Next-Generation *Ab Initio* Symmetry-Adapted No-Core Shell Model and Its Impact on Nucleosynthesis

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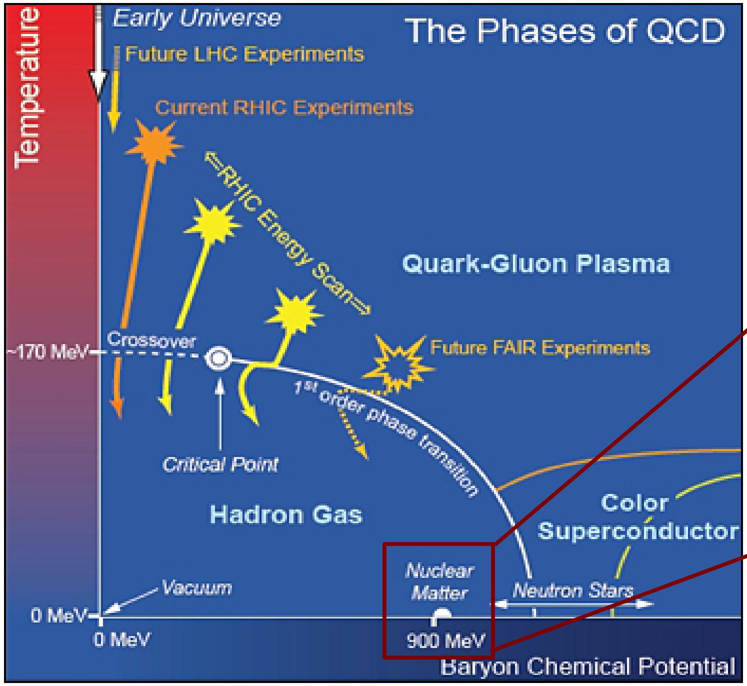
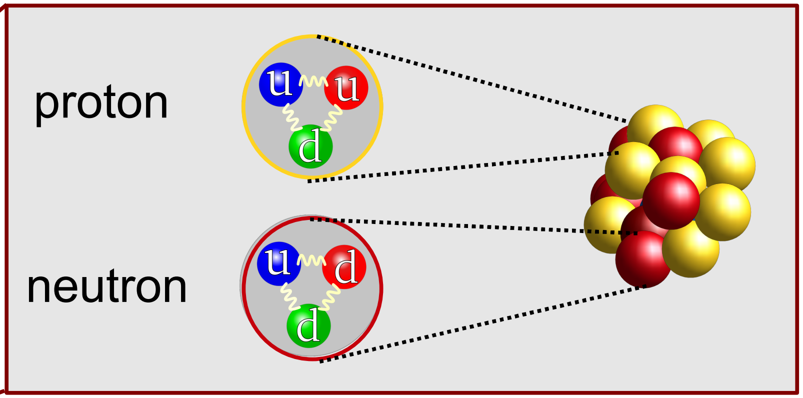
Physics of Atomic Nuclei



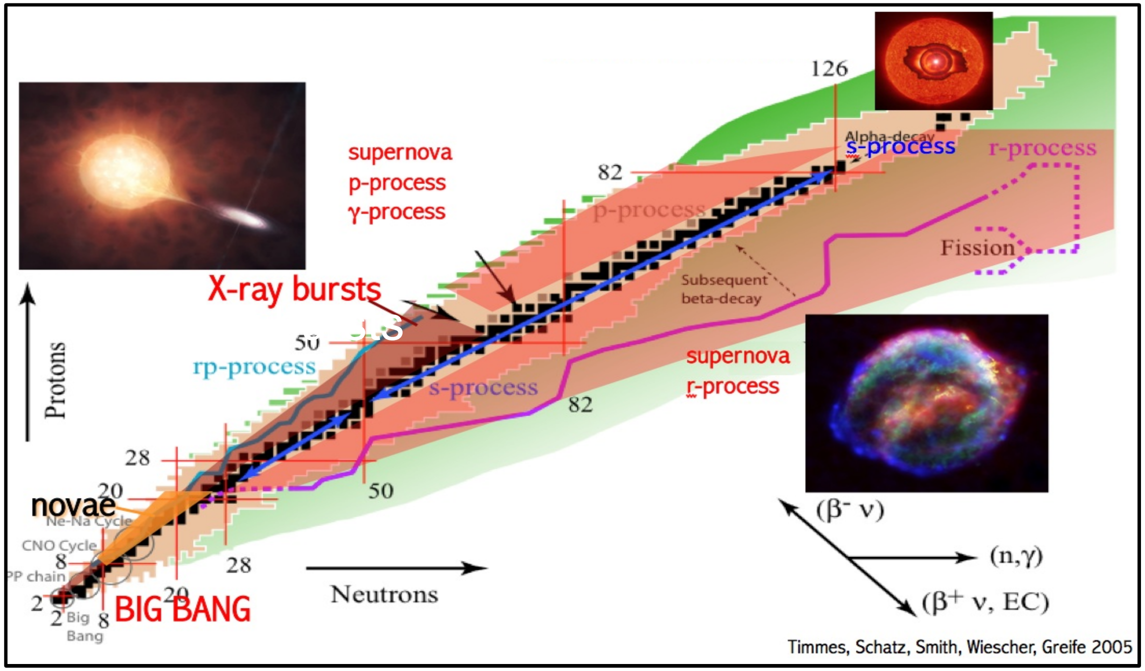


- **Nuclear interactions**
  - Residual strong force $\rightarrow$ highly complex
  - two-, three- and four-body forces

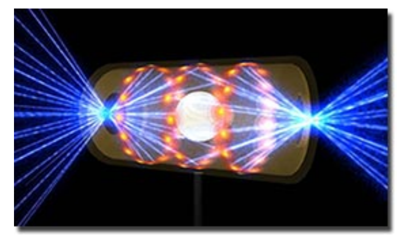
- **Discovery potential in nuclear physics**
  - Universal internucleon interaction derived from QCD
  - Properties and reactions of nuclei at the edge of their existence
  - Accurate tests of fundamentals laws of nature
  - Emergence of simple features from highly complex interactions

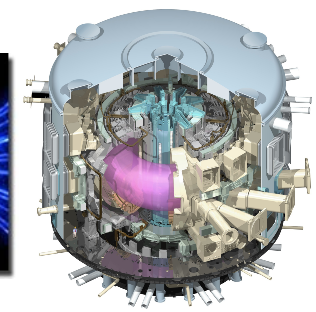
Applications of Nuclear Structure & Reaction Modeling

