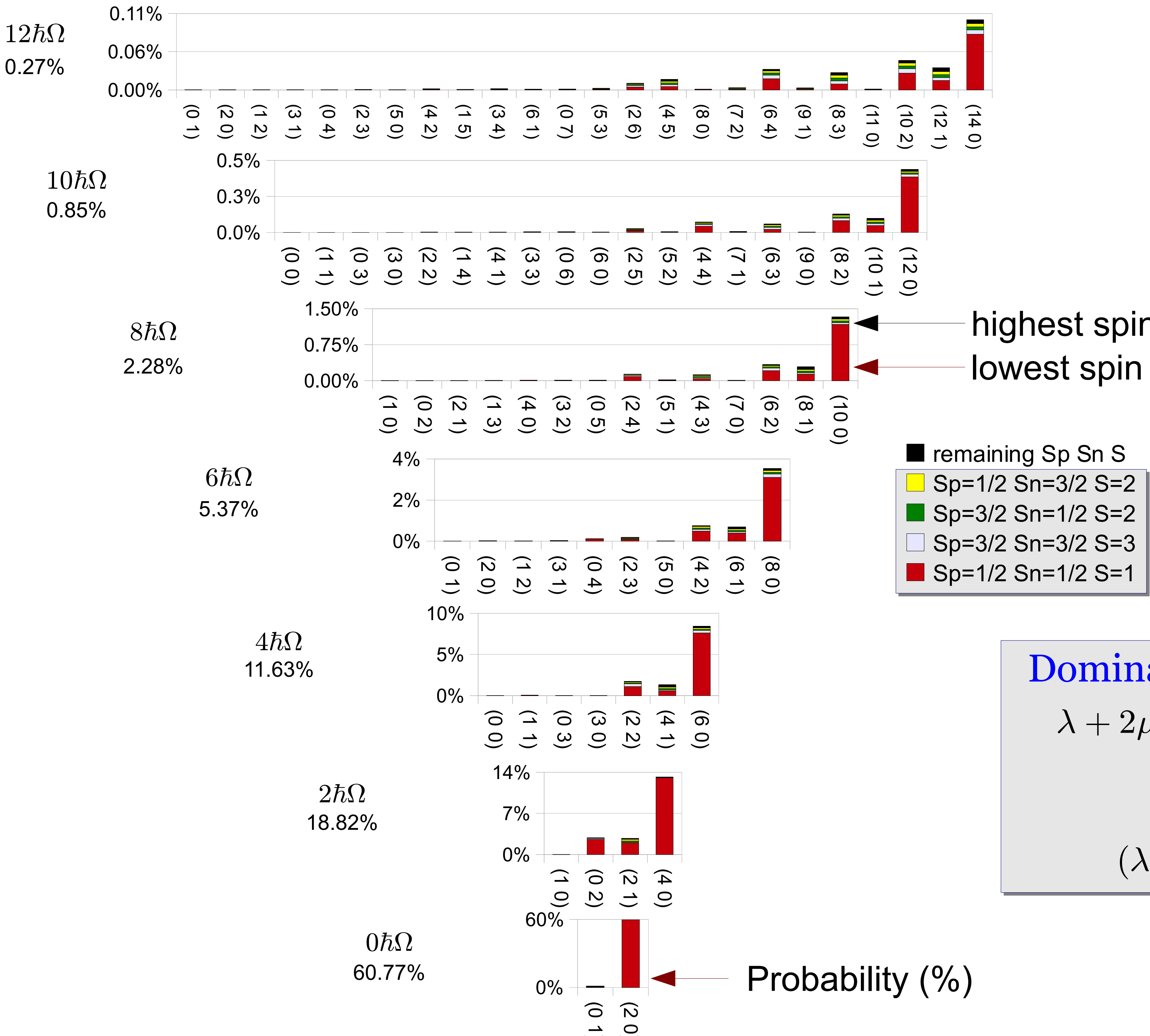
total angular momentum J

- Realistic interactions: mixes all quantum numbers [with the exception of J]

Emergence of Simple Patterns



~99% of ground state

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

$N_{\max} = 12$

JISP16 + Vcoul

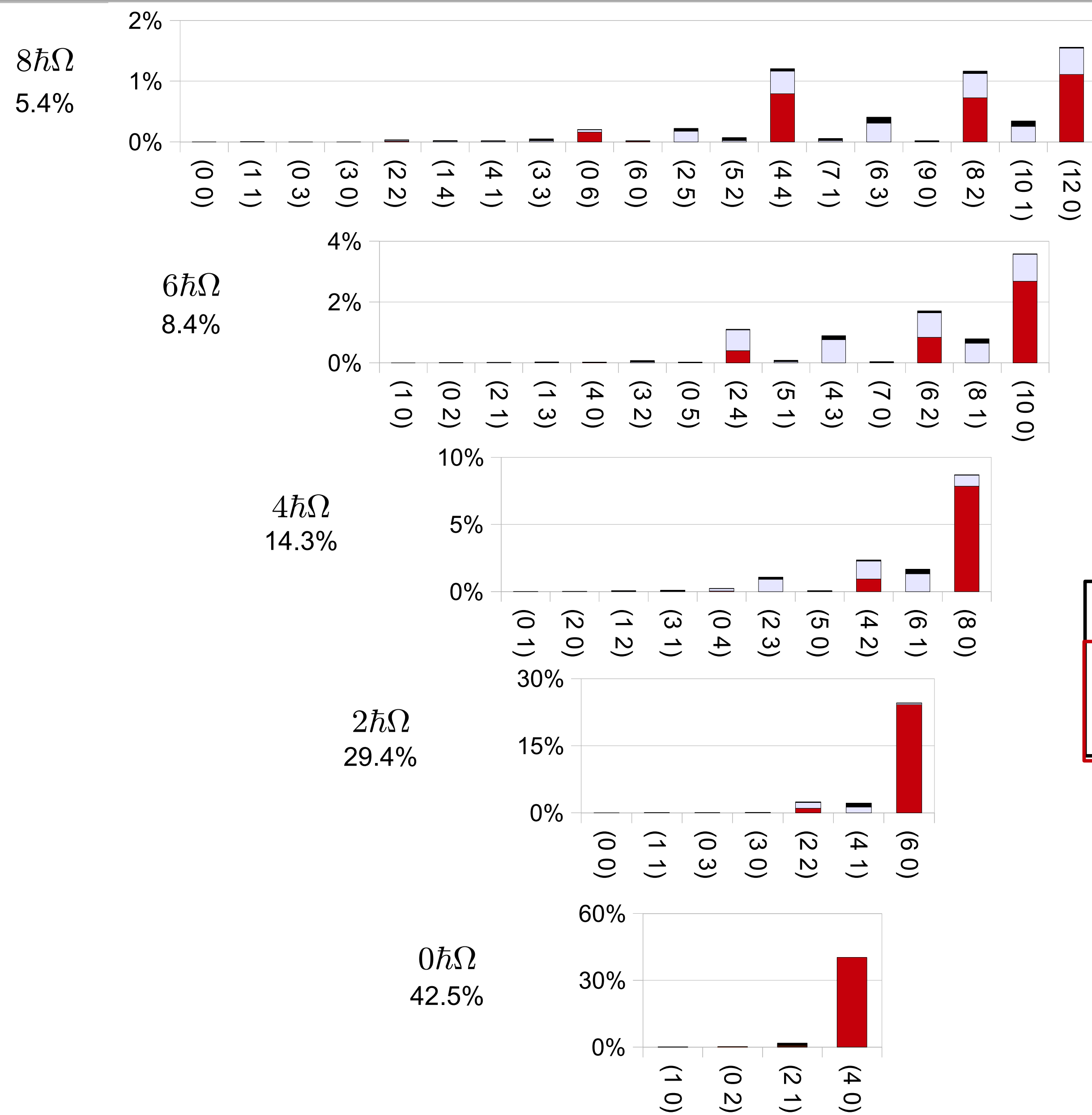
$\hbar\Omega = 20$ MeV

Dominant deformations

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

$$(\lambda_0\, \mu_0) = (2\, 0)$$

Emergence of Simple Patterns



even-even nucleus

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

$N_{\max} = 8$

different interaction

N3LO + Vcoul

$\hbar\Omega = 25\ \mathrm{MeV}$

identical features ...

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

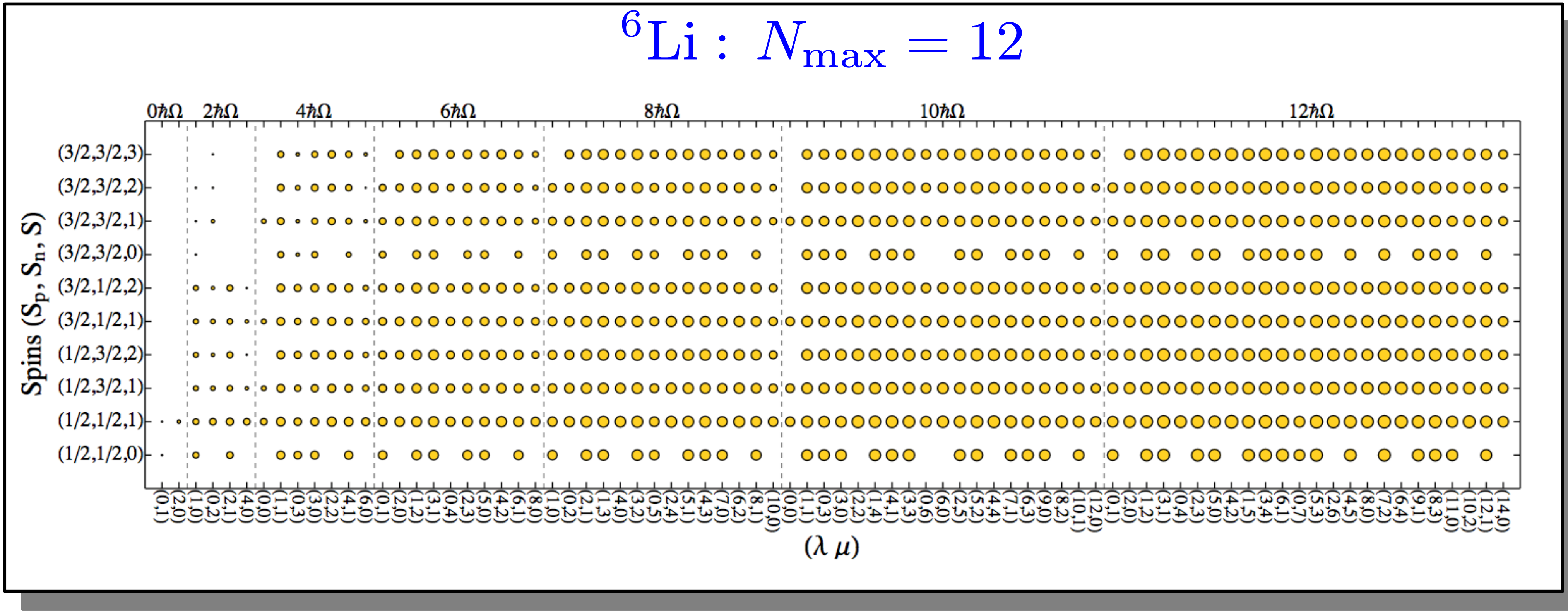
~98% of the ground state

Dominant deformations

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

$$(\lambda_0\,\mu_0) = (4\,0)$$

Nuclear Hilbert Space in SU(3)-coupled Basis



- c.m. spurious states can be removed from each subspace of equivalent configurations exactly

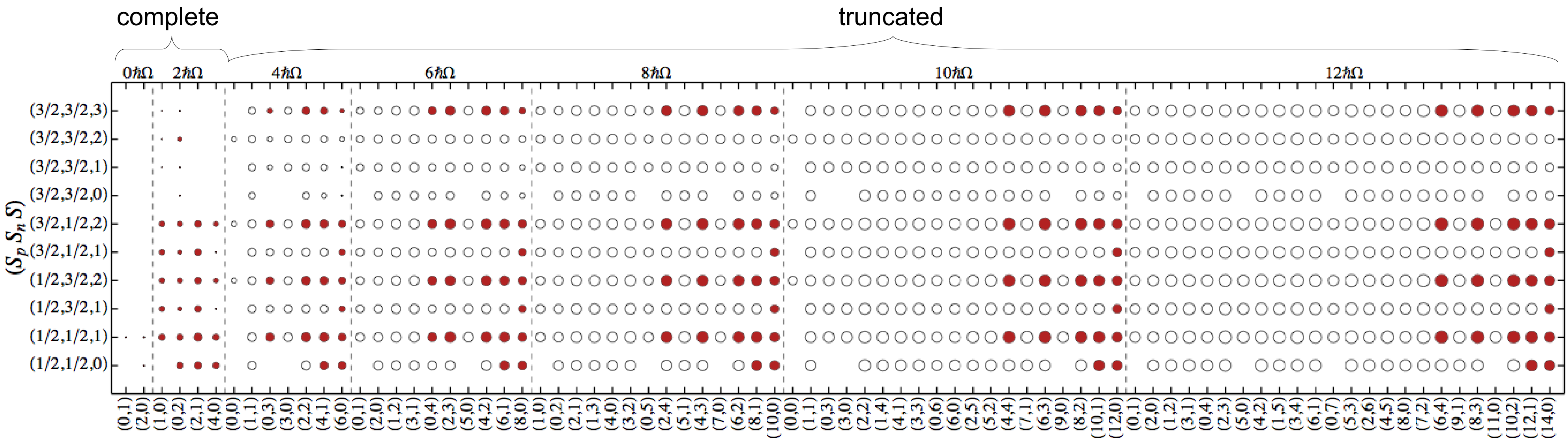
- SU(3)-coupled basis enables truncations according to:

