Symmetry-adapted SU(3) no-core shell model with importance-sampling

František Knapp

IPNP, Charles University, Prague

T. Dytrych

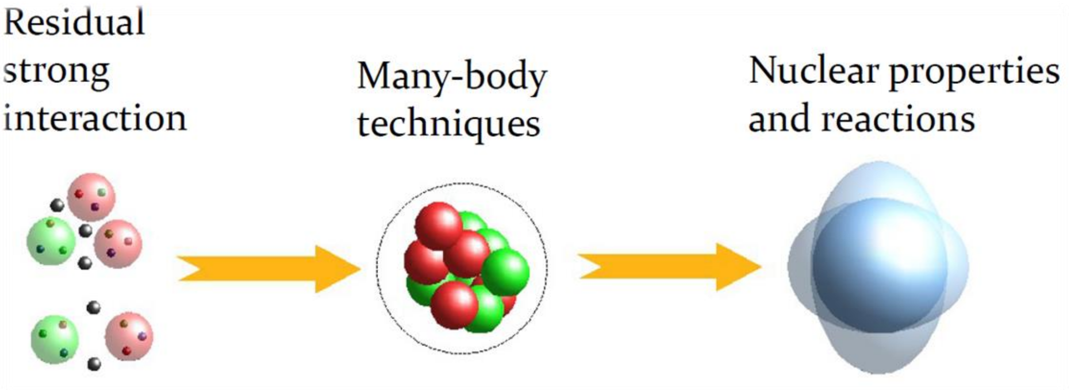
CAS Řež & LSU

D. Langr, T. Oberhuber

CTU, Prague

Ab-initio theory in nuclear physics

- *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: controlled and improvable *ab-initio* many-body computational methods: **No-Core Shell Model** (and extensions), **Coupled-Cluster method, Green Functions many-body theory**, **In-Medium Similarity Renormalization Group Approach** ….
- **No-Core Shell Model (NCSM) and No-Core Full Configuration(NCFC)**

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

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

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
→ Slater determinants constructed from HO s.p. states (with HO length *b*)

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

huge # of basis states needed → HPC (High Performance Computing)

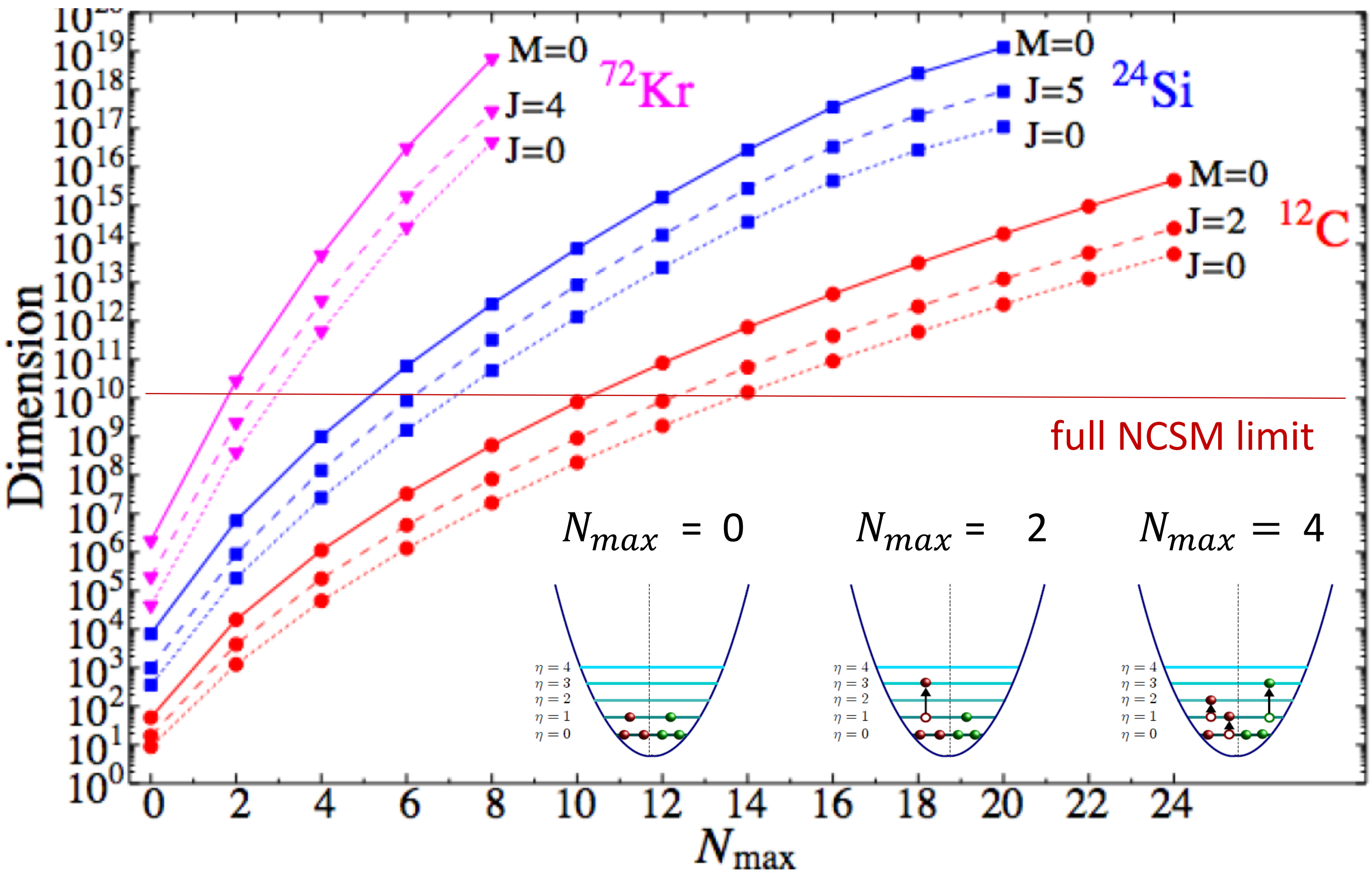
NCSM basis dimensions

- **M-scheme** + trivial construction of basis states + simple calculation of m.e.