Astrophysics: thermonuclear processes in the cosmos

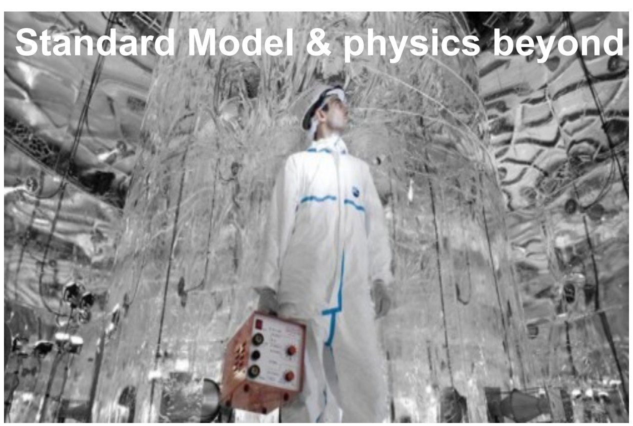


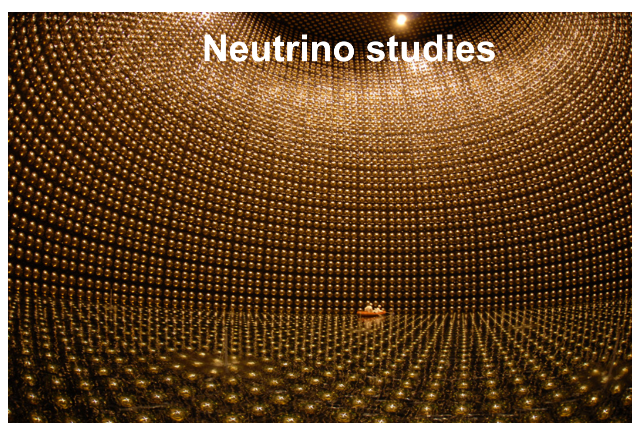
Nuclear reactions for applied energy studies

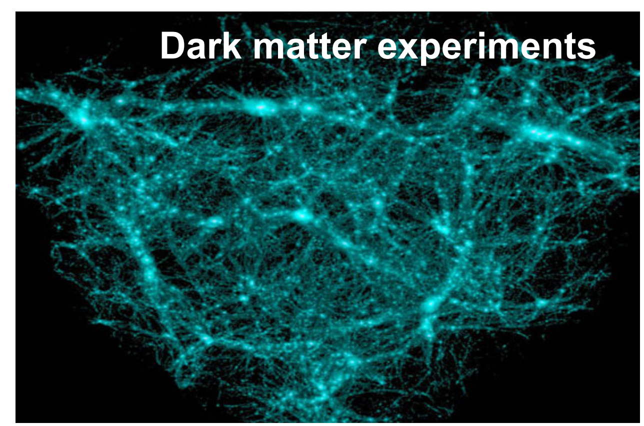




Neutrino & Cosmology research

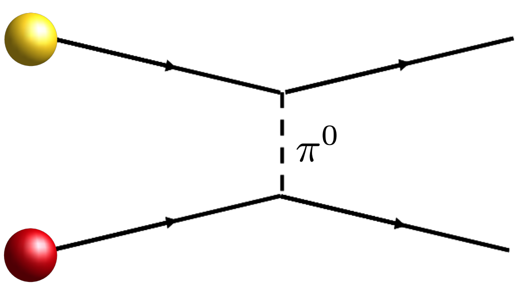






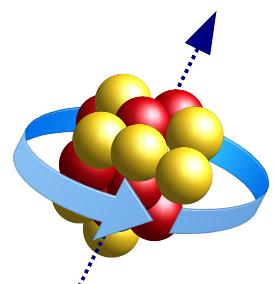
Ab initio Approaches to Nuclear Structure and Reactions

Strong interaction



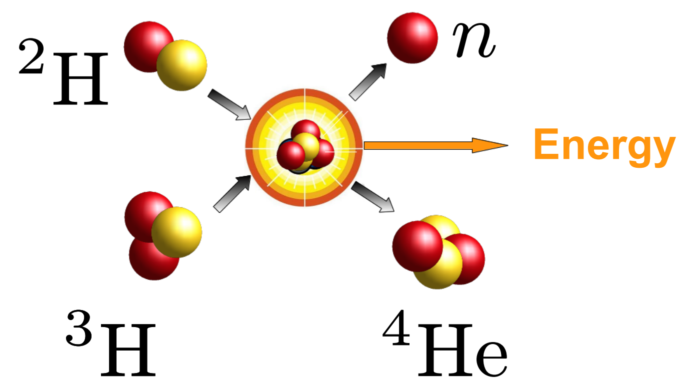
- Realistic nuclear potential models

Many-body dynamics



- wave functions nuclear properties

Nuclear reactions



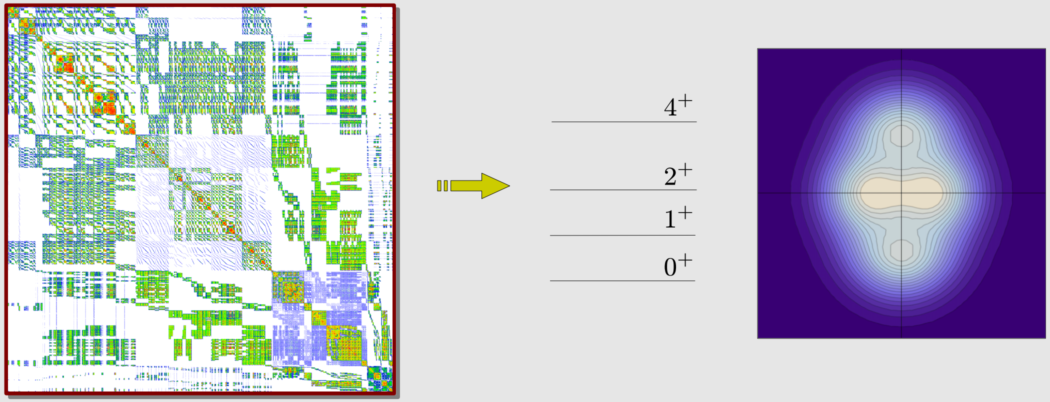
- reaction rates cross sections

Ab Initio No-Core Shell Model

- **Goal:** Solve the non-relativistic quantum problem of A-interacting nucleons

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle \qquad \hat{H} = T + V_{\text{Coul}} + V_{NN} + \ldots$$

