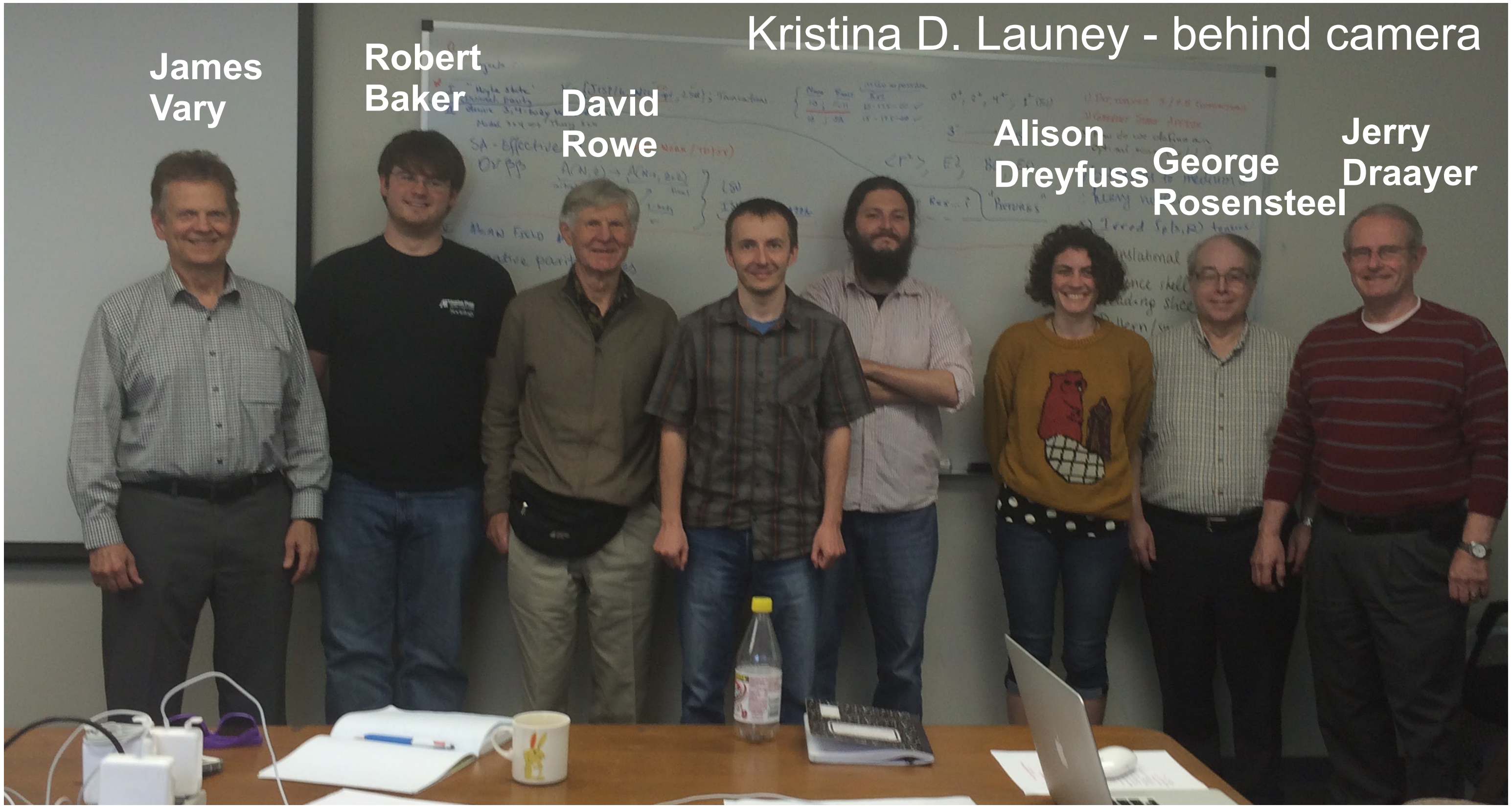
Key role of an emergent symplectic symmetry in atomic nuclei from an ab initio description

Tomáš Dytrych

LOUISIANA STATE UNIVERSITY

Nuclear Physics Institute of
Czech Academy of Sciences

Collaborators



- **University of Notre Dame**

  Anna McCoy, Mark Caprio

- **Czech Technical University**

  Daniel Langr

- **Louisiana State University**

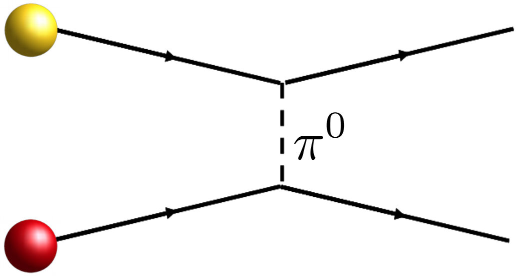
  Grigor Sargsyan

Outline

- Motivation
- Relevant symmetries of Harmonic oscillator: U(3) & Sp(3,R)
- Emergence of symplectic Sp(3,R) symmetry from ab initio perspective
- Recent advances in development of symmetry-adapted tools
- Summary

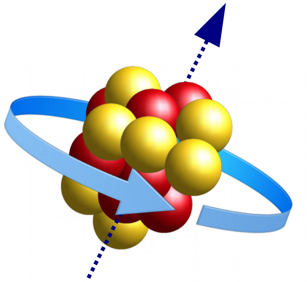
Ab initio Approaches to Nuclear Structure and Reactions

Nuclear interaction



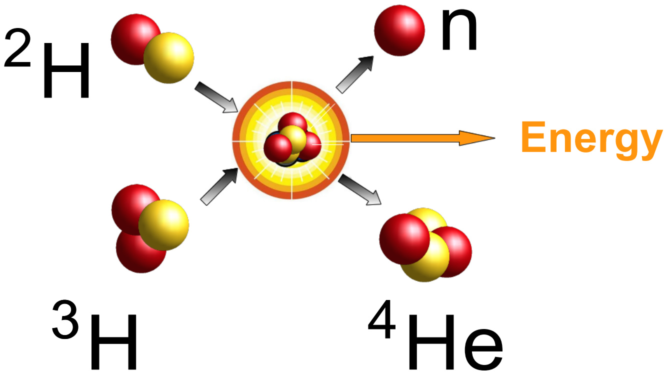
- Realistic nuclear potential models

Many-body dynamics



- wave functions nuclear properties

Nuclear reactions



- reaction rates cross sections

Configuration interaction approach to nuclear many-body problem

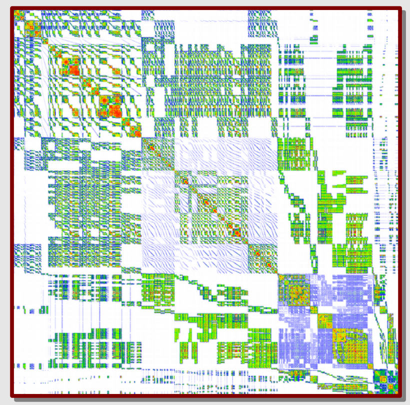
Fundamental task: solve the Schrodinger equation for a system of interacting nucleons

$$\hat{H} = \hat{T} + \hat{V}_{\text{Coul}} + \hat{V}_{NN} + \hat{V}_{3N} \dots$$

1. Choose **physically relevant** model space and construct its basis $\{|\phi_1\rangle, \dots, |\phi_d\rangle\}$

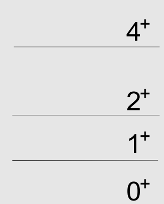
2. Compute Hamiltonian matrix

$$H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle$$



3. Find lowest-lying eigenvalues and eigenvectors $\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$

Lanczos algorithm



eigenvalues

$$|\psi_i\rangle = \sum_{j=1}^{d} c_j |\phi_j\rangle$$

eigenvectors

No-core shell model

- NCSM – most versatile technique for the solution of the *A*-nucleon bound-state problem
  - can use any realistic interaction and applicable to any light nuclear system
  - outcomes can be used for modeling of resonances, continuum states, and nuclear reactions
- NCSM + Resonating Group Method – ab initio nuclear reaction framework
- Model space choice

$$\hat{H}_0 = \sum_{i=1}^{A} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} m\Omega^2 \hat{r}_i^2 \quad \Longrightarrow \quad \hat{H}_0|\phi\rangle = N\hbar\Omega|\phi\rangle$$

  - harmonic oscillator mean field potential ⟹ exact factorization of center-of-mass possible for Nmax cutoff

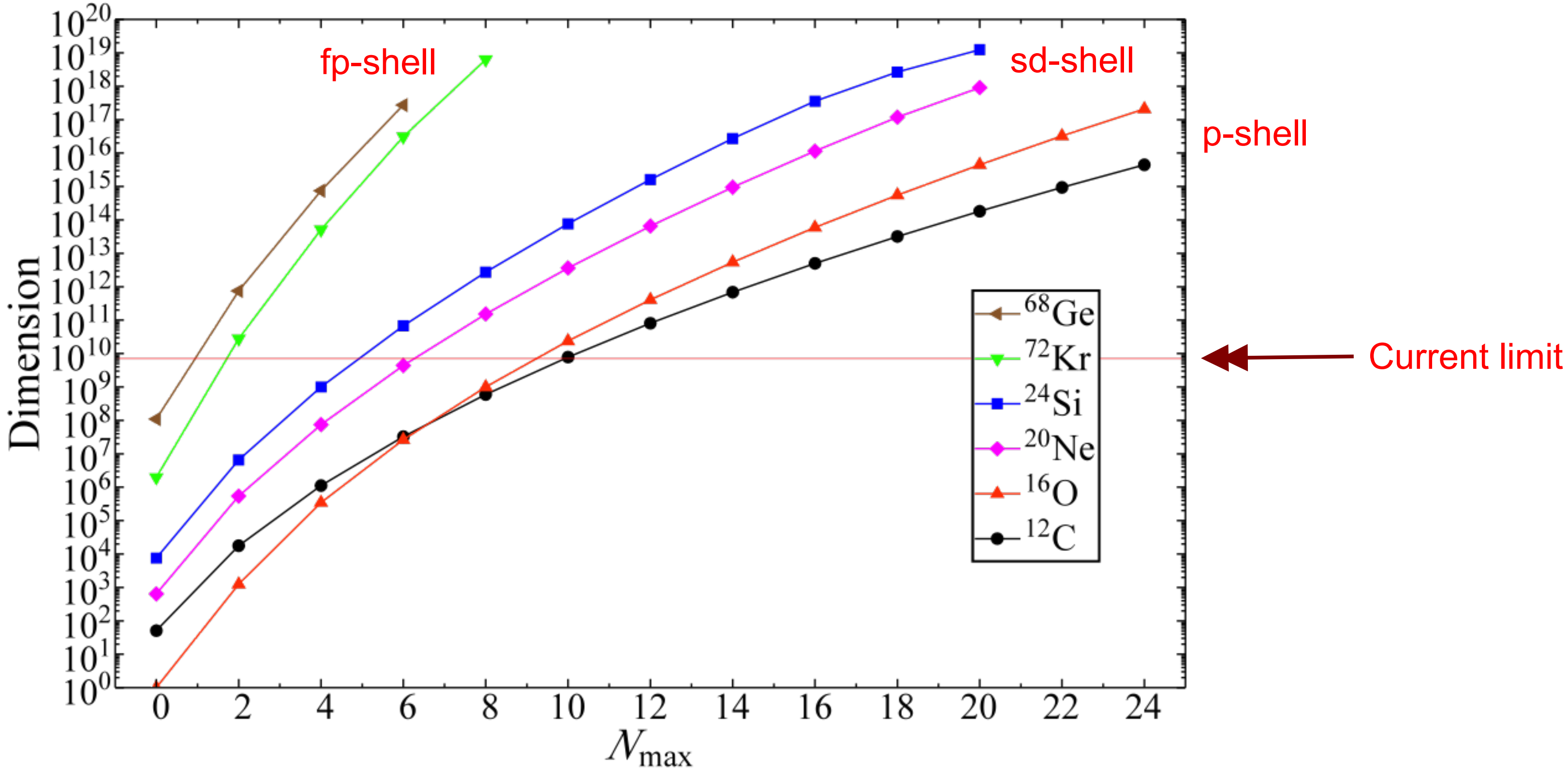
- Standard basis of NCSM **M-scheme basis**

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 oscillator $\varphi_{\eta l j m}(\vec{r}) = R_{\eta l}(r) \left[Y_l(\theta, \phi) \chi_{1/2} \right]_m^j$

Model space scale explosion



- higher Nmax model spaces are needed
  - Description of collective and cluster states
  - shape coexistence
  - Improve nuclear reaction modelling

- NCSM extensions
  - Importance Truncated NCSM
  - Monte-Carlo NCSM
  - alternative single-particle states
  - **Symmetry-adapted NCSM**

Search for relevant degrees of freedom

Exact symmetry considerations

- Both nuclear and many-body harmonic oscillator Hamiltonians are invariant with respect to rotations