  (1) maximal number of total HO quanta Nmax
  (2) intrinsic spins
  (3) deformations

Symmetry-Guided Selection of Model Space

- SU(3) and spin symmetry-guided truncation
  - $\langle N'_{\max}\rangle 12$ complete space up to $N'_{\max}$ and truncated beyond up to $N_{\max} = 12$

- Example: $\langle 2\rangle 12$



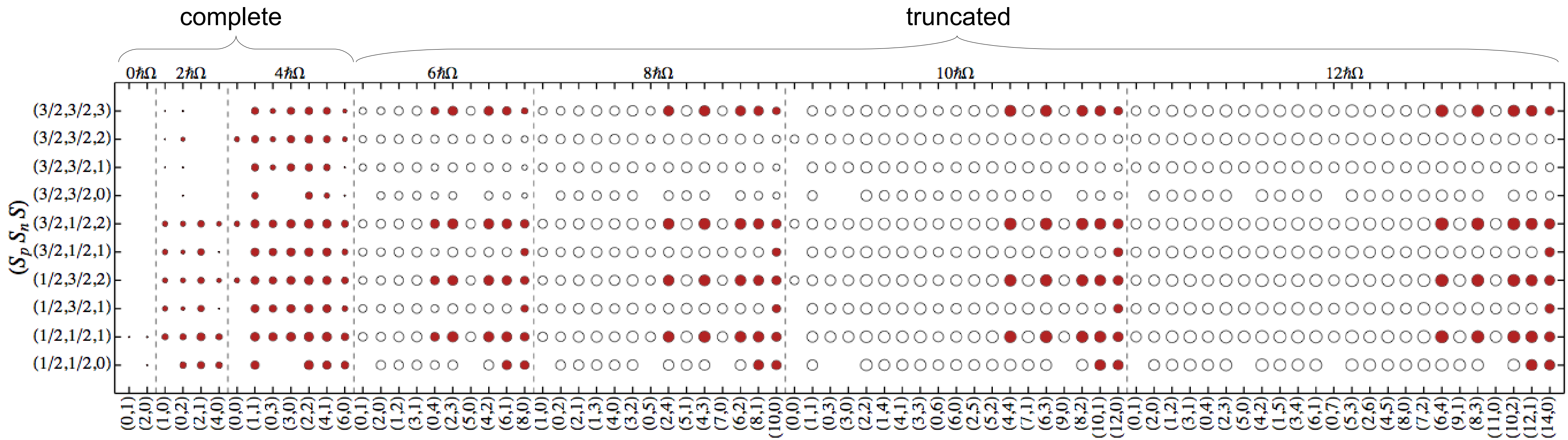
- Study convergence of SA-NCSM solutions for $\langle N'_{\max}\rangle \to 12$

Symmetry-Guided Selection of Model Space

SU(3) and spin symmetry-guided truncation

- $\langle N'_{\max} \rangle 12$ complete space up to $N'_{\max}$ and truncated beyond up to $N_{\max} = 12$

Example: $\langle 4 \rangle 12$

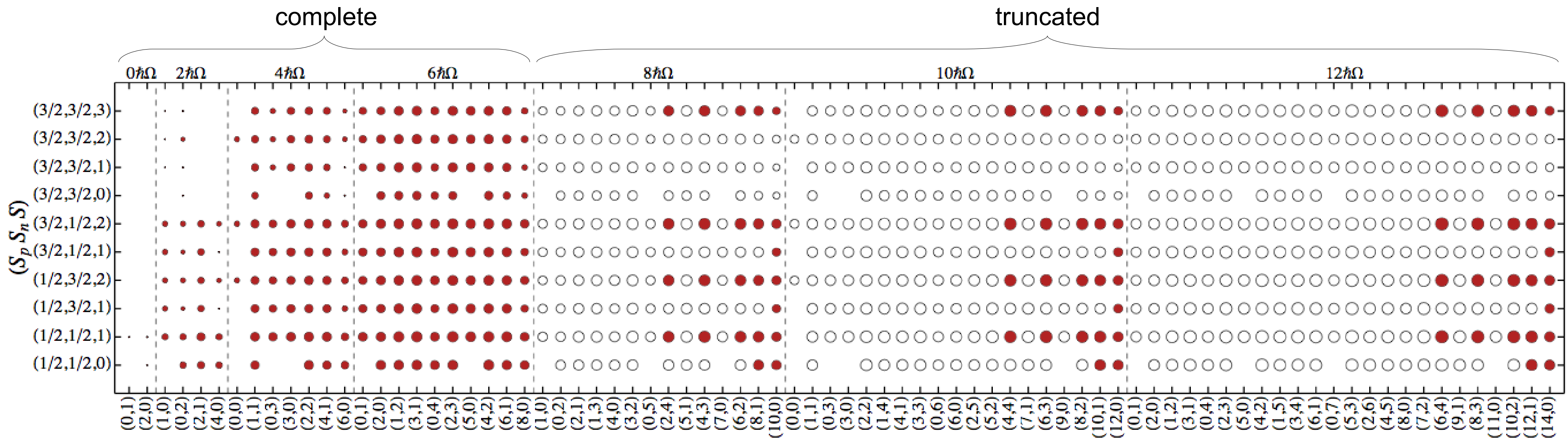


- Study convergence of SA-NCSM solutions for $\langle N'_{\max} \rangle \to 12$

Symmetry-Guided Selection of Model Space

- SU(3) and spin symmetry-guided truncation
  - $\langle N'_{\max} \rangle 12$ complete space up to $N'_{\max}$ and truncated beyond up to $N_{\max} = 12$

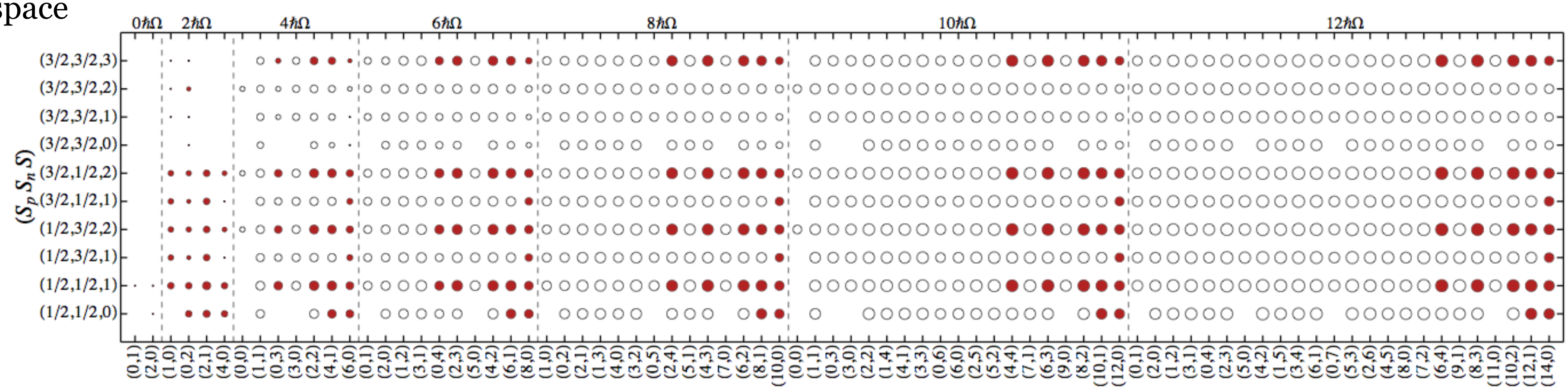
- Example: $\langle 6 \rangle 12$



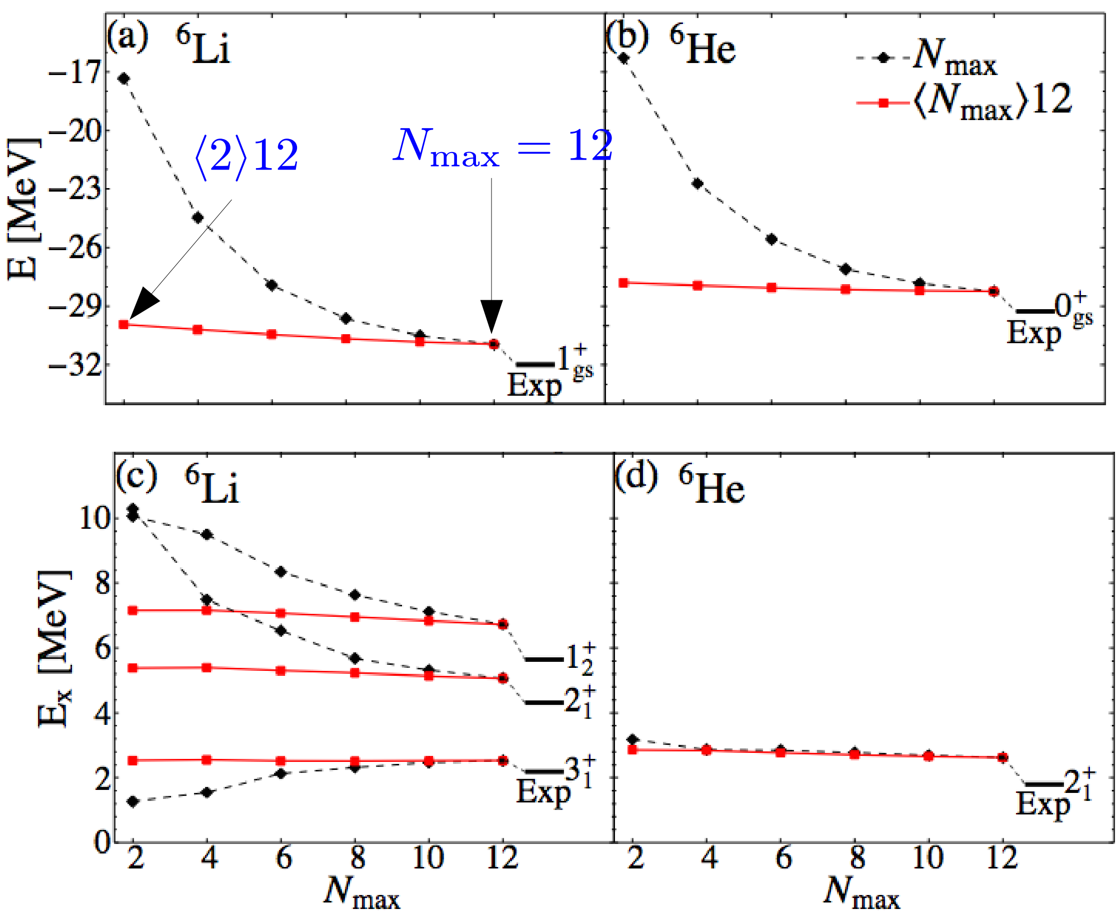
- Study convergence of SA-NCSM solutions for $\langle N'_{\max} \rangle \to 12$

Symmetry-Guided Selection of Model Space

- Model space
  $\langle 2 \rangle 12$



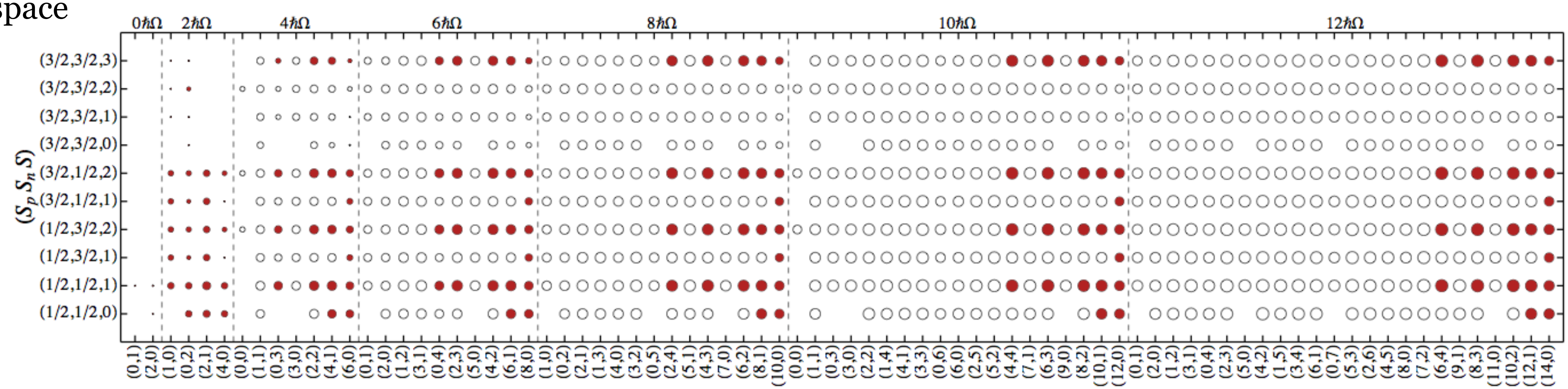
- Interaction: JISP16+Vcoul



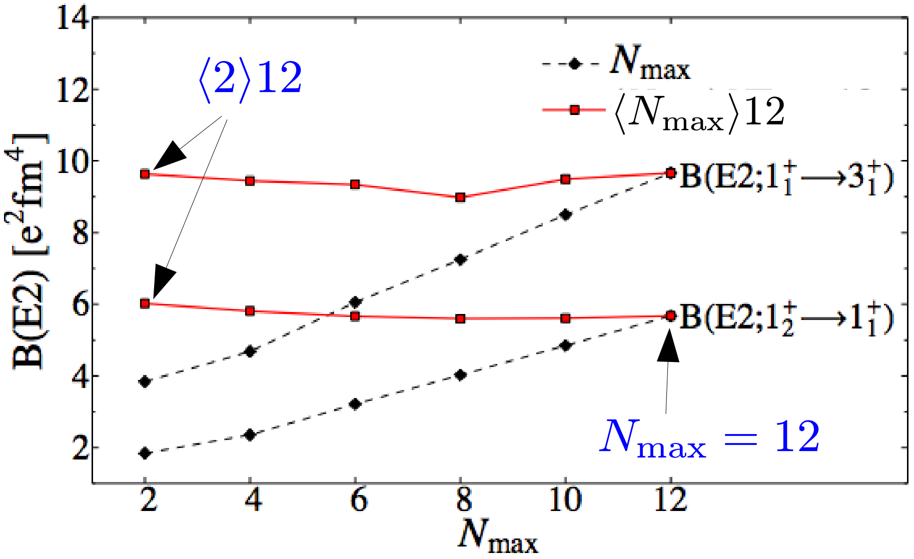
- Selected SU(3) & spins crutial for binding and excitation energies

