High performance computing in nuclear structure studies

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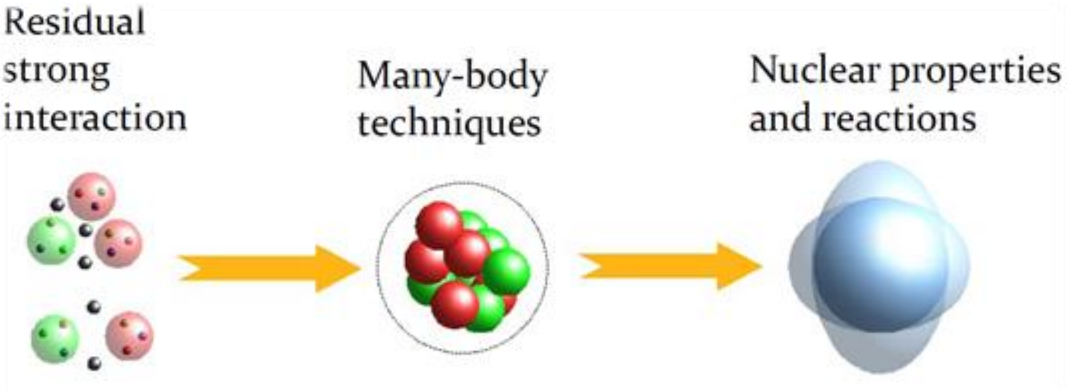
Ab-initio theory from nuclear physics perspective

- *Ab-initio* methods: solution of the nuclear *many-body* problem starting from ***"realistic"*** *inter* -nucleon (**NN+NNN**) (and? NNNN ….) force.



- Exact solution for A $\leq$ 4? (Fadeev, Fadeev-Yakubowski)
- A>4: development of controlled and improvable *ab-initio* many-body computational methods: No-Core Shell Model (and extensions), Coupled-Cluster method, Green Functions many-body theory…

- **No-Core Shell Model (NCSM) and No-Core Full Configuration(NCFC)**

simple, most versatile, access to excited states and transitions, even and odd systems.

NCSM review: *Barrett et al., Progress in Particle and Nuclear Physics 69 (2013).*

NN+NNN interactions

Meson exchange potentials

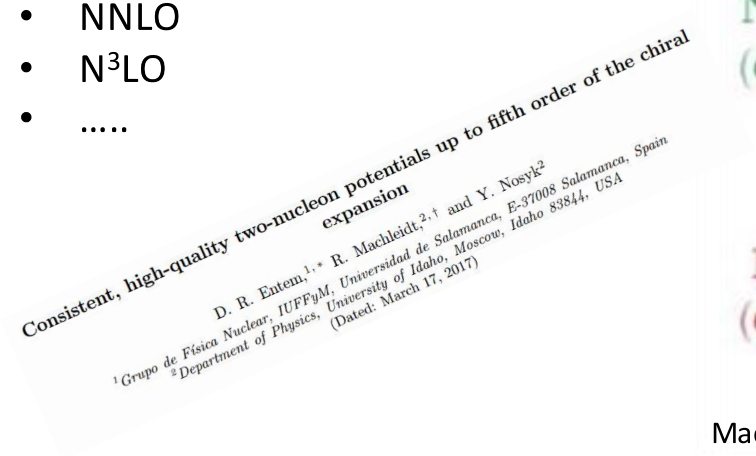
- Bryan Scott (1967-69)
- Paris (*Lacombe et al.* 1980)
- Nijmegen (1994)
- Bonn (Bonn A,CD-Bonn) (*Machleidt et al.*1987-2001)
- Argonne potentials (1995)

modern NN(+NNN) potentials

Chiral Perturbation Theory

links low energy physics to QCD

- NNLO
- N^3LO
- …..

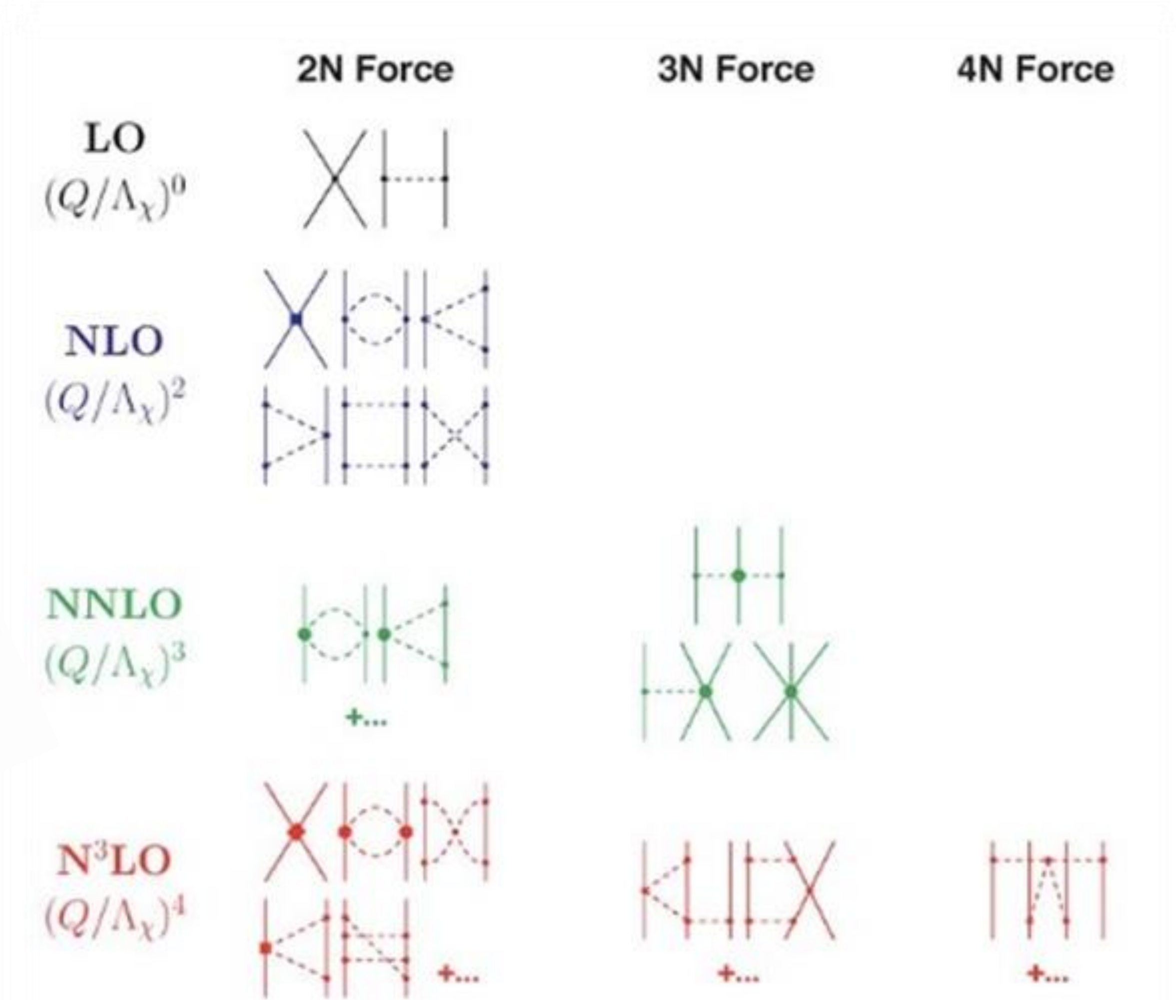

Consistent, high-quality two-nucleon potentials up to fifth order of the chiral expansion

D. R. Entem,[1,*] R. Machleidt,[2,†] and Y. Nosyk[2]

[1]Grupo de Física Nuclear, IUFFyM, Universidad de Salamanca, E-37008 Salamanca, Spain

[2]Department of Physics, University of Idaho, Moscow, Idaho 83844, USA

(Dated: March 17, 2017)



Machleidt et al. 2011

short distance physics not resolved, but captured in short range couplings, fitted to *NN* scattering data, A=3,4 nuclei (recently, heavier systems up to A=16 included)

hierarchy of diagrams, effective 3-, 4- …body forces

NCSM essentials

- Solution of many-body Schrodinger equation for bound states

$$H\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = E\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)$$

for A, (or N,Z) point-like nucleons
NCSM (NCFC) assumes intrinsic non-relativistic Hamiltonian with „realistic“ NN+NNN interaction

$$H_A = \frac{1}{A}\sum_{i<j}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{\mathrm{NN},ij} + \sum_{i<j<k}^{A} V_{\mathrm{NNN},ijk}$$

- All nucleons active (no-core)

- Solution: expansion in 3D spherical harmonic oscillator many-body basis states

$\longrightarrow$ Slater determinants constructed from HO s.p. states (with HO length *b*)

$$\varphi_{nljmm_t}(\vec{r}, \sigma, \tau; b) = R_{nl}(r; b)(Y_l(\hat{r})\chi(\sigma))_m^{(j)}\chi(\tau)_{m_t}$$

- Convergence of observables due to the finite basis expansion is the only source of uncertainty

NCSM essentials

- Slater determinants expansion depends on $\boldsymbol{\Omega}$ (or eq. HO length *b*)

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \sum_k c_k \psi_k(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)$$

determinants Ψ_k are constructed from single particle states of type

$$\varphi_{nljmm_t}(\vec{r}, \sigma, \tau; b) = R_{nl}(r; b)(Y_l(\hat{r})\chi(\sigma))^{(j)}_m \chi(\tau)_{m_t}$$

- Many-body problem transformed to symmetric eigenvalue problem

$$\sum_{k'} H_{kk'} c_{k'} = E c_k$$

$$H_{kk'} = \langle \psi_k | H | \psi_{k'} \rangle$$

- Easy task → find (lowest) eigenvalues and eigenvectors of large **sparse** matrix *H*

→ HPC (High Performance Computing)

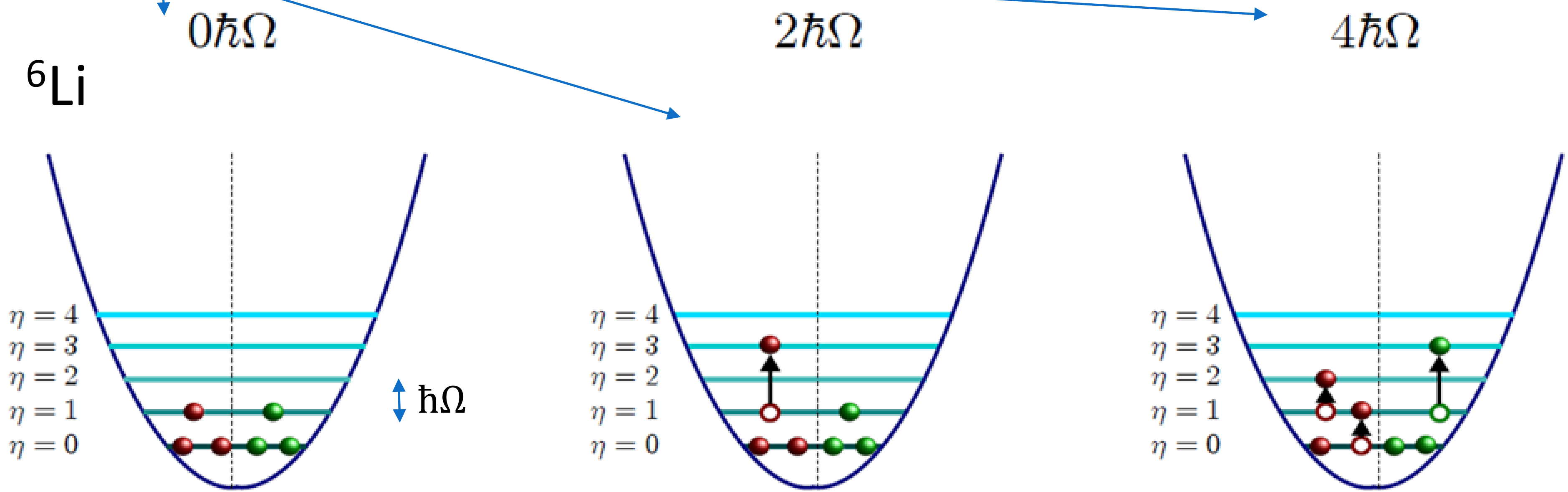
1. *Contruct* $\boldsymbol{H_{kk'}}$
2. *Diagonalize* ***H***
3. *Calculate observables*
4. *Check convergence*

NCSM essentials

- basis construction → *A* nucleons moving independently in spherical 3D HO potential

$$\sum_{i=1}^{A}\left[\frac{\vec{p}_i^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right]$$

$\langle\psi_k|H|\psi_{k'}\rangle$



- Configuration mixing via „residual“ interaction

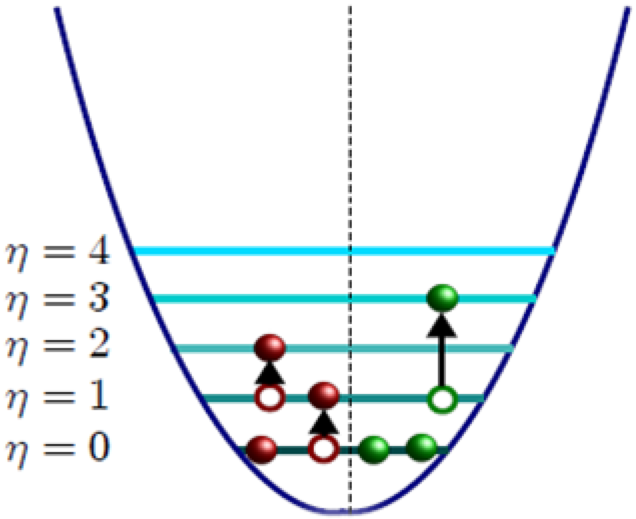
$$\sum_{i<j}^{A}\left[V_{\mathrm{NN},ij}-\frac{m\Omega^2}{2A}(\vec{r}_i-\vec{r}_j)^2\right]+\sum_{i<j<k}^{A}V_{\mathrm{NNN},ijk}$$

NCSM dimensions

- dimension of space grows rapidly for heavier systems

- 3D HO with completely filled major shells up to a principal HO quantum number η contains $n = (\eta+1)(\eta+2)(\eta+3)/3$ single-particle states

$\eta=0$ $n=2$
$\eta=1$ $n=8$
$\eta=2$ $n=20$
$\eta=8$ $n=330$
$\eta=20$ $n=3542$



How to distribute *N,Z* nucleons over n states?