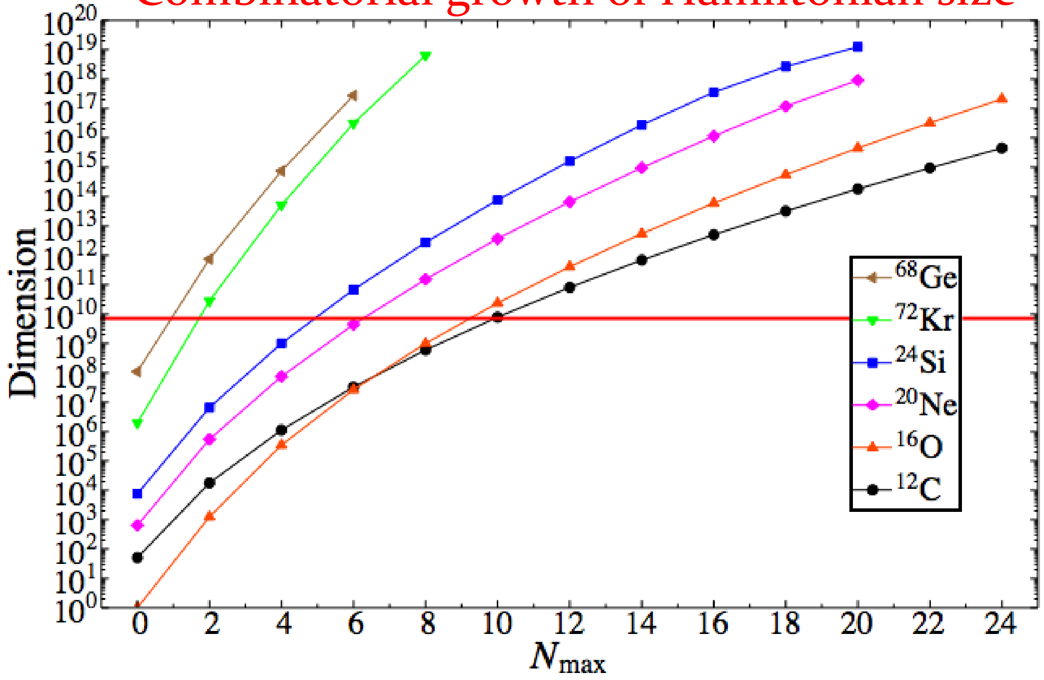
1. Choose **physically relevant** model space and construct its basis $\{|\phi_1\rangle, \ldots, |\phi_d\rangle\}$
2. Compute Hamiltonian matrix $H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$
3. Find lowest-lying eigenvalues and eigenvectors [Lanczos algorithm]

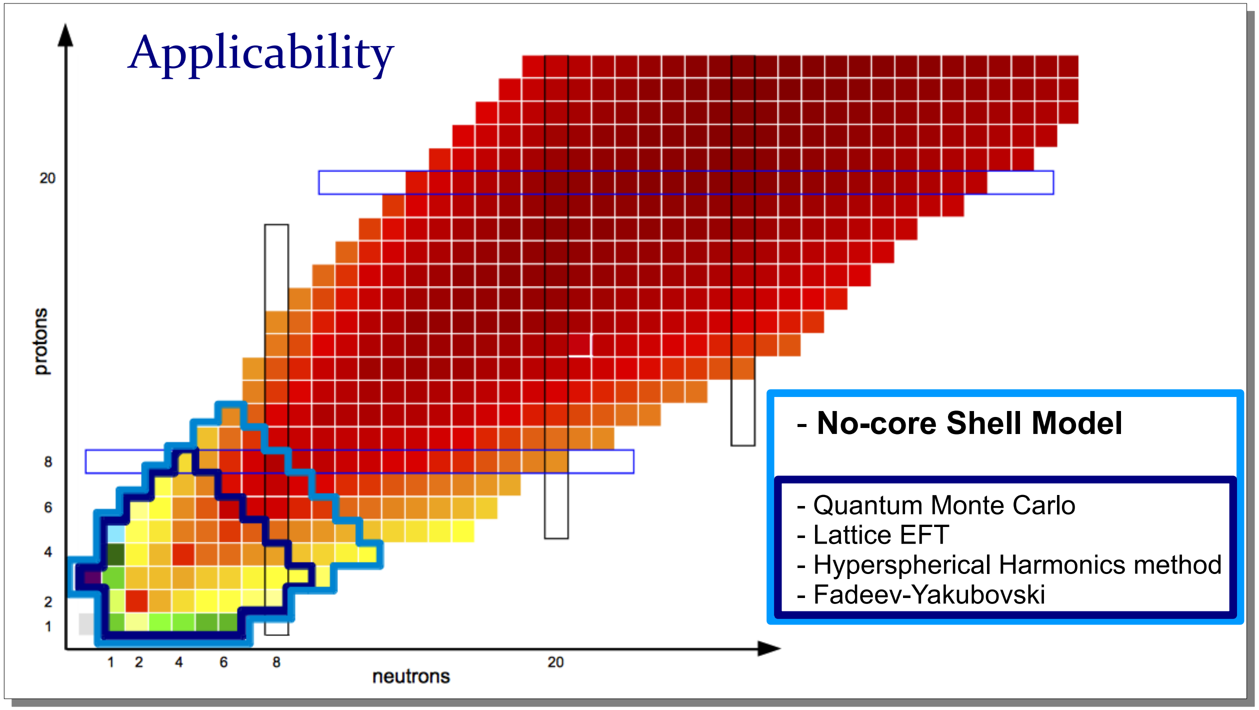


- **Resulting wave functions:**
  - obey Pauli exclusion principle
  - exact separation between intrinsic and center-of-mass motion

Computational Challenge: Scale Explosion

Combinatorial growth of Hamiltonian size



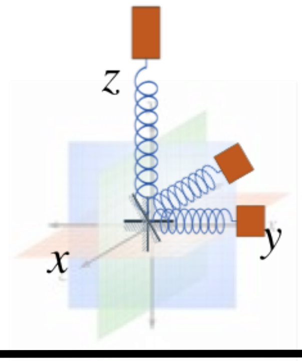
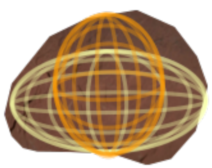


Computational Scale Explosion

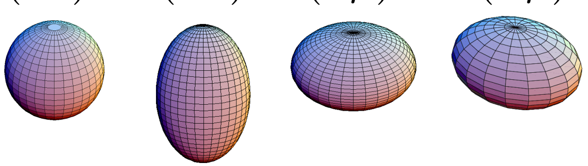
- Applicability limited to light nuclei
- Memory bound

Symmetry-Adapted No-Core Shell Model

- Many-nucleon basis natural for description of many-body dynamics of nuclei

number of HO excitations			N
total proton, total neutron and total intrinsic spins			$S_p\, S_n\, S$
deformation	SU(3)		$(\lambda\,\mu)$
rotation	SO(3)		L