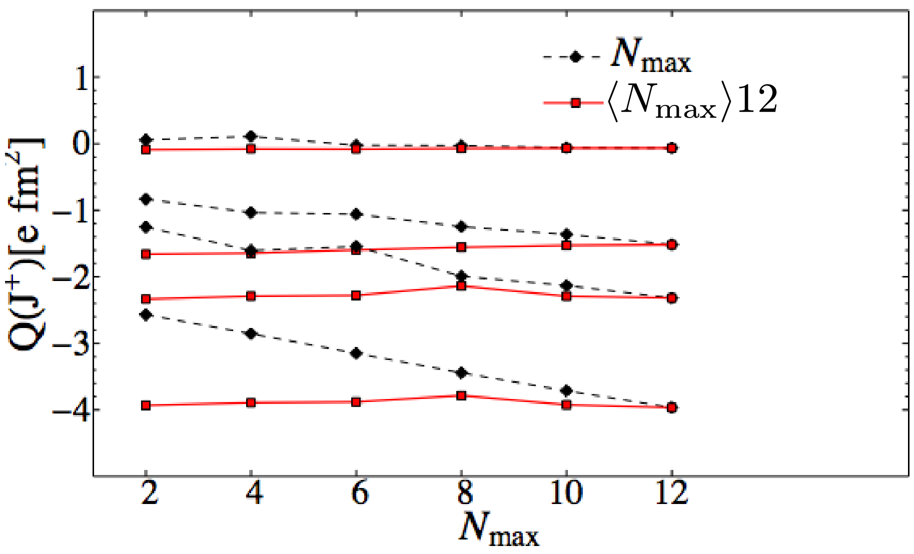
Symmetry-Guided Selection of Model Space

- Model space
  $\langle 2 \rangle 12$



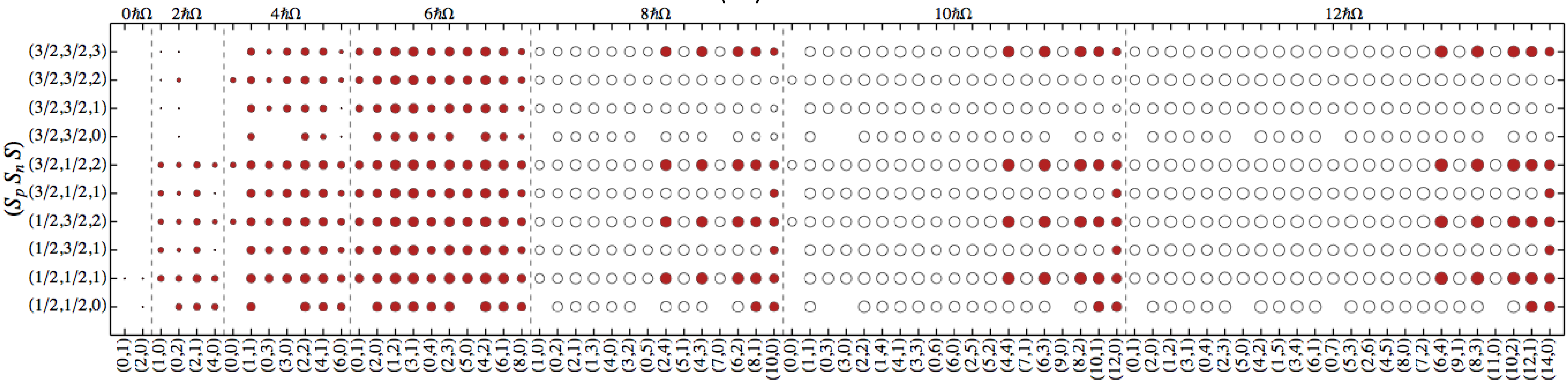
- Selected SU(3) & spins crutial for E2 transitions and quadrupole moments

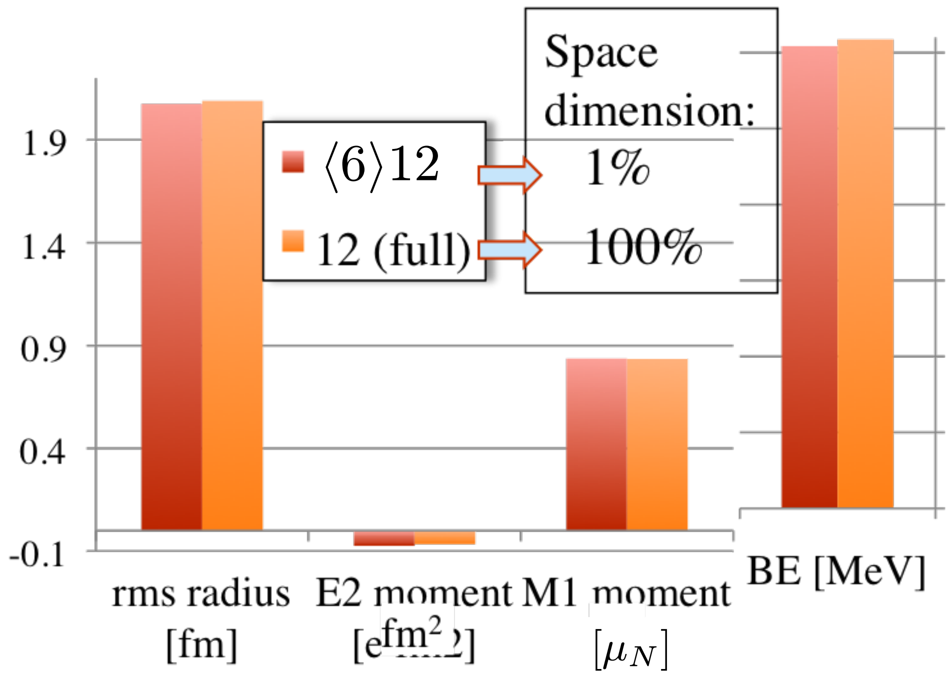




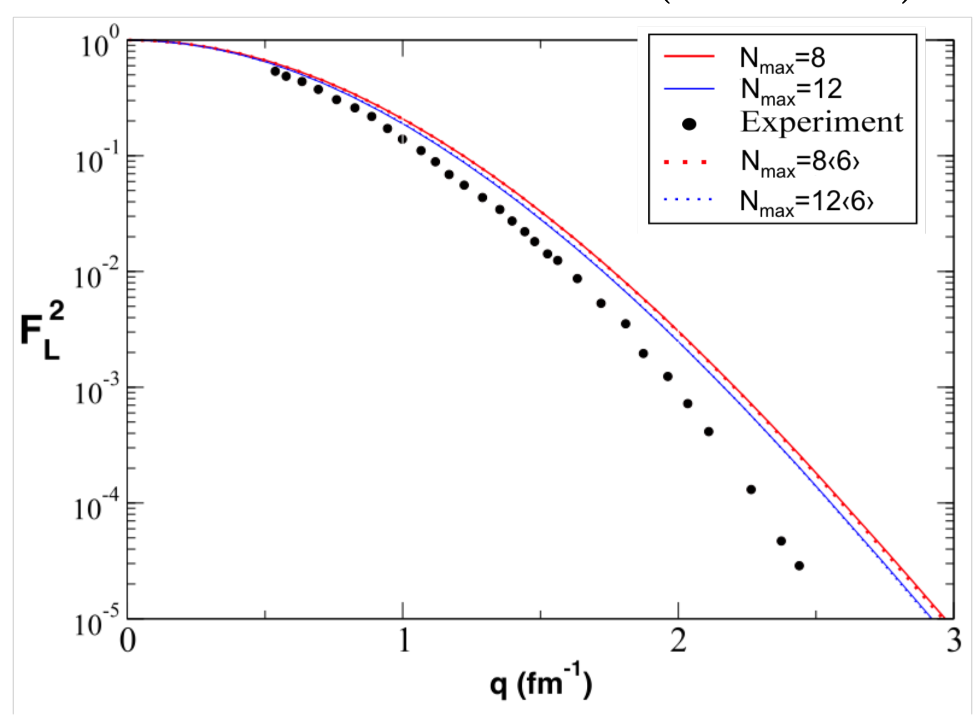
Symmetry-Guided Selection of Model Space

$\langle 6 \rangle 12$





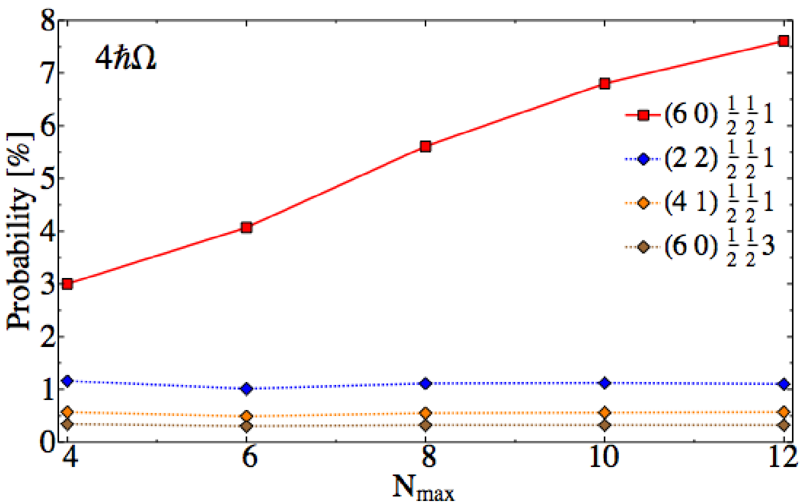
Electron scattering ^{6}Li $(1^+ \to 1^+)$