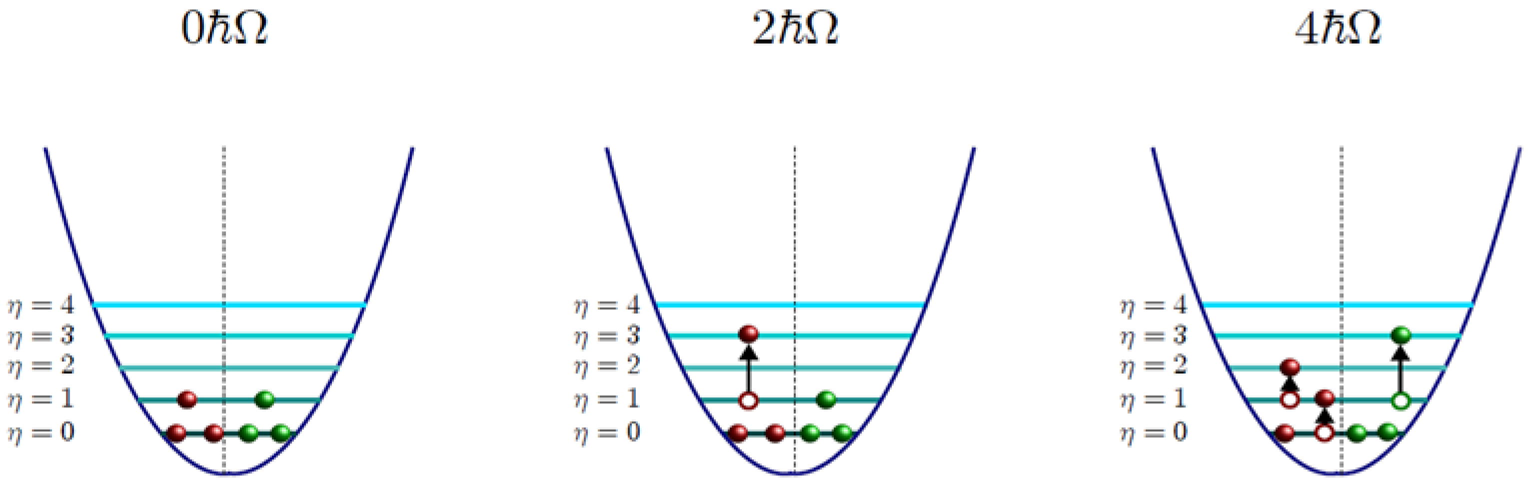
dim= $\binom{n}{N} \times \binom{n}{Z}$

	^{12}C	^{16}O
$\eta=1$	1120	1
$\eta=6$	$7.\ 10^{5} \times 7.\ 10^{5}$	$1.\ 10^{12} \times 1.\ 10^{12}$
$\eta=8$	$3.\ 10^{11} \times 3.\ 10^{11}$	$3.\ 10^{15} \times 3.\ 10^{15}$

NCSM dimensions

- In practice, we truncate basis

In the NCSM states with *N=0* HO quanta up to N_{max} above lowest configuration are included (preserves centre-of-mass factorization)



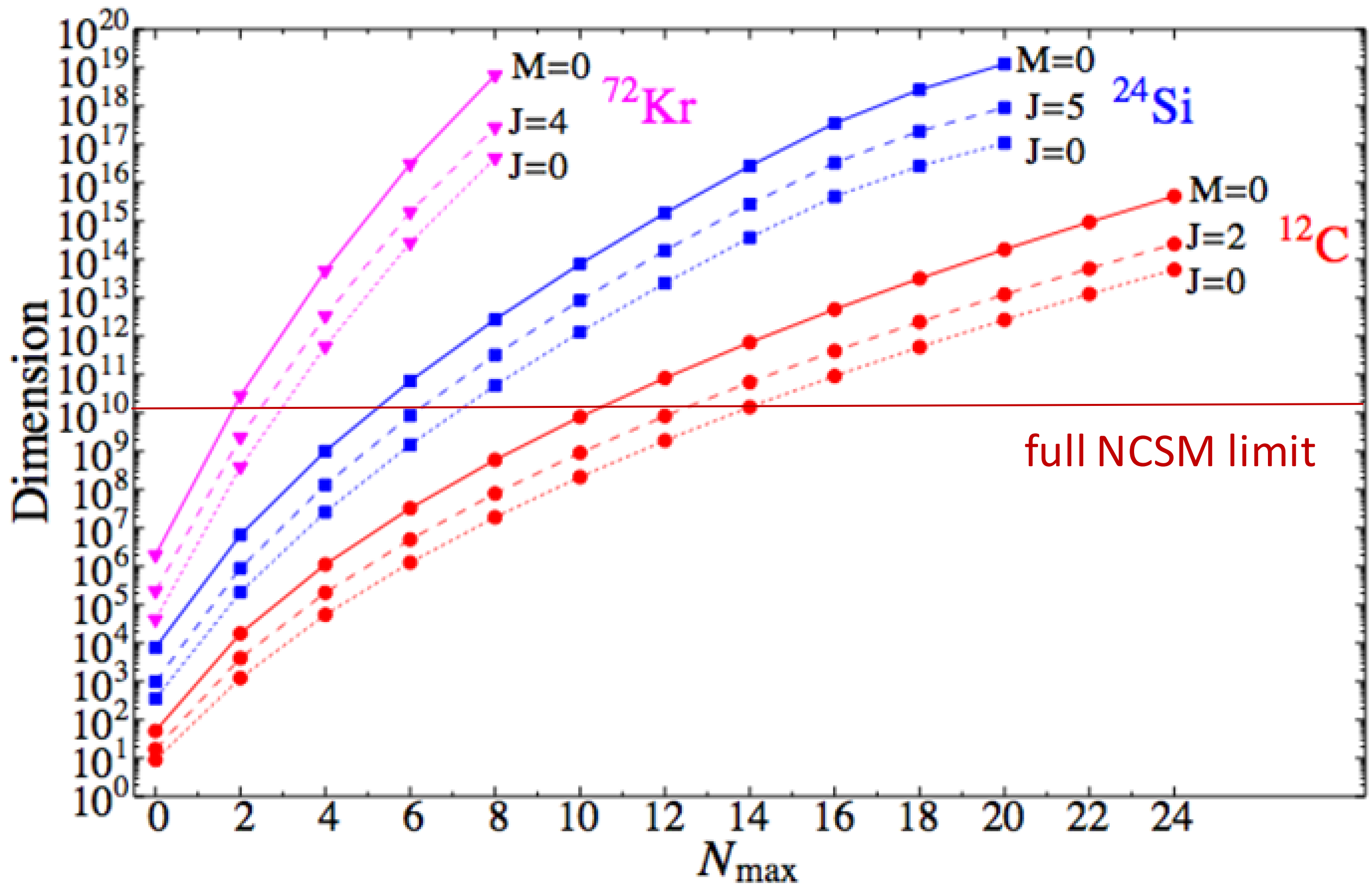
Moreover, one can assume symmetries of the Hamiltonian and construct basis states with required symmetry

$$[\boldsymbol{H}, \boldsymbol{J_z}] = 0 \qquad [\boldsymbol{H}, \boldsymbol{J^2}] = 0$$

projection of total angular momentum $\longrightarrow$ **M - scheme**
magnitude of total angular momentum $\longrightarrow$ **J - scheme**

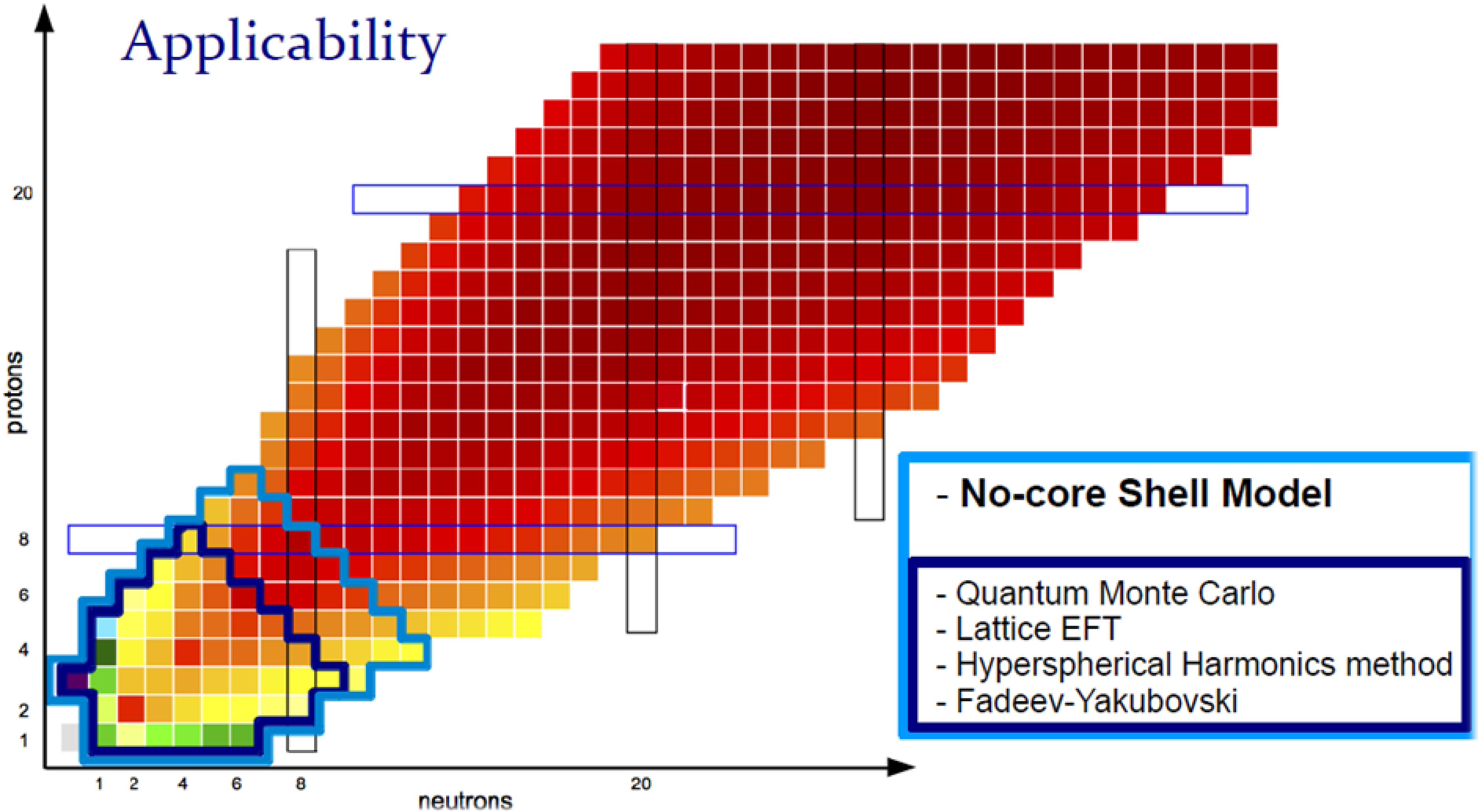
NCSM dimensions

- **M-scheme** + trivial construction of basis states (Fock space |110010011010….>)
  + simple calculation of m.e.
  - larger dimension of matrices
- **J-scheme** + few orders od magnitude reduction
  - involved calculation of m.e., more dense matrix



Ab-initio theory from nuclear physics perspective

- complete NCSM calculations manageable up to $N_{max} = 8$ in ^{16}O
- ground state energy converged for „soft“ interactions, not for excited states



How to diagonalize large (huge) matrix? Lanczos algorithm

Lánczos Kornél (1893-1974)

Idea: construct orthogonal basis which turns **H** to tridiagonal form

Algorithm :

i=1, β_1=0, p_1 *with* $||p_1||$=1 (pivot vector)

do while convergence

$p = Hp_i$

$\alpha_i = p_i^T H p_i$

k=p-$\alpha_i p_i$-$\beta_i p_{i-1}$ (ortog k w.r.t. p_i)