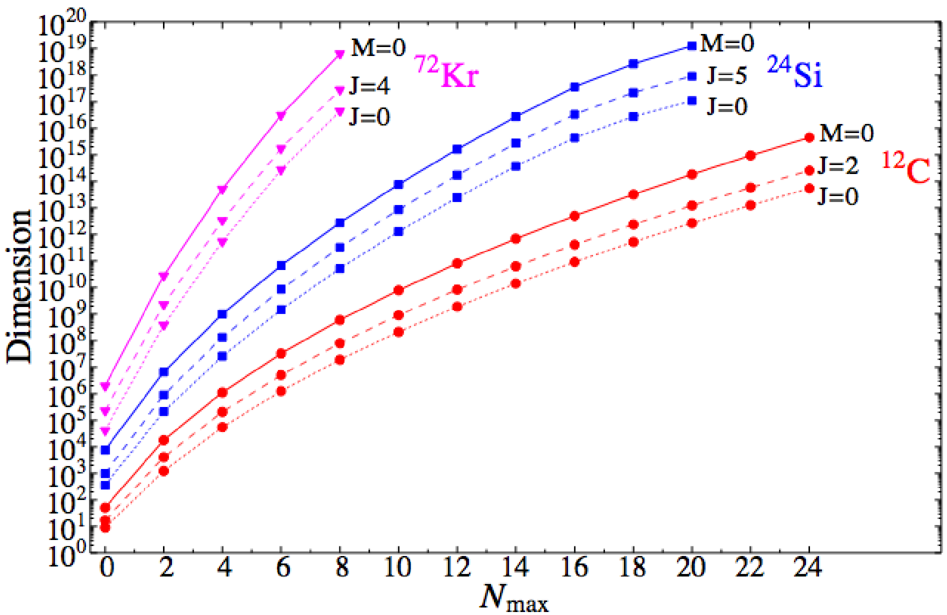
$$\left[\hat{H}, \hat{J}^2\right] = 0$$ ⇒ Nuclear wave functions carry a definite total angular momentum

$$\left[\hat{H}_0, \hat{J}^2\right] = 0$$ ⇒ Harmonic oscillator wave functions carry a definite total angular momentum

NCSM in J-coupled basis

- NCSM model space cutoff:

$$N \leq N_{\max}$$
$$J$$



The good:

- Model space dimension reduced

The bad:

- Hamiltonian matrix becomes much denser
- takes more memory compared to m-scheme

Elliott's SU(3) model

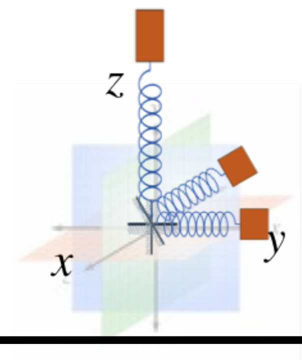
- origin of deformed rotational states in light and sd-shell nuclei

$$\hat{H} = \hat{H}_0 - \frac{1}{2}\chi Q^a \cdot Q^a$$

$$\mathrm{U}(\Omega) \supset \mathrm{SU}(3) \supset \mathrm{SO}(3)$$

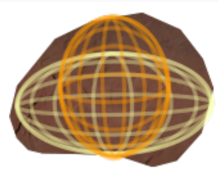
- Quantum labels of basis states

number of HO excitations



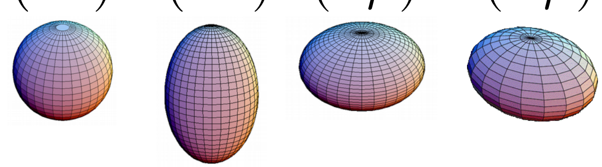
N

deformation SU(3)

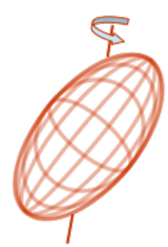


$(\lambda\,\mu)$

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



rotation SO(3)



L

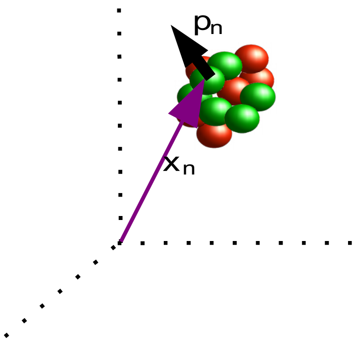
Symplectic model of nuclear collective motion

Symplectic Sp(3,R) model

G. Rosensteel and D. J. Rowe, Phys. Rev. Lett. 38 (1977) 10

- Microscopic realization and generalization of Bohr-Mottelson model

- Sp(3,R): smallest Lie algebra that contains both kinetic energy & quadrupole moments



21 Generators

$Q_{ij} = \sum_n x_{ni} x_{nj}$	monopole and quadrupole moments
$S_{ij} = \sum_n (x_{ni} p_{nj} + p_{ni} x_{nj})$	generators of monopole & quadrupole deformations
$L_{ij} = \sum_n (x_{ni} p_{nj} - p_{ni} x_{nj})$	generators of rotations
$K_{ij} = \sum_n p_{ni} p_{nj}$	generators of quadrupole flow (kinetic energy)

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

- Symplectic states realize nuclear collective modes

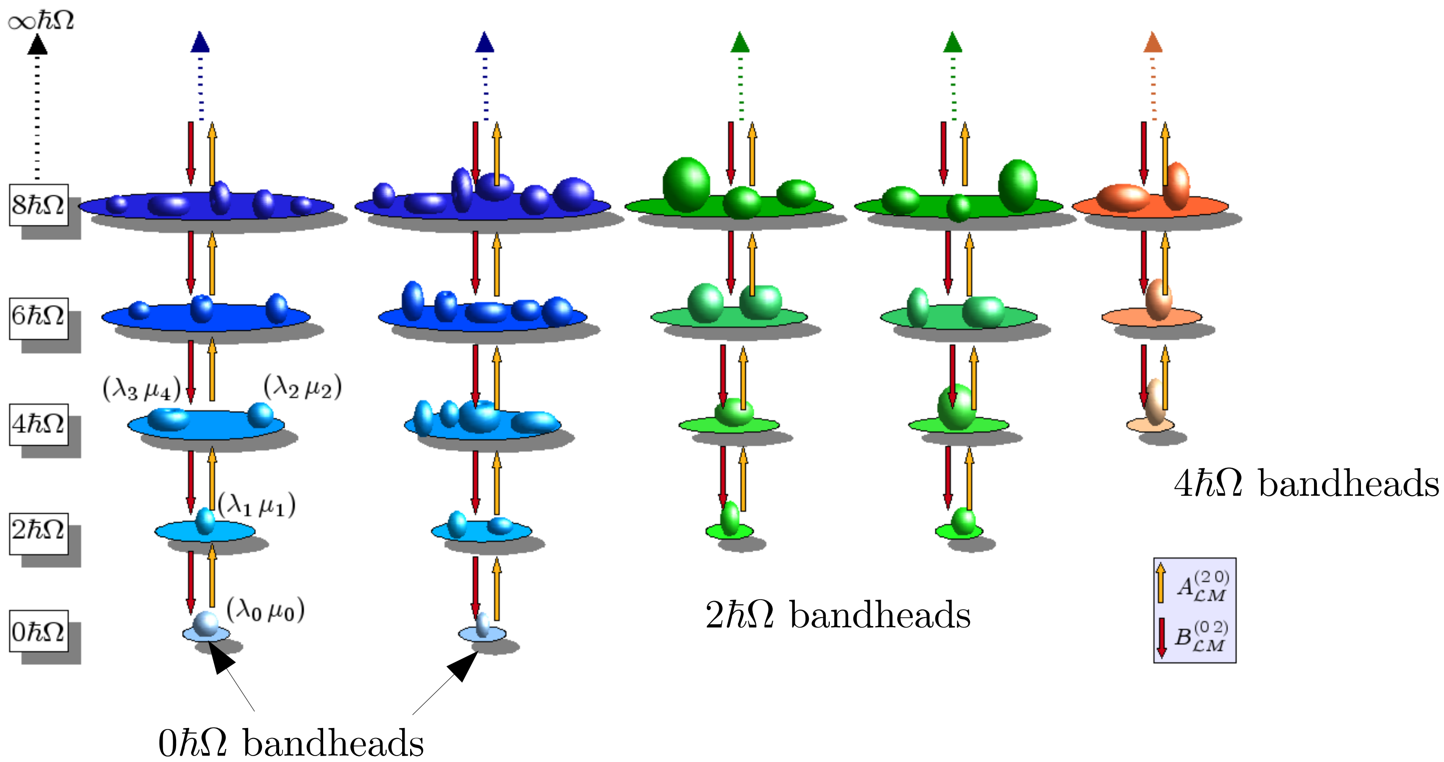
  low-lying rotational bands

  beta and gamma vibrations

  giant monopole and quadrupole resonances

  shape coexistence

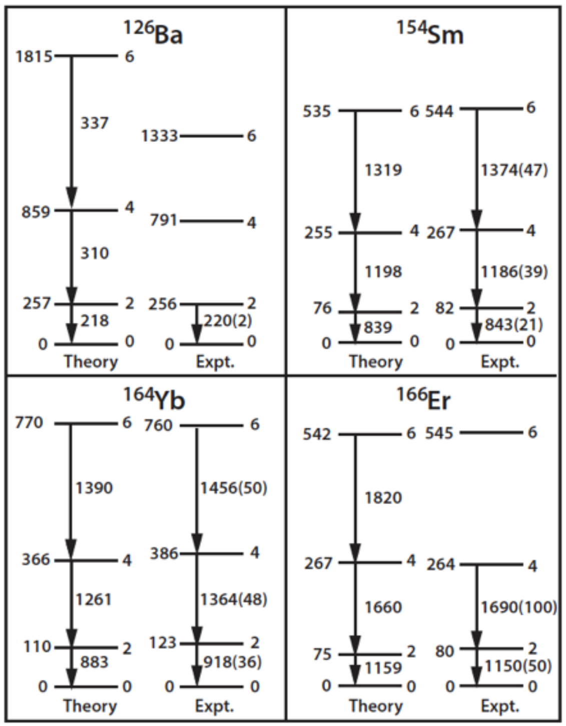
Shell model space decomposition by Sp(3,R) symmetry



- Sp(3,R) irreps and their basis states
  - Generated from a single U(3) irrep (“bandhead”) by action of symplectic raising operators
  - Carry the parity of their bandhead
  - Carry the spin/isospin of their bandhead
- Symplectic basis states can be expanded in basis of no-core shell model (m-scheme basis)

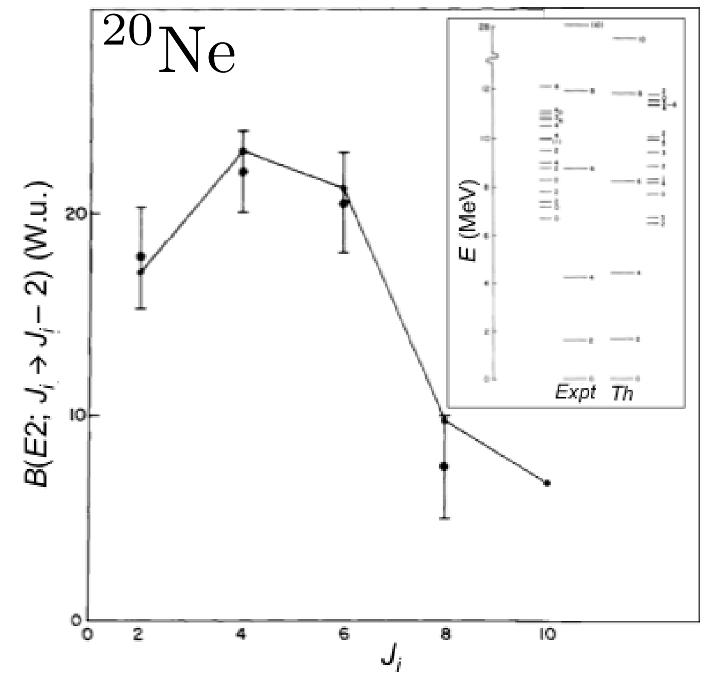
Earlier studies

- Model space spanned by few irreps + symmetry-preserving interaction



P. Parker, et al., Nucl. Phys. A414 (1984) 93

D. J.. Rowe, Rep. Prog. Phys. 48 (1985) 48



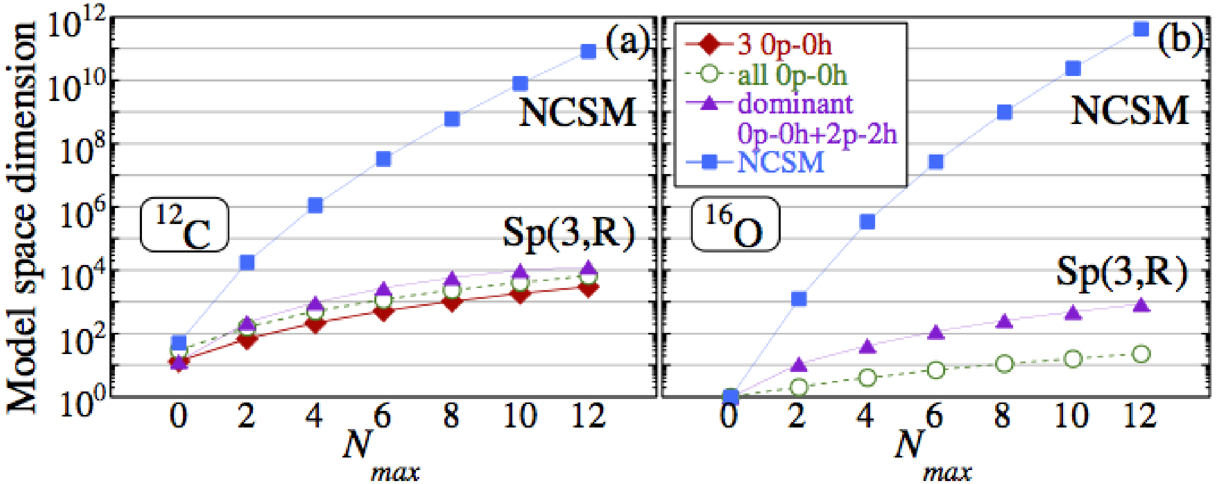
J. P. Draayer, et al., Nucl. Phys. A419 (1984) 1