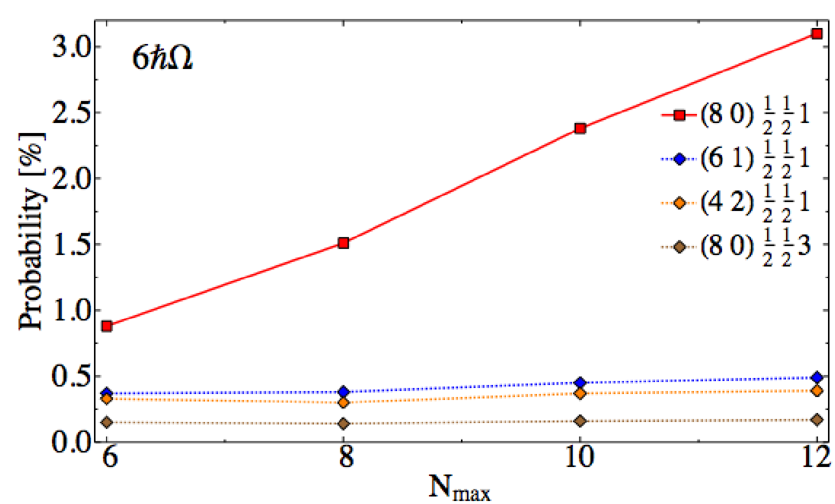


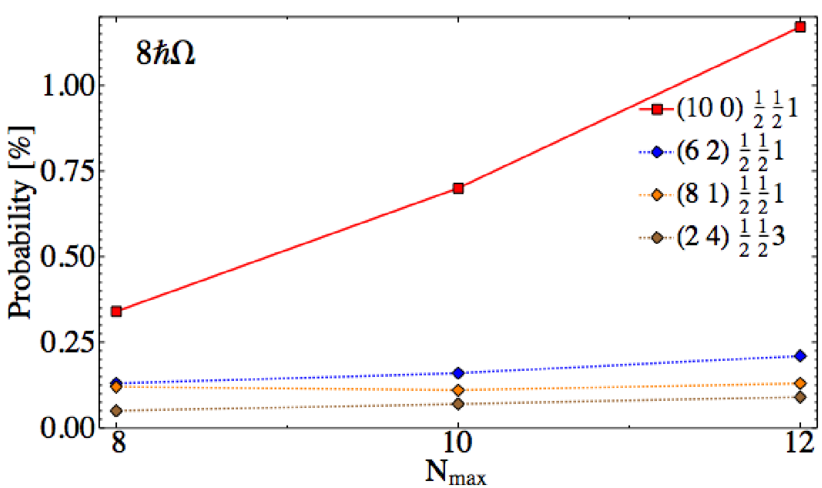
Increasing Nmax - Enhancing Deformation

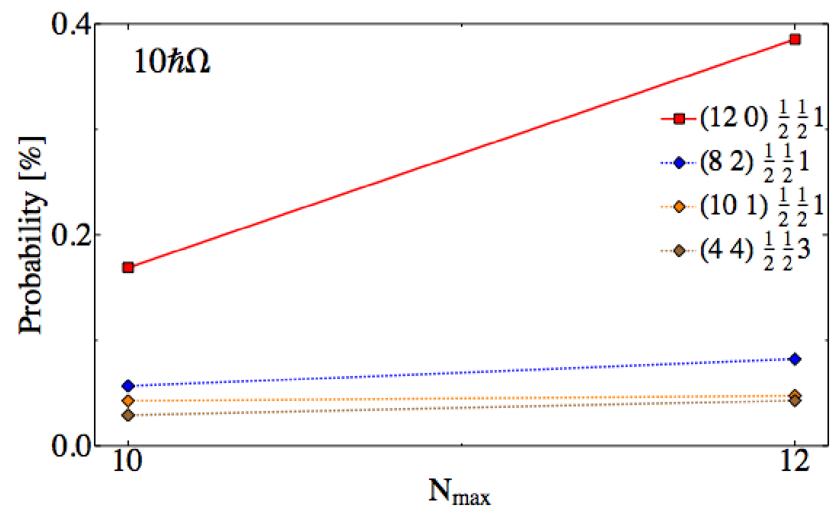
Effects of higher $N_{\max}$

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

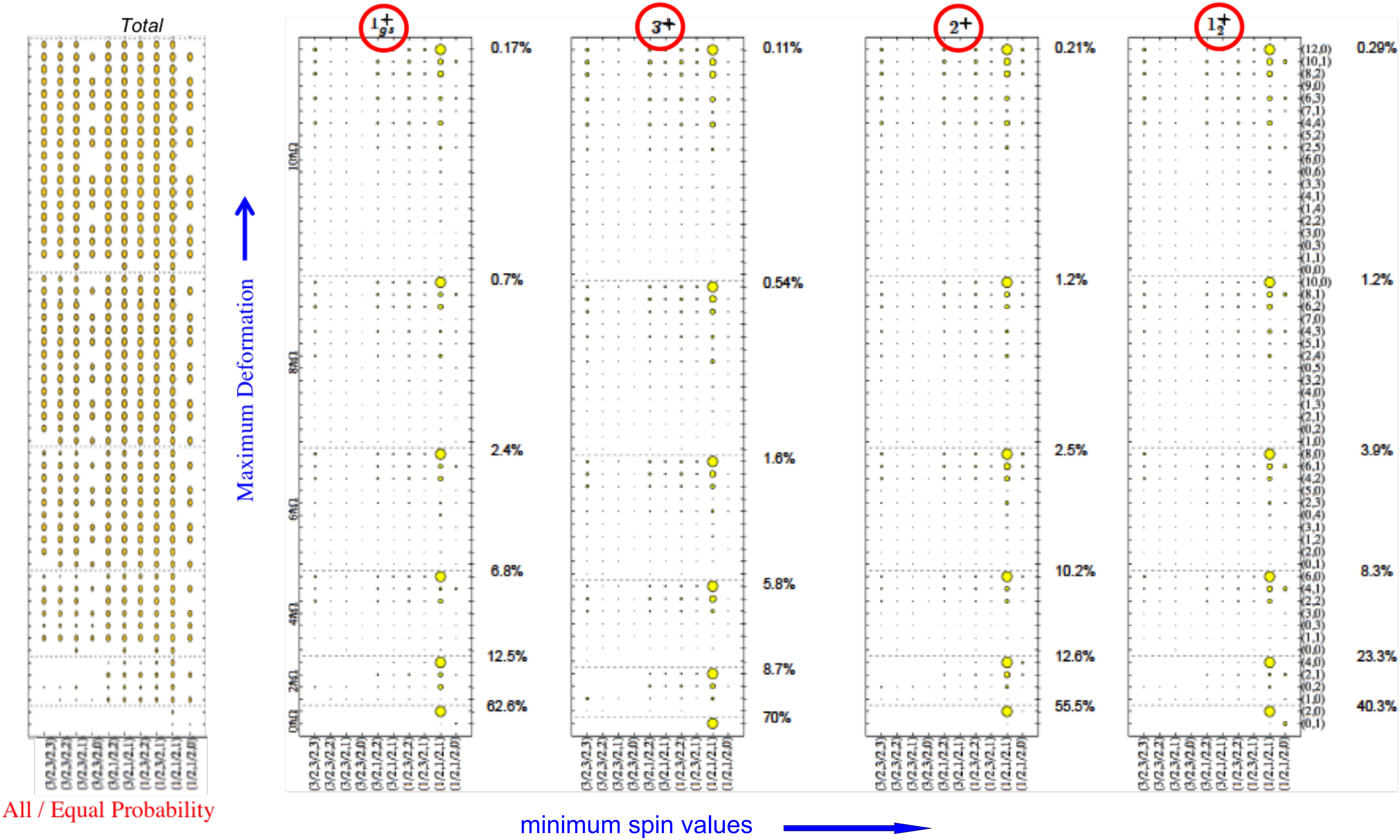




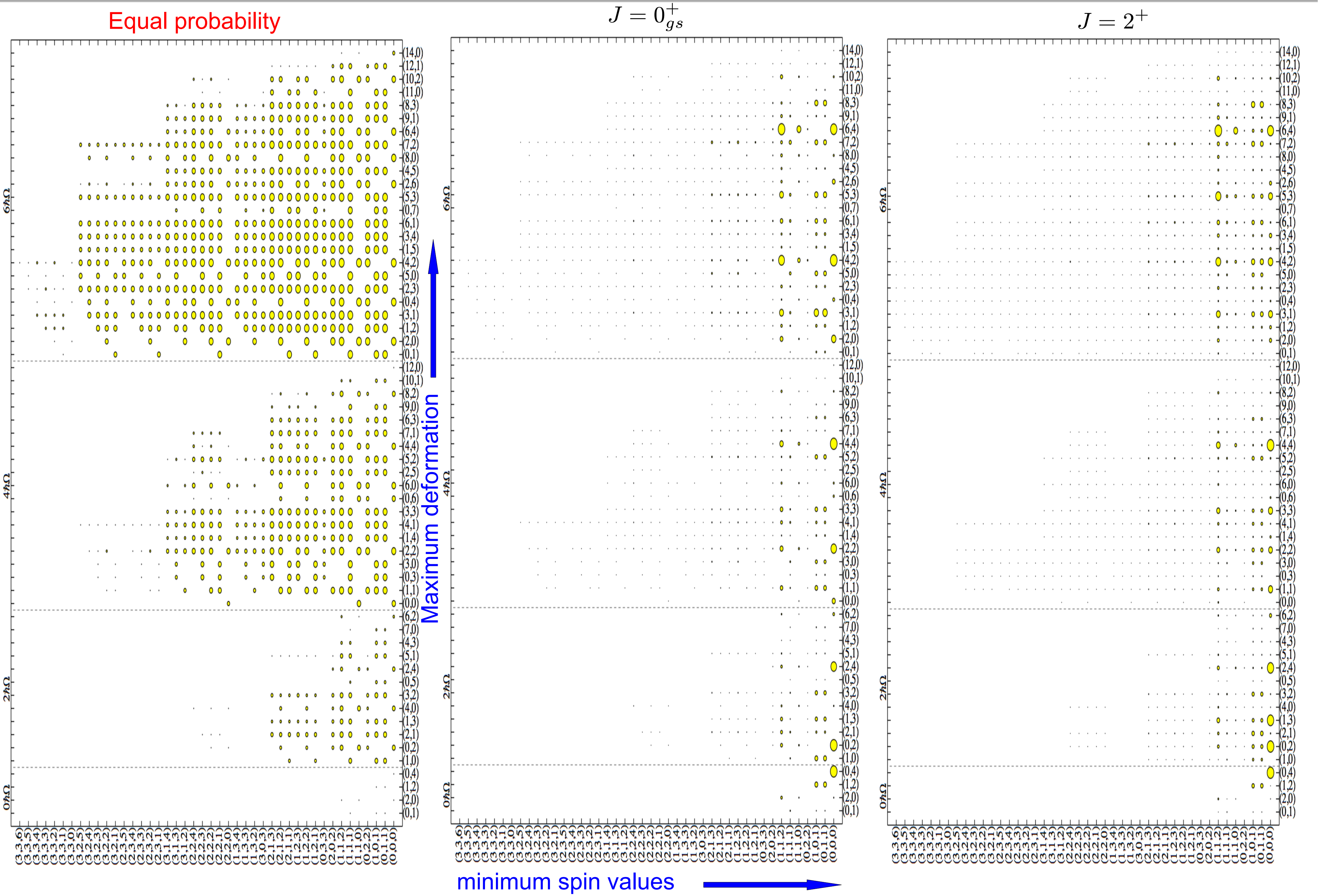




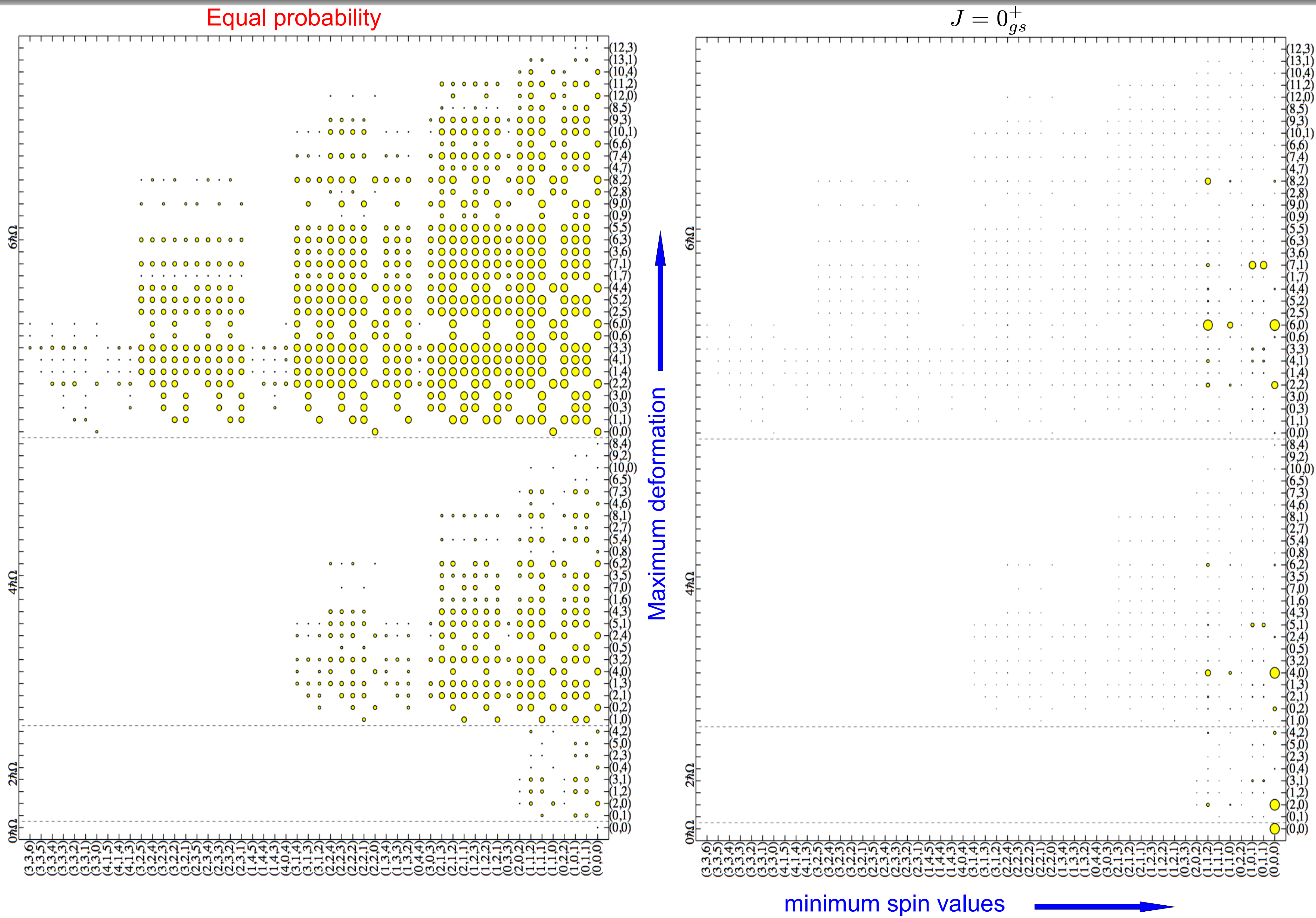
^{6}Li - coherent structure of T=0 states