$\beta_{i+1} = ||k||$

p_i=k/β_{i+1}

i=i+1

diagonalize tridiagonal matrix T

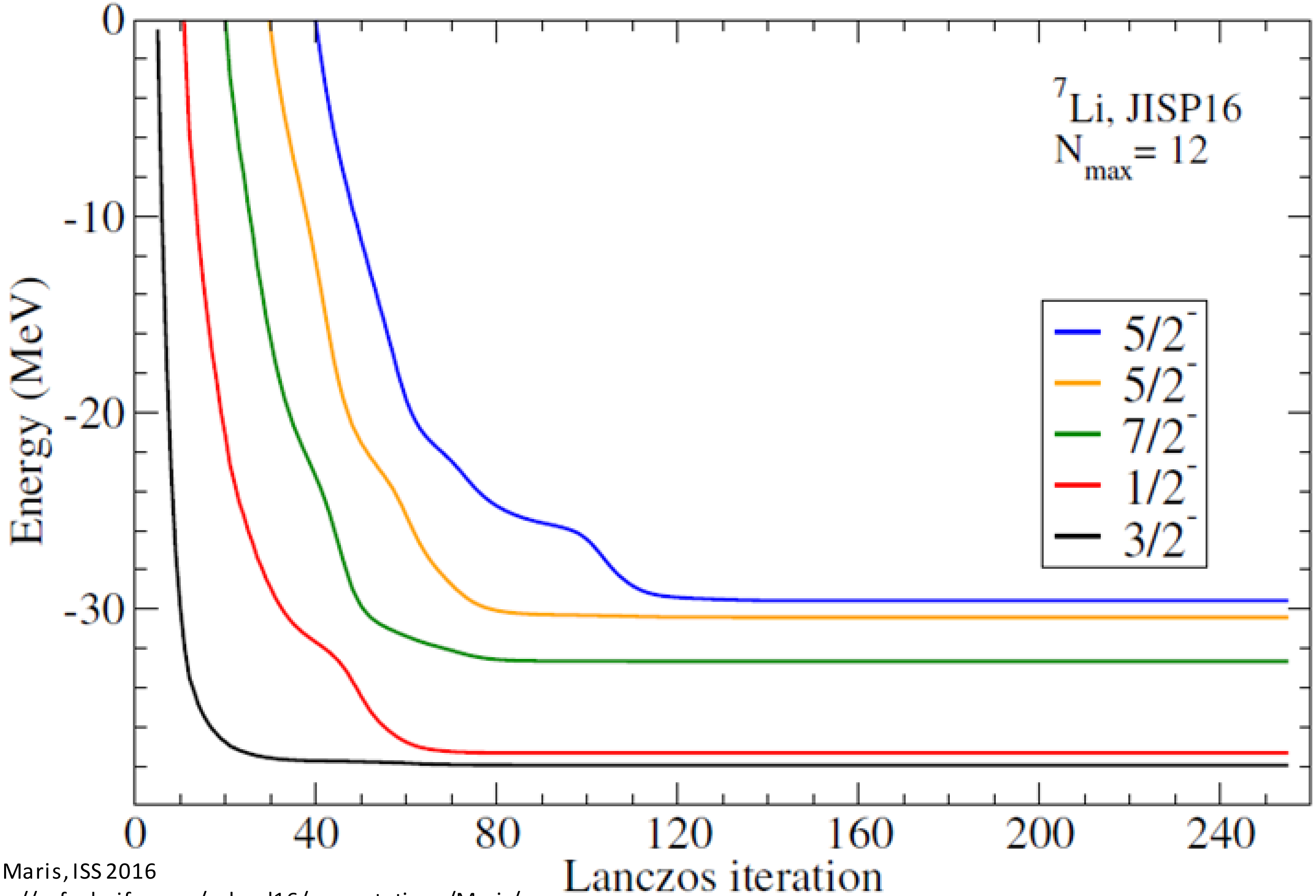
check convergence of lowest eigenvalues

end do

$$T = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \beta_4 & \\ & & \beta_4 & \alpha_4 & \beta_5 \\ & & \cdots & & \end{bmatrix}$$

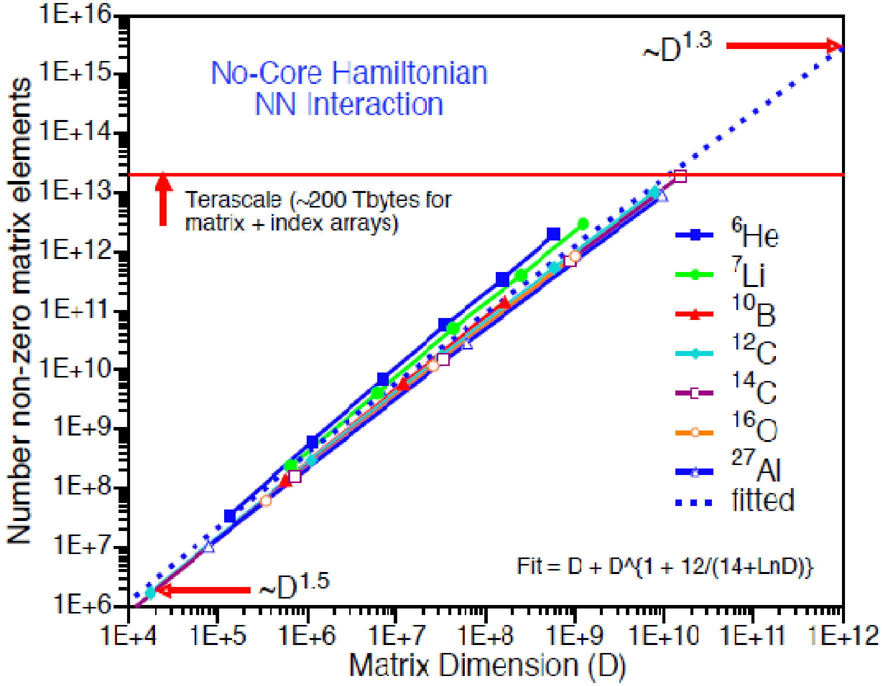
Lanczos algorithm - convergence

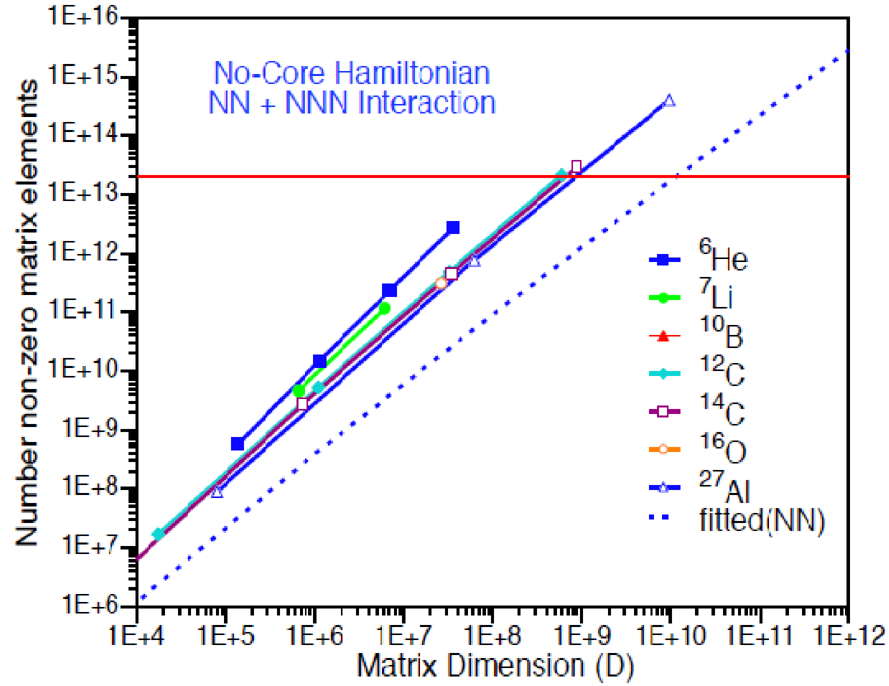
- matrix dimension 252.10^6 with 4.10^{11} n.n.z. matrix elements
- highly optimized parallel code *MFDn*
- 124 nodes using 496 MPI ranks with 6 OpenMP threads/MPI
- total runtime less than 10 minutes (scales up to 100 000 cores!)



P. Maris, ISS 2016
http://rafael.ujf.cas.cz/school16/presentations/Maris/

No-core shell model – storage





nucleus	$N_{\max}$	dimension	2-body	3-body	4-body
^{6}Li	12	$4.9 \cdot 10^{6}$	0.6 GB	33 TB	590 TB
^{12}C	8	$6.0 \cdot 10^{8}$	4 TB	180 TB	4 PB
^{12}C	10	$7.8 \cdot 10^{9}$	80 TB	5 PB	140 PB
^{16}O	8	$9.9 \cdot 10^{8}$	5 TB	300 TB	5 PB
^{16}O	10	$2.4 \cdot 10^{10}$	230 TB	12 PB	350 PB
^{8}He	12	$4.3 \cdot 10^{8}$	7 TB	300 TB	7 PB
^{11}Li	10	$9.3 \cdot 10^{8}$	11 TB	390 TB	10 PB
^{14}Be	8	$2.8 \cdot 10^{9}$	32 TB	1100 TB	28 PB
^{20}C	8	$2 \cdot 10^{11}$	2 PB	150 PB	6 EB
^{28}O	8	$1 \cdot 10^{11}$	1 PB	56 PB	2 EB

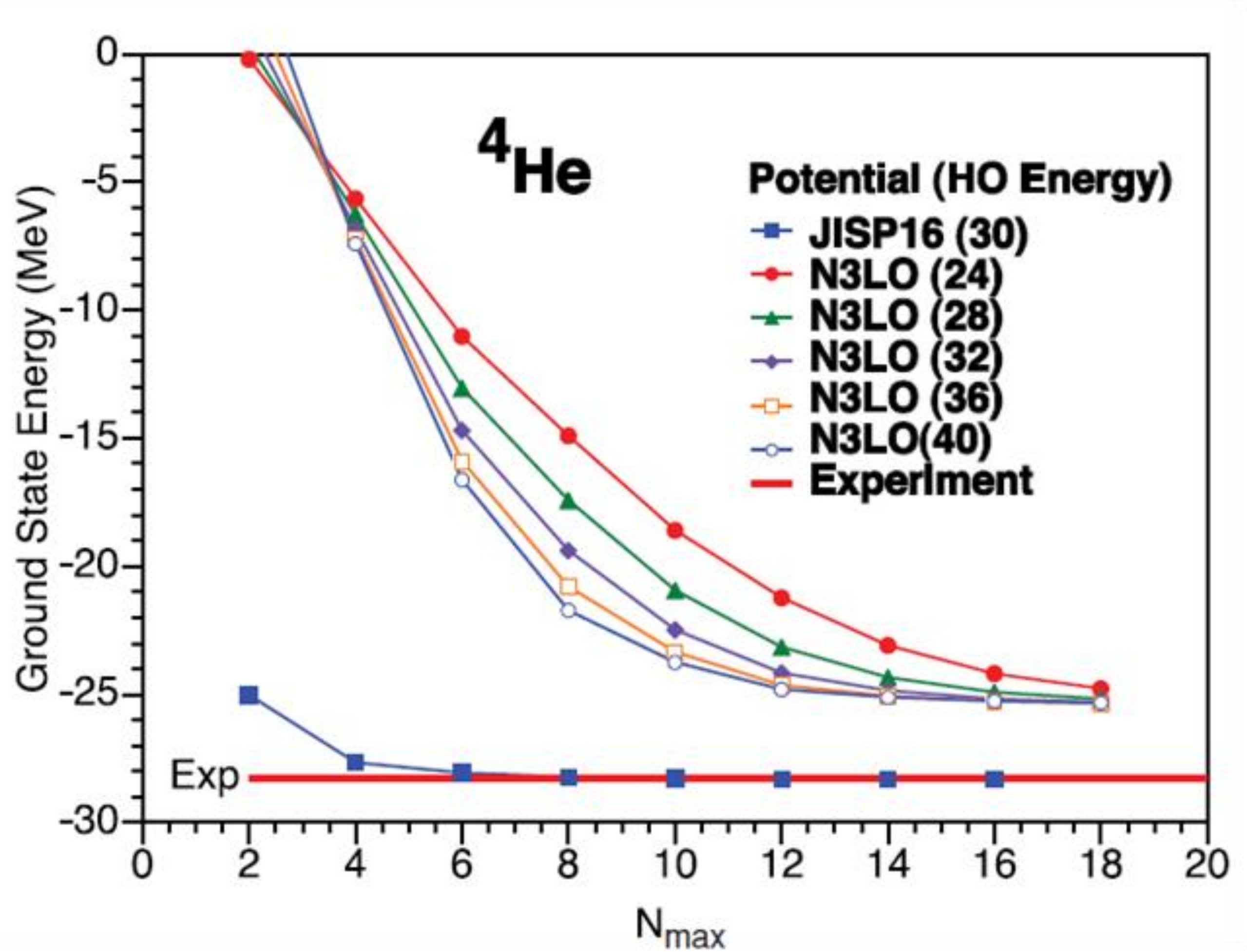
J. Vary et al, Journal of Physics: Conference Series **180** (2009) 012083

No-core shell model – selected results

- interaction determines convergence rate!
- for “soft“ interactions smaller space is needed