  - large dimension of matrices

- **J-scheme** + few orders od magnitude reduction

  - involved calculation of m.e., more dense matrix

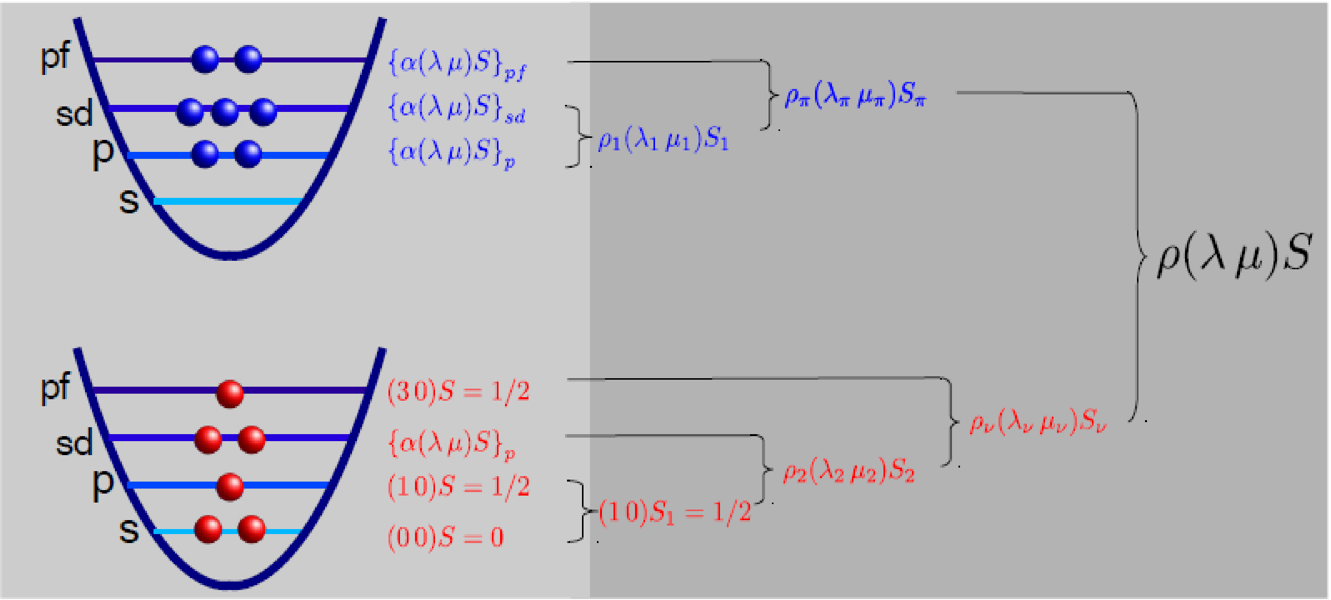


- **Symmetry-adapted basis - SU(3)**

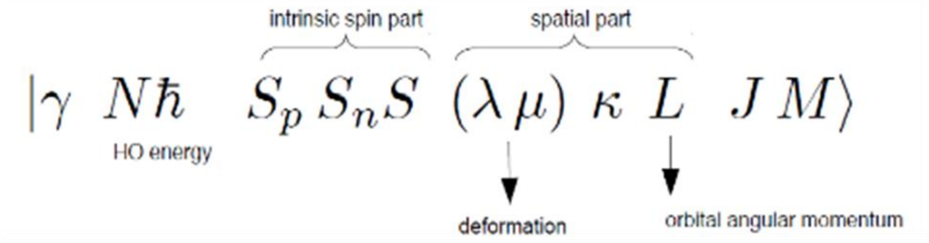
Symmetry-adapted NCSM

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.

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



many-nucleon basis state

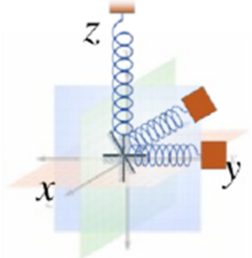


$$|\gamma\;\underbrace{N\hbar}_{\text{HO energy}}\;\overbrace{S_p\,S_n S}^{\text{intrinsic spin part}}\;\overbrace{\underset{\substack{\downarrow\\ \text{deformation}}}{(\lambda\,\mu)}\;\kappa\;\underset{\substack{\downarrow\\ \text{orbital angular momentum}}}{L}}^{\text{spatial part}}\;\;J\,M\rangle$$

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

Symmetry-adapted NCSM

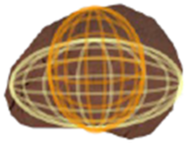
number of HO excitations



N

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

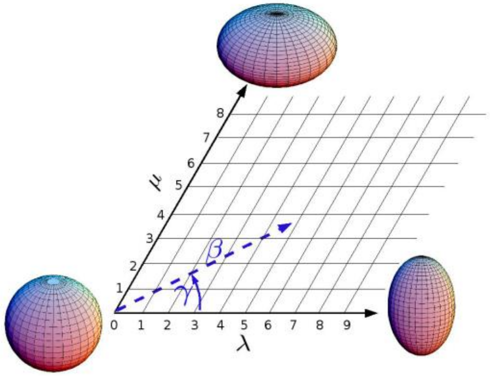
deformation SU(3)



$(\lambda\,\mu)$

rotation SO(3)

L

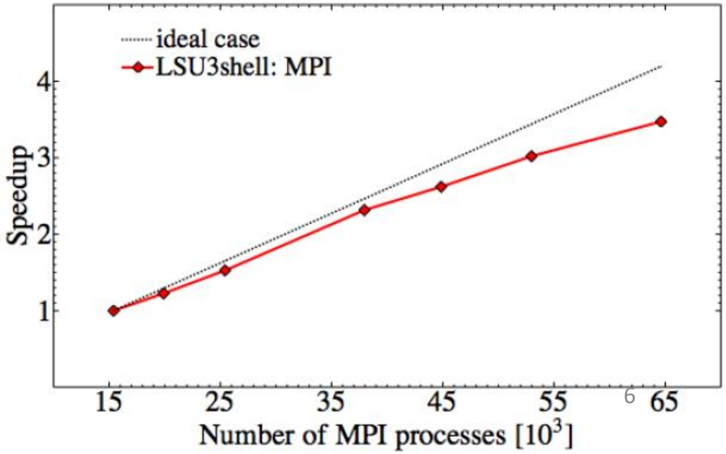


total angular momentum J

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

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

- highly nontrivial calculation of matrix elements 95% of runtime! (current version: two-body interaction)



SA-NCSM on Blue Waters

BLUE WATERS

total performance ≈ 1 Pflop/s (on a sustained basis)
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)

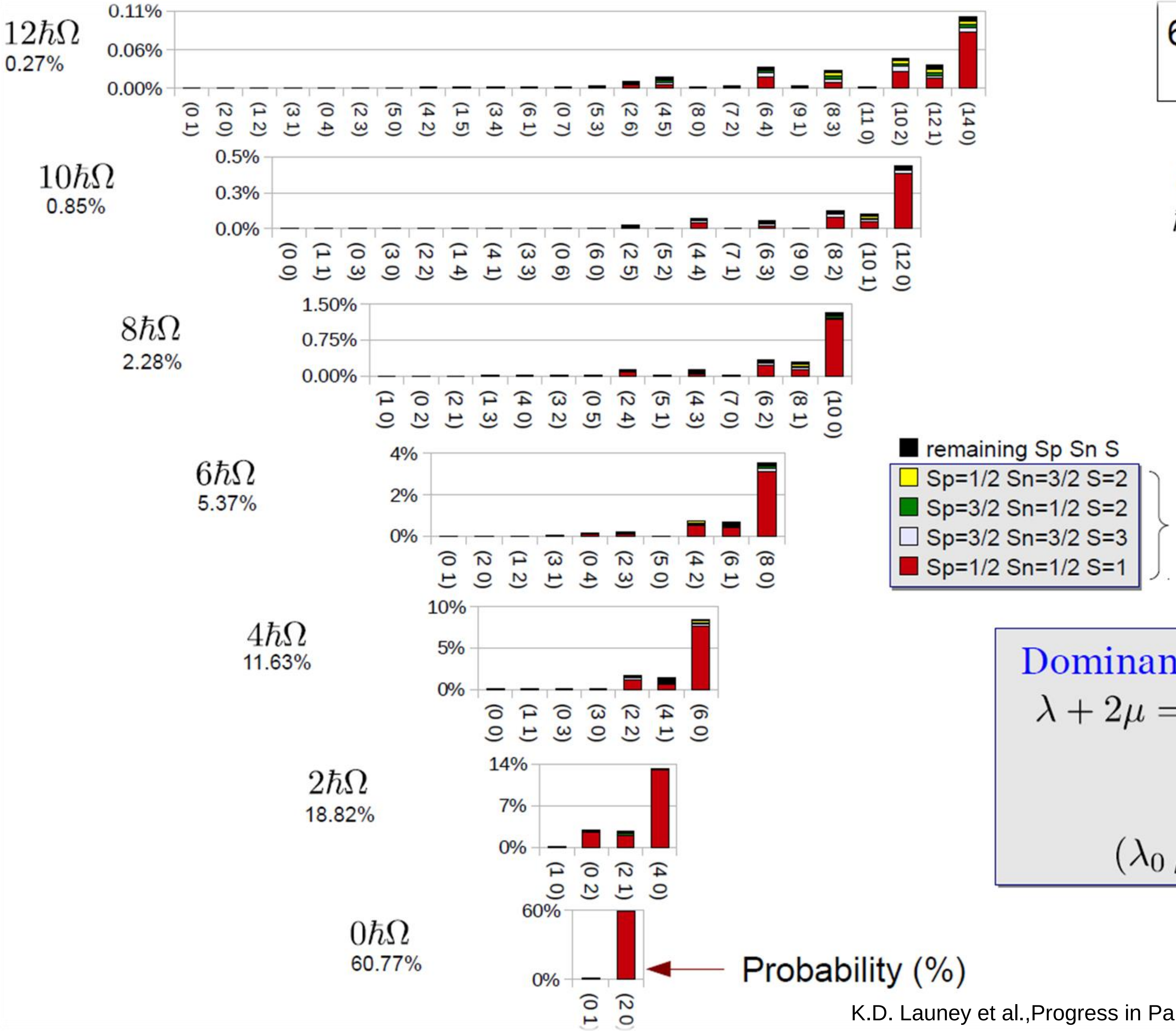
Computing time: US National Science Foundation grant.
Collaborative Research: Advancing first-principle symmetry-guided nuclear modeling for studies of nucleosynthesis and fundamental symmetries in nature
(PI J. Draayer, LSU)

example: $J^{\pi} = 2^{+}$ in ^{20}Ne in N_{max} = <4>8 space

- dim. ≈ 8.10^{7}
- runtime ≈ 1 hour for calculation of Hamiltonian + diagonalization
  by using ≈ 22 000 nodes (≈ 350 000 cores)
- matrix storage: 139 TB in VBC