^{12}C : model space decomposition

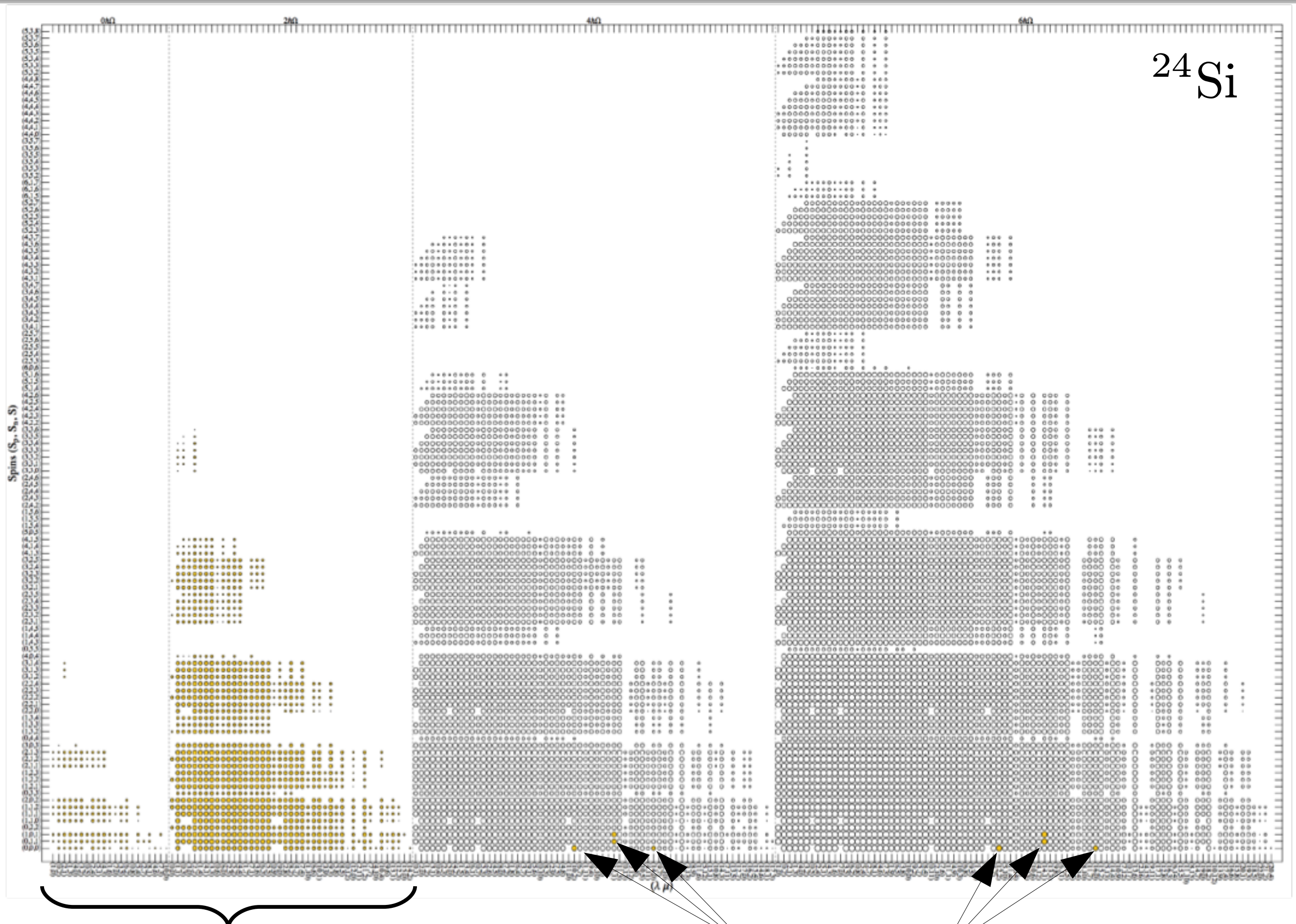


^{16}O



Equal probability
$J = 0^+_{gs}$
Maximum deformation
minimum spin values

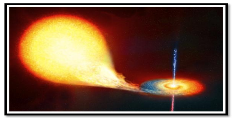
SA-NCSM: reaching towards medium mass nuclei



complete selected

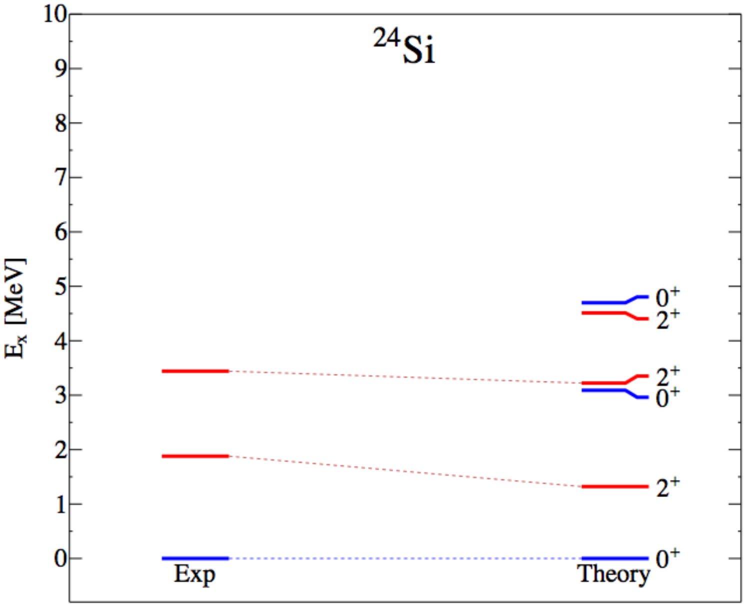
dimension: 3×10^6

Complete space dimension: 7×10^{10}



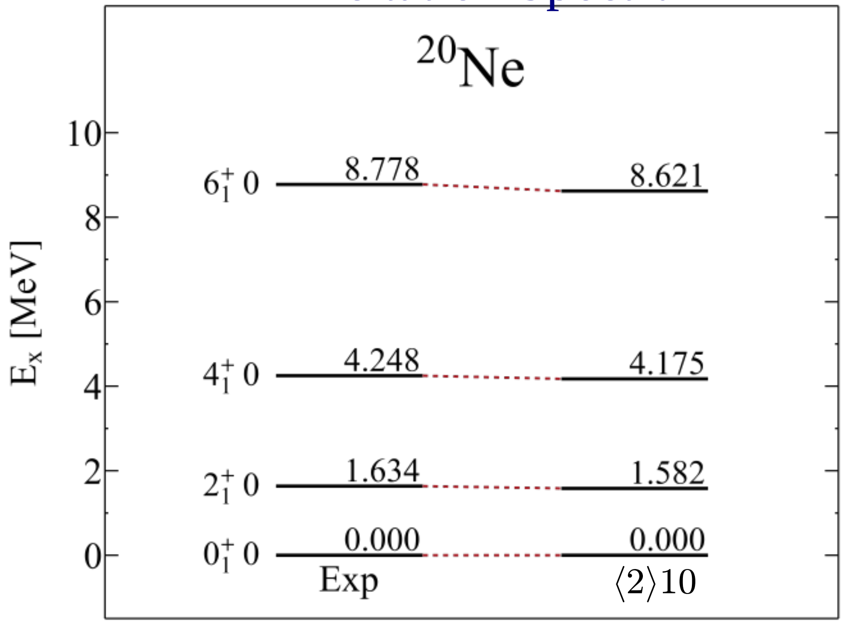
Novae and X-ray bursts

$^{23}\mathrm{Al}(p,\gamma)^{24}\mathrm{Si}$

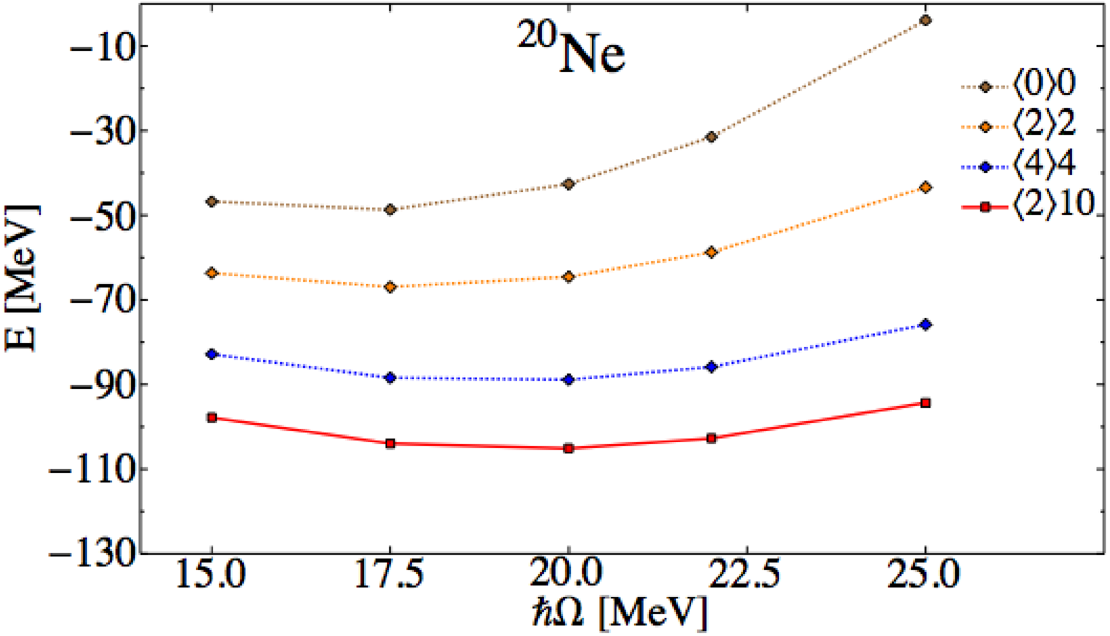


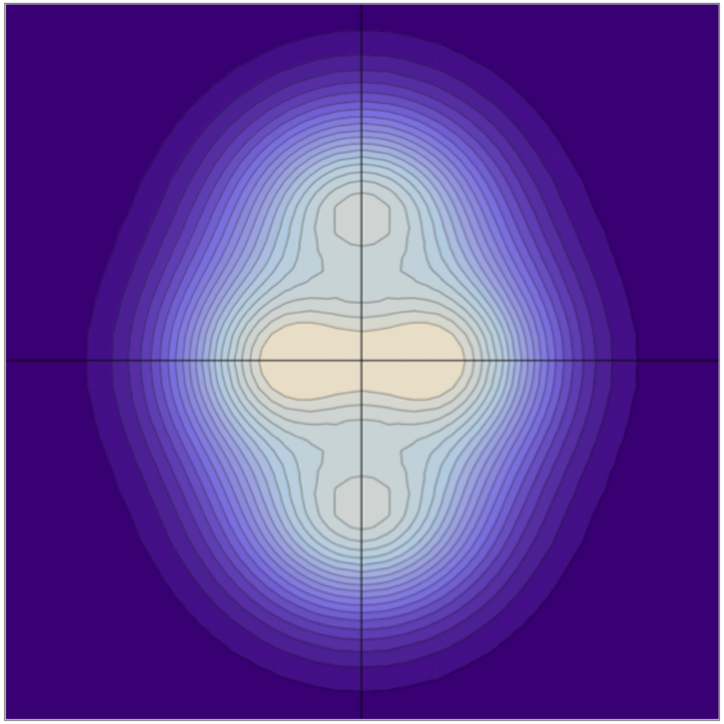
SA-NCSM: reaching towards medium mass nuclei

Excitation Spectrum



Binding energy





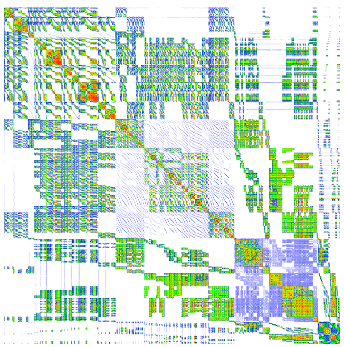
Matter density of leading SU(3) state

Complete space: 4×10^{12}

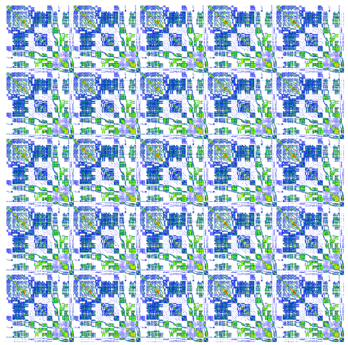
Symmetry-adapted space: 1×10^{7}

MPI/OpenMP Implementation of SA-NCSM

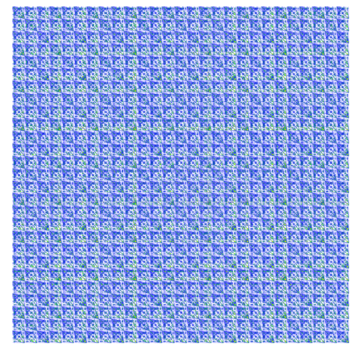
- **Computational effort**
  - 95% - computing matrix elements → Embarassingly parallel problem
  - 3% - solving eigenvalue problem
- **Load balanced computations**