- Describe spectrum and B(E2) without effective charges

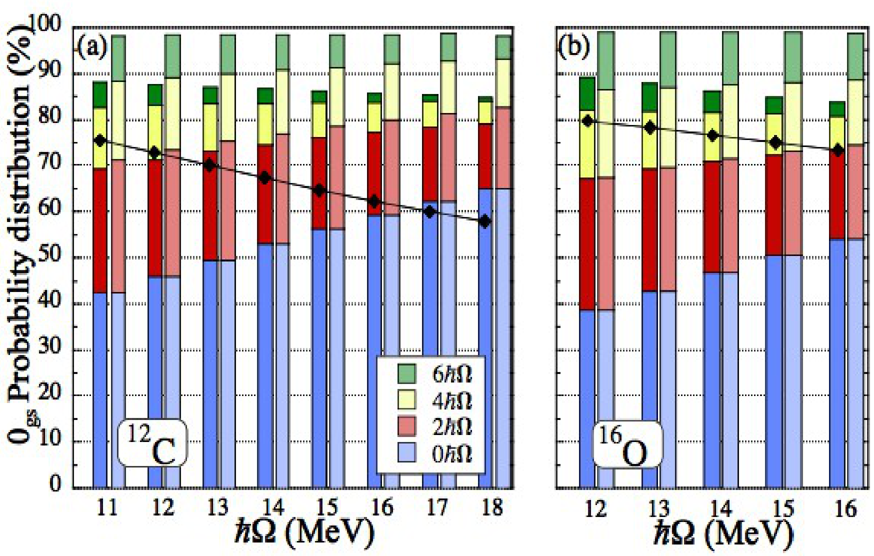
- realistic nuclear interactions break Sp(3,R) symmetry!

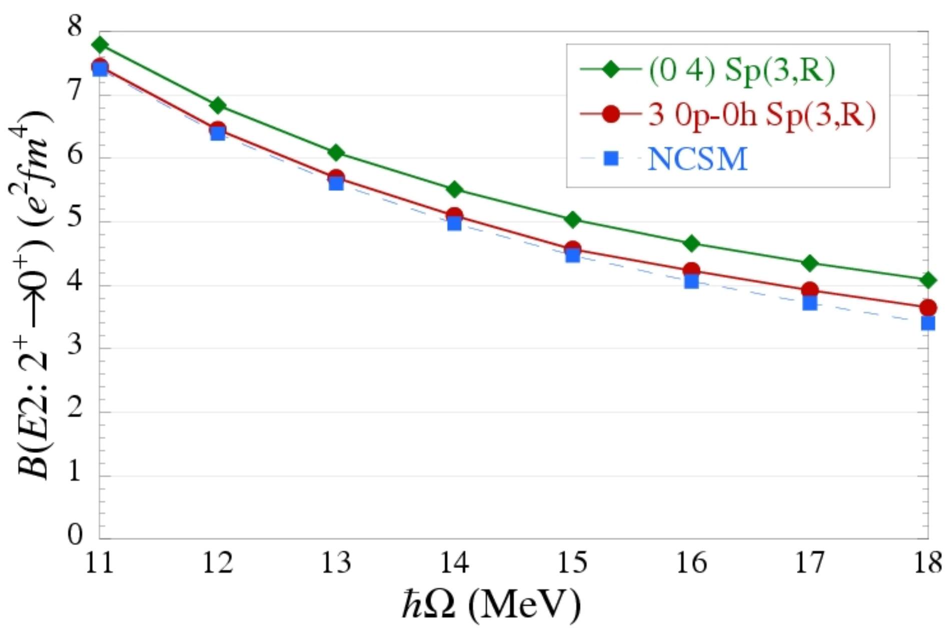
Early evidence for Sp(3,R) symmetry in NCSM results

- Proof-of-principle study $^{12}\mathrm{C} : 0^+_{gs}, 2^+_1, 4^+_1$ $^{16}\mathrm{O} : 0^+_{gs}$
  - Expand Sp(3,R) irreps in m-scheme basis
  - Project NCSM states to Sp(3,R) irreps



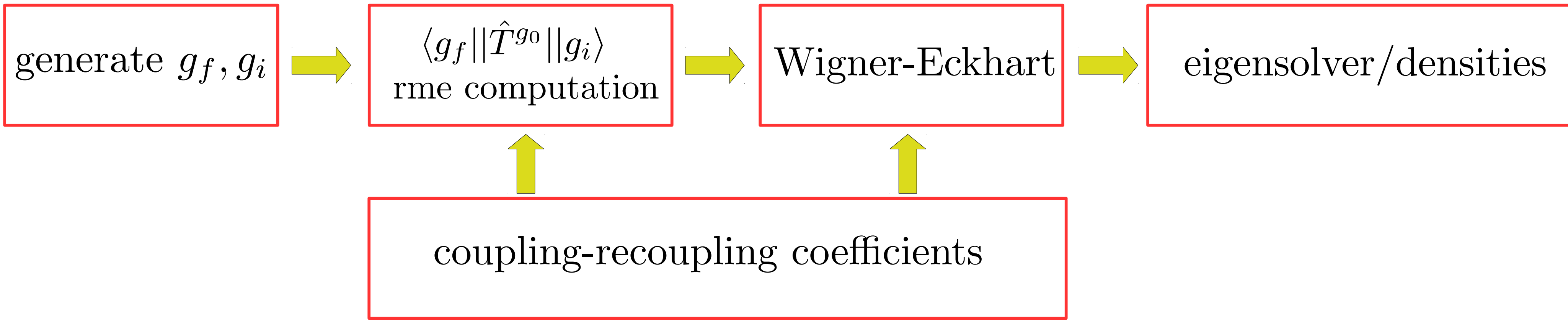
- Results:
  - few Sp(3,R) irreps -- 85-80% of wave functions
  - 3 irreps reproduce NCSM results for B(E2)



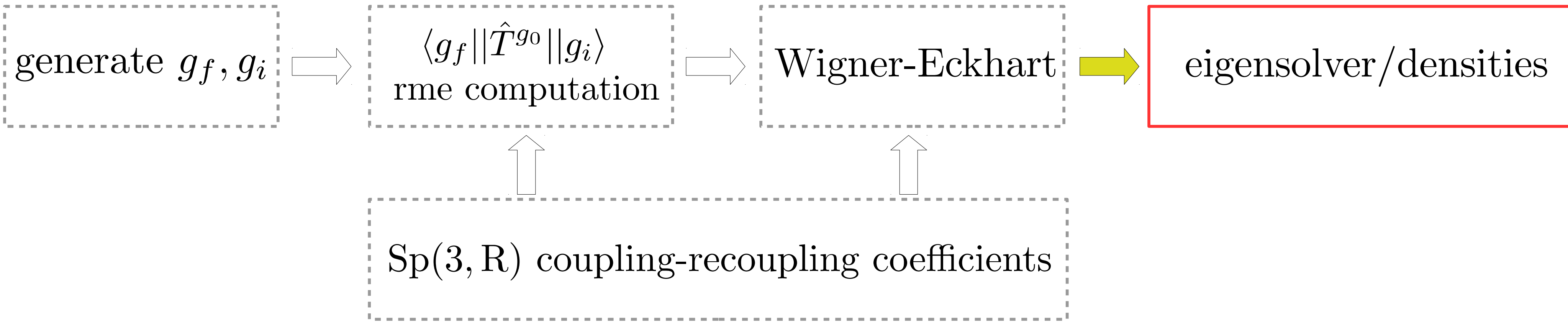


Dytrych, Launey, Bahri et al., Phys. Rev. Lett. 98 (2007) 162503

Symmetry-adapted NCSM framework

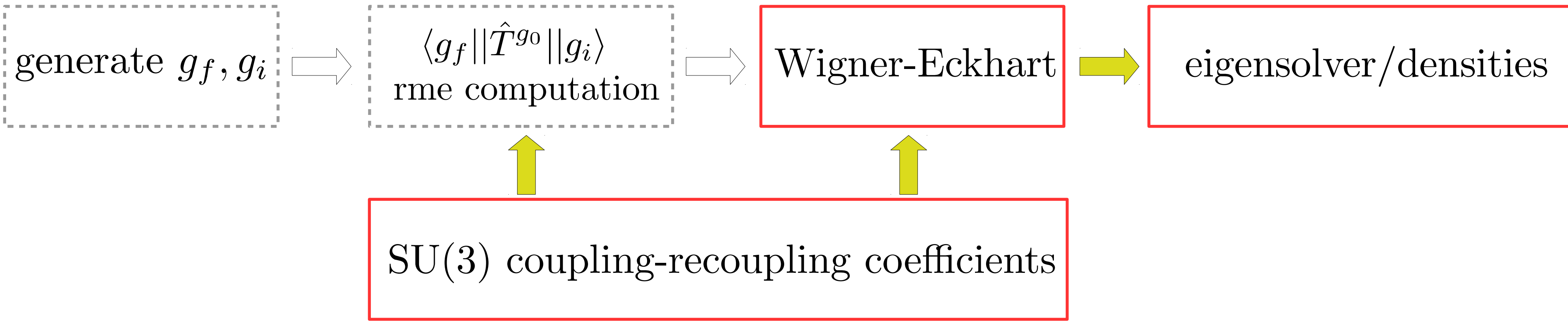


SA-NCSM in Sp(3,R) basis



- Two ingredients were missing:
  - Sp(3,R) coupling-recoupling coefficients
  - Sp(3,R) reduced matrix elements are in fact “just” SU(3) reduced matrix elements

SA-NCSM in SU(3) basis

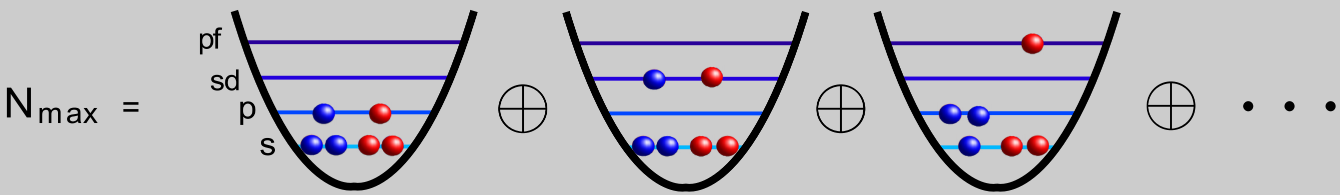


- Solution: take advantage of SU(3) subgroup of Sp(3,R)
  - SU(3) coupling-recoupling coefficients available since 1973 work of Draayer and Akyiama
  - alternative approaches to evaluate matrix elements in Sp(3,R) basis rely on SU(3) techniques

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

Step 1

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



Step 2

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

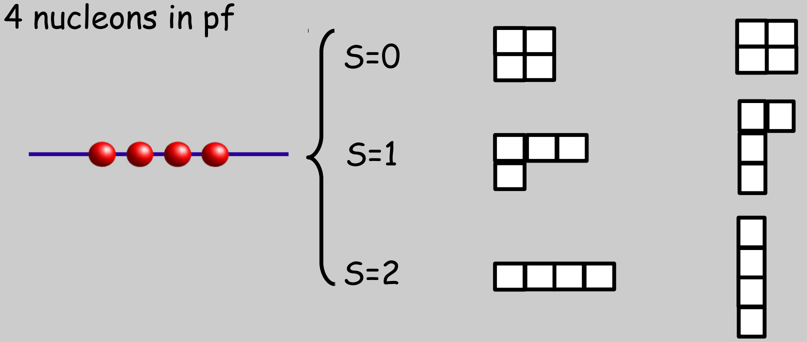
Step 3

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

U(2) ⊗ U(10) ⊃ SU(3)

quantum labels: S [f] α $(\lambda\,\mu)$

- Example:
  4 nucleons in pf



S=0: ⊃ {(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: ⊃ {(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)}