  “hard“ interactions → “renormalization“ techniques

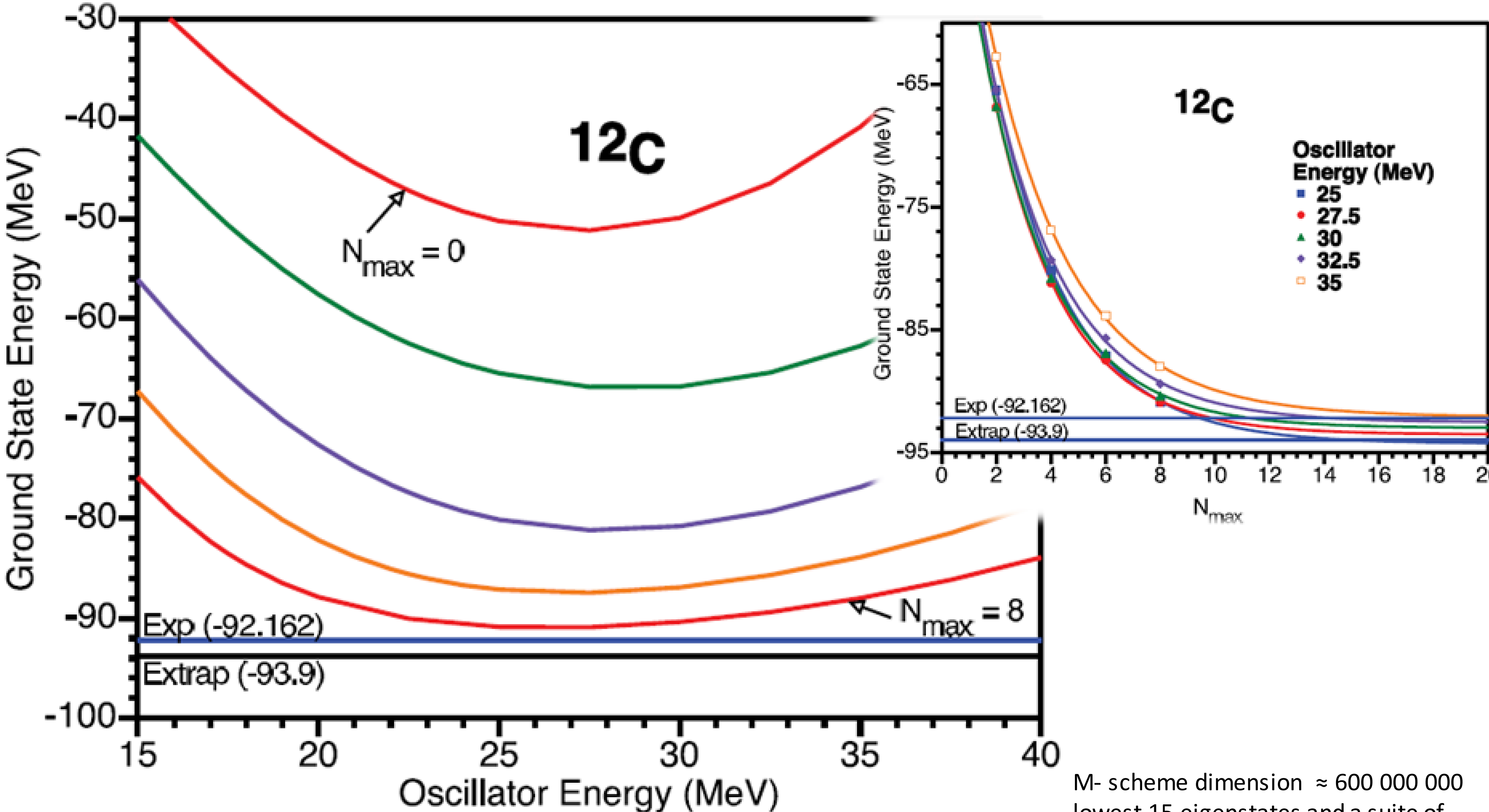
  (transformation of “bare“ interaction → many body forces)



P. Maris et al, Phys. Rev C. 79, 014308 (2009)

No-core shell model – selected results

- for heavier nuclei fully converged results are not available → extrapolation



M- scheme dimension ≈ 600 000 000 lowest 15 eigenstates and a suite of observables obtained in 2.3 hours on 12,720 processors using the Jaguar supercomputer at Oak Ridge National Laboratory (ORNL).

P. Maris et al, Phys. Rev C. 79, 014308 (2009)

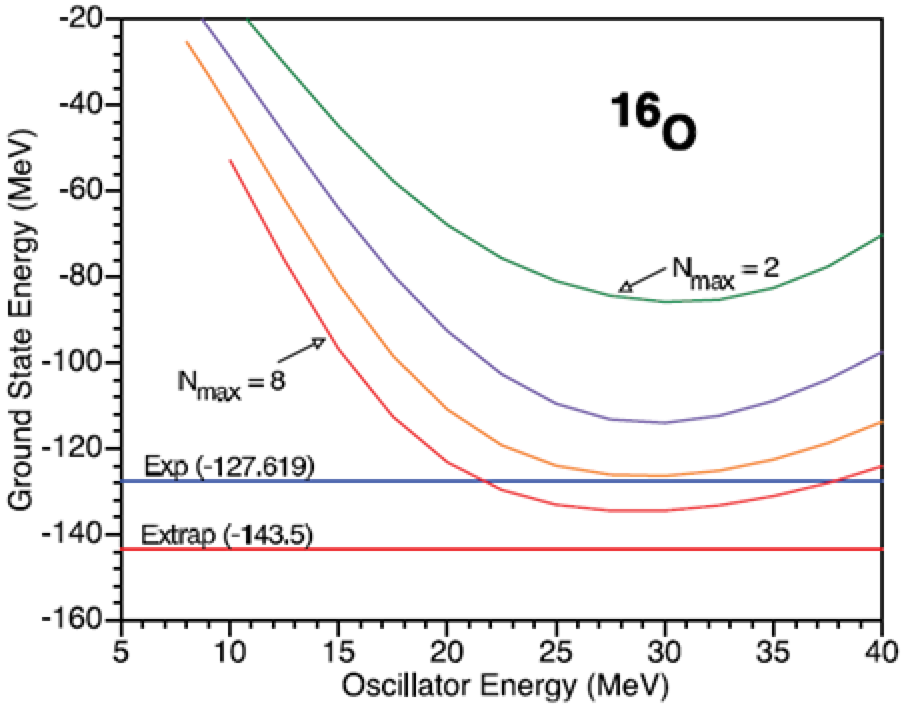
No-core shell model – selected results

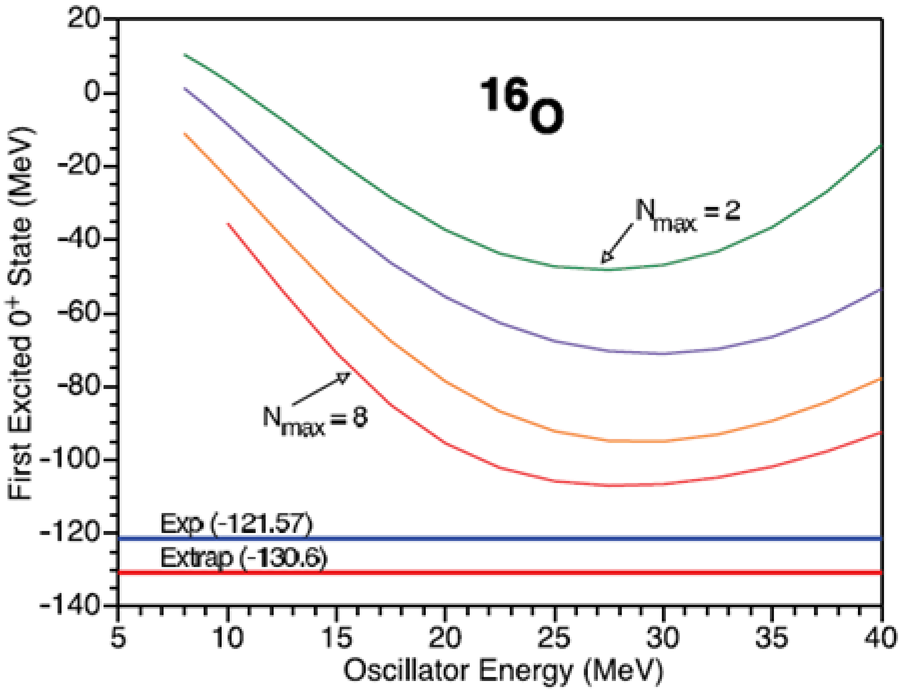
- some excited states converge very slowly in HO S.D. basis
- typical examples are cluster states in ^{16}O and ^{12}C

N_{max} =8
matrix dim. 996,878,170
n.n.z 805,811,591,748 (assuming symmetric matrix)
storage of one vector 4.0 GB

Matrix 6.5 TB

lowest 8 eigenstates and a suite of observables obtained in 4.5 hours on 12,090 processors @Franklin supercomputer at the National Energy Research Supercomputer Center (NERSC).





P. Maris et al, Phys. Rev C. 79, 014308 (2009)

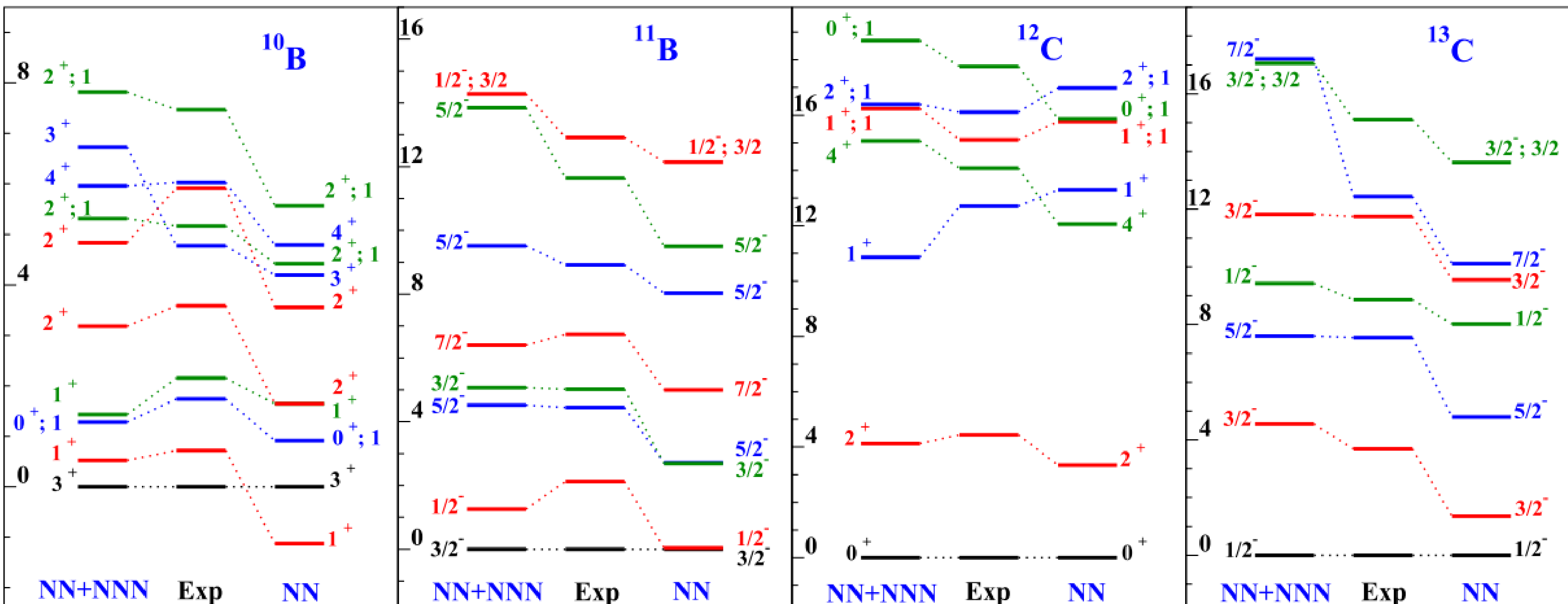
No-core shell model – selected results

- Nevertheless NCSM can test different NN (+NNN) potentials.

Do three-body forces enter the description?
How large are three-body forces?