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



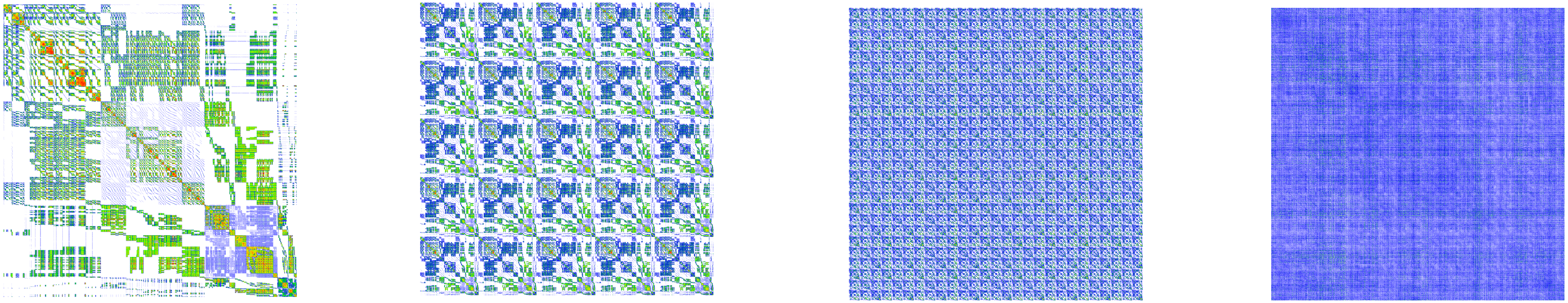
- Three pillars of Symmetry-Adapted No-Core Shell Model
  - Computational group theory
  - Nuclear physics
  - High performance computing

MPI/OpenMP Implementation of Symmetry-Adapted No-Core Shell Model

Computational effort

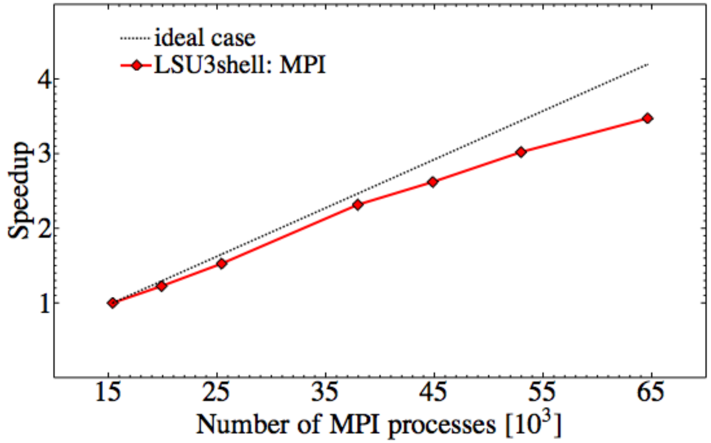
- 95% - computing matrix elements ⟶ Embarassingly parallel problem
- 3% - solving eigenvalue problem