Symmetry-adapted NCSM

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



~99% of ground state

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

N_{max} = 12

JISP16 + Vcoul

$\hbar\Omega = 20$ MeV

Dominant deformations

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

$$\uparrow$$

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

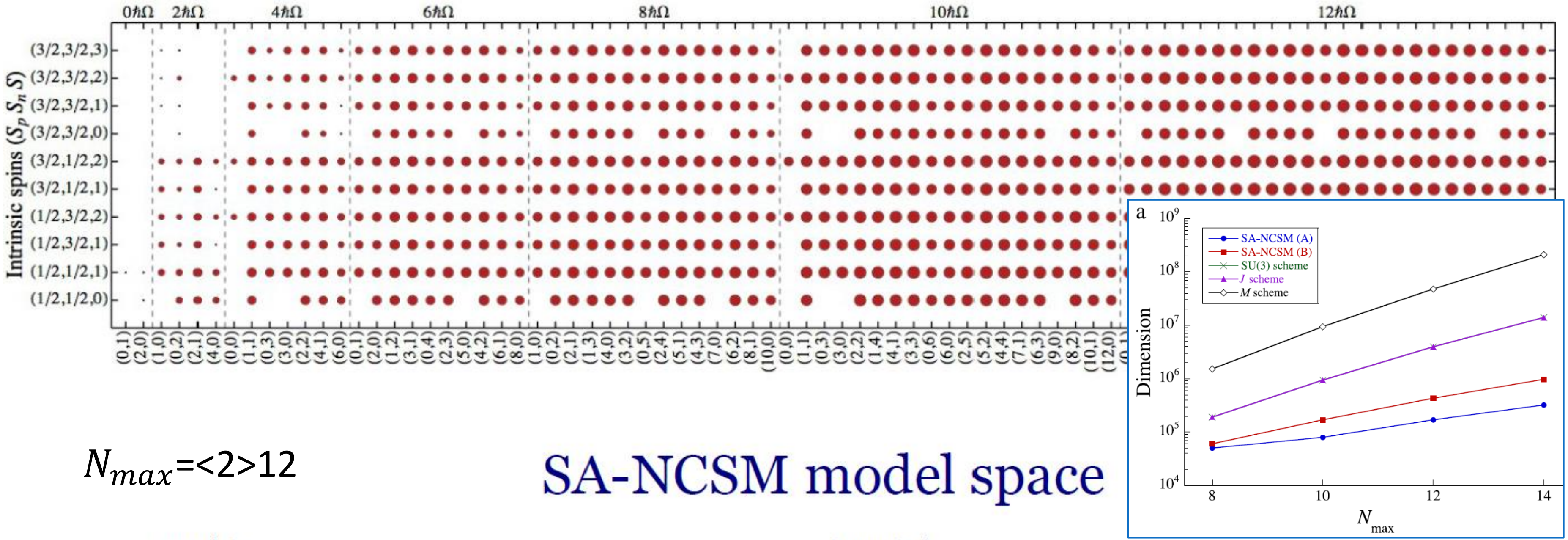
K.D. Launey et al.,Progress in Particle and Nuclear Physics 89 (2016)