- NCSM calculations with chiral NN and NNN potential

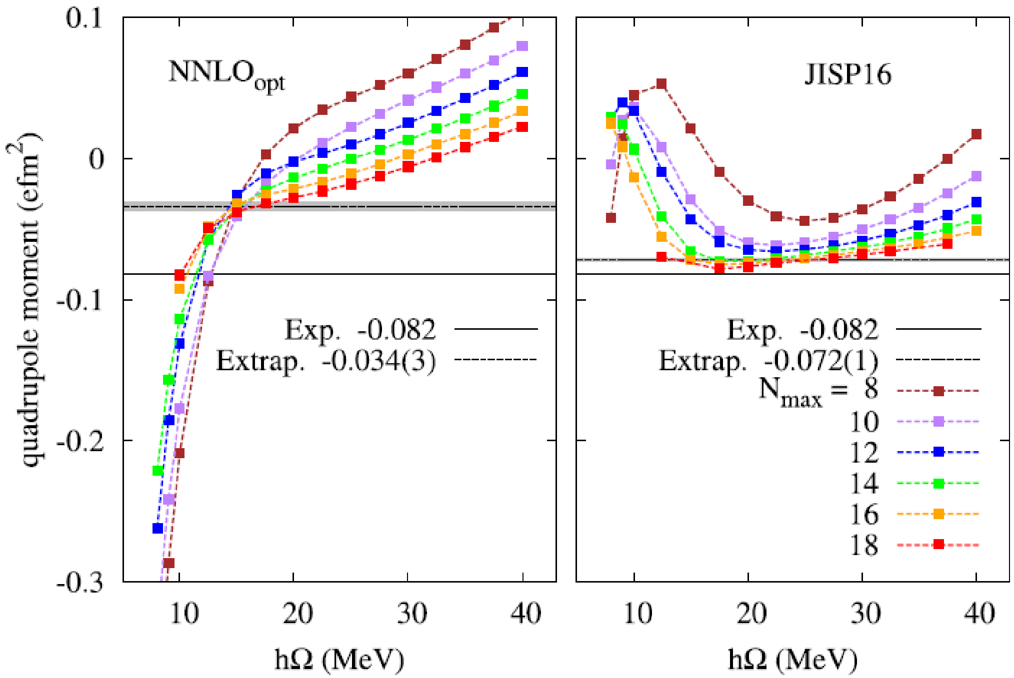
→ role of NNN forces in inversion of 3^+ and 1^+ in ^{10}B



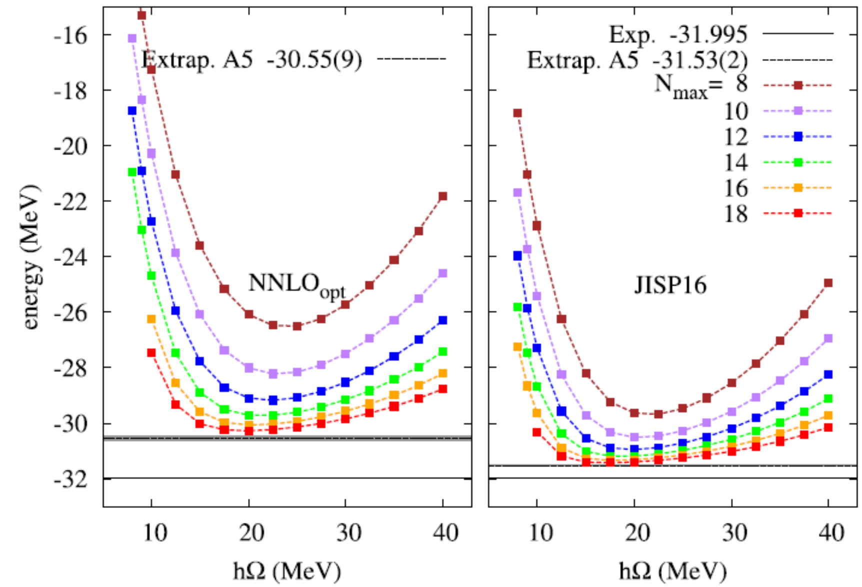
P. Navrátil et al.,Phys. Rev. Lett. 99 (2007) 042501

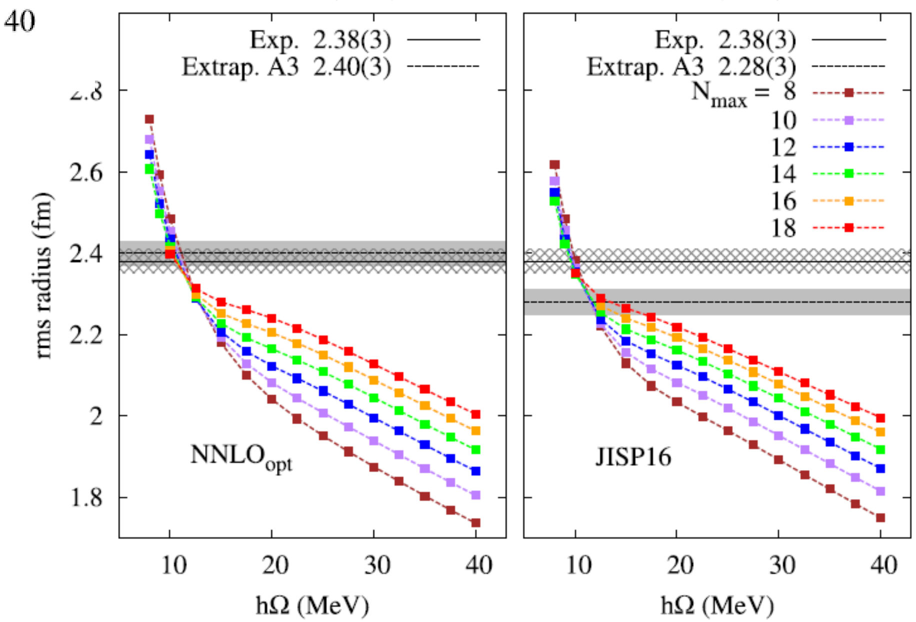
No-core shell model – selected results

But, what about other observables? Well, it depends .....



Shin et al. J. Phys. G. 44 (2017) 075103.





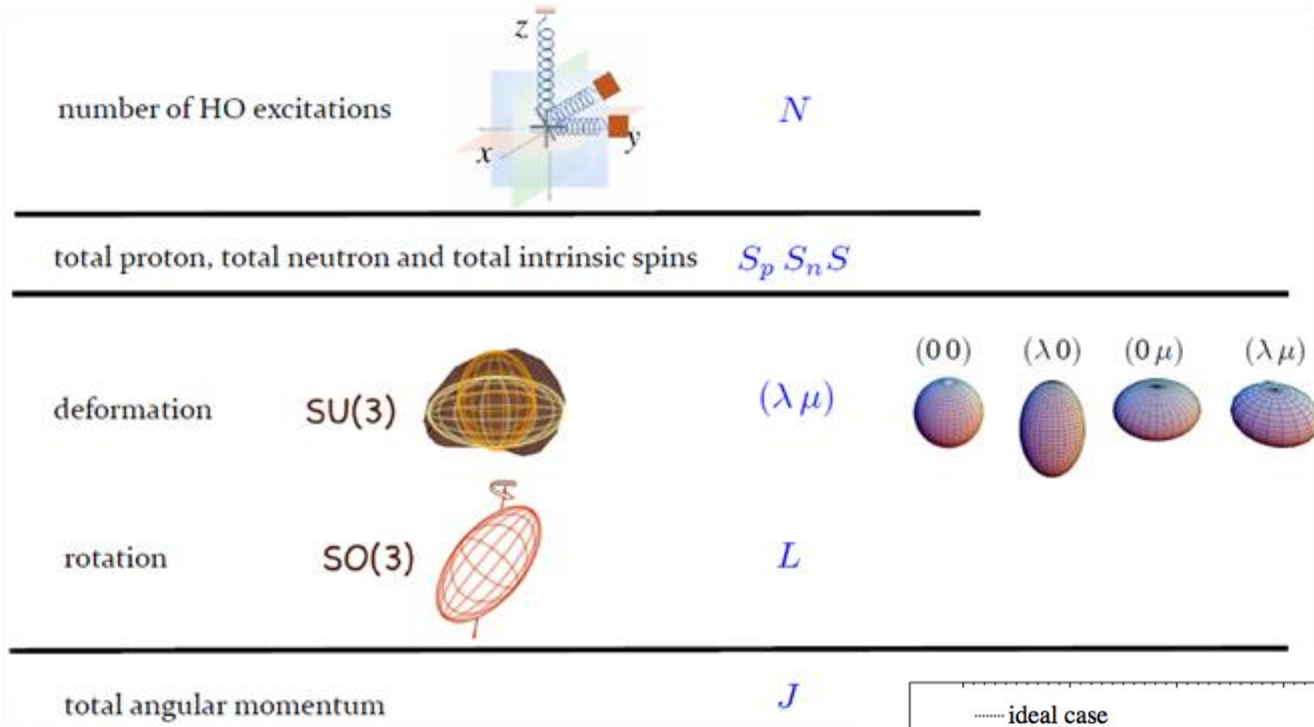
- radii, quadrupole moments, B(E2) transition probabilities converge more rapidly for different value of **ħΩ** than energies ☹

Symmetry-adapted NCSM

Symmetry-adapted NCSM (SA-NCSM)-combines algebraic techniques with the NCSM

- multishell extension of Elliot SU(3) model

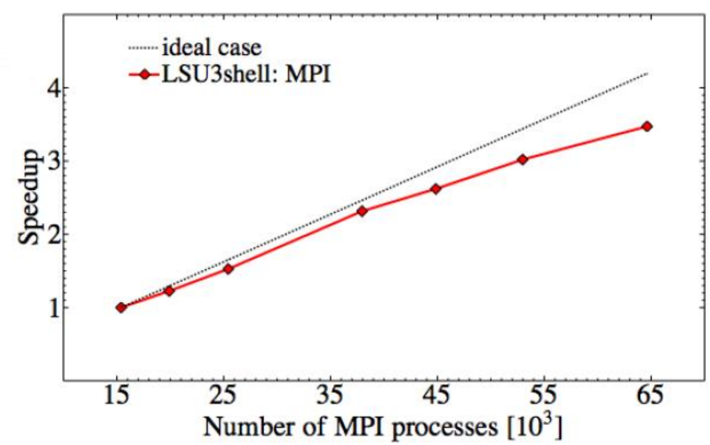
T. Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501.



- **LSU3Shell** code – MPI/OpenMP implementation of SA-NCSM (T. Dytrych)

https://sourceforge.net/projects/lsu3shell/

- involved calculation of matrix elements 95% of runtime!

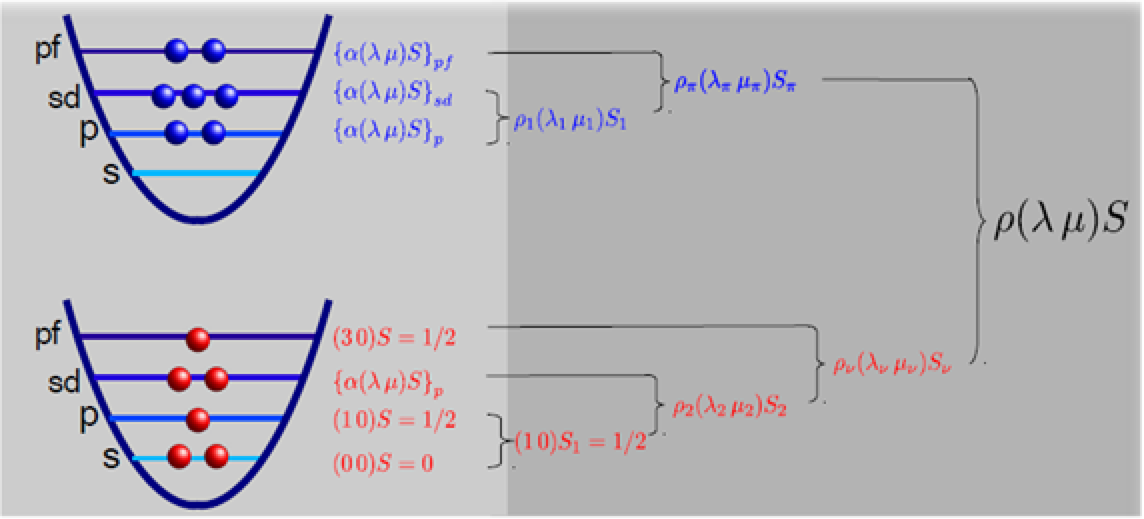


Symmetry-adapted NCSM

- SU(3) clasification scheme for spatial part → LS coupling → **J=L+S**

Step 1: SU(3) coupling of succesive shells

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



many-nucleon basis state

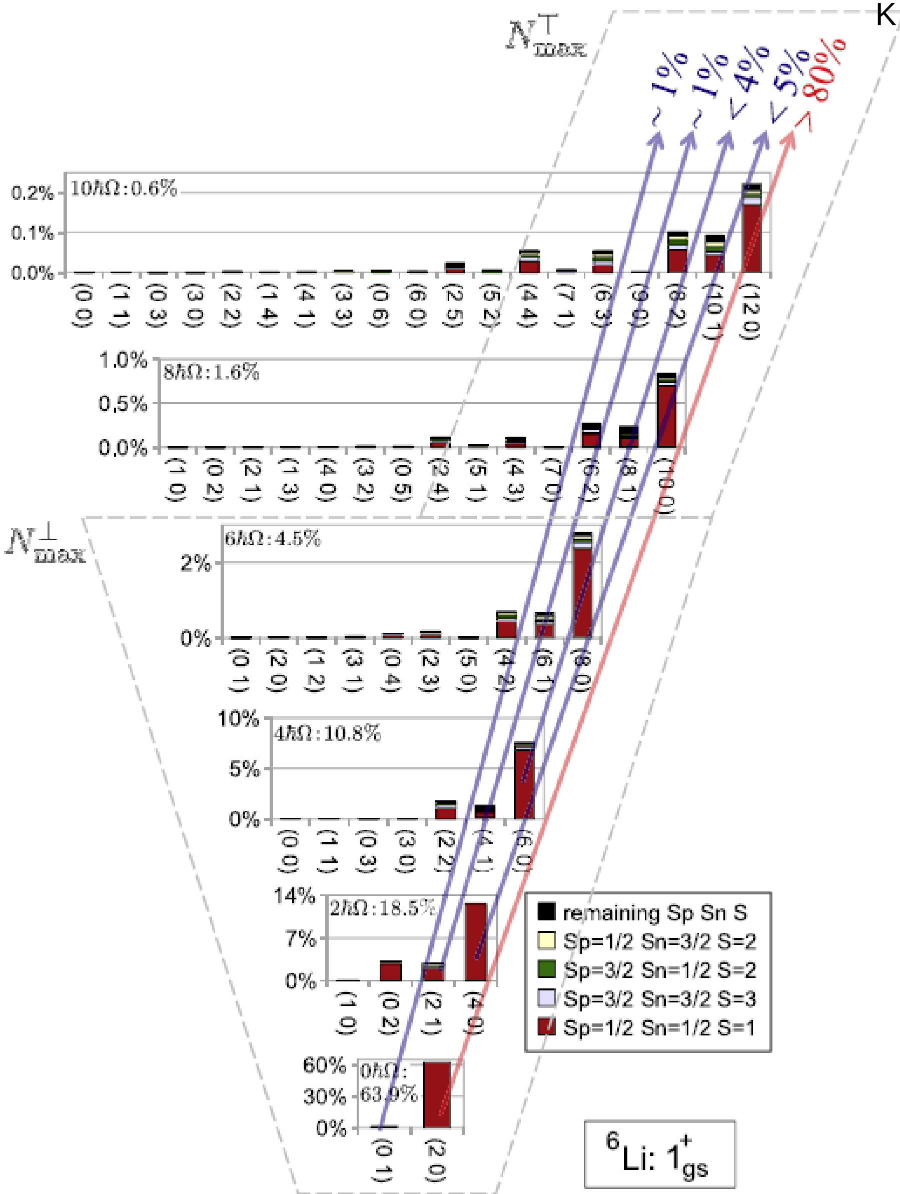
$$|\gamma\ N\hbar\ \ S_p\,S_n S\ (\lambda\,\mu)\ \kappa\ L\ \ J\,M\rangle$$