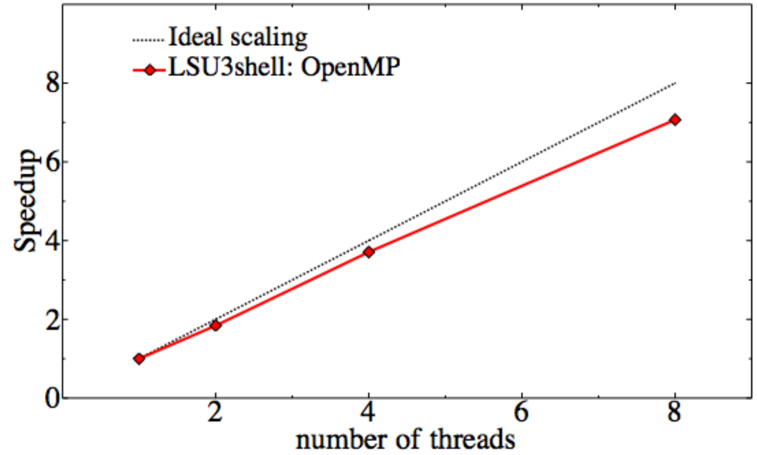
Load balanced computations



1 process — 15 processes — 378 processes — 37,950 processes

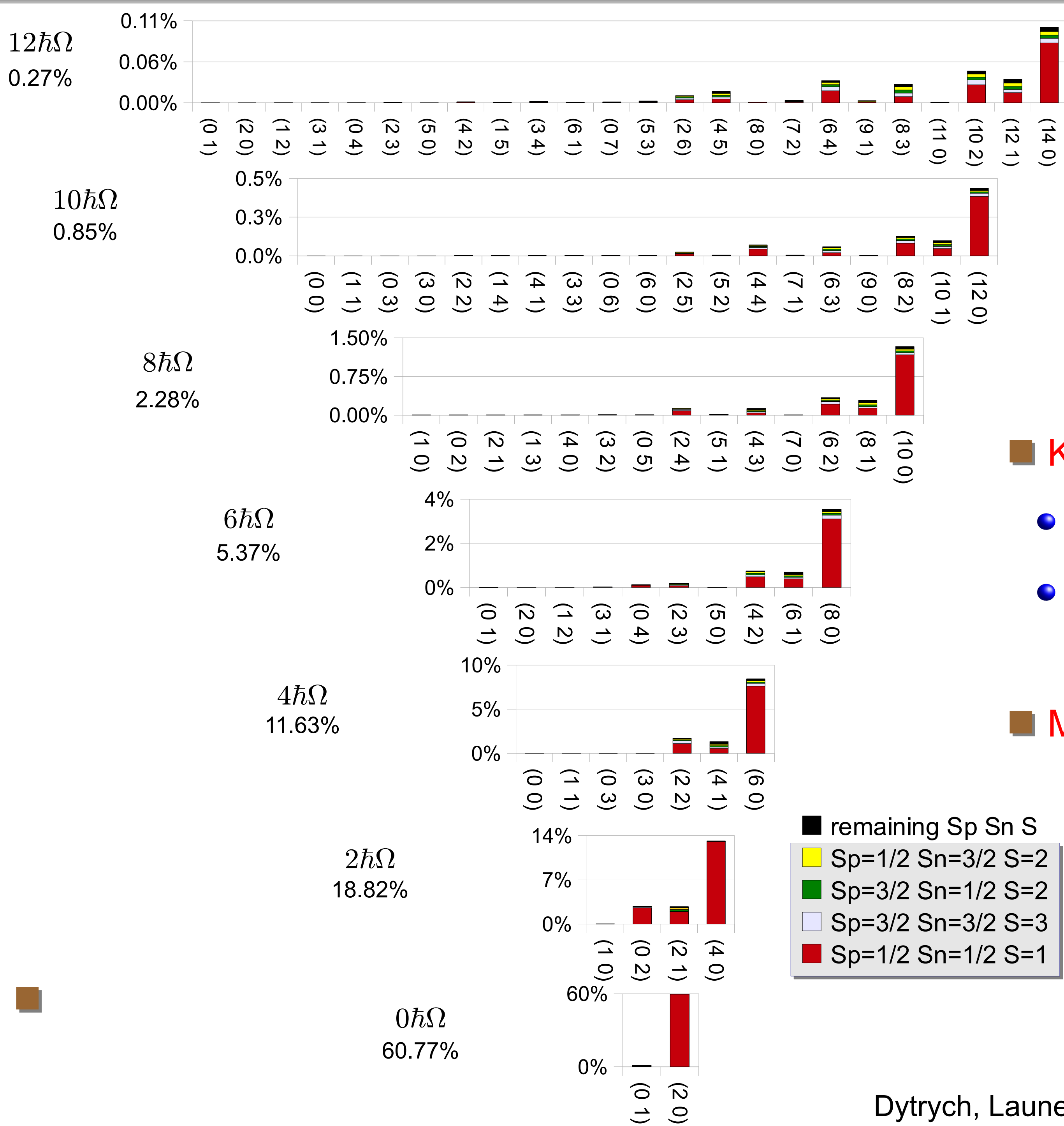
Excellent scalability





Discovery: Emergence of Simple Patterns in Complex Nuclei

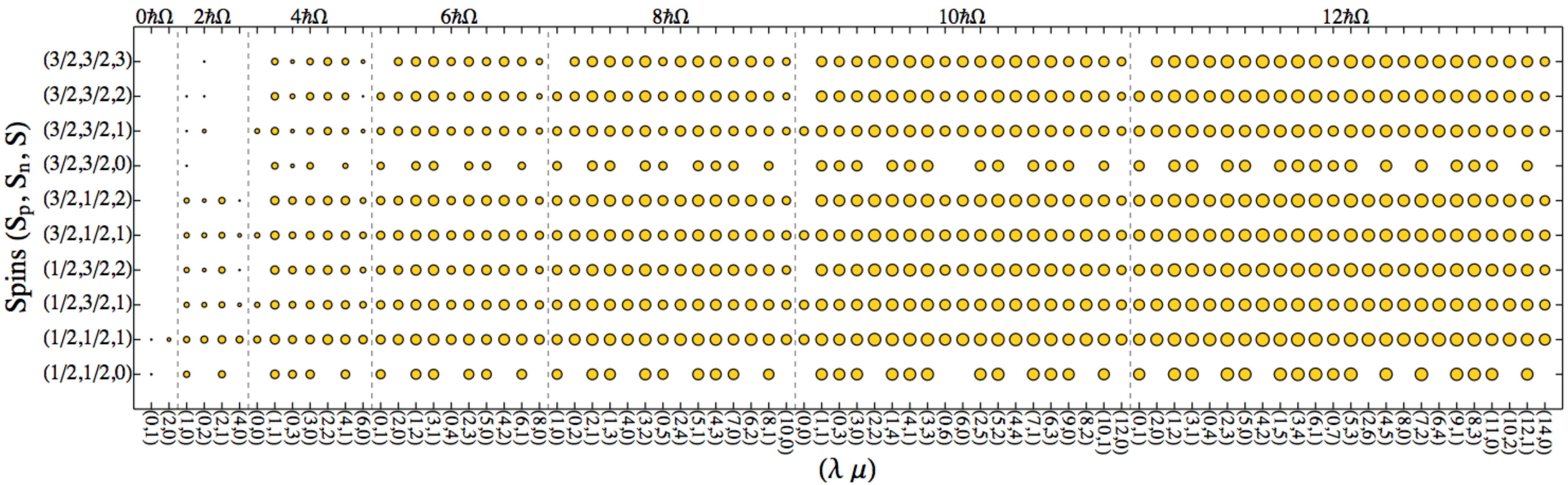
$^{6}\mathrm{Li} : 1^{+}_{gs}$



- Key features of nuclear structure
  - Low spin
  - Large deformation
- Model space truncation

Dytrych, Launey, Draayer, et al., PRL 111 (2013) 252501

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



- $N\hbar\Omega$ space: direct sum of subspaces [●] of states carrying the same $(\lambda\ \mu)$ and $S_p S_n S$