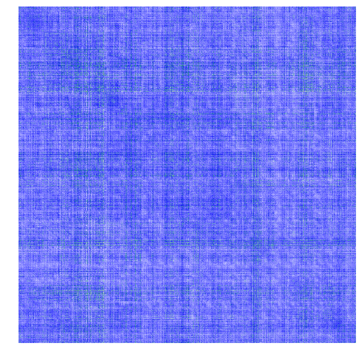
1 process



15 processes

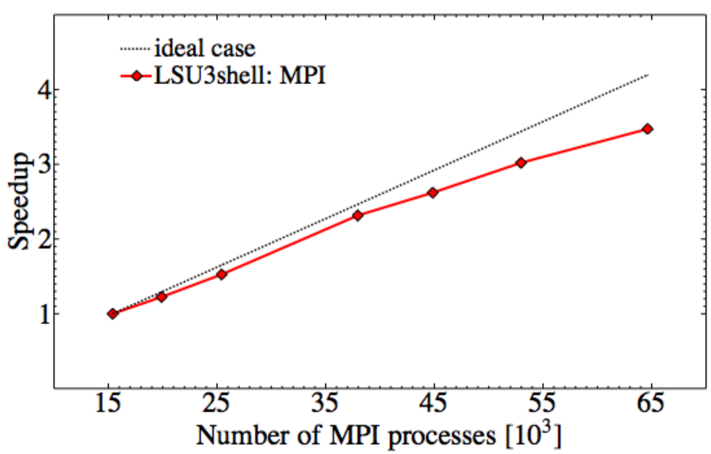


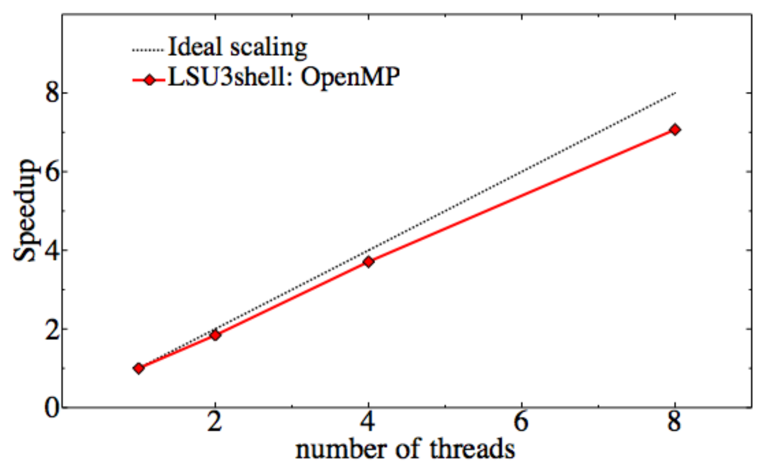
378 processes



37,950 processes

- **Good scalability**





- **Publicly available:** https://sourceforge.net/p/lsu3shell/home/Home/

Construction of Sp(3,R) States in SA-NCSM

- Diagonalize Sp(3,R) Casimir operator

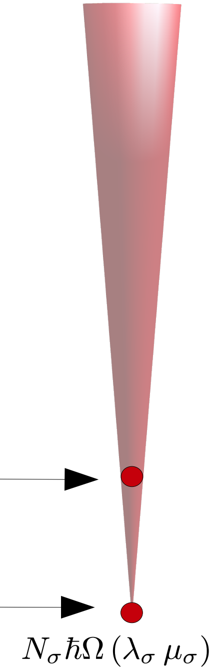
Sp(3,R) generators

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

HO laddering operators

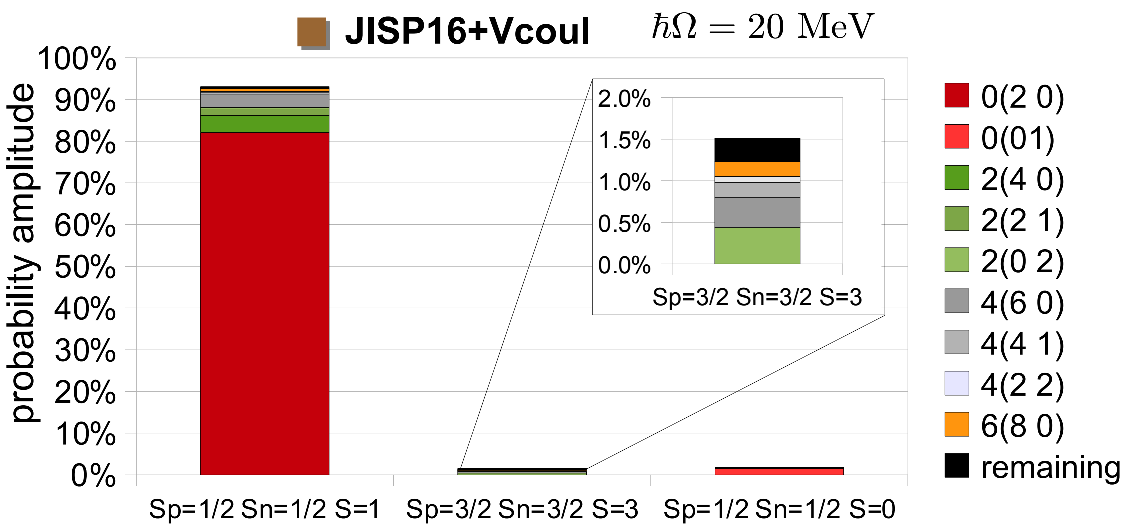
- $\hat{T}^{(0\,0)}$
  - Block diagonal in SU(3)-basis $N\hbar\Omega\,(\lambda\,\mu)$
  - Eigenvalues are analytical function of Sp(3,R) quantum labels
  - Eigenvectors are Sp(3,R) basis states

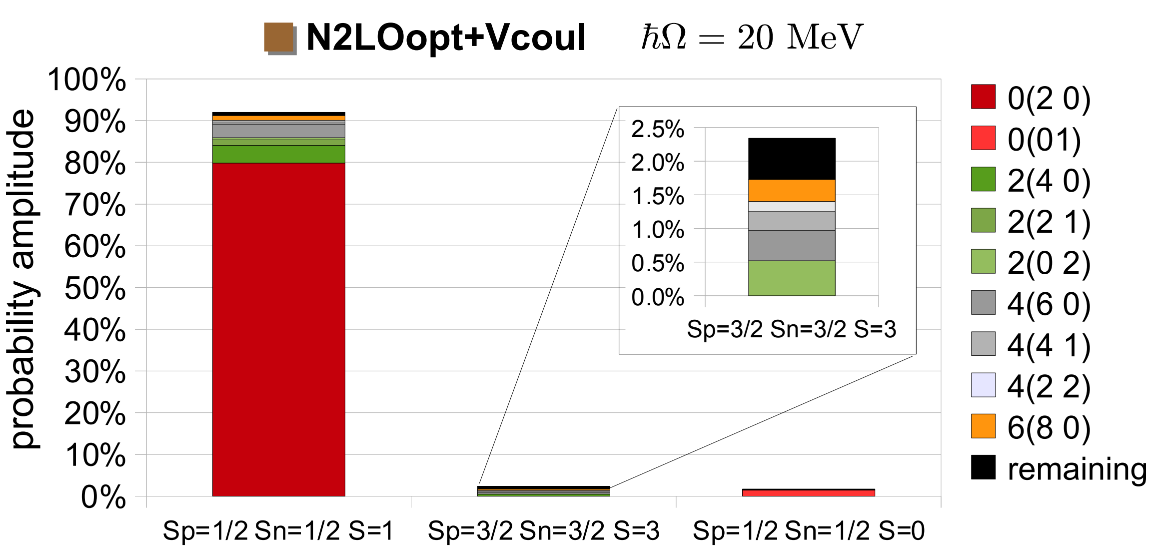
$$\hat{T}^{(0\,0)}|v\rangle = \lambda|v\rangle \begin{cases} \lambda < 0 & \text{Symplectic basis state} \\ \lambda = 0 & \text{bandhead} \\ \lambda > 0 & \text{excited center-of-mass} \end{cases}$$