Symmetry-adapted NCSM

^{6}Li model space 1^+

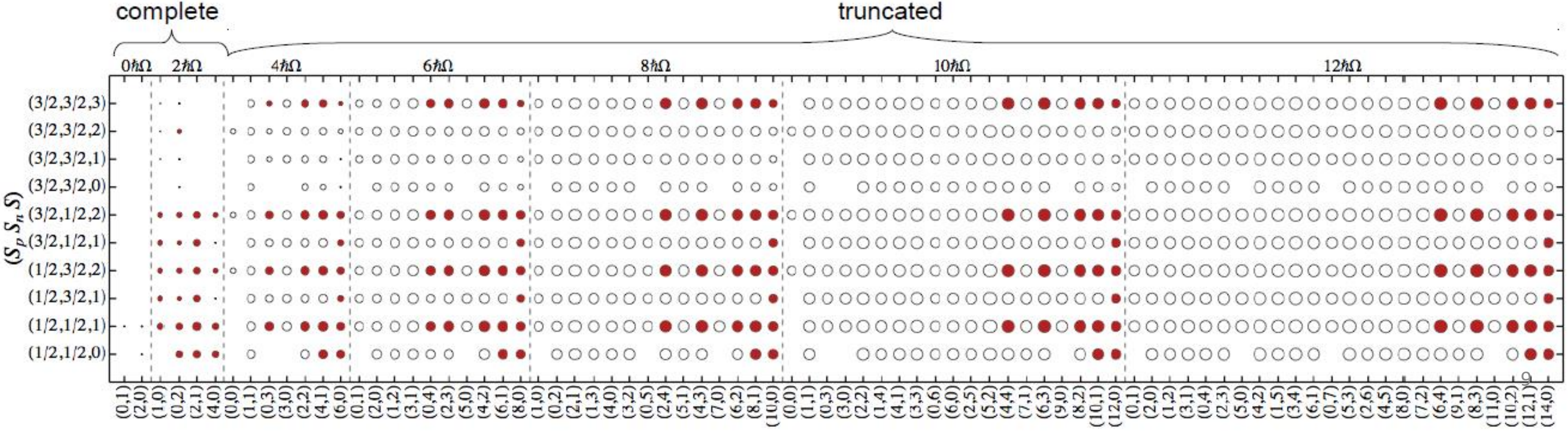
N_{max}=12

NCSM model space



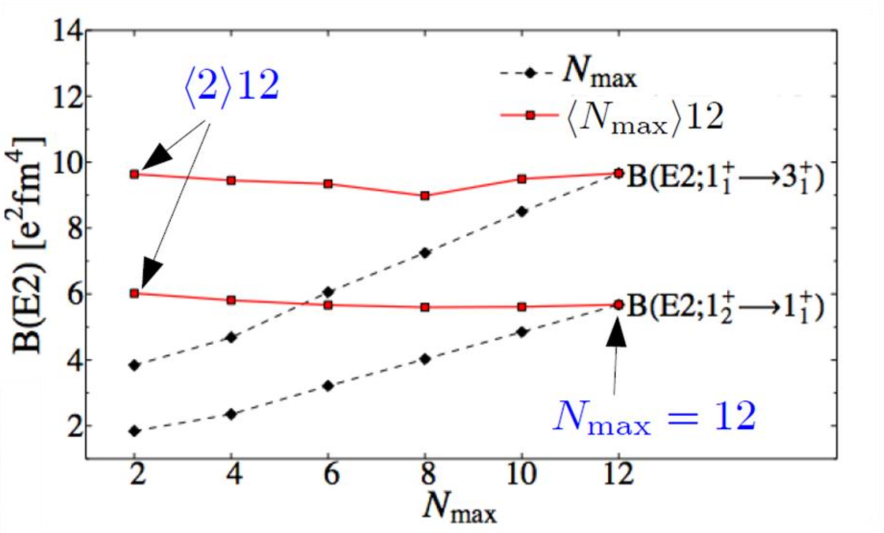
N_{max}=<2>12

SA-NCSM model space



Symmetry-adapted NCSM

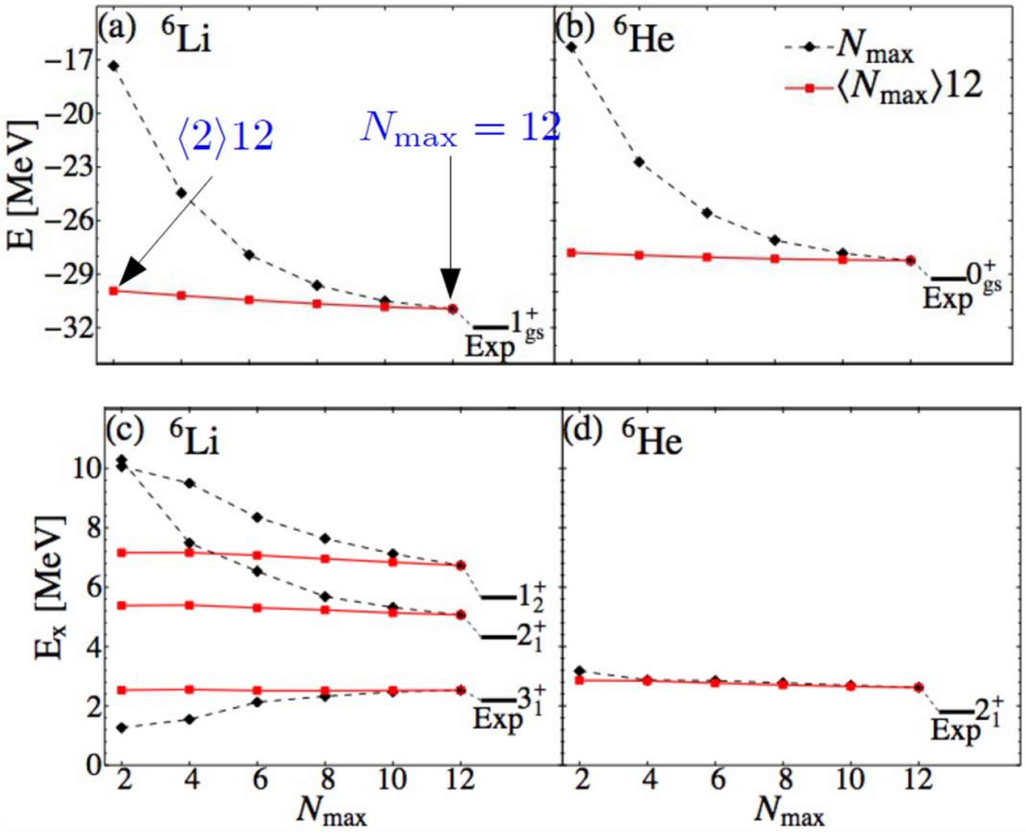
- simple patterns in the structure of low-lying states in light nuclei
- dominance of **high deformation**
  (λμ) = (20) (40) (60) (80) ….
  and **low spins** $S_p\ S_n\ S = \frac{1}{2}\ \frac{1}{2}\ 1$ ….



- drastic reduction of space

  5-10% of the total dimension

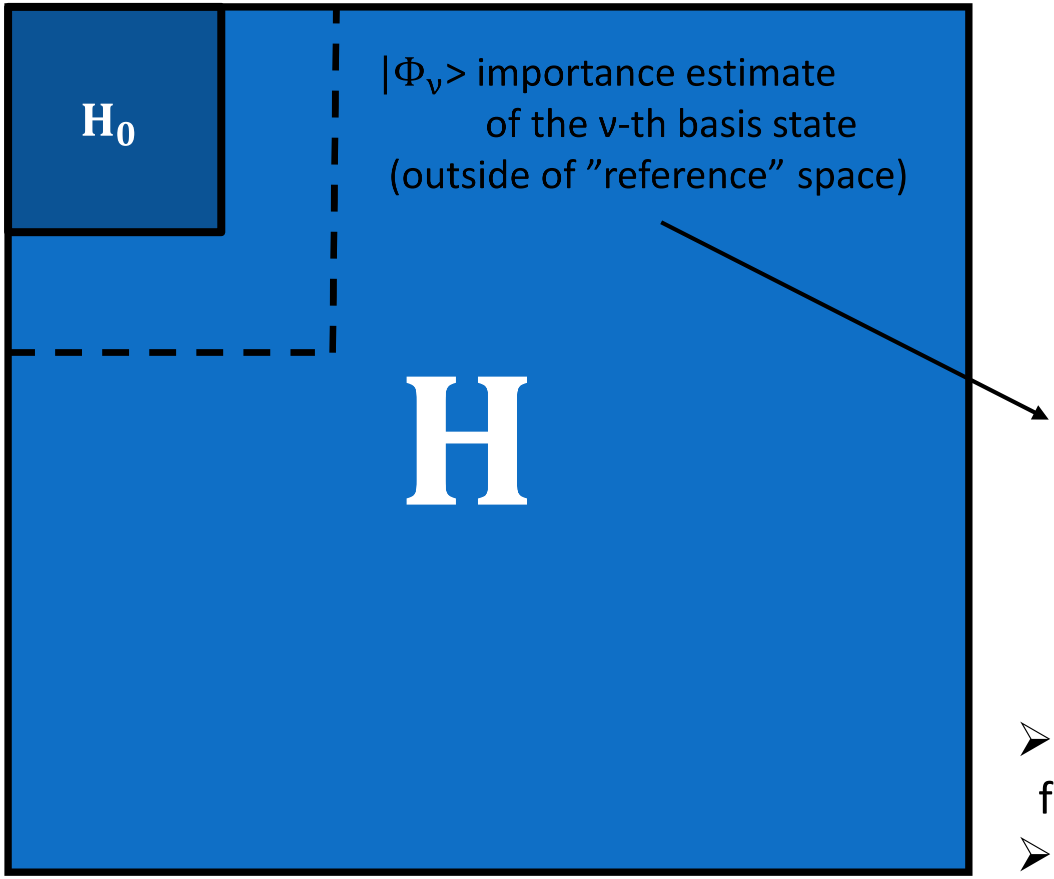
- good convergence of electric quadrupole (E2) transitions and quadrupole moments