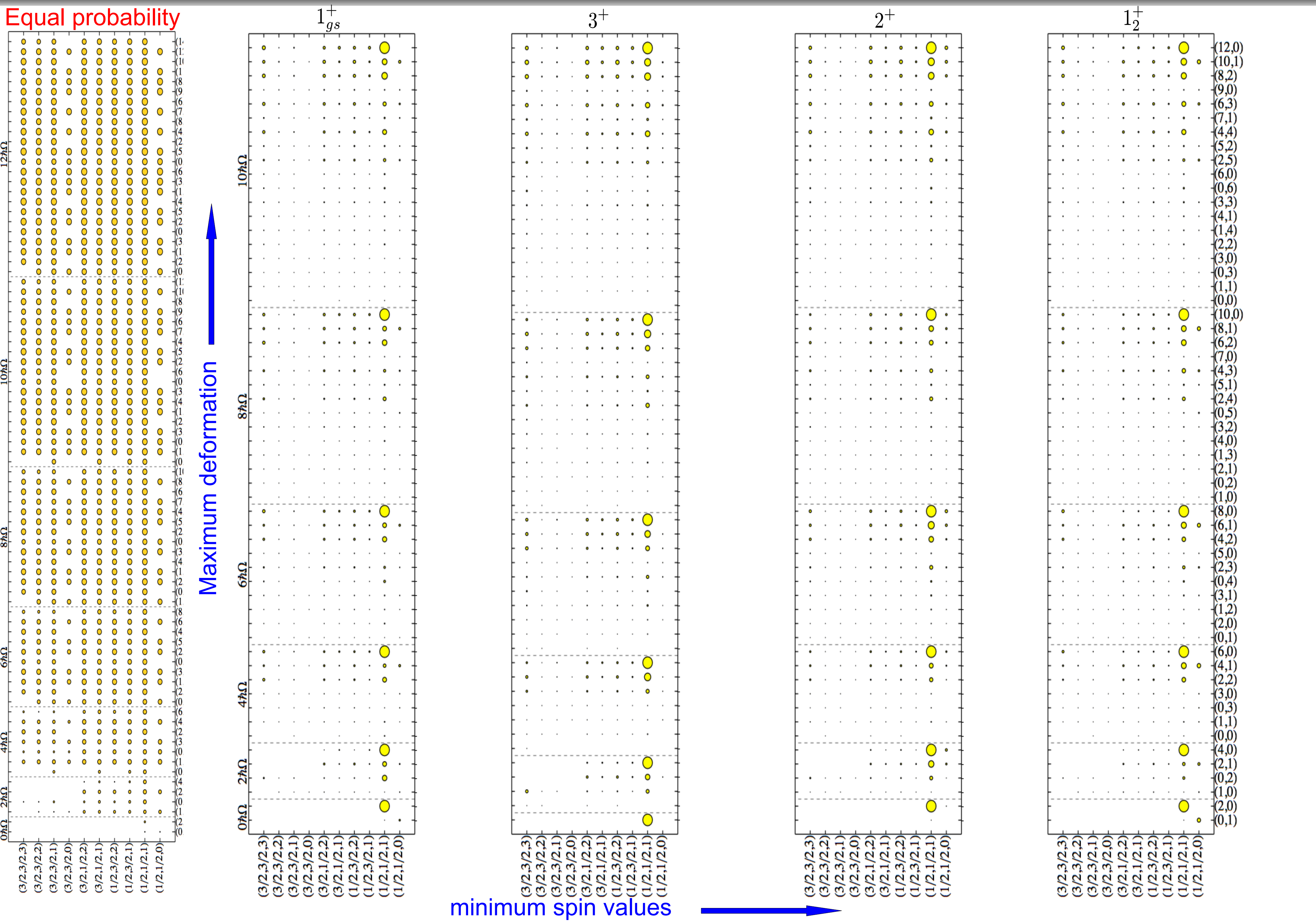
■ Symmetry-Adapted Truncation Scheme

(1) maximal number of total HO quanta Nmax

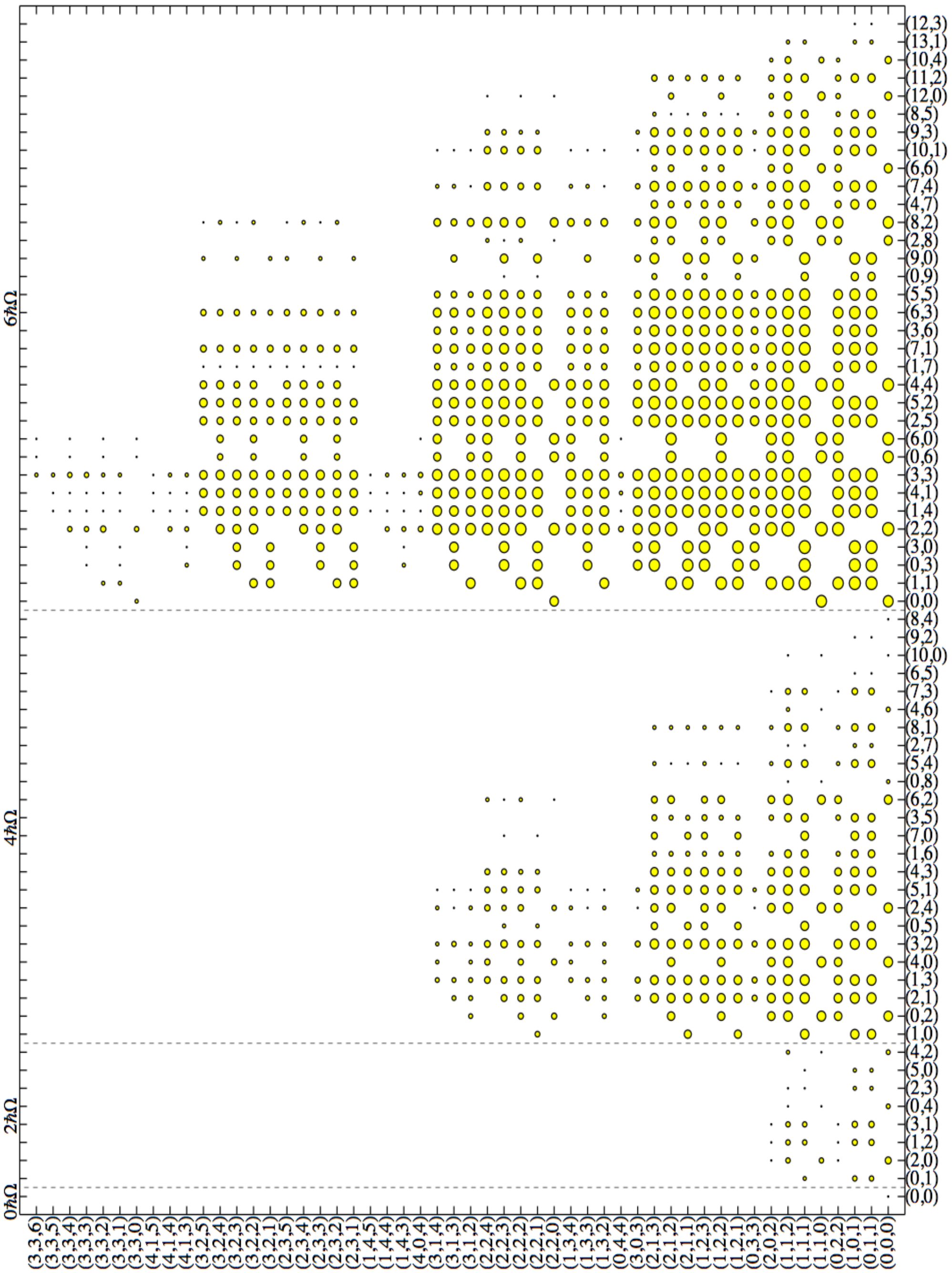
(2) intrinsic spins $S_p\, S_n\, S$

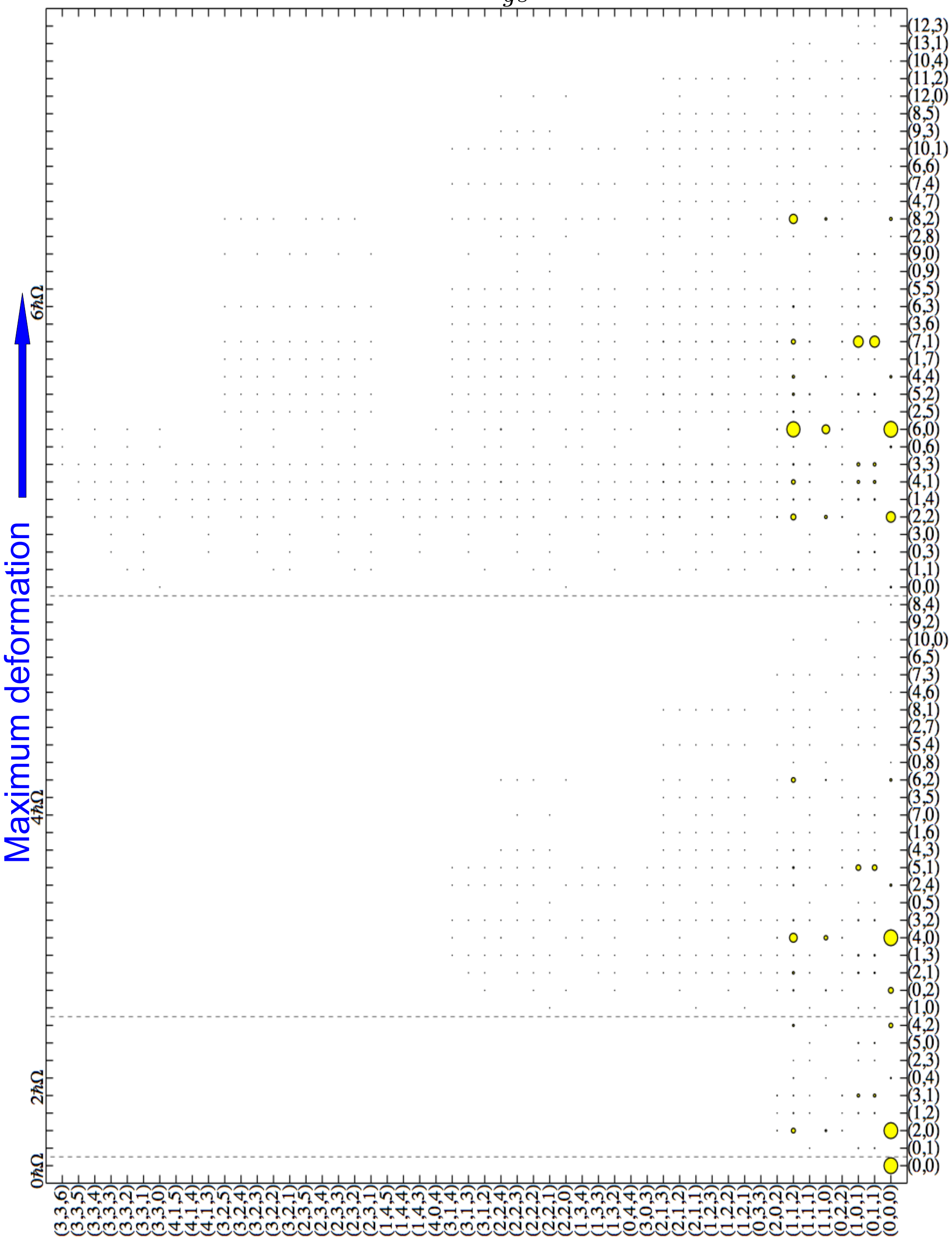
(3) deformations $(\lambda\ \mu)$

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



^{16}O

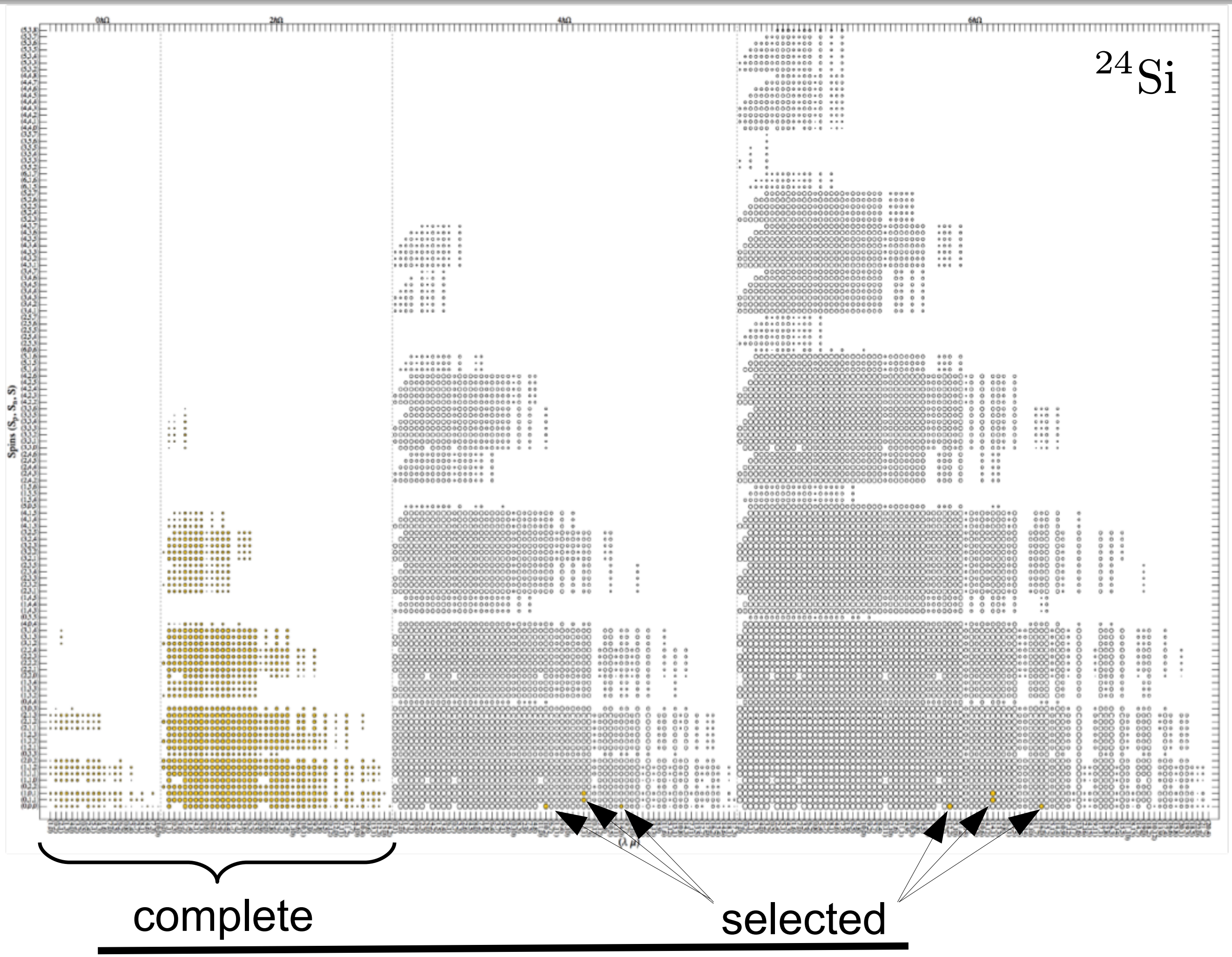




Maximum deformation