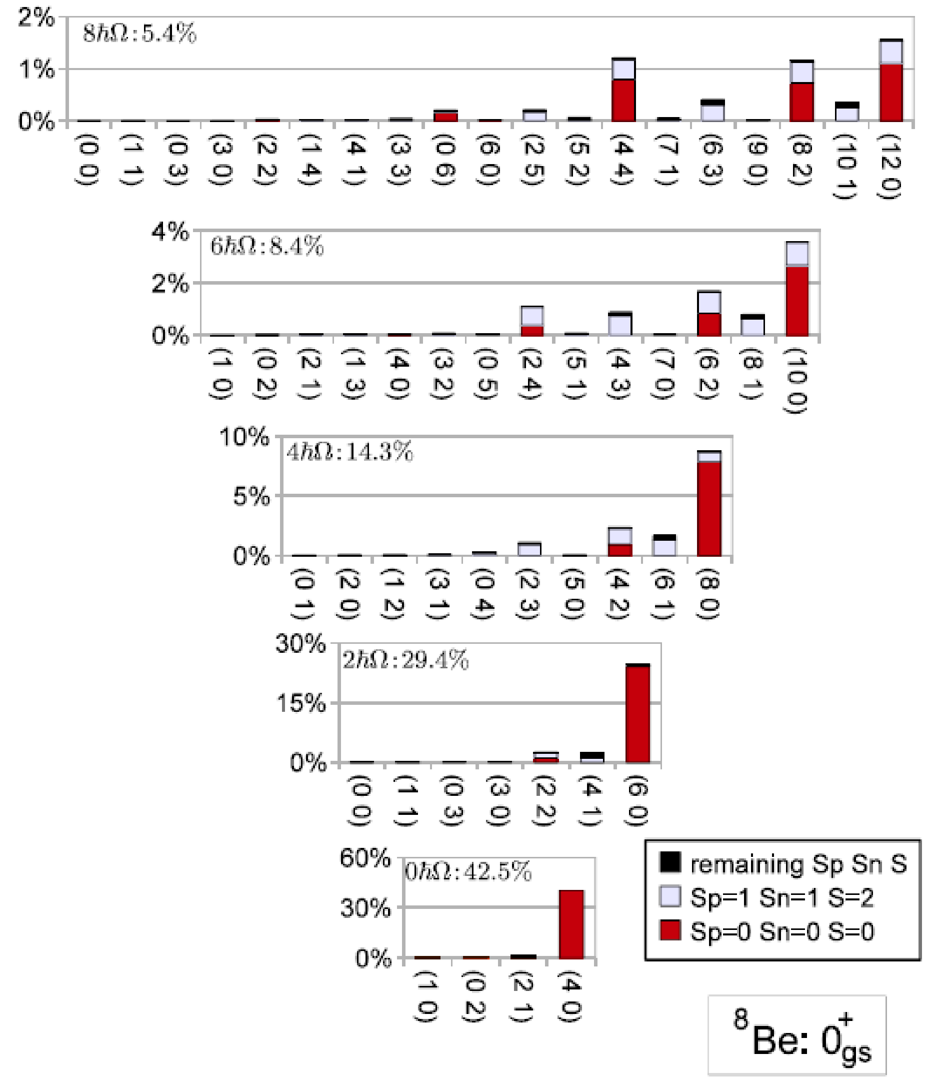
Why SU(3) coupling scheme? **truncation of the model space**

Symmetry-adapted NCSM

- decomposition of NCSM model space → dominant components in the w.f. → truncation

K.D. Launey et al.,Progress in Particle and Nuclear Physics 89 (2016)

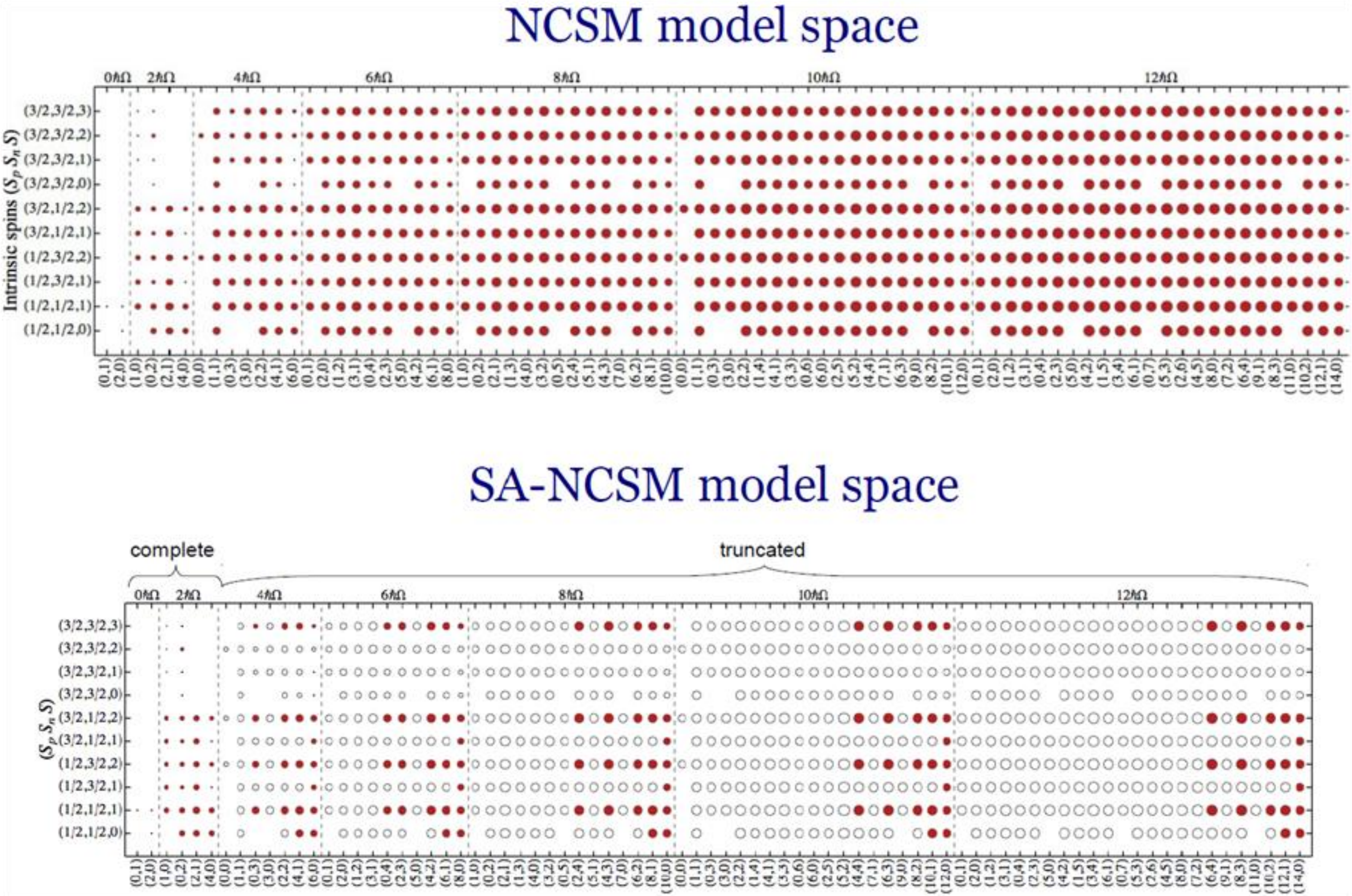




Symmetry-adapted NCSM

^{6}Li model space

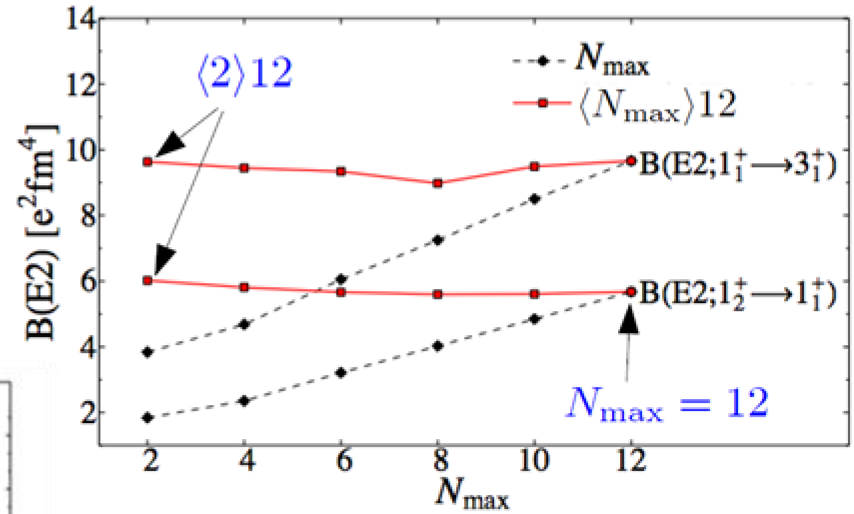
K.D. Launey et al.,Progress in Particle and Nuclear Physics 89 (2016)

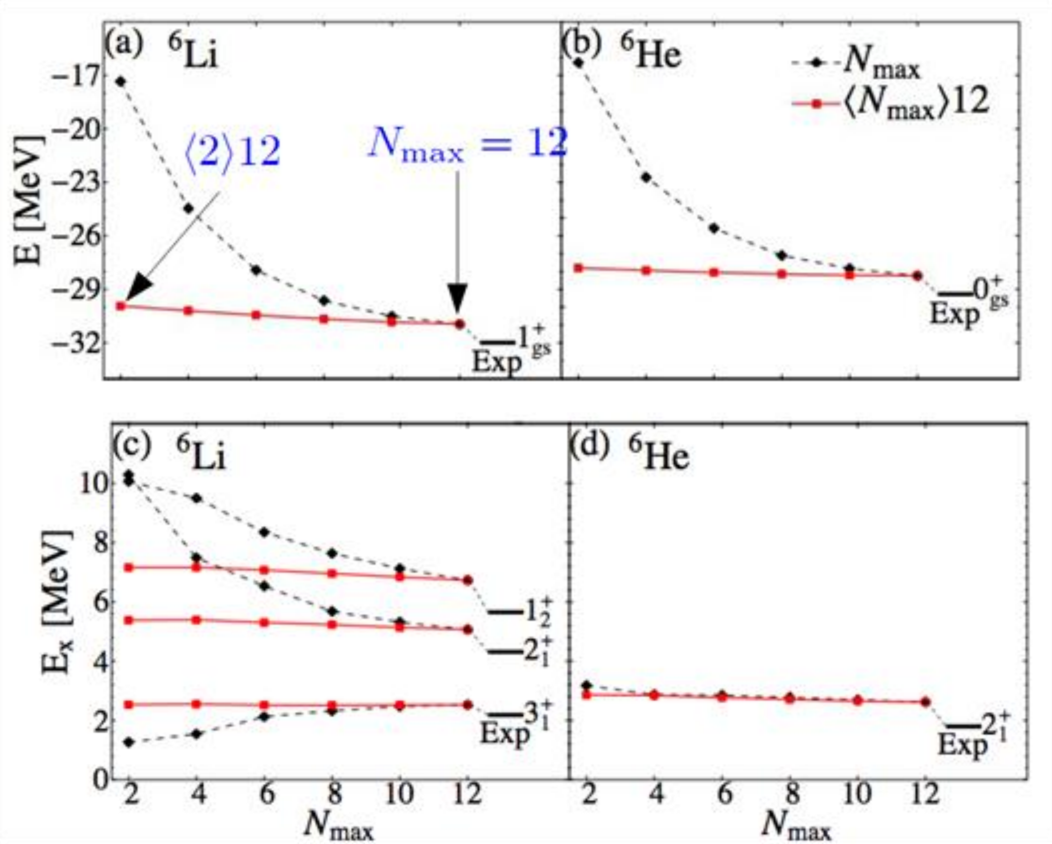


Symmetry-adapted NCSM

- simple patterns in the structure of low-lying nuclear states

dominance of **high deformation**
(λμ) = (20) (40) (60) (80) ….
and **low spins** S_p S_n S =1/2 1/2 1 ….