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

SA-NCSM with importance truncation

- additional reduction of model space for heavier systems urgent
- quantitative justification of basis states selection → **Importance Truncation (IT)** estimation based on 1st order many-body perturbation theory



$|\Phi_\nu>$ importance estimate of the ν-th basis state (outside of ”reference” space)

lowest eigenstate(s) in the 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

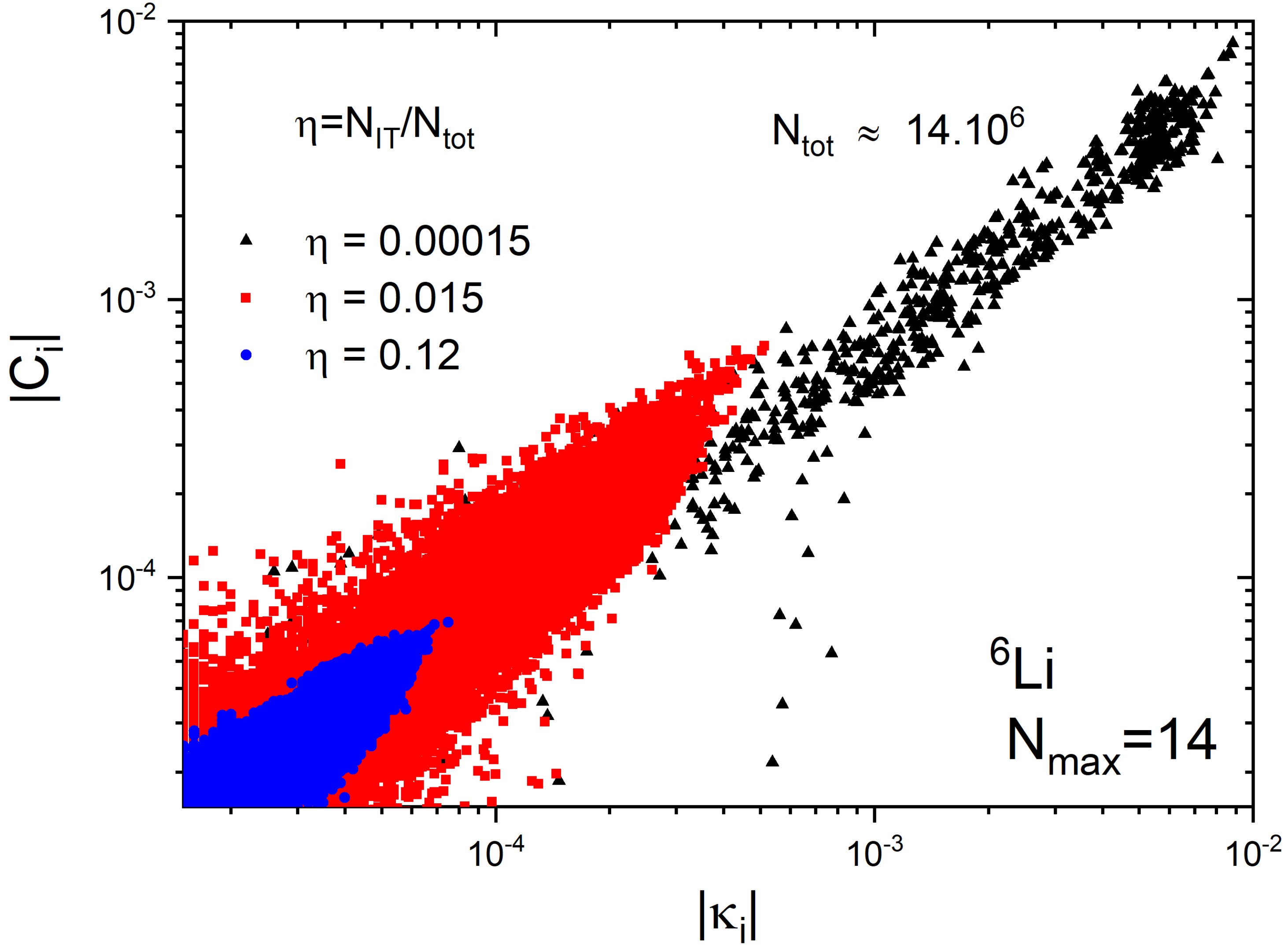
$$\boxed{\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}}$$