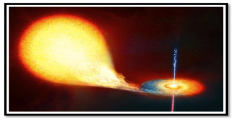
minimum spin values

SA-NCSM on BlueWaters: reaching towards medium mass nuclei



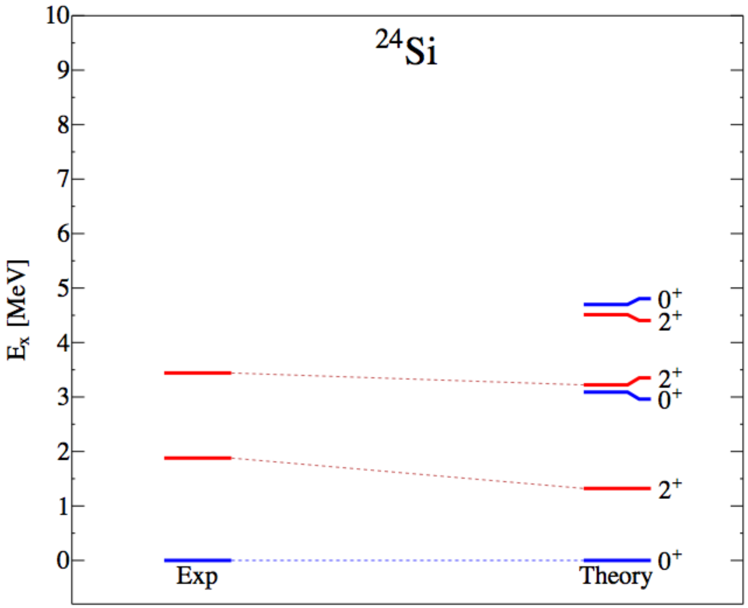
dimension: 3×10^6

Complete space dimension: 7×10^{10}



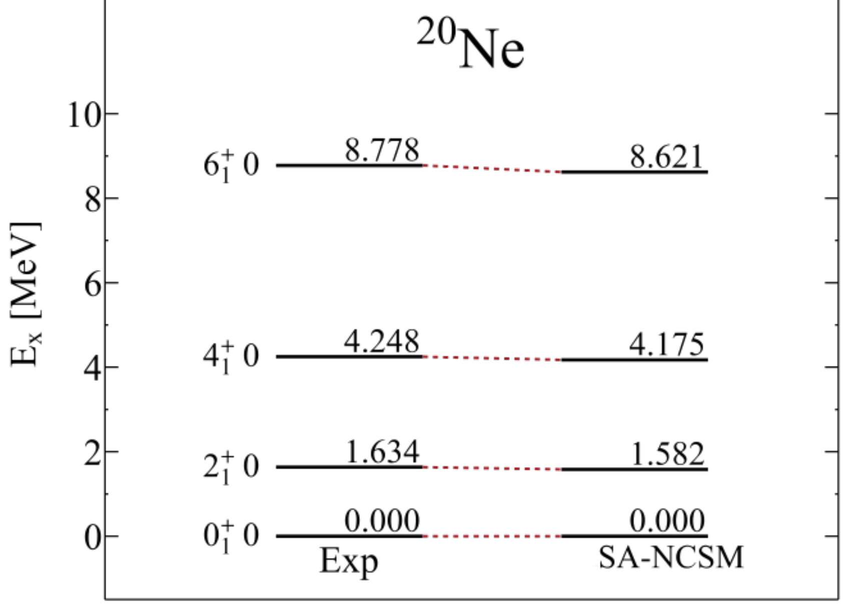
Novae and X-ray bursts

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

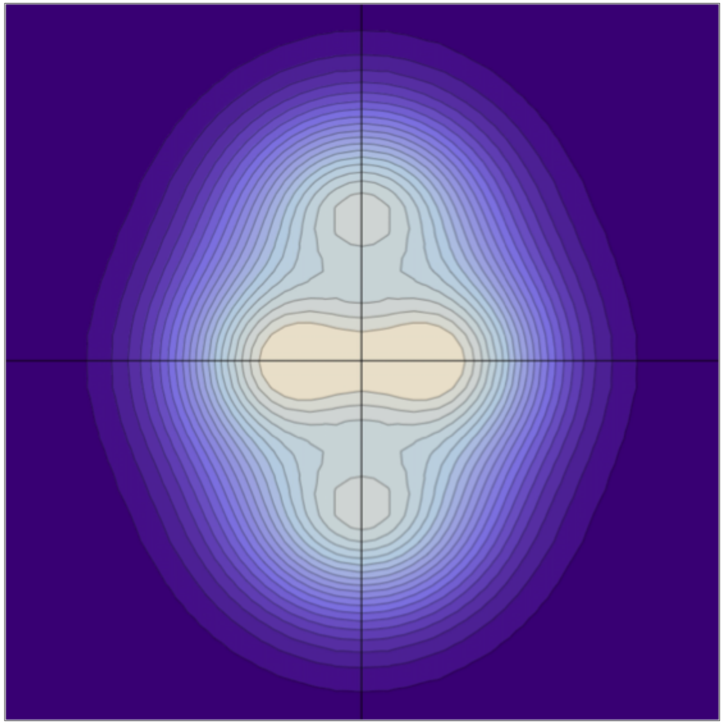


SA-NCSM on BlueWaters: reaching towards medium mass nuclei