- drastic reduction of space

  5-10% of the total dimension

- good convergence of electric quadrupole (E2) transitions and quadrupole moments

K.D. Launey et al.,Progress in Particle and Nuclear Physics 89 (2016)

Computer resources

BLUE WATERS

- Fastest supercomputer at university campus

total performance ≈ 1 Pflop/s (on a sustained basis)
total peak performance 13.24 Pflop/s
total system memory 1.634 PB

- 22,640 Cray XE6 nodes each 64 GB RAM, 16 cores
- 4,228 Cray XK7 nodes 32 GB RAM, 16 cores +2688 CUDA

(≈ 400 000 cores)

- 26 PB storage quick access
- 380 PB long term data storage

Computing time: US National Science Foundation (NFS) grant.

Collaborative Research: Advancing first-principle symmetry-guided nuclear modeling for studies of nucleosynthesis and fundamental symmetries in nature (PI J. Draayer, LSU)

3,430,000 node hrs in 08/2017-08/2018

note: Salomon – most powerful supercomputer in the CR @IT4Innovations: 24 192 cores, 129 TB RAM

SA-NCSM@BlueWaters

- large calculation: ^{20}Ne – beyond reach of NCSM

≈ 22 000 nodes (≈ 700 000 cores)
runtime ≈ 1 hour for calculation of Hamiltonian + diagonalization

- example: $J^{\pi} = 2^{+}$

dim. ≈ $80 \, . \, 10^{6}$

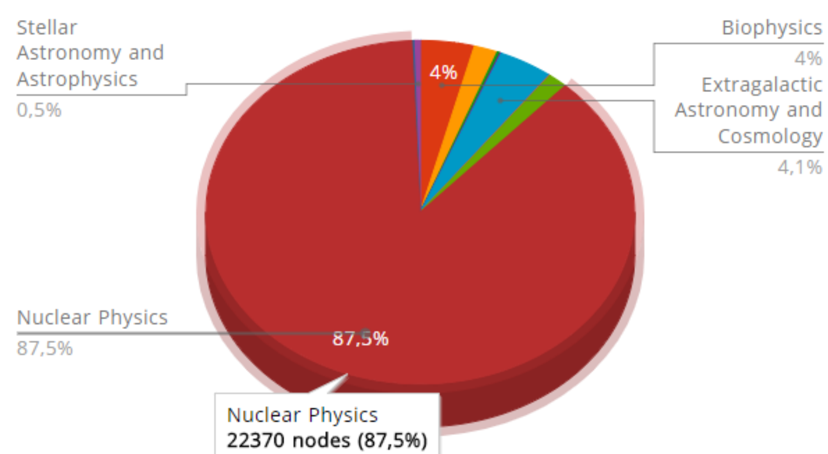
n.n.z. m.e. ≈ $28. \, 10^{12}$

matrix storage:

139 TB in VBC
211 TB in CSR

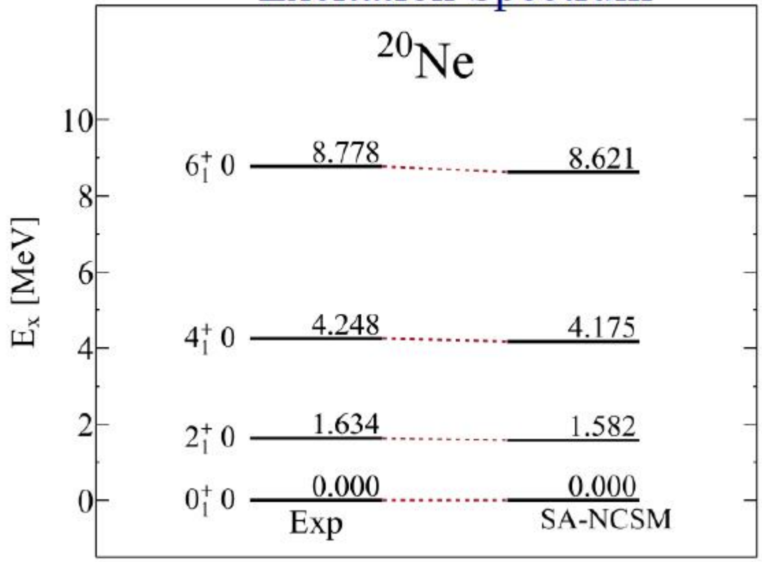
Collaborative Research: Advancing first-principle symmetry-guided nuclear modeling for studies of nucleosynthesis and fundamental symmetries in nature (**Jobs:**1) **PI:** Jerry Draayer, Louisiana State University	XE	715712	202,288.04
GPU-enabled General Relativistic Simulations of Jetted Tidal Disruptions of Stars by Supermassive Black Holes (**Jobs:**4) **PI:** Alexander Tchekhovskoy, University of California, Berkeley	XK	16880	2,980.98
Unveiling the functions of the HIV-1 and hepatitis B virus capsids through the computational microscope (**Jobs:**1) **PI:** Juan Perilla, University of Illinois at Urbana-Champaign	XK	7200	1,269.00
Probing New Physics in Galaxy Formation at Ultra-High Resolution (**Jobs:**2) **PI:** Philip Hopkins, California Institute of Technology	XE	2560	446.51
More Power to the Many: Scalable Ensemble-based Simulations and Data Analysis (**Jobs:**1) **PI:** Shantenu Jha, Rutgers, the State University of New Jersey	XE	1920	160.27

CURRENT RUNNING JOBS BY SCIENCE AREA

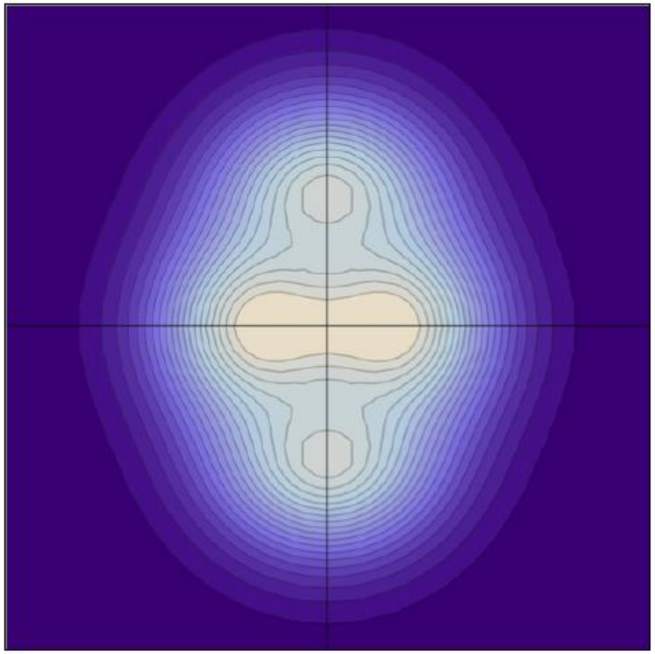


SA-NCSM@BlueWaters

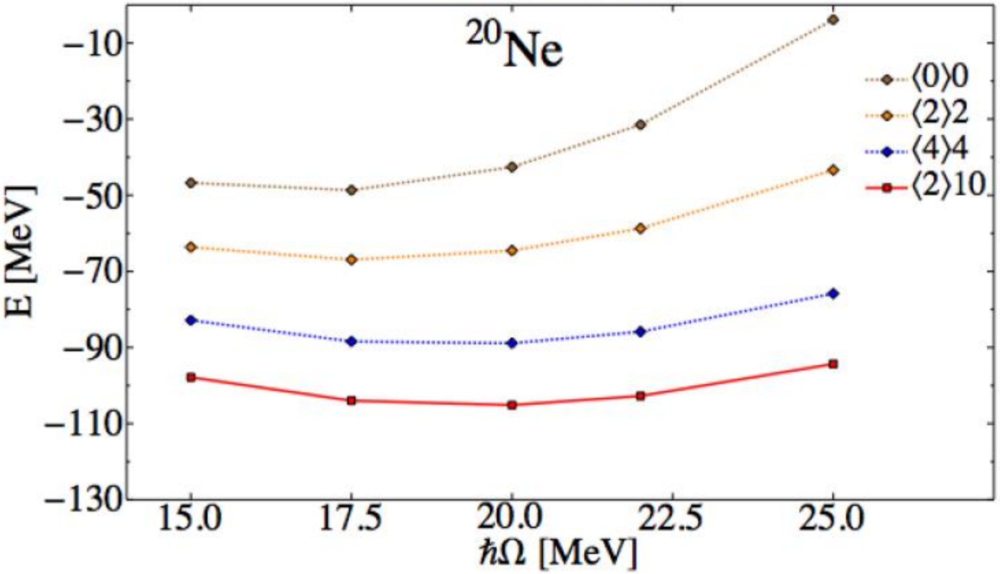
Excitation Spectrum



Nuclear density



Binding energy



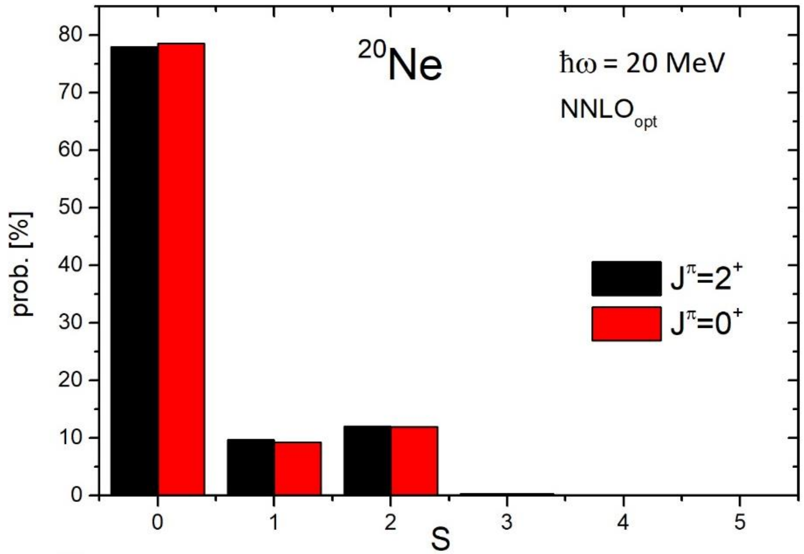
Complete space: 4×10^{12}

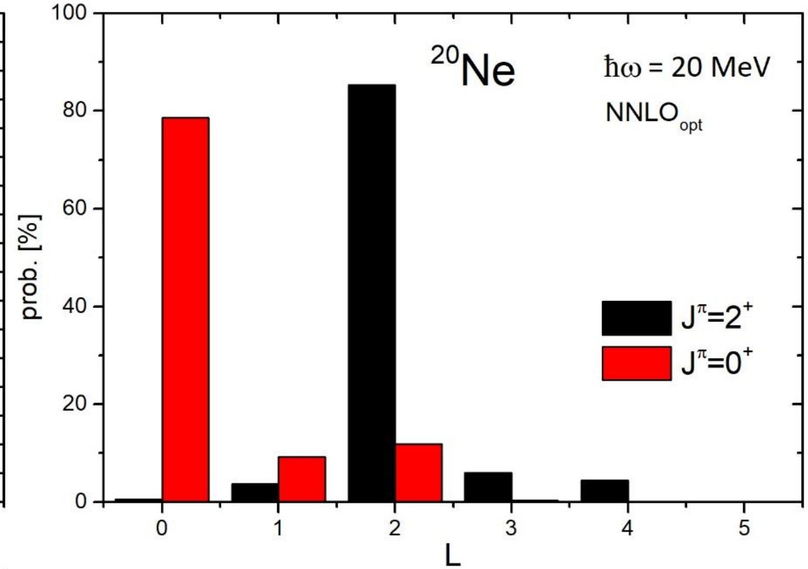
Symmetry-adapted space: 1×10^{7}

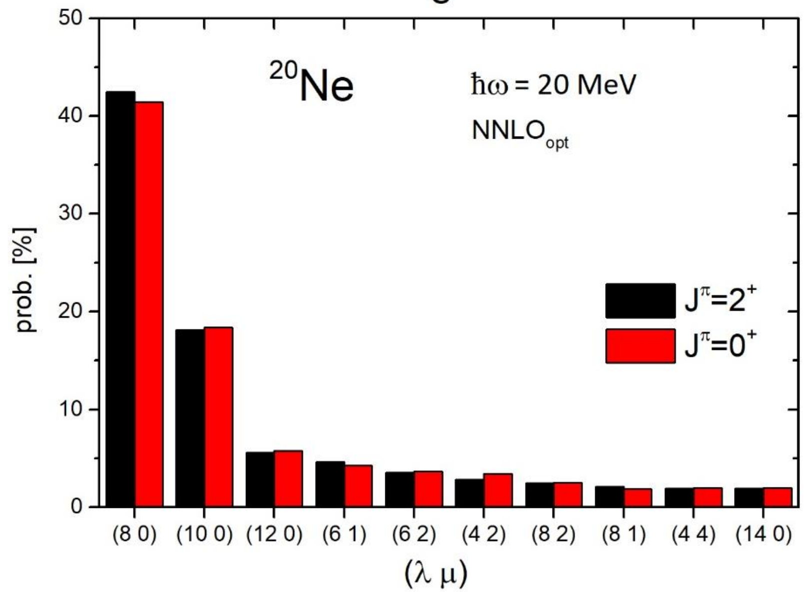
T. Dytrych

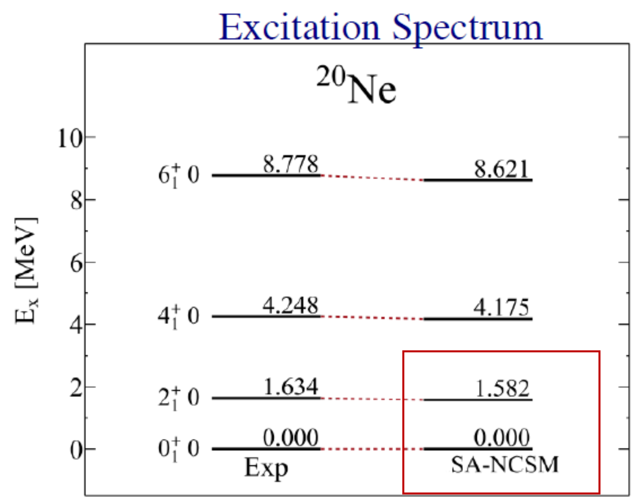
SA-NCSM@BlueWaters

- LS decomposition of w.f. → interpretation of state as rotation of deformed shape nuclear spin **J=L+S**