- Calculate importance measure κ_ν for the states outside the reference space
- Accept state(s) if $|\kappa_\nu| < \kappa_{min}$
- Rediagonalize H in larger space → new reference state(s)
- Decrease κ_{min} and repeat

Implemented in the IT-NCSM
R. Roth, P. Navrátil Phys. Rev. Lett. 99 (2007)
R. Roth, Phys. Rev. C 79, 064324 (2009)
Kruse et al. Phys. Rev. CC 87, 044301 (2013)

SA-NCSM with importance truncation

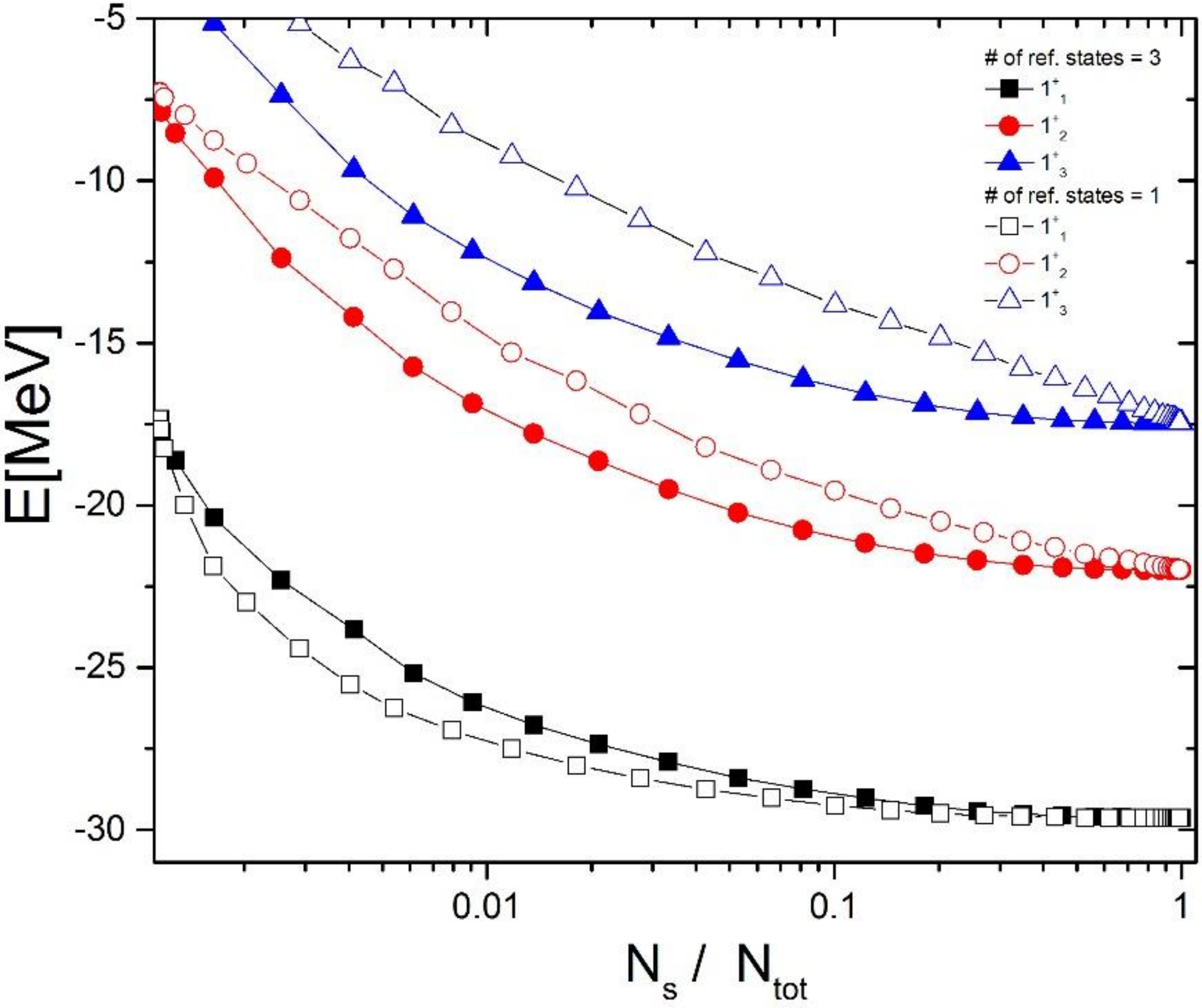
- Example: correlation between importance measure $|\kappa_i|$ and amplitudes $|C_i|$ of the i-th SA-NCSM basis components in the g.s. wave function of ^{6}Li.



SA-NCSM with importance truncation

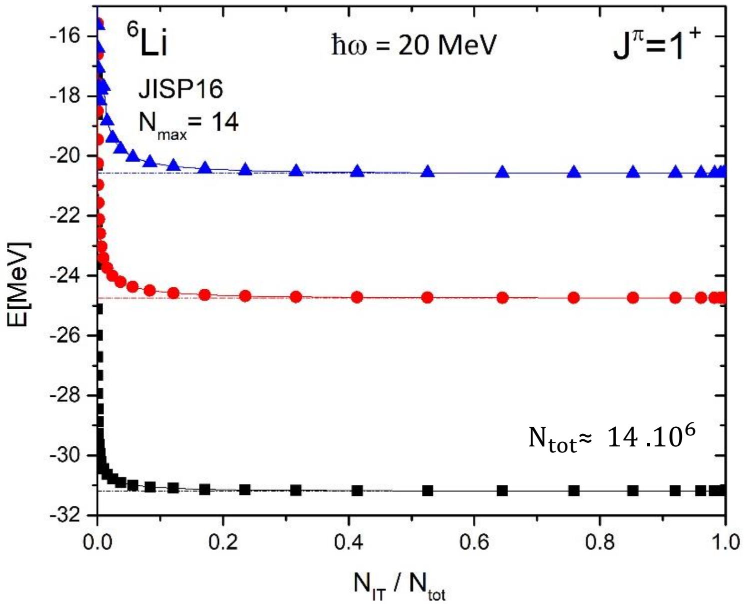
- Single vs. multi-reference IT?
- Multi-reference IT scheme more suitable for excited states

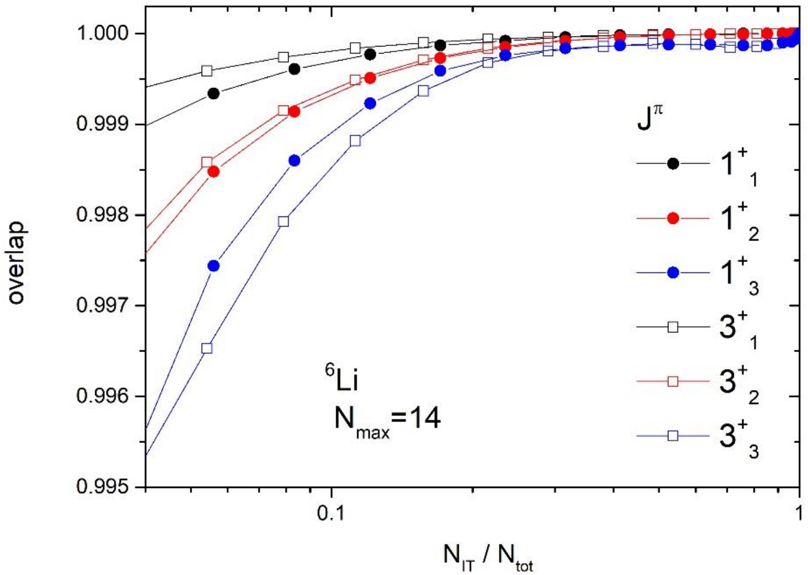
$$\kappa_{\nu} = -\frac{\langle \Phi_{\nu} | H | \Psi_{\text{ref}} \rangle}{\epsilon_{\nu} - \epsilon_{\text{ref}}}$$