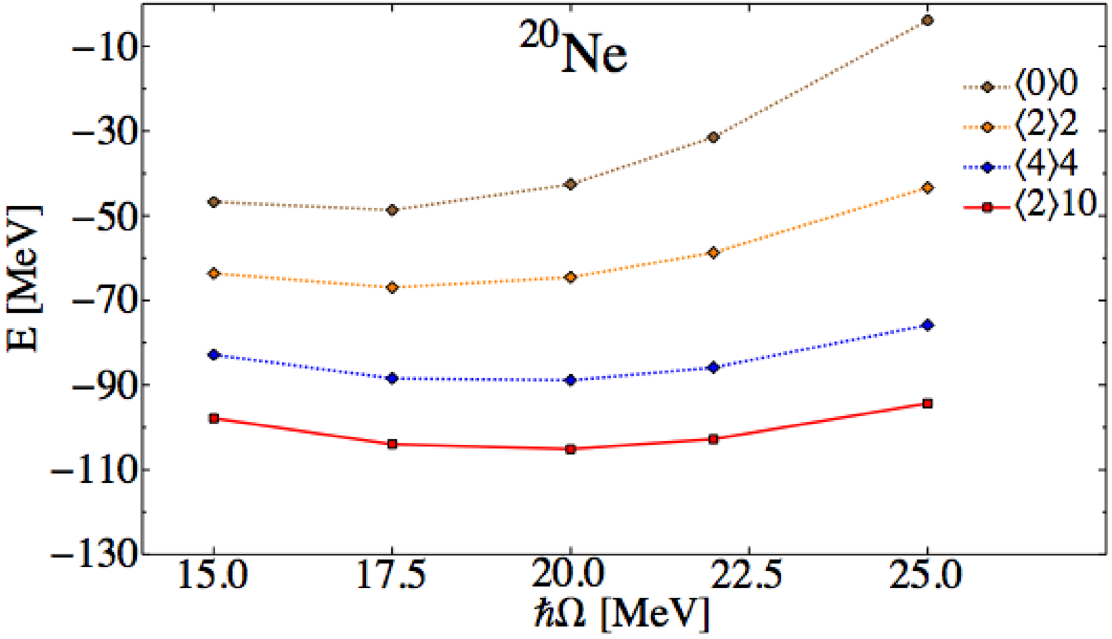
Excitation Spectrum



Nucleon Density



Binding energy



Complete space: 4×10^{12}

Symmetry-adapted space: 1×10^{7}

Summary

Symmetry-Adapted No-Core Shell Model on Blue Waters

- Collective modes emerge from first principles
- Physically relevant model spaces for ab initio modeling of nuclear structure
- First applications of ab initio theory to open shell medium mass nuclei