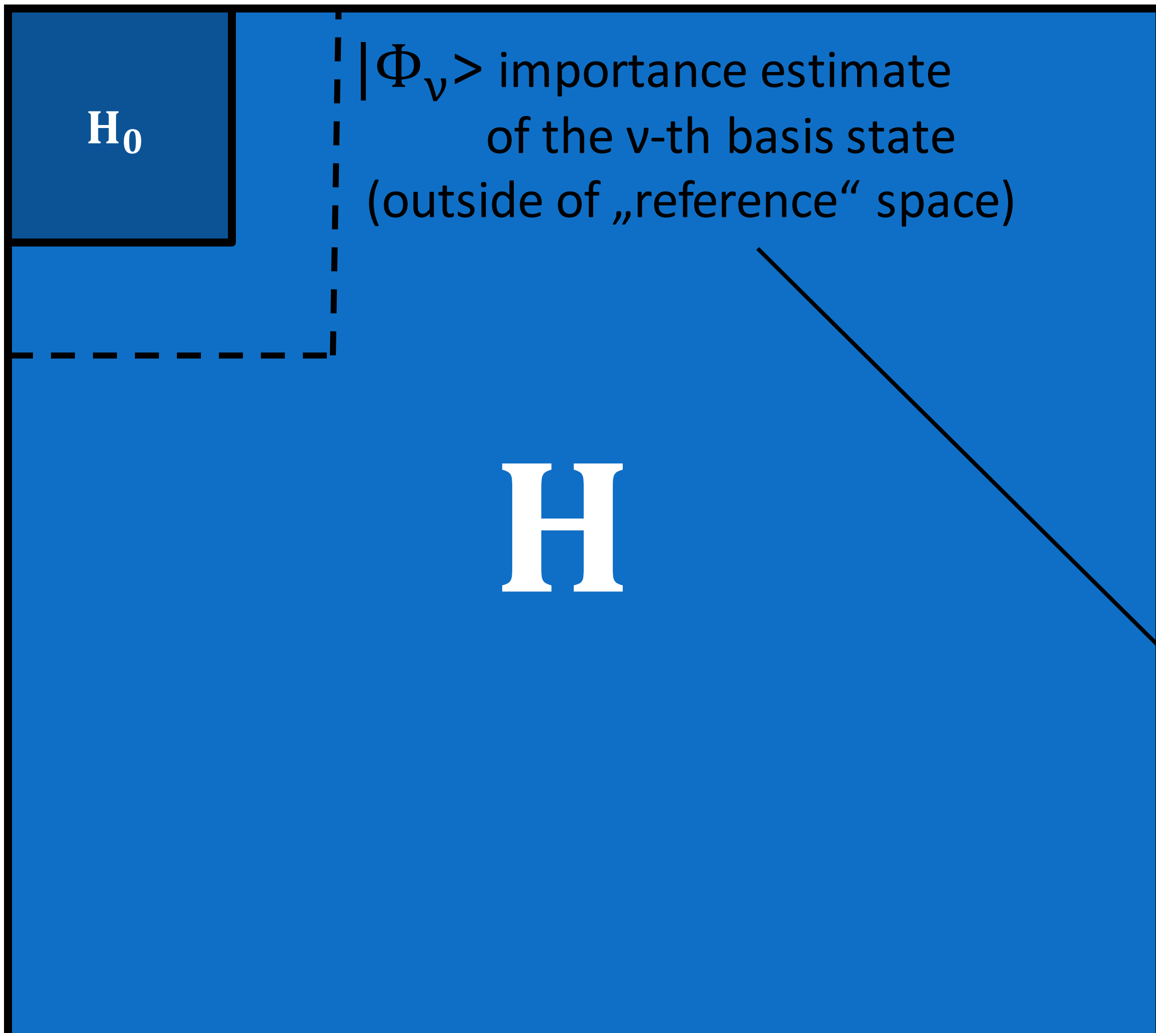






SA-NCSM with importance truncation

- additional reduction of model space for heavier systems necessary
- quantitative justification of truncation $\longrightarrow$ **Importance Truncation (IT)** based on 1[st] order many-body perturbation theory



- lowest eigensolution in a small space → reference state

$$H_0|\Psi_{\text{ref}}\rangle = \epsilon_{\text{ref}}|\Psi_{\text{ref}}\rangle$$

$$\epsilon_\nu = \langle\Phi_\nu|\,H\,|\Phi_\nu\rangle$$

Importance measure parameter

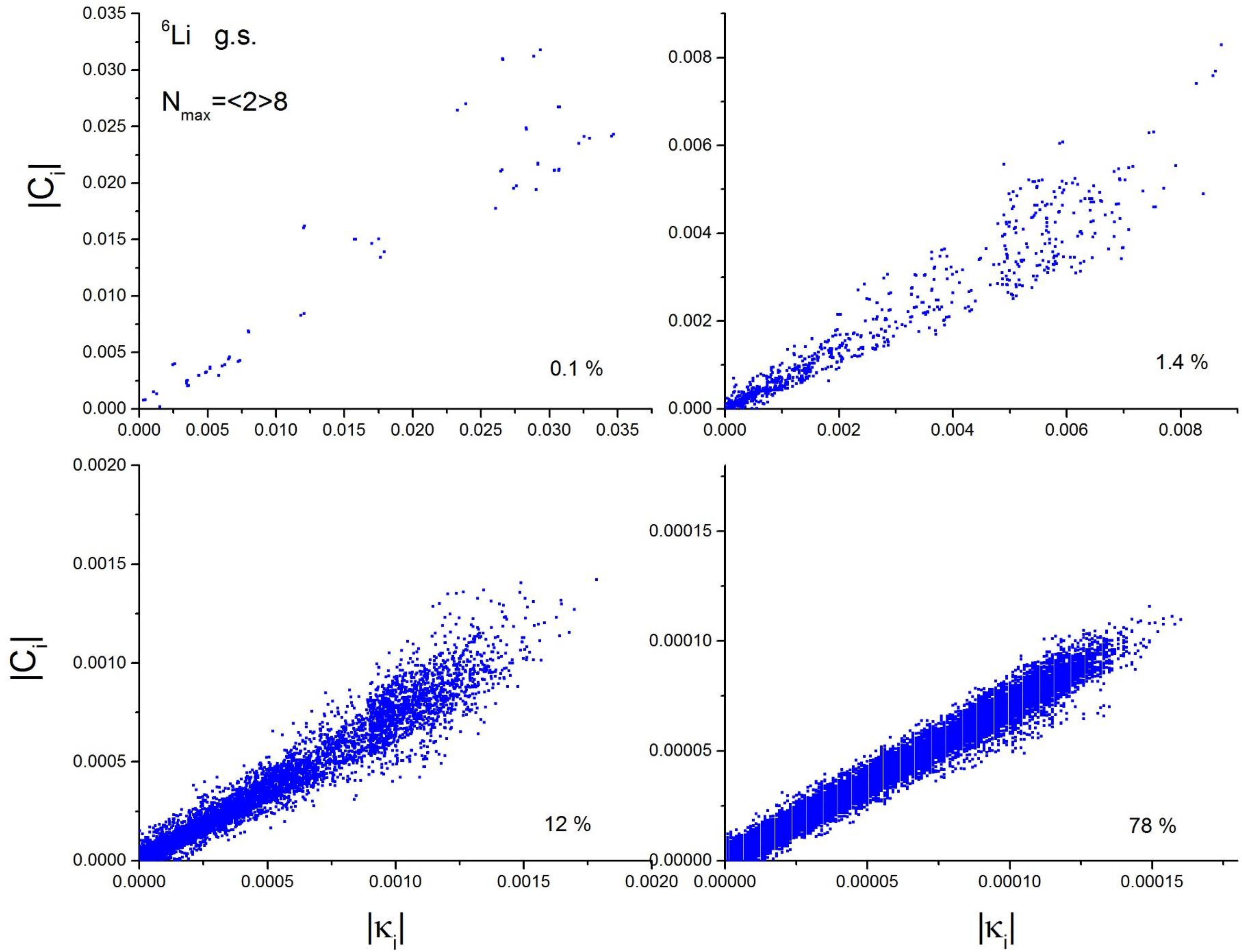
$$\kappa_\nu = -\frac{\langle\Phi_\nu|H|\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

IT-NCSM implementation:

R. Roth, P. Navrátil Phys. Rev. Lett. 99 (2007)
R. Roth, Phys. Rev. C 79, 064324 (2009)

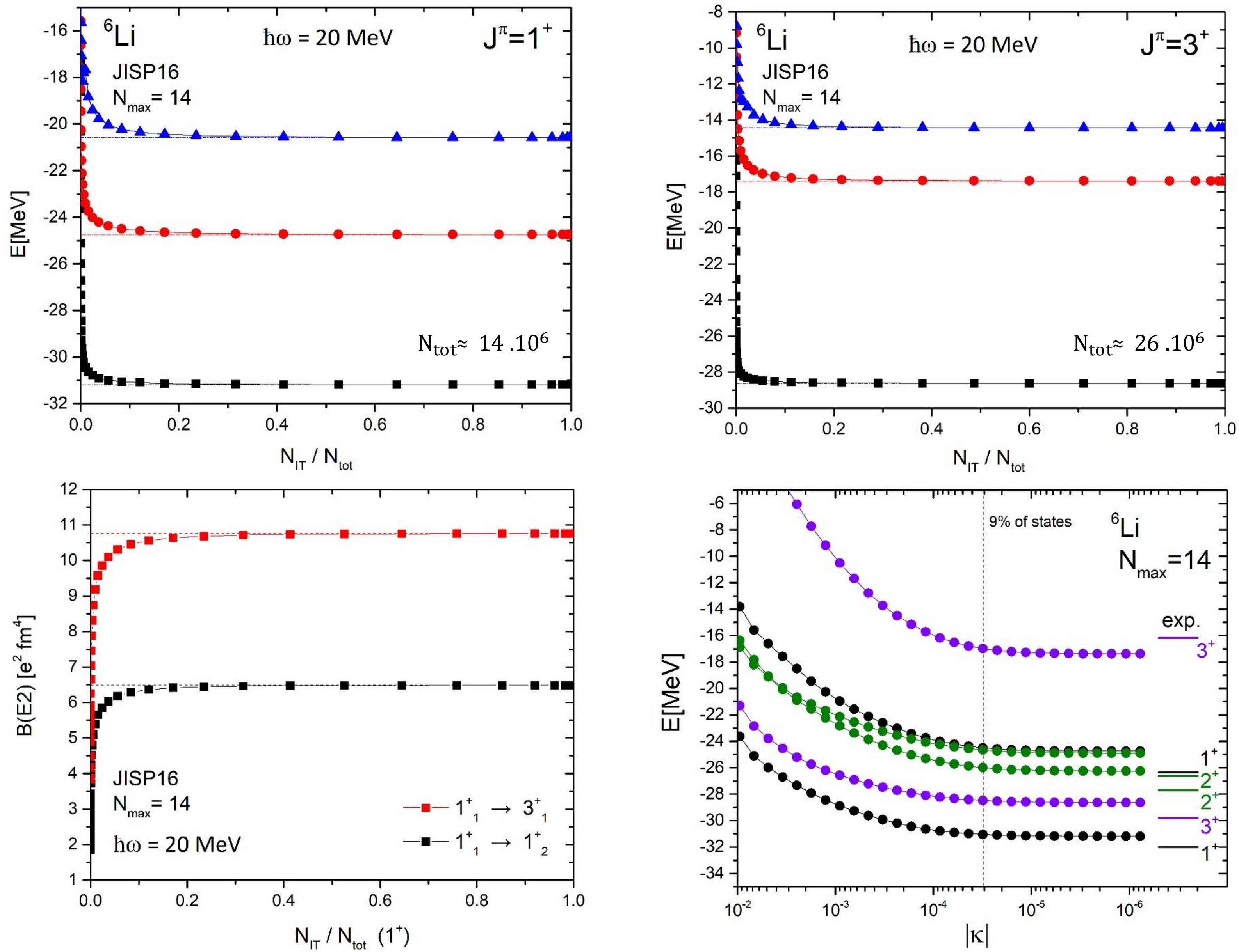
SA-NCSM with importance truncation

- correlation between importance measure $|\kappa_i|$ and amplitudes $|C_i|$ for i-th component



SA-NCSM with importance truncation

- fast convergence of observables → reduction of basis dimensions



Thank you!