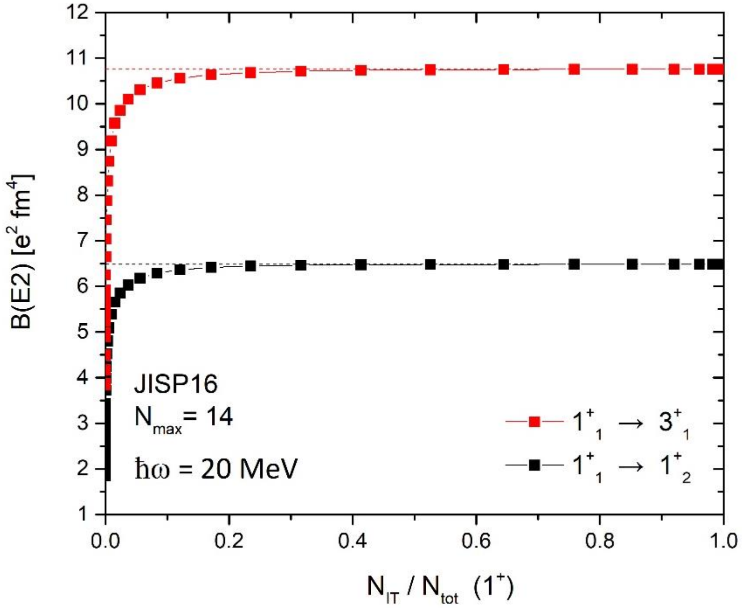


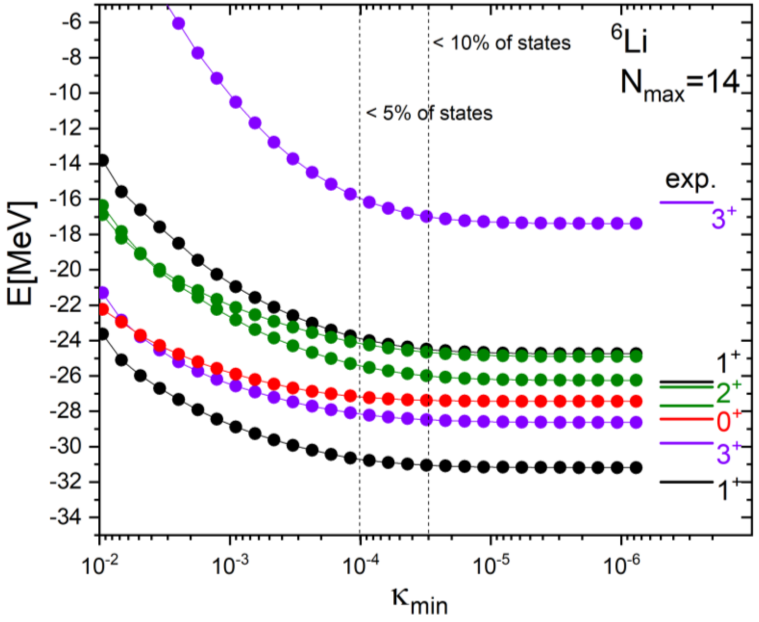
SA-NCSM with importance truncation

- fast convergence of energies and B(E2) ! → reduction of basis dimensions





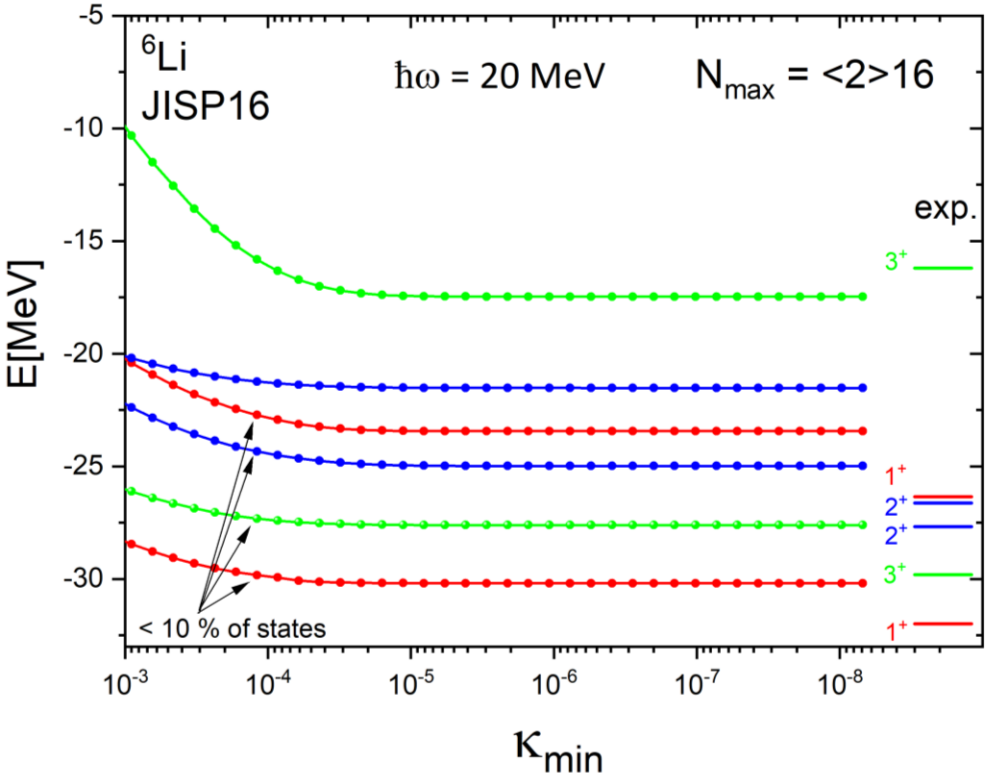


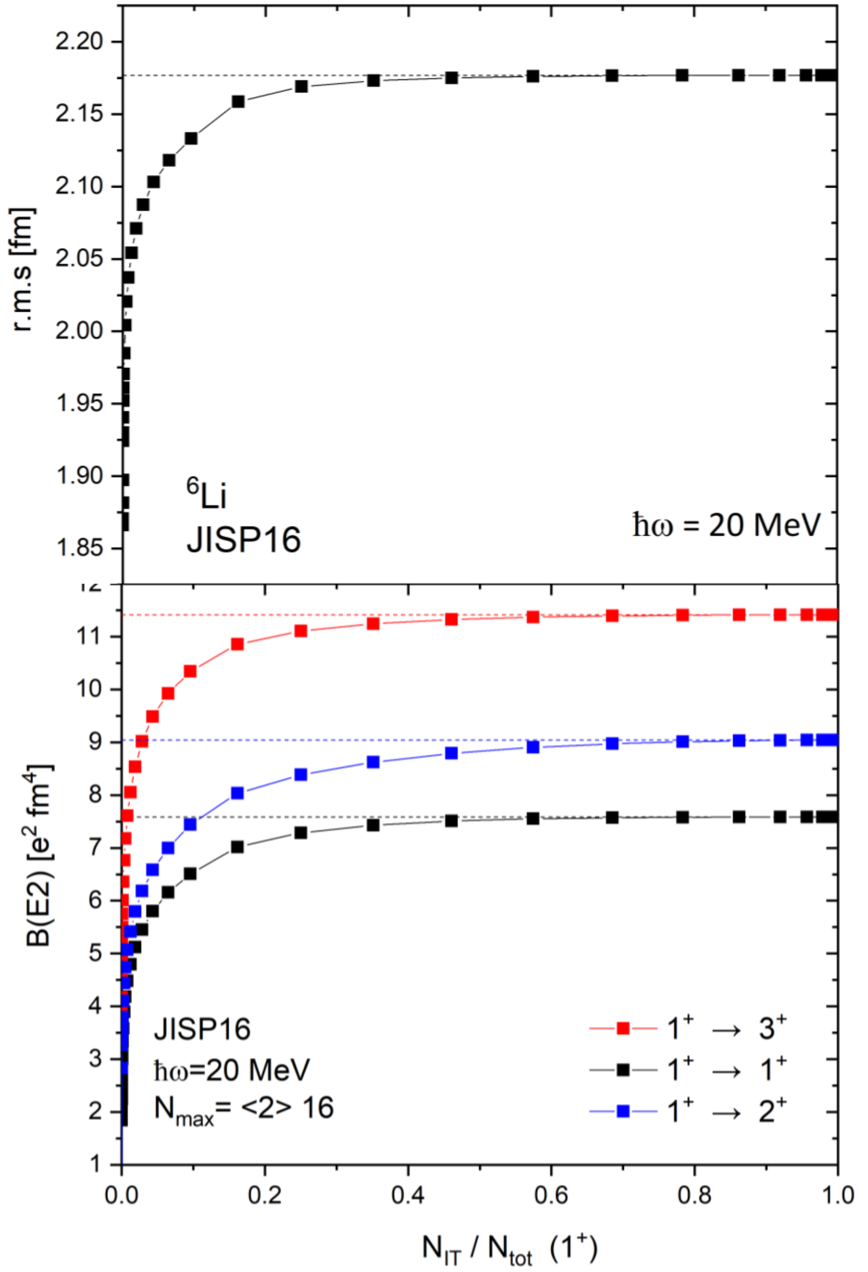


SA-NCSM with importance truncation

- Can be (truncated) SA-NCSM space even more reduced with the importance truncation estimate?

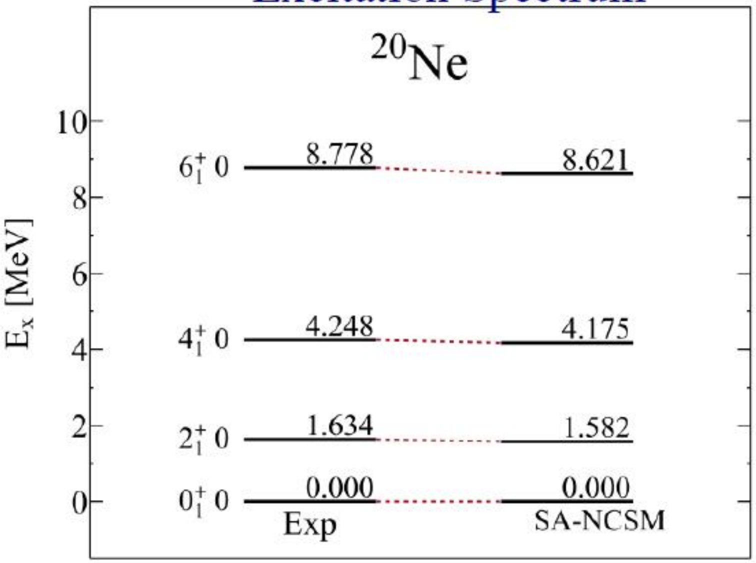
Yes, it can!