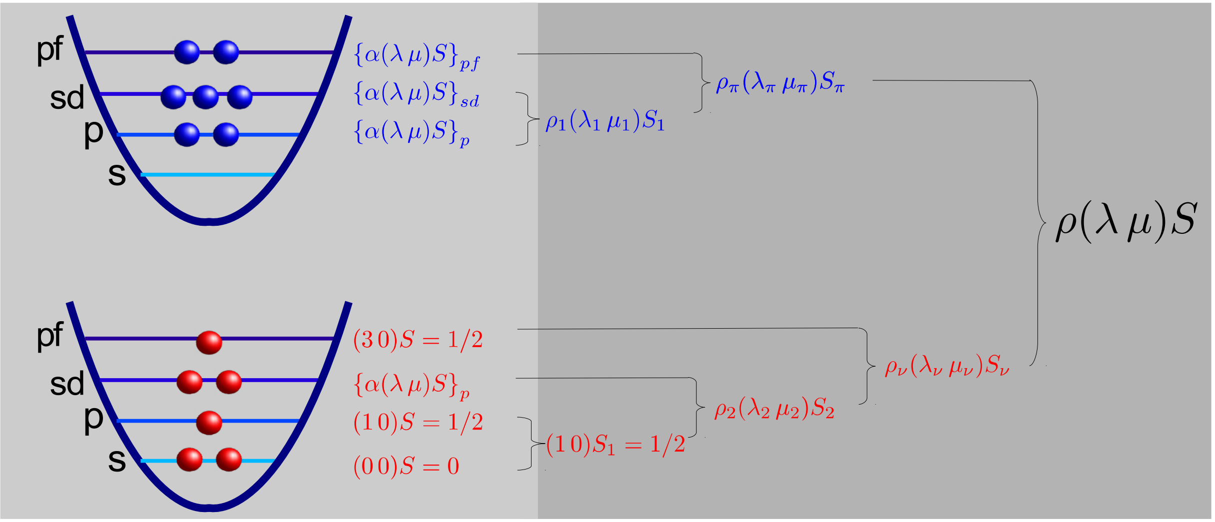
S=2: ⊃ {(5 2) (0 6) (3 3) (2 2) (3 0)}

"single-shell" SU(3)xSU(2) irreps

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

Step 1: SU(3) coupling of succesive shells

Step 2: SU(3) coupling of protons and neutrons



Many-nucleon basis states of SA-NCSM

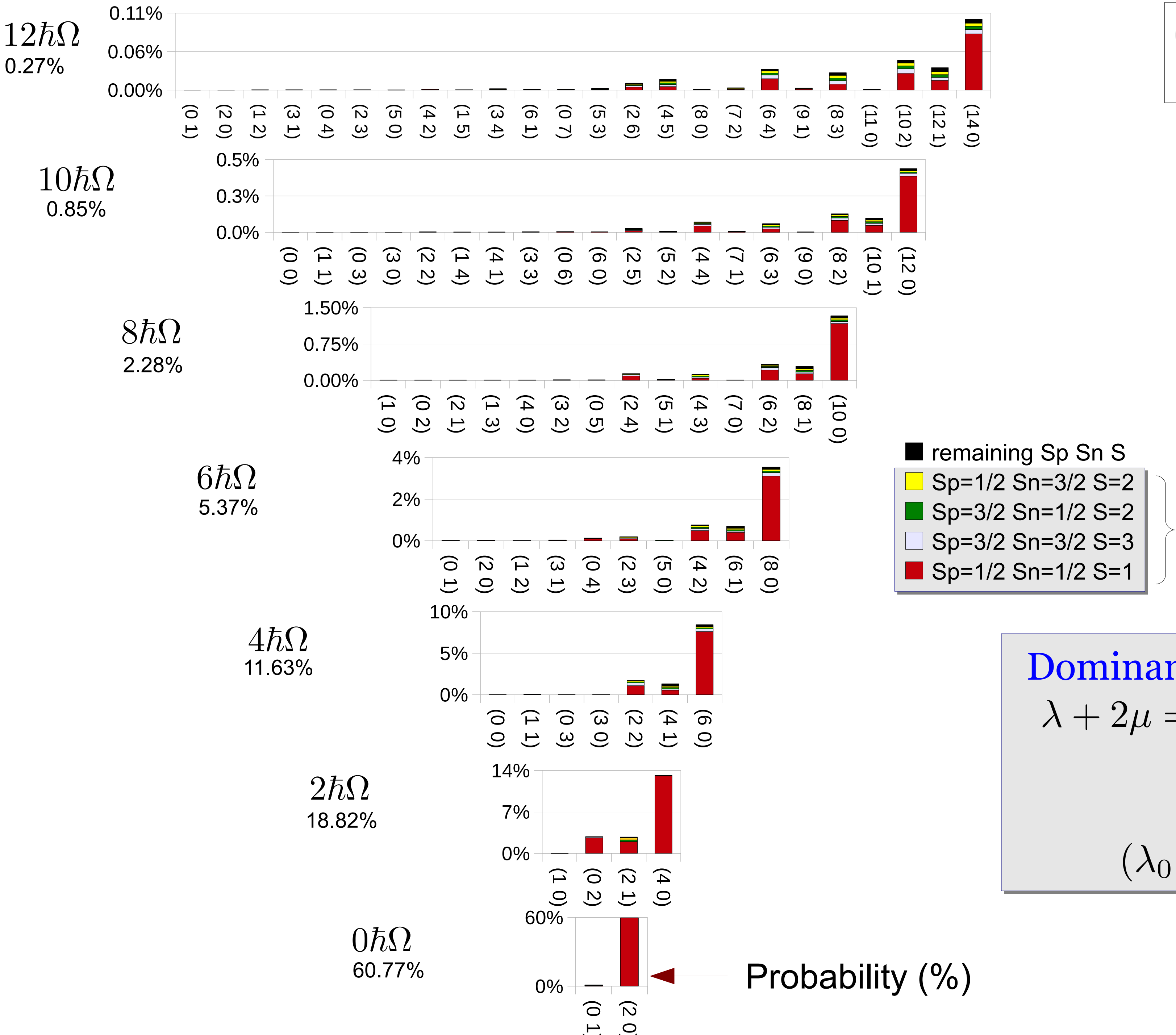
$$|\gamma\;\; N\hbar\Omega\;\; \overbrace{S_p\, S_n S}^{\text{intrinsic spin part}}\;\; \overbrace{(\lambda\,\mu)\;\;\kappa L}^{\text{spatial part}}\;\;\; J\, M\rangle$$

HO energy

deformation

orbital angular momentum

Emergence of Simple Patterns



^{6}Li : 1^{+}_{gs}

$N_{max} = 12$

JISP16 + Vcoul

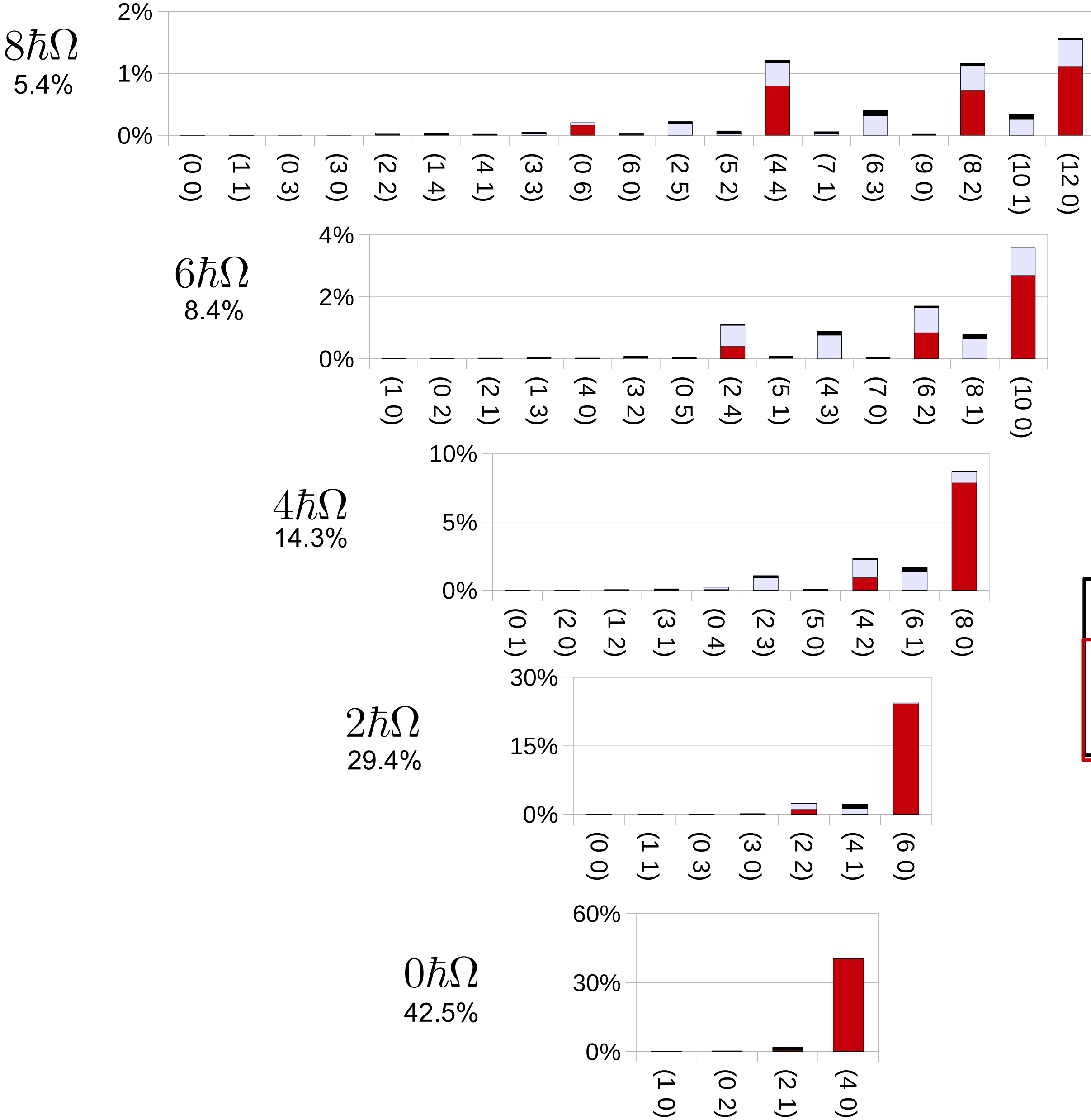
$\hbar\Omega = 20$ MeV

Dominant deformations

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

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

Emergence of Simple Patterns



even-even nucleus

different interaction

identical features ...