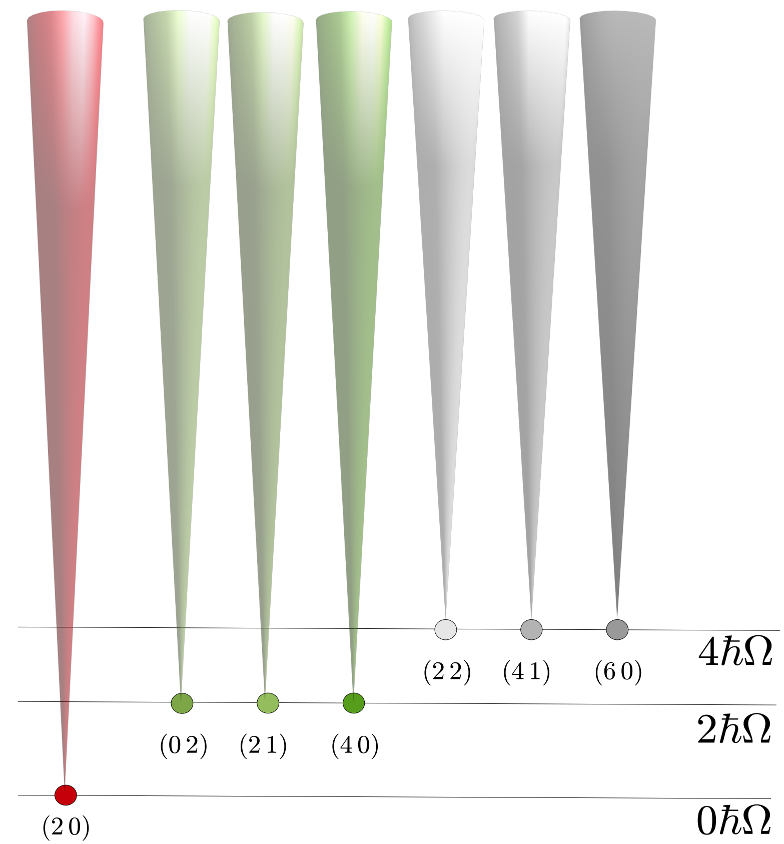


Dominance of Symplectic Basis States

- Contribution of dominant symplectic slices to the ground state of 6Li

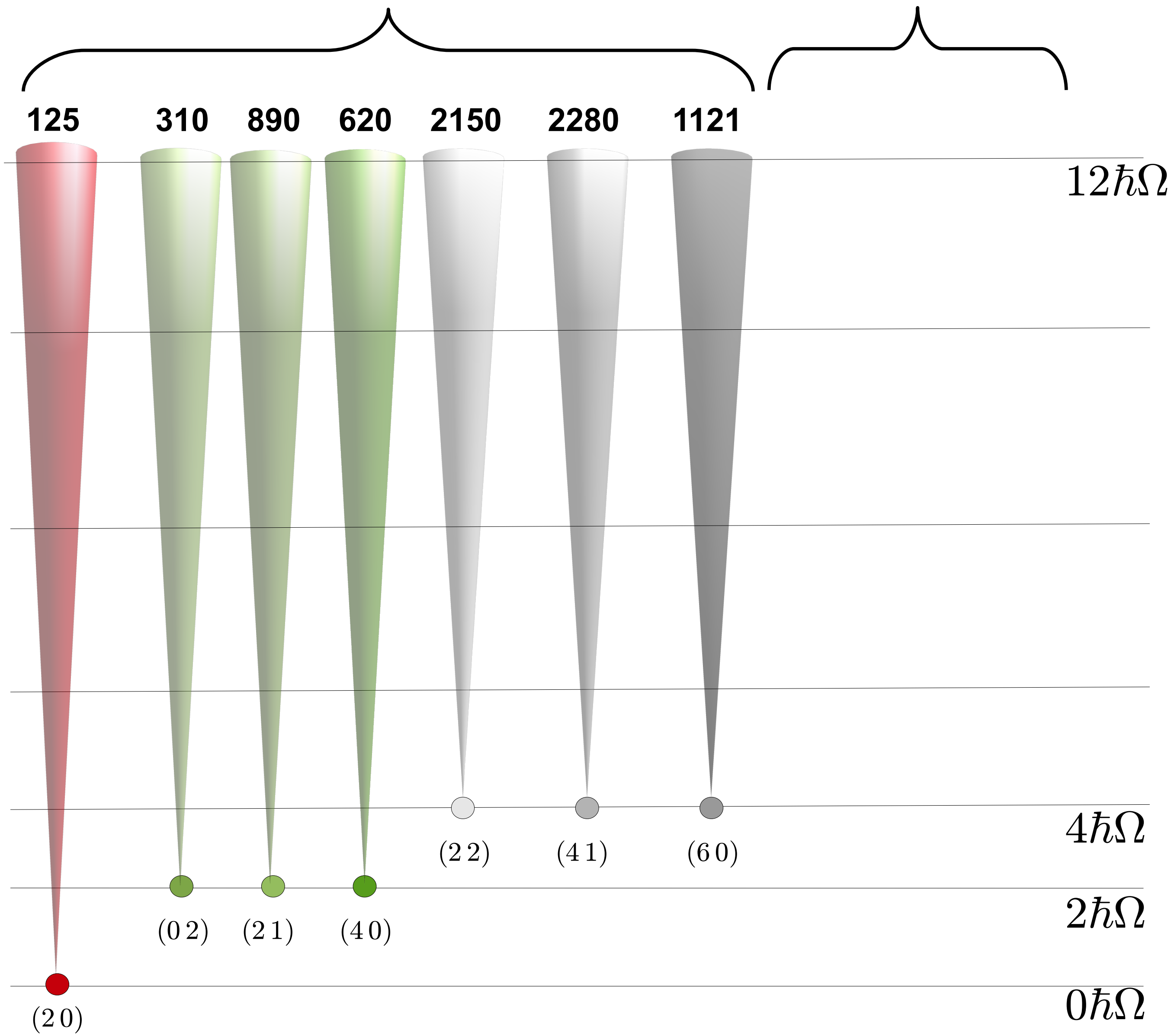






Symplectic Model Space: Sp=1/2 Sn=1/2 S=1

Projection:	92%	1%
Dimension [J=1 states]:	7,496	890,000



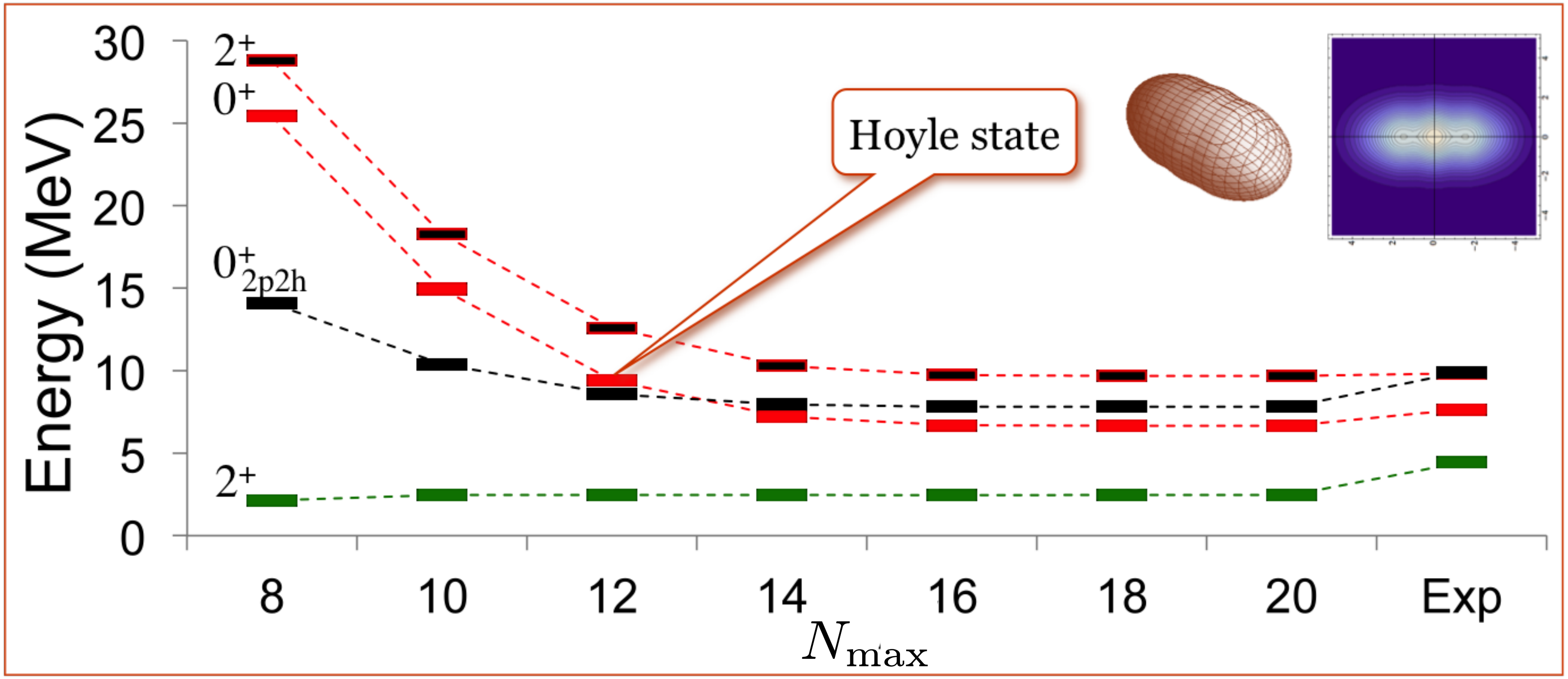
Collective & Cluster Modes in Symplectic Basis

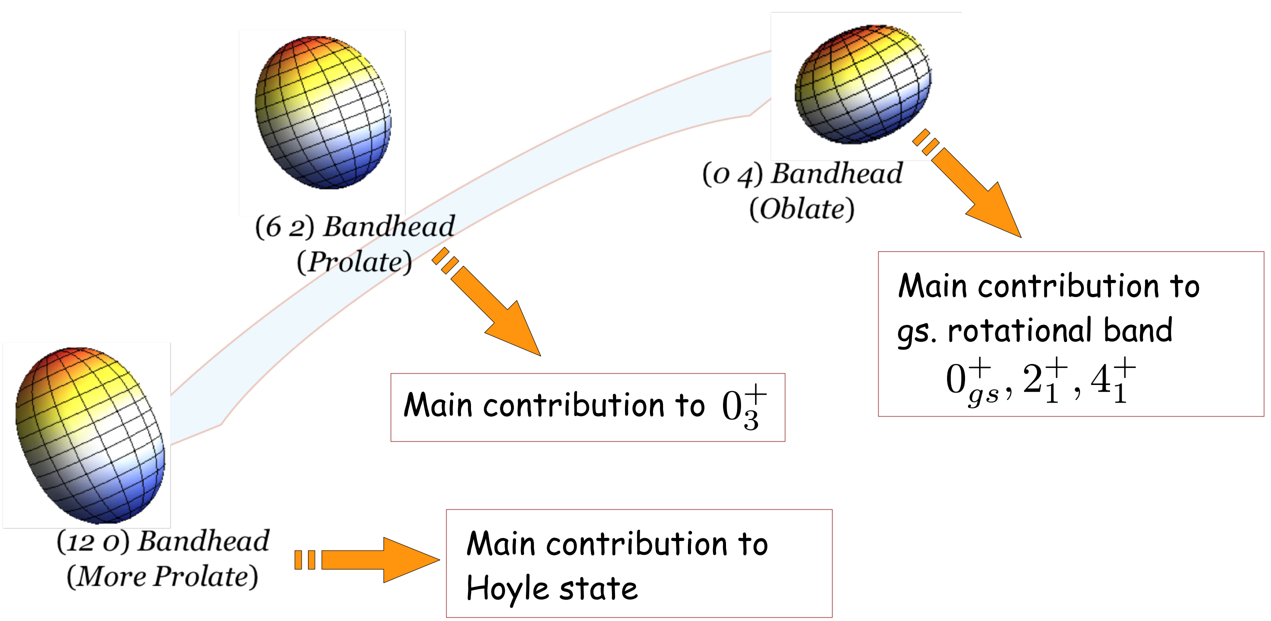
- Single parameter Hamiltonian for cluster & collective modes

$$H_\gamma = H_0 - \frac{\chi}{2}\frac{\left(e^{\gamma Q\cdot Q} - 1\right)}{\gamma} - \frac{20}{A^{2/3}}\sum_{i=1}^{A} l_i s_i$$

- $\chi = \frac{\hbar\Omega}{\sqrt{N_f N_i}}$
- $\gamma \to 0$ and valence space : Hamiltonian of Elliott model $H_0 - \frac{\chi}{2} Q \cdot Q$
- Matrix elements analytical in Sp(3,R) basis
- Spin-orbit term breaks SU(3) & Sp(3,R) symmetries

Importance of Large Model Spaces

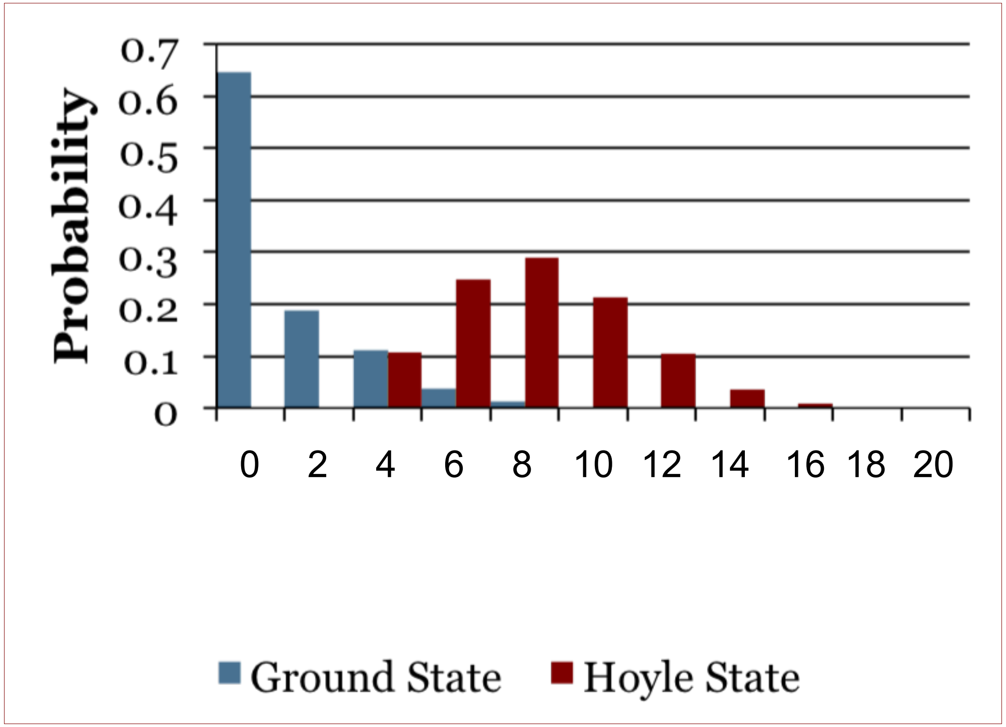




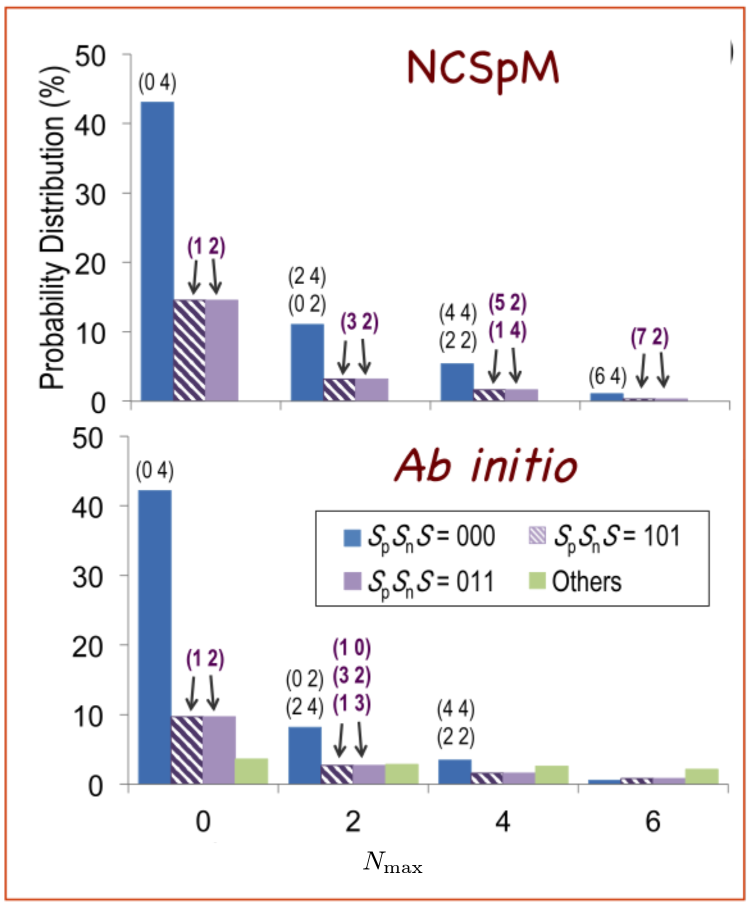
- BE2, Q, rms radii looks reasonably well