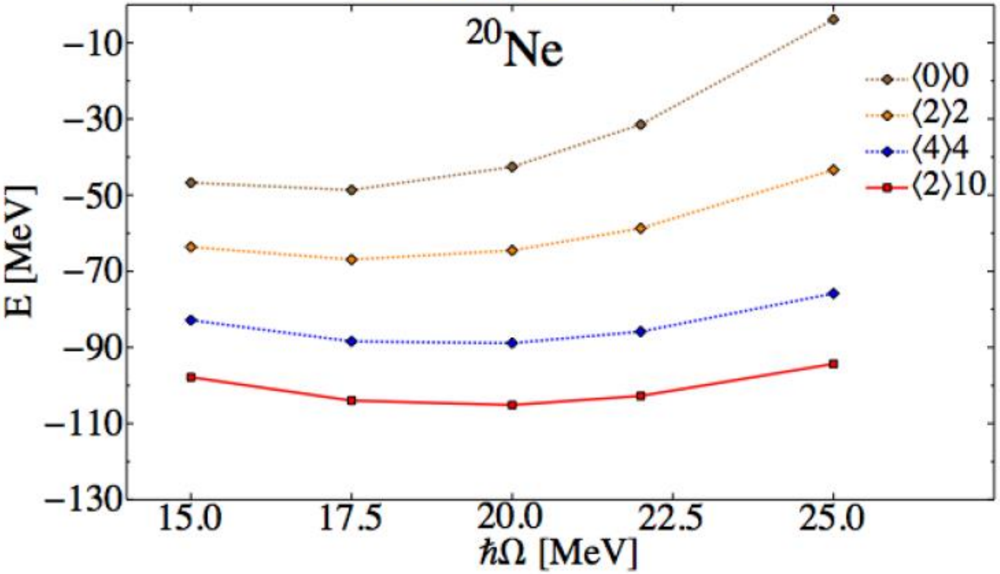


SA-NCSM with importance truncation

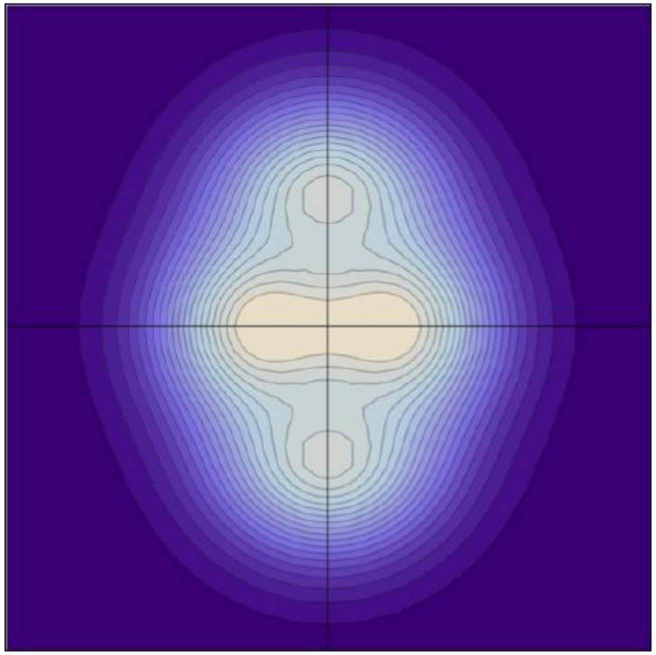
Excitation Spectrum



Binding energy



Nuclear density



Complete space: 4×10^{12}

Symmetry-adapted space: 1×10^{7}

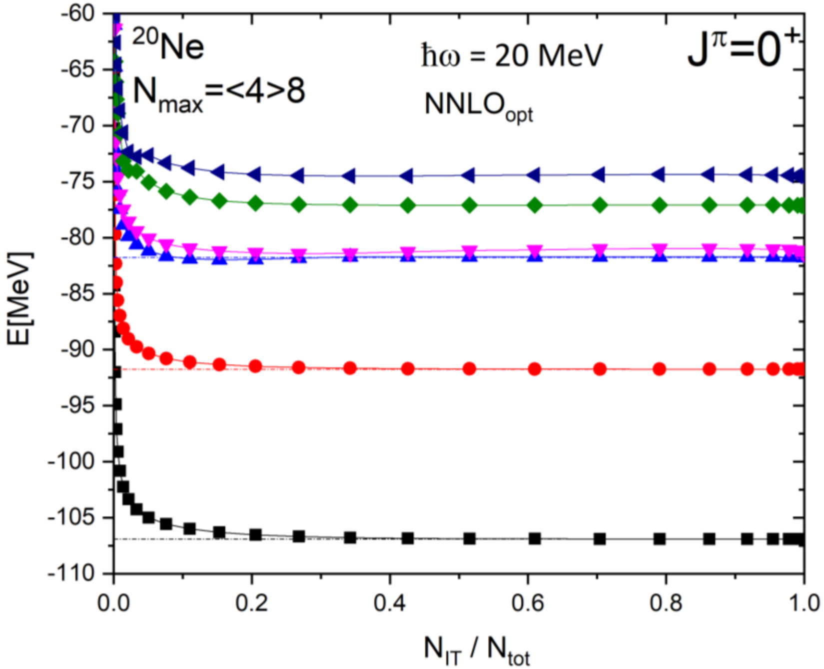
T. Dytrych

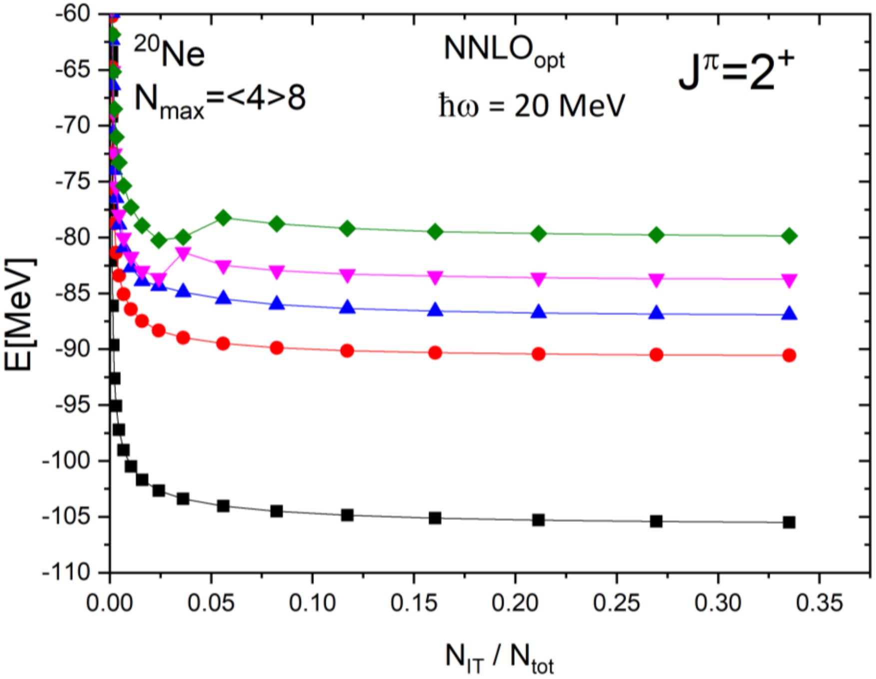
SA-NCSM with importance truncation

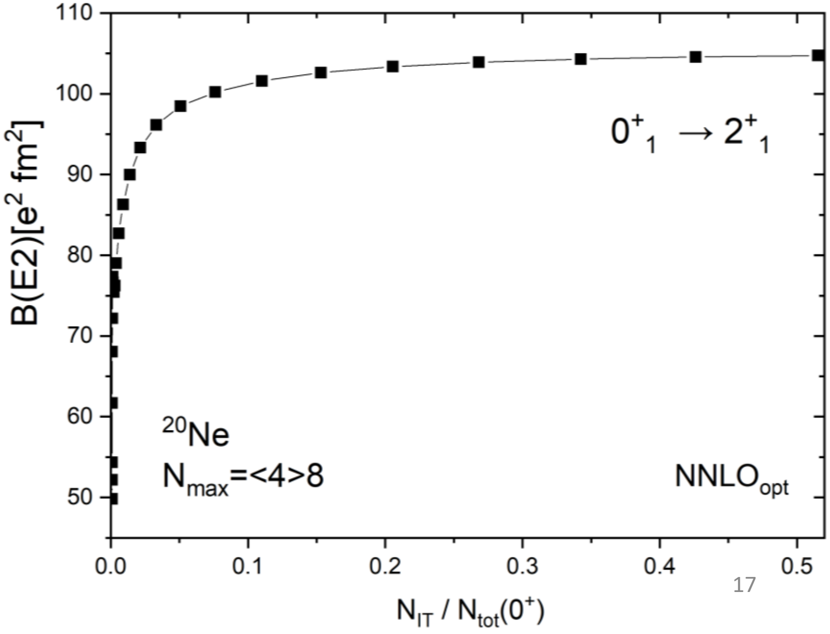
- test: additional truncation of very reduced SA-NCSM model space for heavier system ^{20}Ne

  N_{max} = <4>8 , dim $\sim 10^7$
  (N_{max}= 8 , dim $\sim 10^{12}$)

- fast convergence of energies and B(E2) values (10 % states)

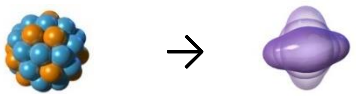


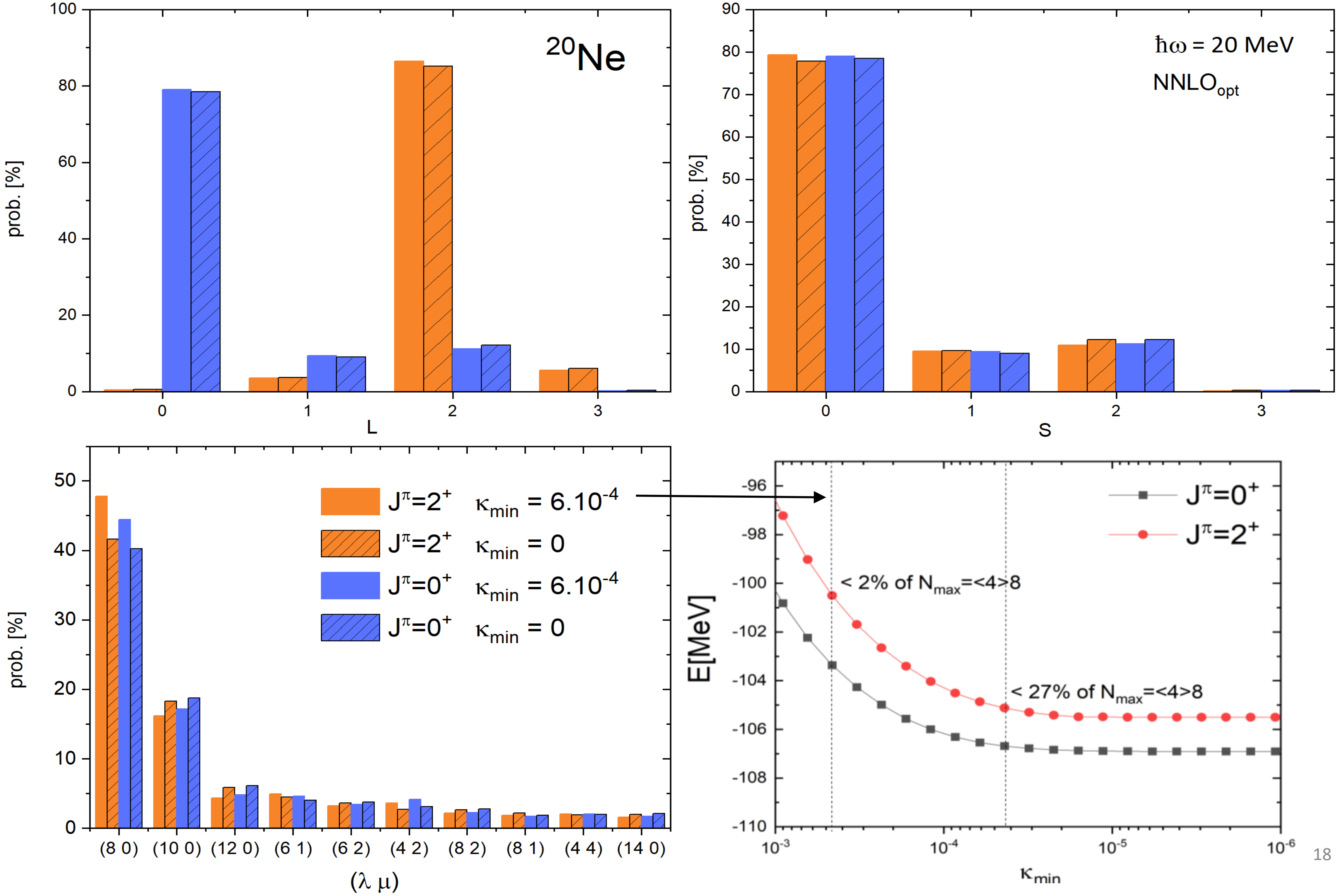




SA-NCSM with importance truncation

- LS decomposition of SA-NCSM w.f. **J=L+S**
  ab-initio description of lowest rotational states





Summary

- SA-NCSM: powerful tool for selection of physically relevant model spaces in *ab-initio* calculations based on symmetry arguments

- Emergence of collective features in light nuclei from *ab-initio* calculation

- Importance truncation: very effective scheme in SA-NCSM (energies, radii, transition probabilities).

Goals…

- Redesign *LSU3shell* to speed-up computation of m.e. and to avoid the storage of irrelevant m.e. → importance truncation in heavier systems

- NNN interactions: derivation of formalism and implementation to *LSU3shell*