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

$N_{max} = 8$

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 deformations

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

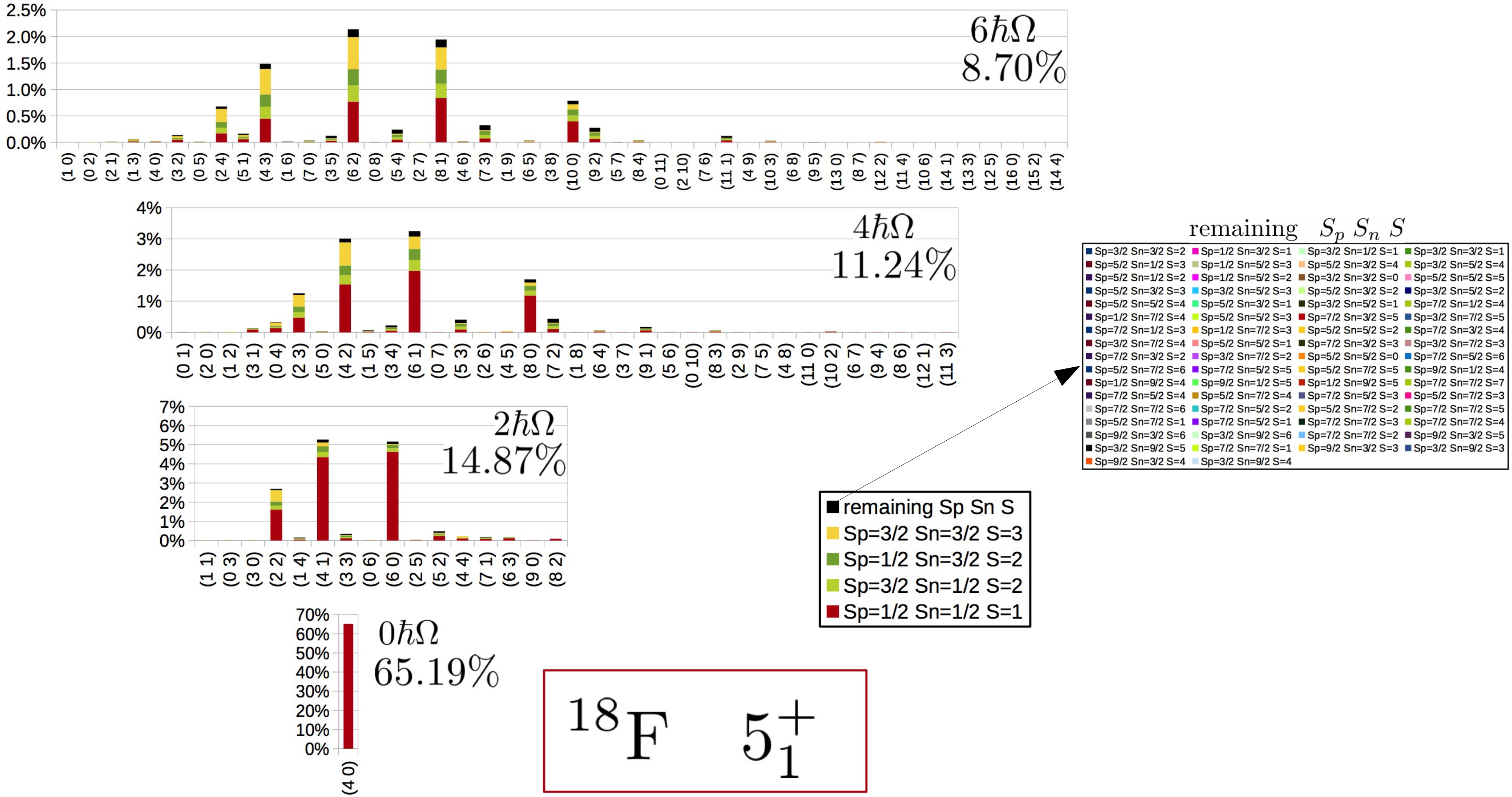
$$(\lambda_0\,\mu_0) = (4\,0)$$

Emergence of Simple Patterns

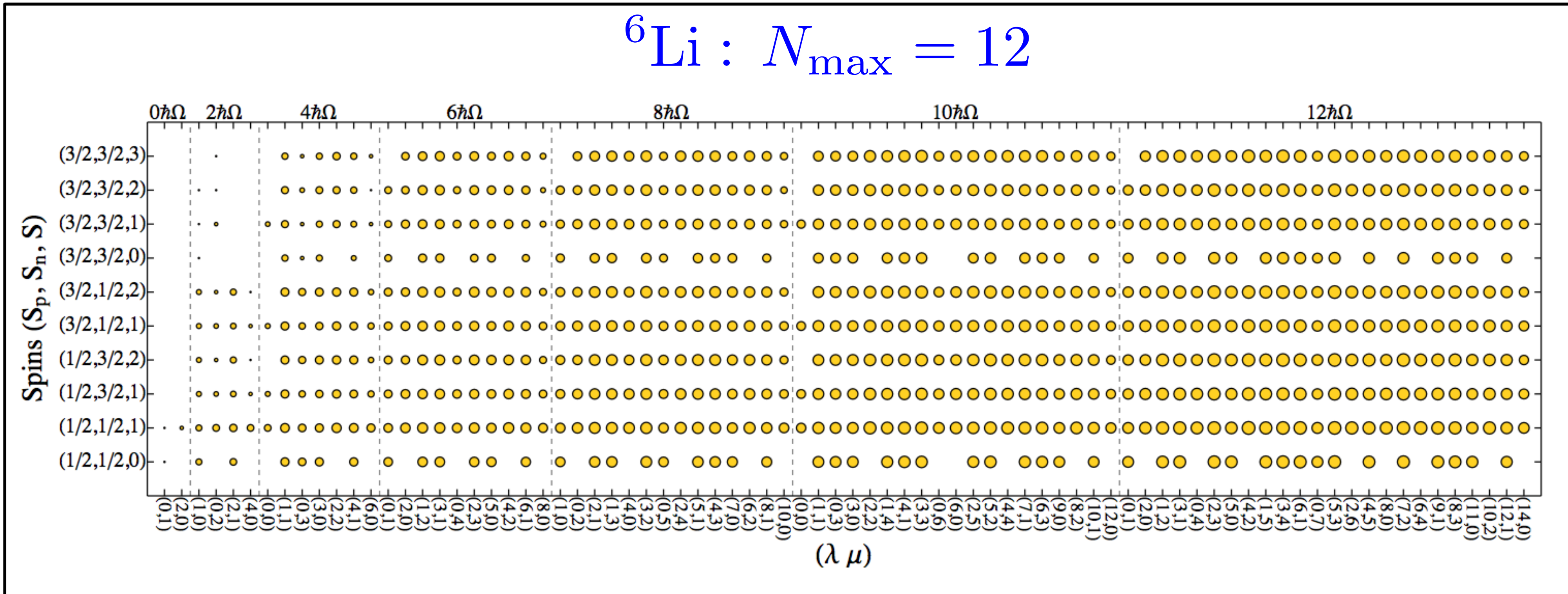
$N_{max} = 12$

N2LOopt + Vcoul

$\hbar\Omega = 20$ MeV



NCSM model space in SU(3)-coupled Basis

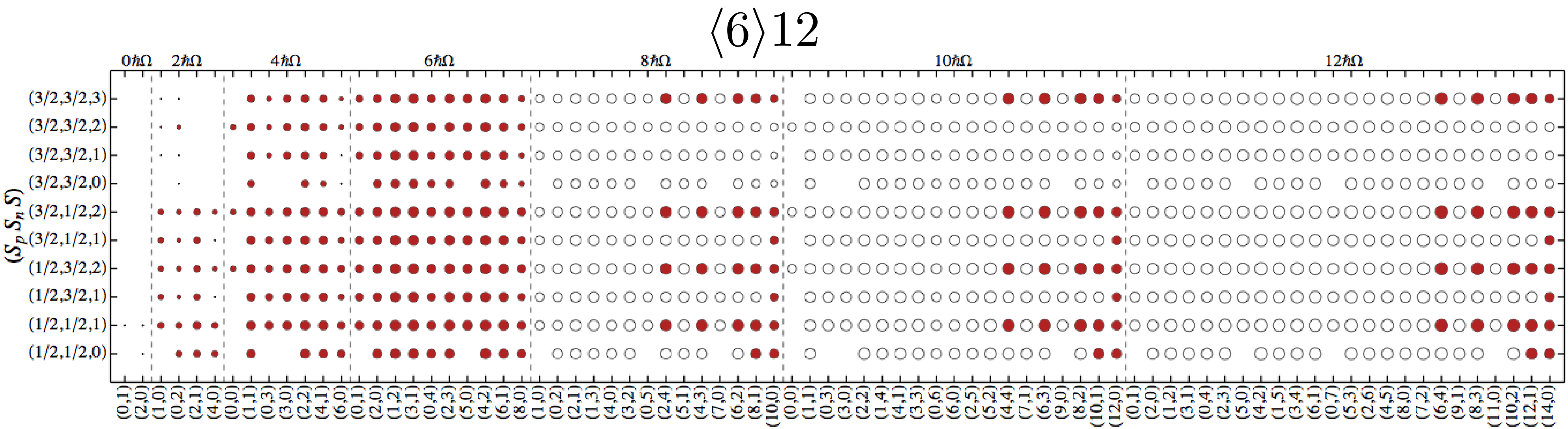


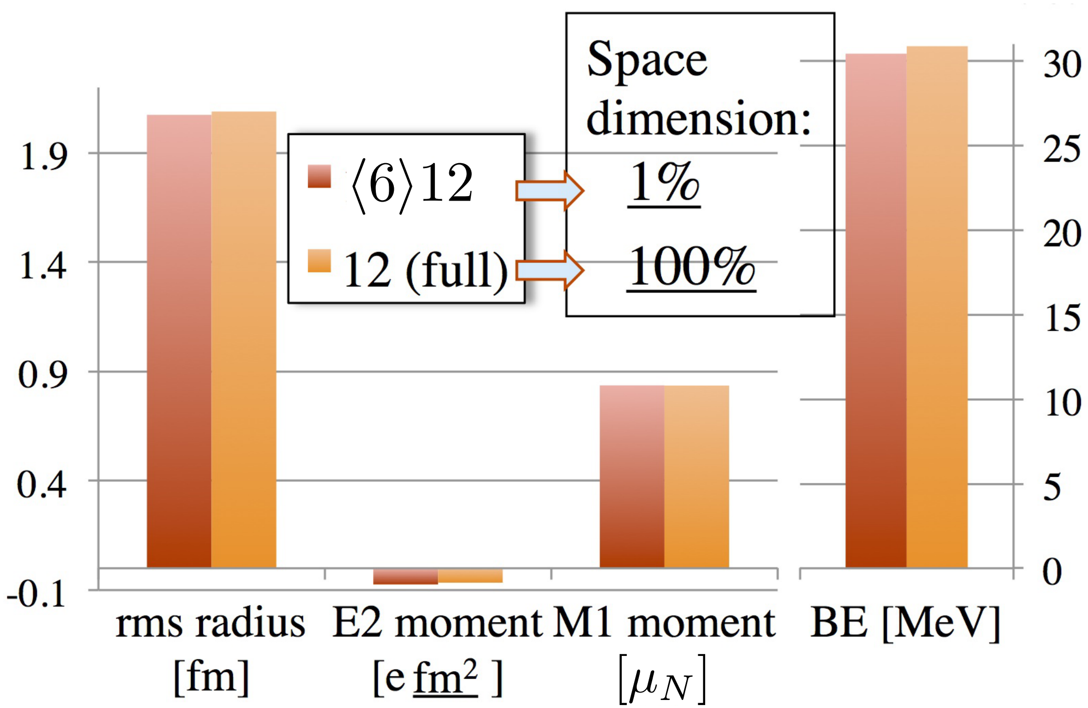
- c.m. spurious states can be removed from each subspace of equivalent U(3)xSU(2) irreps exactly

- 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





T. Dytrych, K. D. Launey, J. P. Draayer et al, Phys. Rev. Lett. 111 (2013) 252501

Applications of SA-NCSM in SU(3) basis scheme

- Robert B. Baker

  Electromagnetic sum rules in SA-NCSM to study EM reactions for light and medium-mass nuclei

- Alison C. Dreyfuss

  Clustering and alpha-capture reaction rates from SA-NCSM description of 20Ne

- Grigor Sargsyan

  Large-scale ab initio SA-NCSM studies of nuclear structure for physics beyond the standard model

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

- Diagonalize Sp(3,R) Casimir operator

Sp(3,R) generators

$$\hat{A}_{ij} = \sum_n b^\dagger_{ni} b^\dagger_{nj}$$

$$\hat{B}_{ij} = \sum_n b_{ni} b_{nj}$$

$$\Rightarrow \quad \hat{T}^{(0\,0)} := -\left[\hat{A} \times \hat{B}\right]^{(0\,0)} + \gamma \hat{N}_{\mathrm{cm}}$$

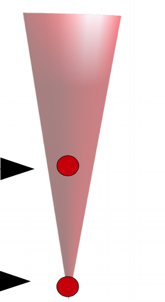
- Eigenvectors: Sp(3,R) basis states
- Sp(3,R) quantum labels can be determined from eigenvalues

$$\hat{T}^{(0\,0)}|v\rangle = \lambda |v\rangle$$

$\lambda < 0$ Sp(3,R) basis state →

$\lambda = 0$ Sp(3,R) bandhead →

$\lambda > 0$ excited center-of-mass



$N_\sigma \hbar\Omega\,(\lambda_\sigma\,\mu_\sigma)$

- Simplification: construction done in subspaces of equivalent U(3) irreps $N\hbar\Omega\,(\lambda\,\mu)$
- Resulting expansion: $|v\rangle = \sum_i c_i |i\, N(\lambda\,\mu)\rangle$ does not depend on quantum numbers k L J.

Approach

- Generate Sp(3,R) irreps
  - $^6\mathrm{Li},^8\mathrm{He}: N_{\max} = 12$
  - $^{20}\mathrm{Ne}: N_{\max} = 8$

$$
\begin{array}{lll}
 & ^6\mathrm{Li} & \\
48,887,656 \rightarrow & \dim N_{\max} = 12 & \\
293,642 \rightarrow & \dim |N_\sigma(\lambda_\sigma\,\mu_\sigma) N(\lambda\,\mu)\, S_p S_n S\rangle & \mathrm{Sp}(3,\mathrm{R}) \supset \mathrm{SU}(3)\ \text{irreps} \\
36,878 \rightarrow & \dim |N_\sigma(\lambda_\sigma\,\mu_\sigma) S_p S_n S\rangle & \mathrm{Sp}(3,\mathrm{R})\ \text{irreps}
\end{array}
$$

- Problem size reduction
  - **500,000 GB** needed to store expanded Sp(3,R) J-coupled states in m-scheme basis
  - **10 GB** needed to store this expansion in terms in SU(3) irreps

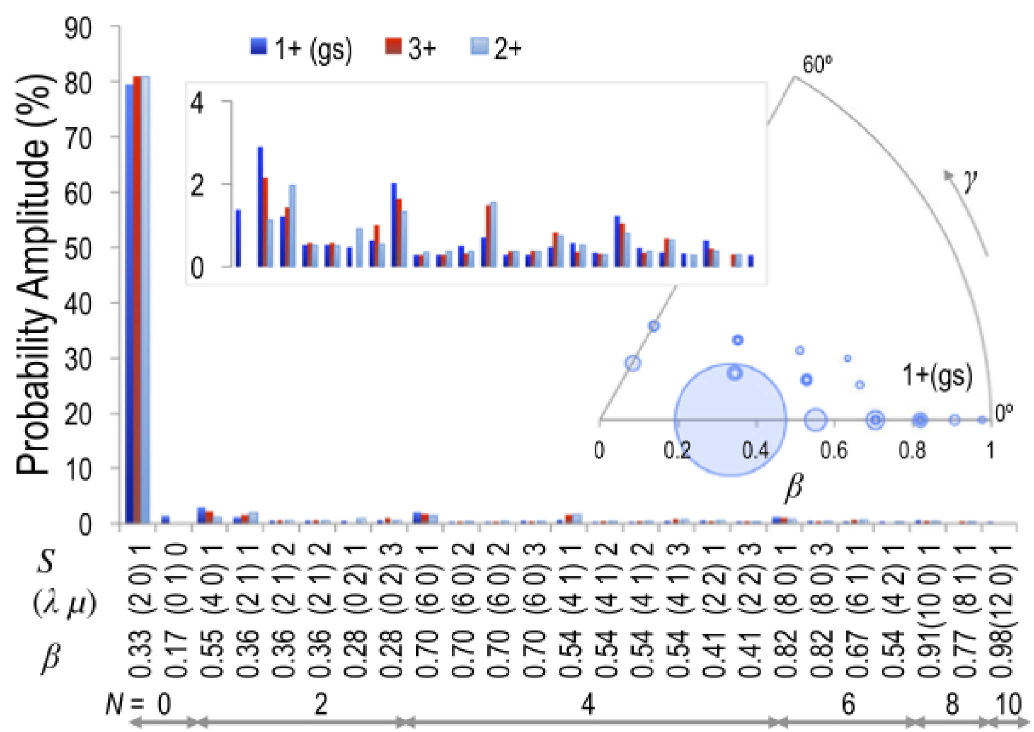
- We use SA-NCSM in SU(3)-coupled basis scheme with N3LO, NNLOopt and JISP16 interactions