Probability Distributions

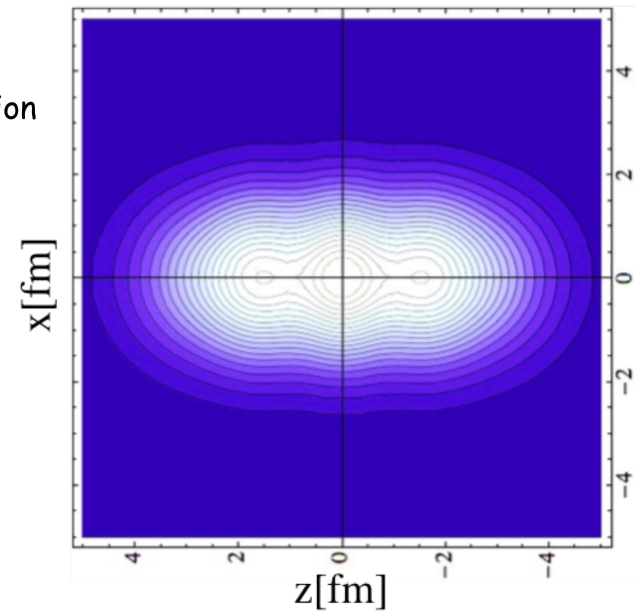
- Ground state peaks at $0\hbar\Omega$ extends to $\sim 10\hbar\Omega$
- Hoyle state peaks at $8\hbar\Omega$ and extends to $\sim 18\hbar\Omega$



- Comparing with ab initio SA-NCSM results



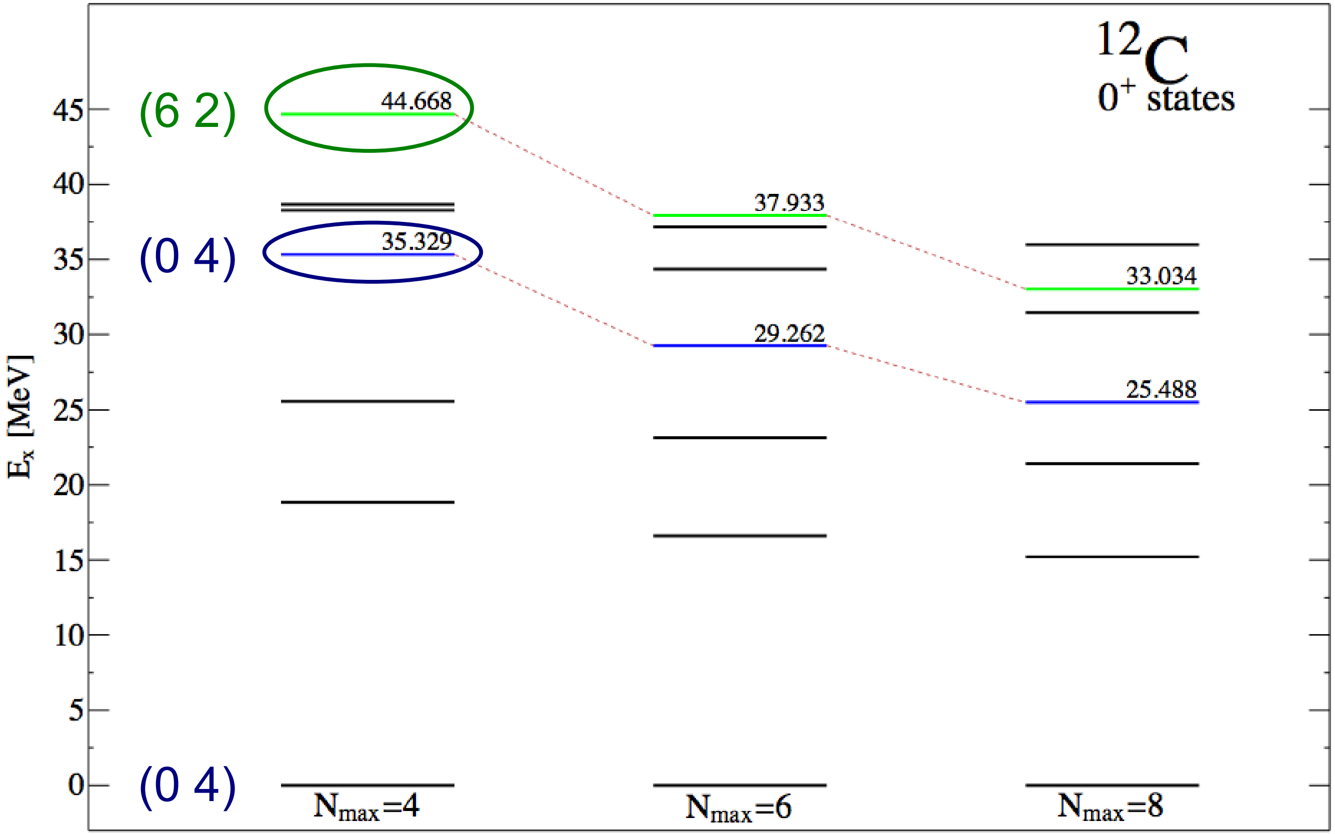
- Matter density of the leading configuration in Hoyle state



Ab Initio SA-NCSM Study: Complete Space

- Interaction: JISP16 + Vcoul, $\hbar\Omega = 20\ \mathrm{MeV}$

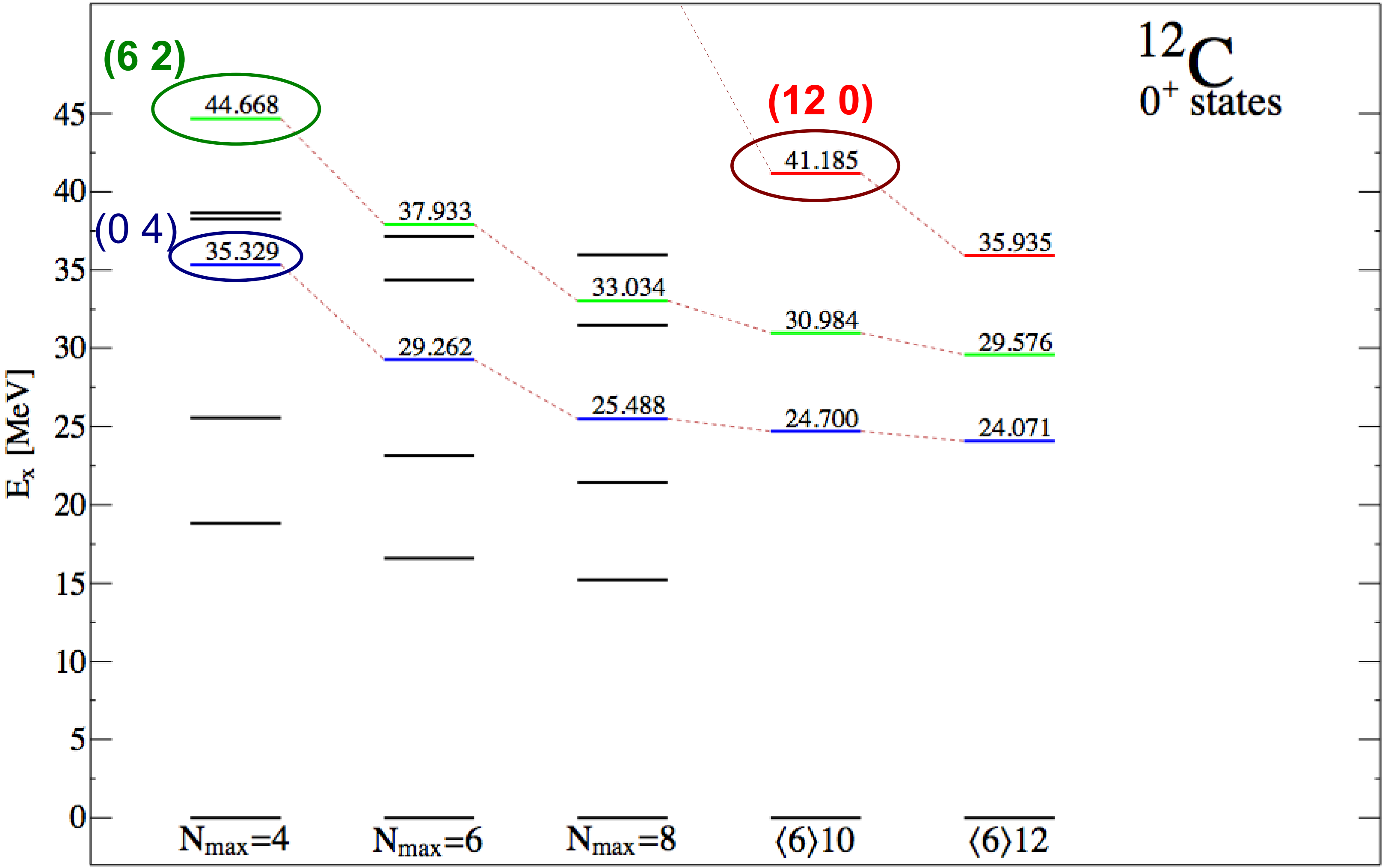
- 2 states with dominant $2\hbar\Omega$ configurations



- No state dominated by (12 0) configuration between lowest 25 excited states in Nmax=8 complete space.

Ab Initio SA-NCSM Study

- Construct symmetry-truncated model space that extends up to Nmax=12
- State dominated by (12 0) Sp(3,R) band identified at <6>10 model space



Summary & Outlook

Summary

Simple patterns of collective modes emerge from first principles

Provide physically relevant model spaces for ab initio modeling of nuclear structure

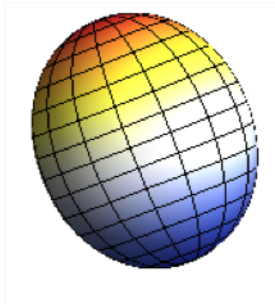
Observed emergence of symplectic symmetry could further expand reach of SA-NCSM

Outlook

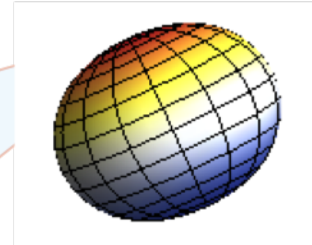
Computational improvement of SU(3)-based techniques SA-NCSM

Augment SA-NCSM with symplectic basis

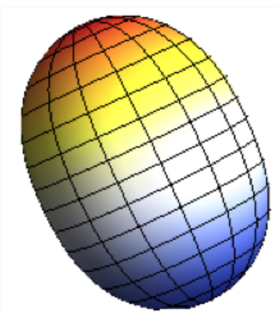
Model Space



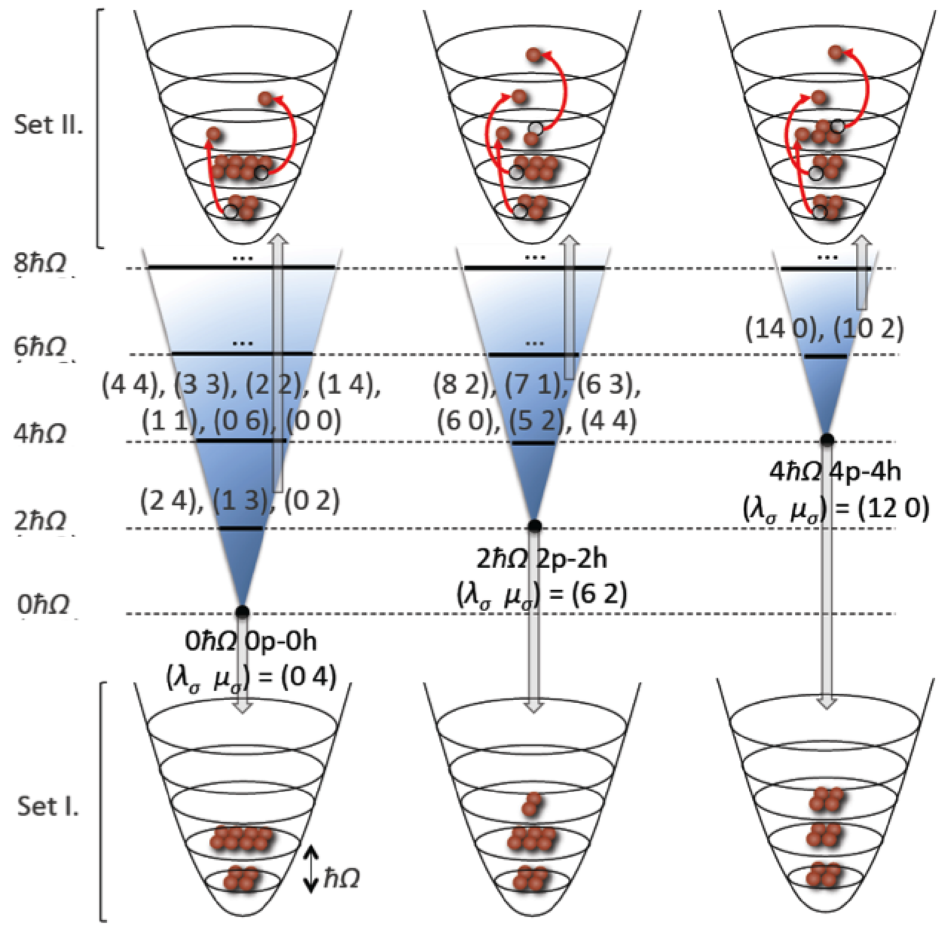
(6 2) Bandhead
(Prolate)



(0 4) Bandhead
(Oblate)



(12 0) Bandhead
(More Prolate)



Model Space

- Symplectic Sp(3,R) slices expanded up to Nmax=20
- Intertwining shell and cluster picture