- SA-NCSM wave functions are projected on Sp(3,R) basis states

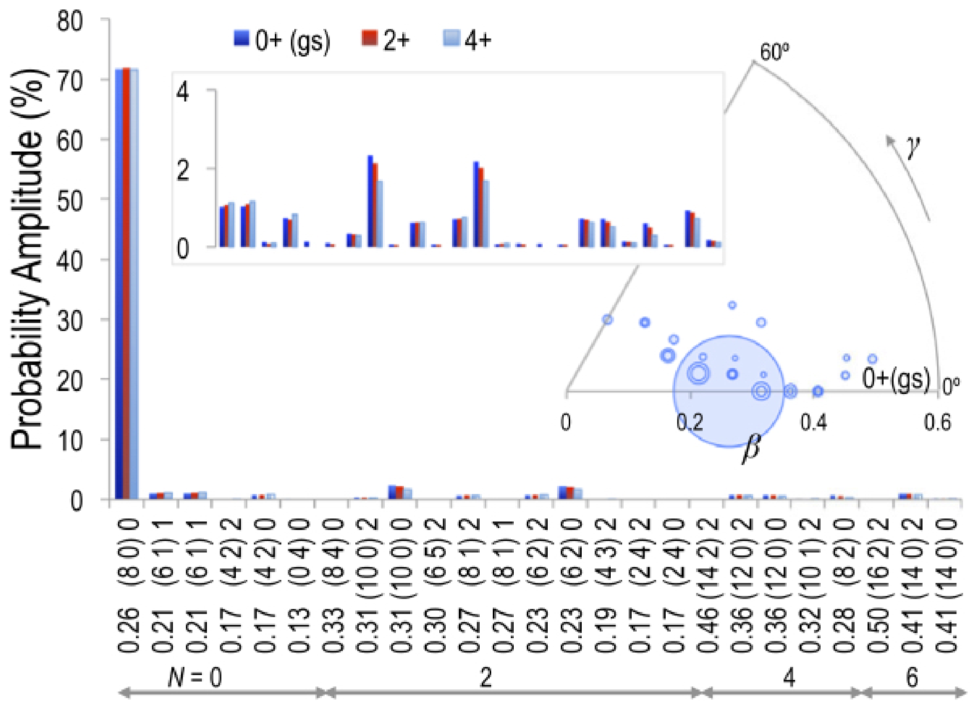
Emergence of symplectic symmetry from ab initio studies

- Typically just a few Sp(3,R) irreps dominates (70%-80%) wave functions
  - single dominant Sp(3,R) irrep: ^{6}Li ^{8}Be ^{16}O ^{20}Ne
  - two or three dominant Sp(3,R) irreps: ^{8}He ^{12}C
- Manageable number of Sp(3,R) irreps contribute by 1%-4%
- Emerging symplectic structure does not depend on interaction used
- Members of a rotational band have the same intrinsic structure ⇒ indentify rotational band members

(a) ^{6}Li, EM-N^{3} LO NN

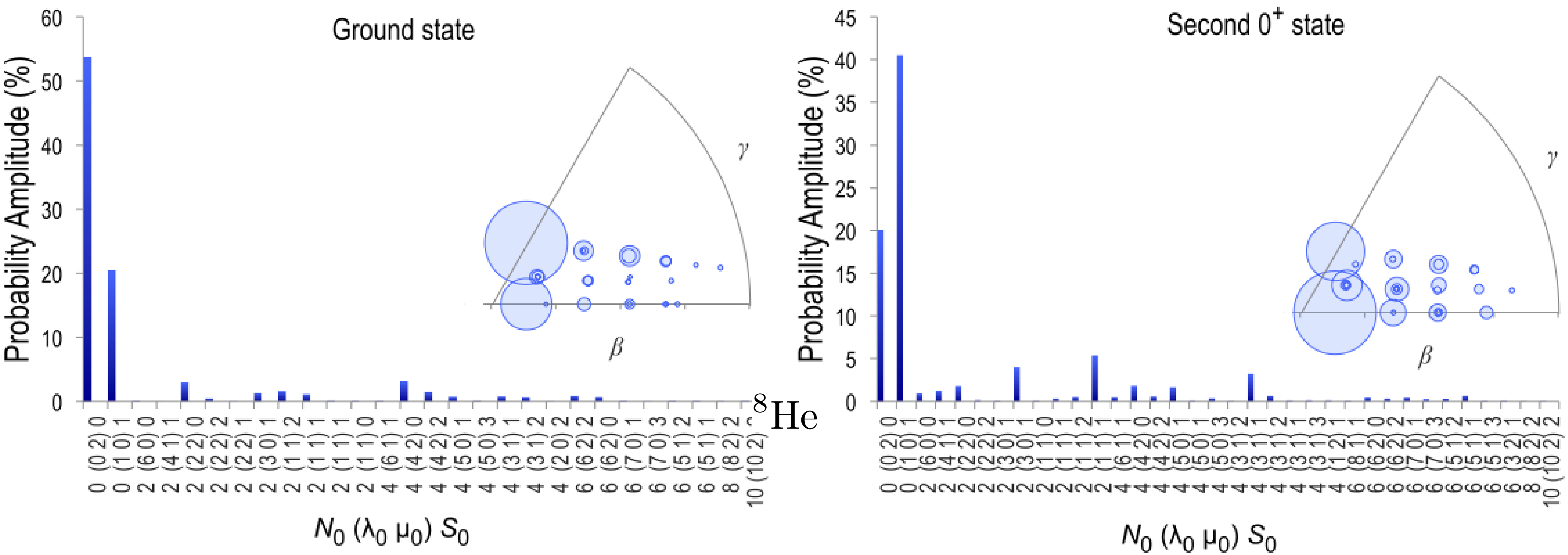


^{20}Ne, EM-N^{3}LO NN



Emerging symplectic structure in 0+ states of 8He

$^{8}\text{He NNLO}_{\text{opt}}$

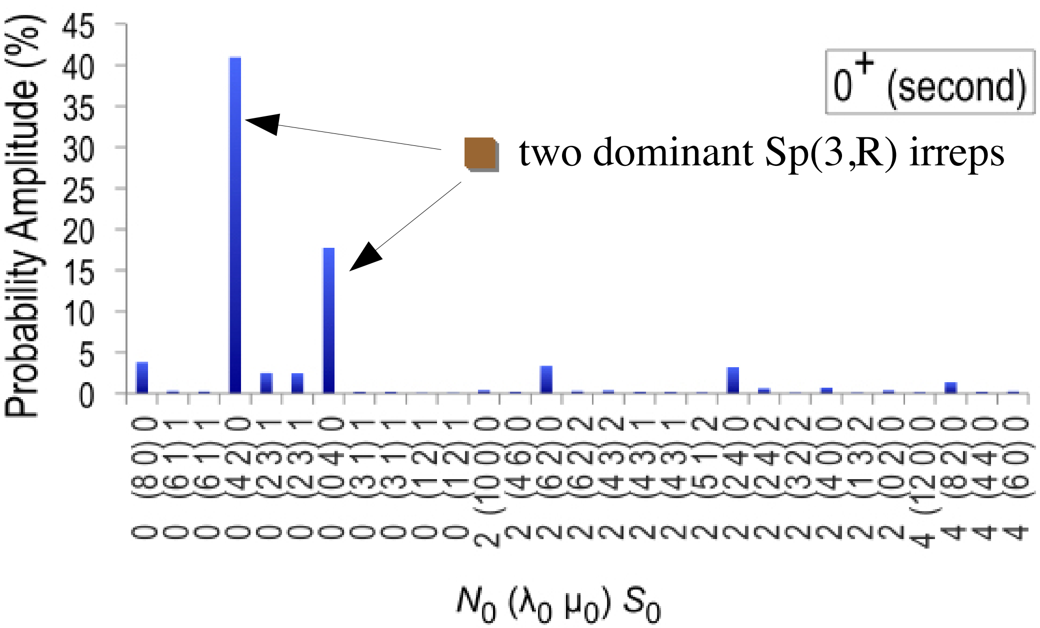


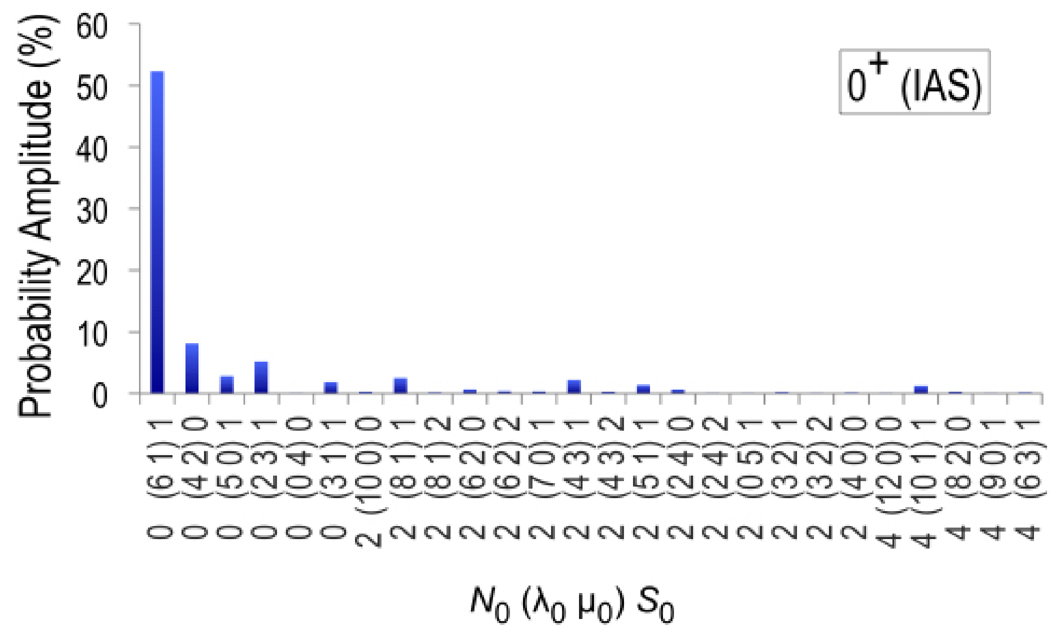
- structure of 8He is dominated by two Sp(3,R) irreps with different deformation
    - oblate 0 (0 2) S=0
    - prolate 0 (1 0) S=1
- both shapes add constructively to B(E2) strength from J=2 rotational state

T. Dytrych, K. D. Launey, J. P. Draayer et al, Phys. Rev. Lett. 124, 042501 (2020)

Emerging symplectic structure in 0+ states of 20Ne

- project 20 lowest-lying 0+ wave functions of 20Ne obtained in Nmax=8 model space to Sp(3,R) states



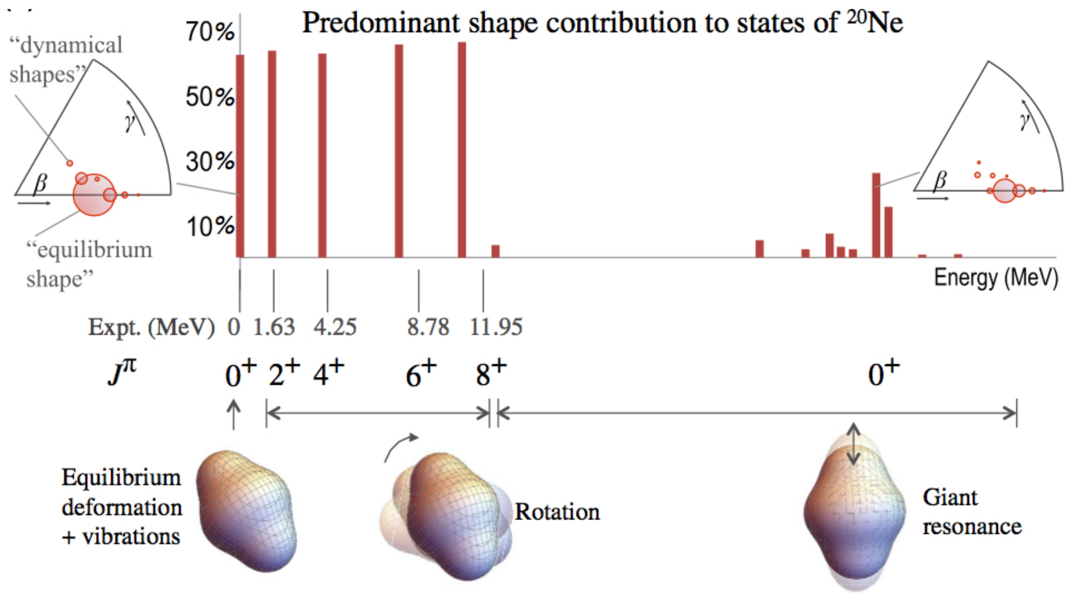


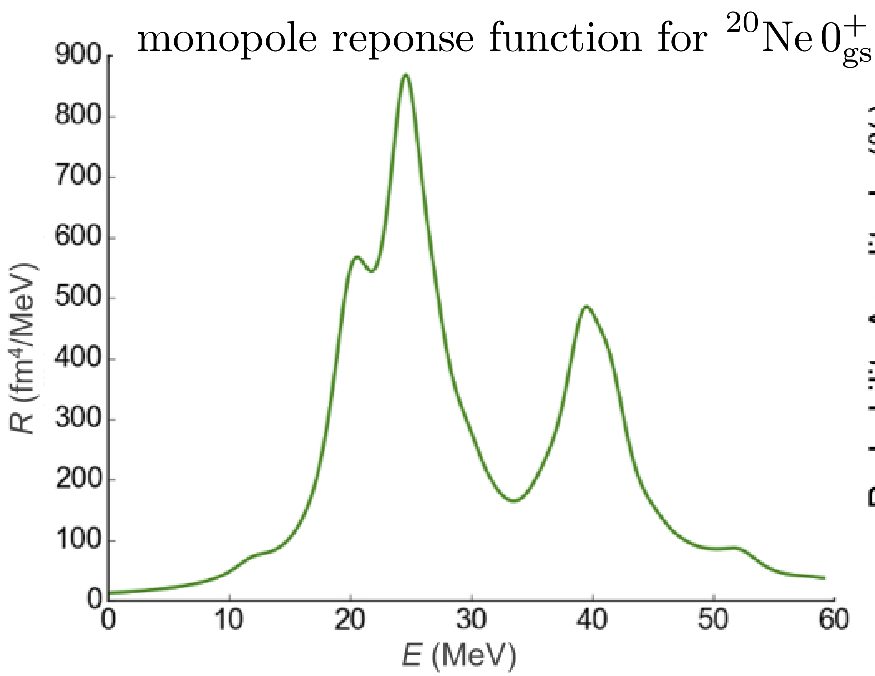
- coherent mixing of Sp(3,R) irreps
  - observed for members of rotational bands
  - emergence of quasi-dynamical symmetry – David Rowe described its mathematical structure and physical significance

- same structure as lowest 0+ in 20F and 20Na

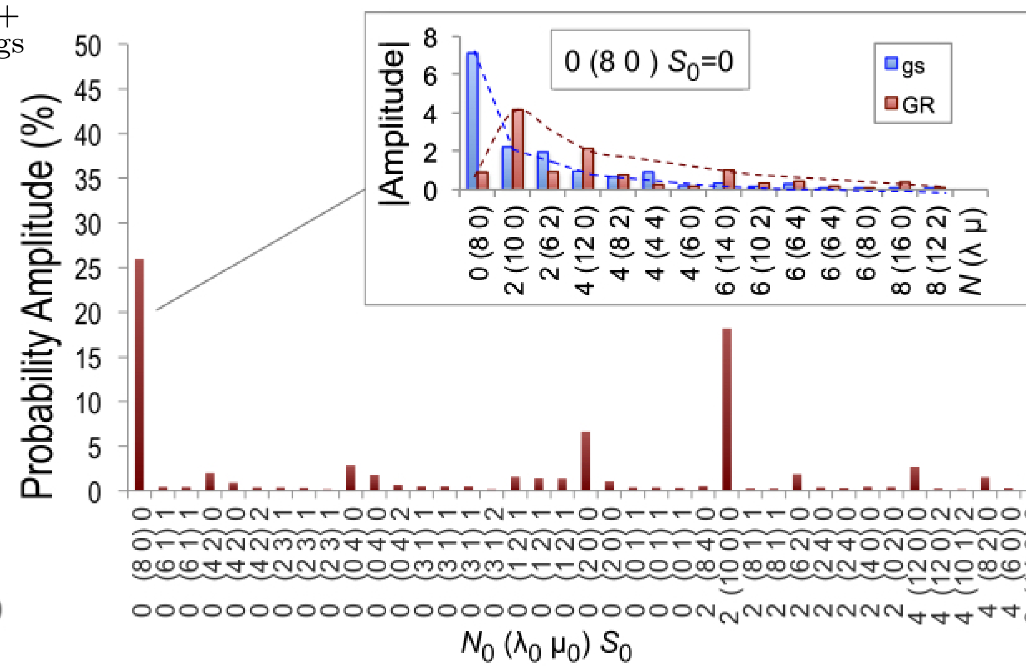
T. Dytrych, K. D. Launey, J. P. Draayer et al, Phys. Rev. Lett. 124, 042501 (2020)

Monopole resonance in 20Ne





(a)

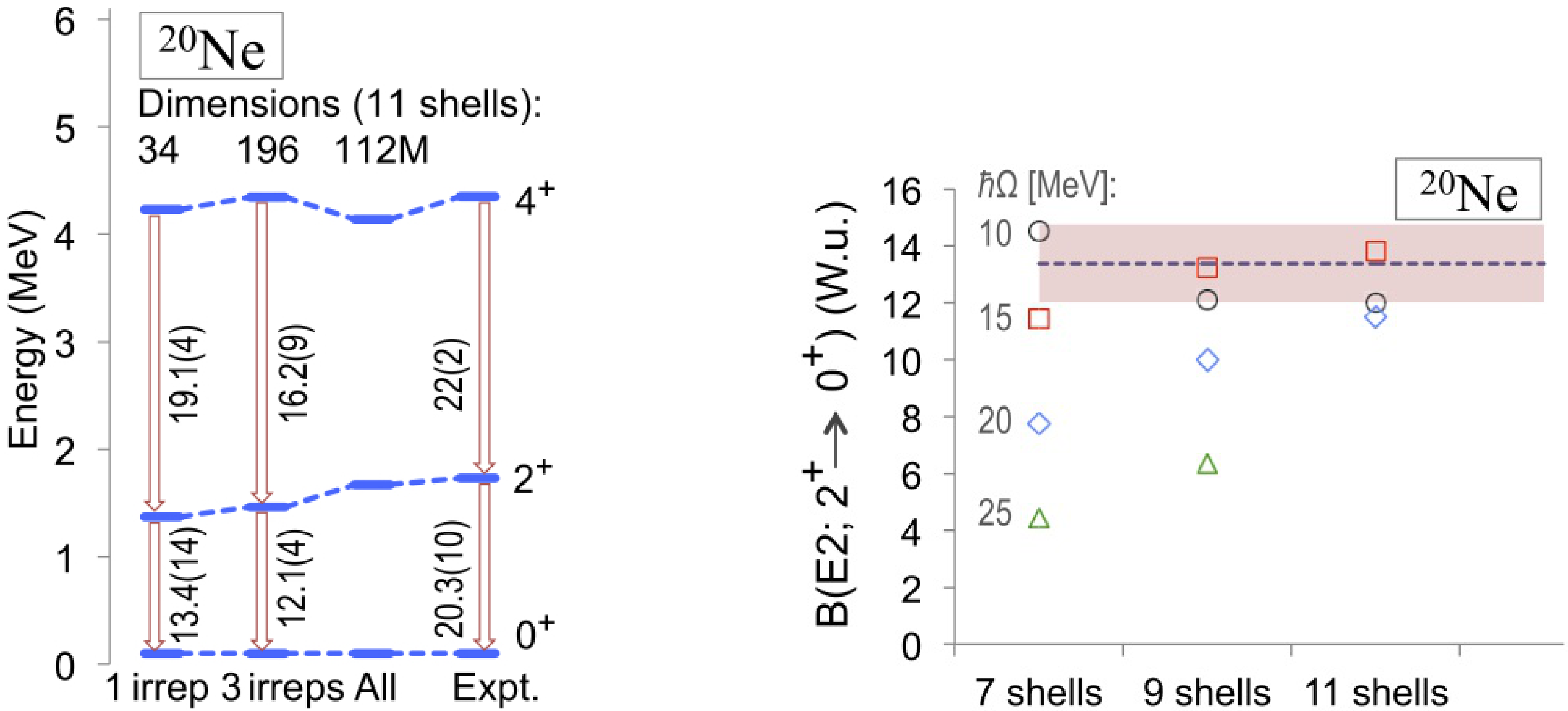


(b)

T. Dytrych, K. D. Launey, J. P. Draayer et al, Phys. Rev. Lett. 124, 042501 (2020)

SA-NCSM in Sp(3,R) basis

- We implemented SA-NCSM in Sp(3,R) basis



- B(E2), rms, excitation energies are on a good converging trend
- Results extrapolated to infinite shells

T. Dytrych, K. D. Launey, J. P. Draayer et al, Phys. Rev. Lett. 124, 042501 (2020)

SA-NCSM in Sp(3,R) basis

- Alternative method for computing matrix elemets in Sp(3,R) basis proposed in 80's
  - Y. Suzuki and K. T. Hecht, Nucl. Phys. A 455, 315 (1986).
  - Y. Suzuki and K. T. Hecht, Prog. Theor. Phys. 77, 190 (1987).
- Matrix elements are computed recursively from reduced matrix elements of Sp(3, R) bandheads
- Anna E. McCoy (Notre Dame): Ab Initio Multi-Irrep Symplectic No-Core Configuration Interaction Calculations

- Requirements:
  - SU(3) coupling-recoupling coefficients ... available
  - rmes of Sp(3,R) bandheads ... available

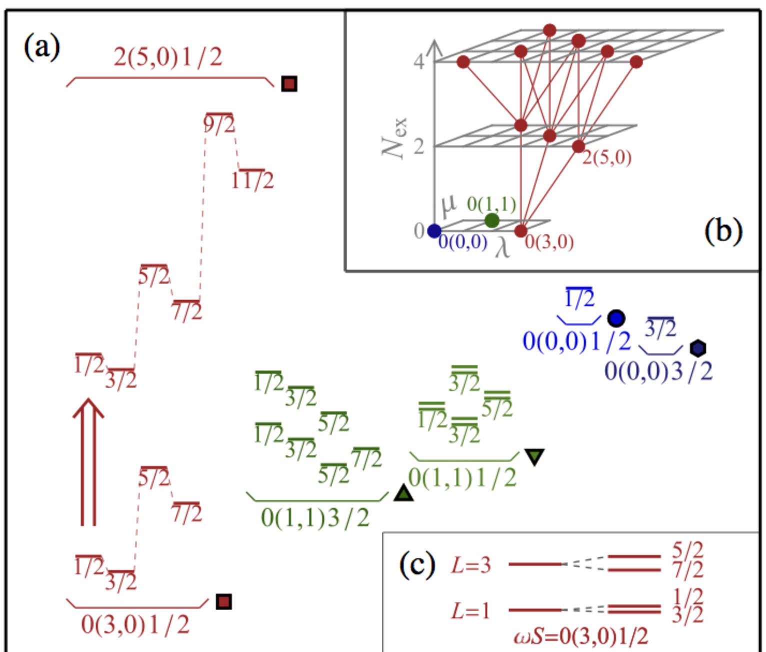
A. E. McCoy, M. A. Caprio, T. Dytrych and P. Fasano, Phys. Rev. Lett. 125, 102505 (2020)

Emergence of Sp(3,R) symmetry in low-lying states of 7Be

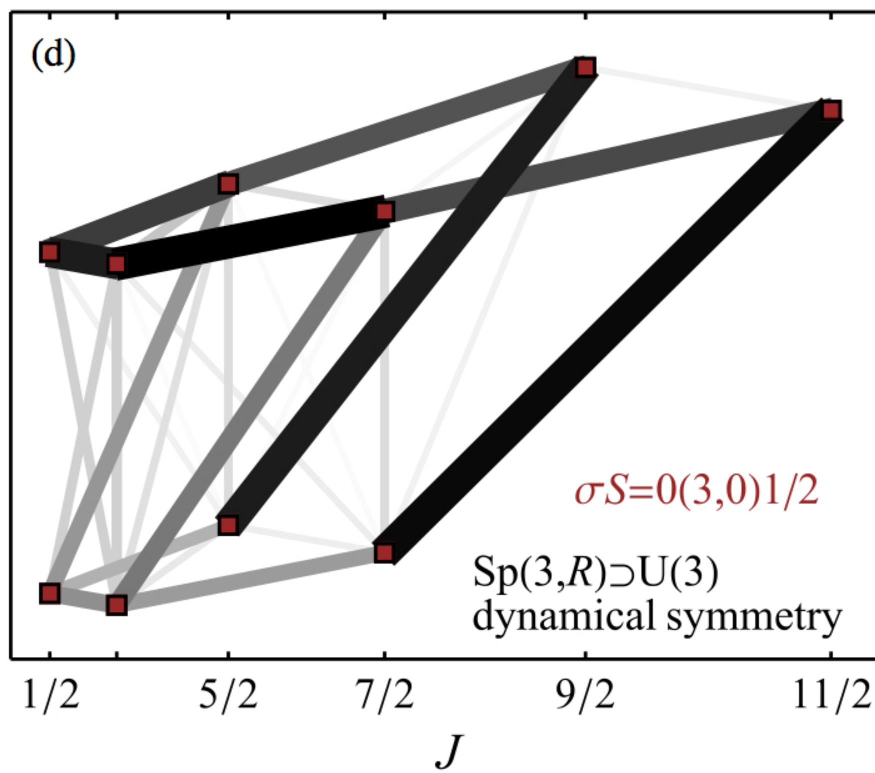
- Complete Nmax=6 model space calculation for 7Be with Deajon16 interaction in Sp(3,R) basis
- Confirms ubiquity of symplectic symmetry in low-lying states
- Low-lying states in 7Be are underpinned by emergent $\mathrm{Sp}(3,\mathrm{R}) \supset \mathrm{SU}(3)$ dynamical symmetry

$$H = \alpha C_{\mathrm{Sp}(3,\mathbb{R})} + \varepsilon H_0 + \beta C_{\mathrm{SU}(3)} + a_L \mathbf{L}^2 + a_S \mathbf{S}^2 + \xi \mathbf{L}\cdot\mathbf{S}.$$

spectrum

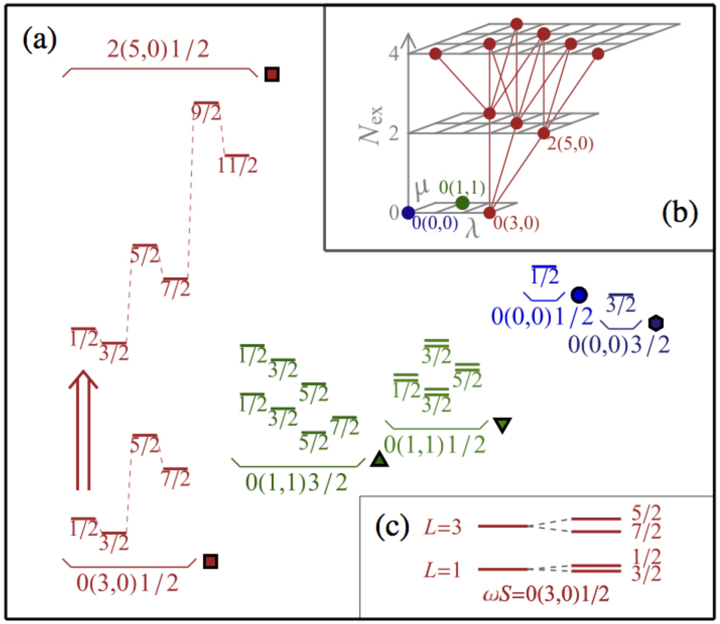


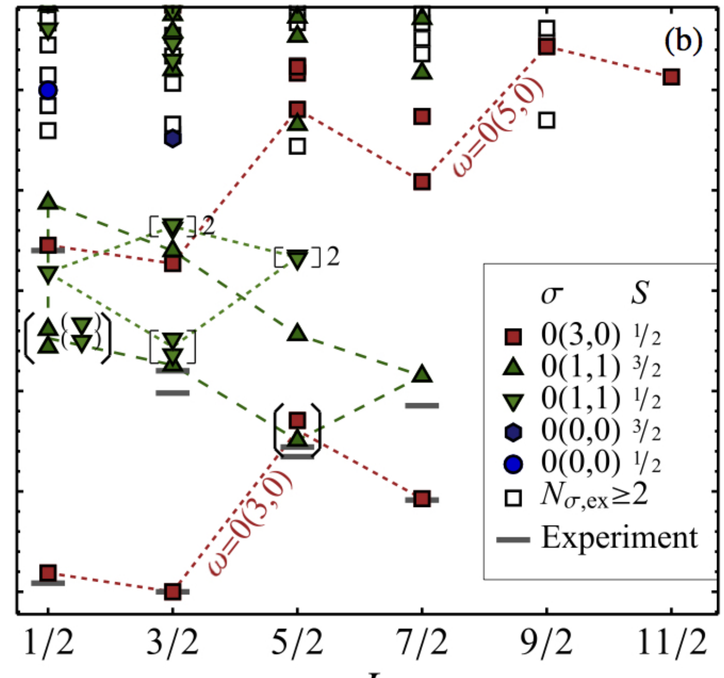
B(E2) transitions

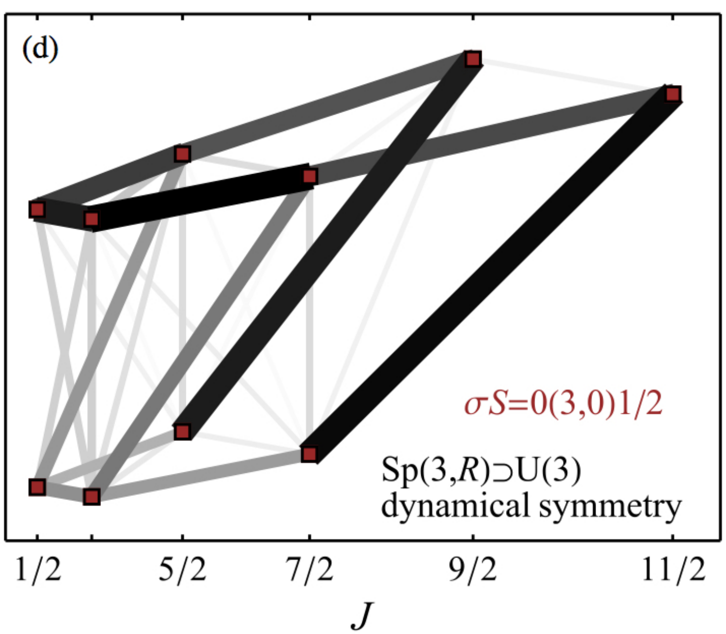


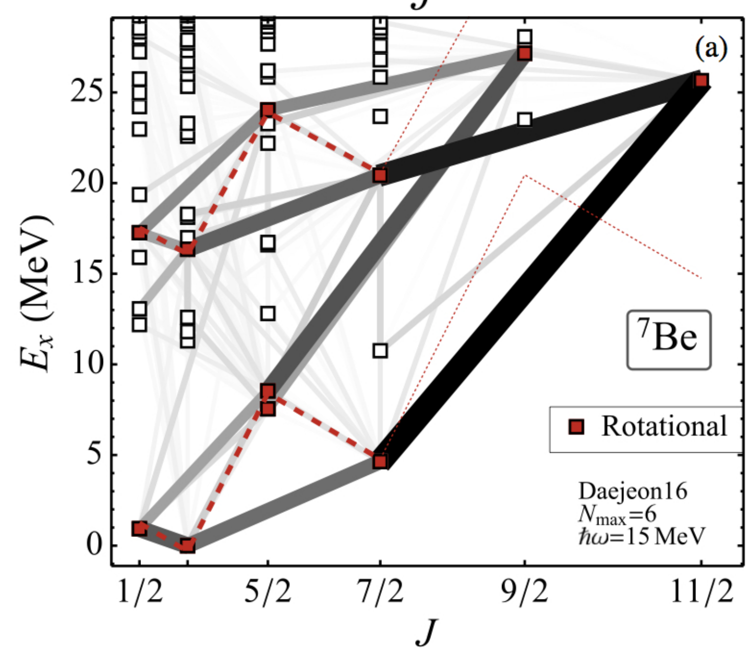
A. E. McCoy, M. A. Caprio, T. Dytrych and P. Fasano, Phys. Rev. Lett. 125, 102505 (2020)

Emergence of Sp(3,R) symmetry in low-lying states of 7Be









A. E. McCoy, M. A. Caprio, T. Dytrych and P. Fasano, Phys. Rev. Lett. 125, 102505 (2020)

Computational advances and development

- in collaboration with Daniel Langr, Czech Technical University in Prague.
- Goal: extend the reach of SA-NCSM formalism towards heavier nuclear systems
- Approach: express the elegant language of group theory in form of efficient and scalable algorithms

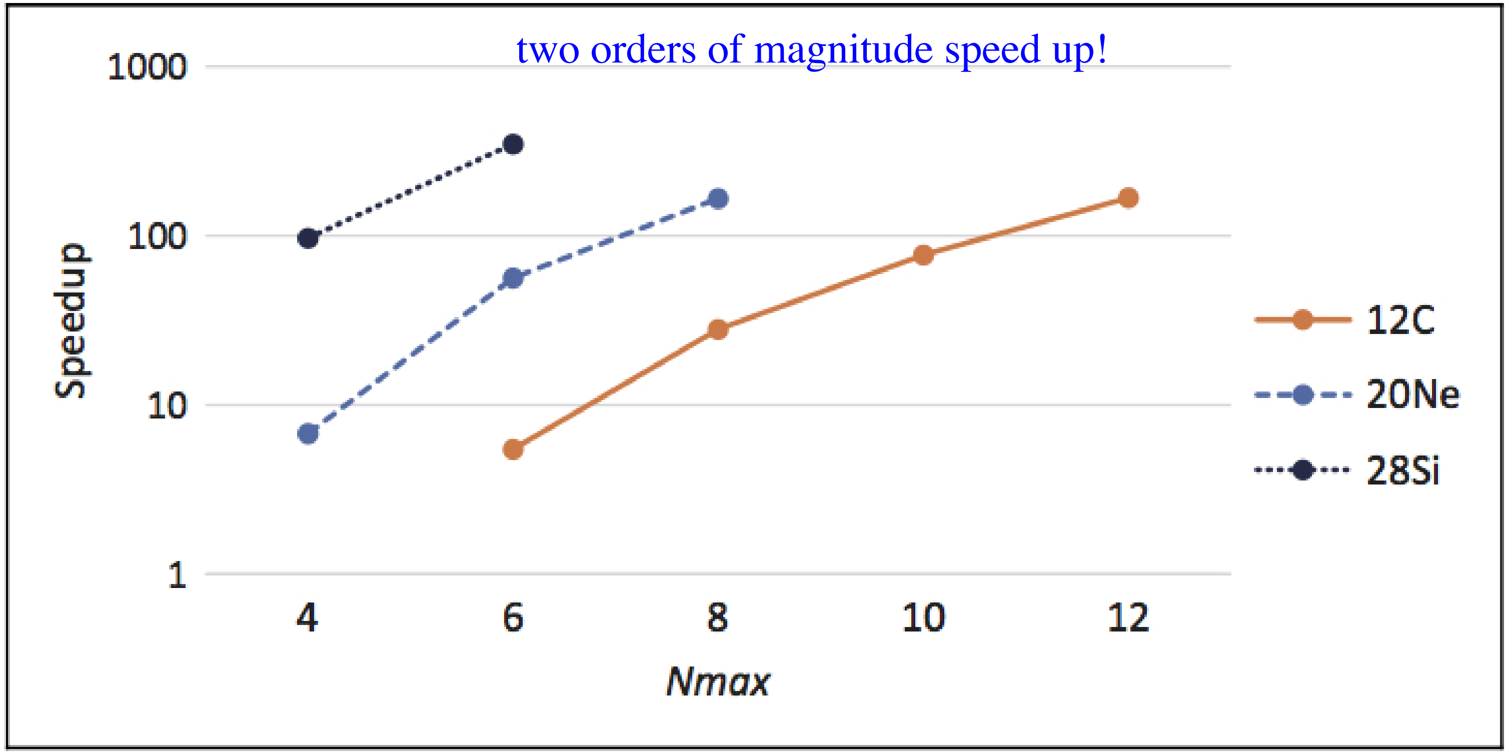
- Challenges set. Challenges met.
  - $\mathrm{U}(\Omega) \rightarrow \mathrm{SU}(3)$ reduction for heavier nuclei
  - Generation of SU(3)-scheme many-nucleon basis for heavier systems
  - Accurate SU(3) coefficients for large irreps and outer multiplicities

Computational advances and development

- $\mathrm{U}(\Omega) \rightarrow \mathrm{SU}(3)$ reduction
  - a new efficient and scalable algorithm -- two orders of magnitude speed up

  D. Langr, T. Dytrych, J. P. Draayer et al., Computer Physic Comunication 244, 442 (2019)

- Generation of SU(3) coupled many-nucleon basis
  - Efficient and scalable algorithm implemented in hybrid MPI/OpenMP parallel approach



- U(3) symmetry-adapted basis generation reduced to a fraction (< 0.2%) of total computing time

  D. Langr, T. Dytrych, J. P. Draayer et al, Int. J of High Perf. Comp. App. 33(3), 42 (2019).

Computational advances and development

- SU3lib: A C++ library for accurate computation of Wigner and Racah coefficients of SU(3)
  - Publicly available: https://gitlab.com/tdytrych/su3lib
  - Modern C++ implementation of Draayer and Akyiama method
  - provides accurate results for large SU(3) irreps and multiplicities heretofore inaccessible

Major enabling feature for SA-NCSM framework

T. Dytrych, D. Langr, J. P. Draayer et al., Computer Physic Comunication 269, 108137 (2021)

- LSU3shell: implementation of SA-NCSM for U(3) and Sp(3,R) adapted basis
  - Publicly available: https://gitlab.com/tdytrych/lsu3shell

Summary

- Modern SU(3) based SA-NCSM framework developed
  - It's implementation scales well runs efficiently on modern supercomputers
  - New applications of ab initio SA-NCSM for structure and reactions modeling emerging
- Ab initio SA-NCSM framework with Sp(3,R) basis developed
- Key role of emergent symplectic Sp(3,R) symmetry unveiled in light and medium-mass nuclei
- Dramatic improvement of foundational algorithms of SA-NCSM approach