Alpha clustering in light nuclei

Structure of low-lying states of ^{12}C

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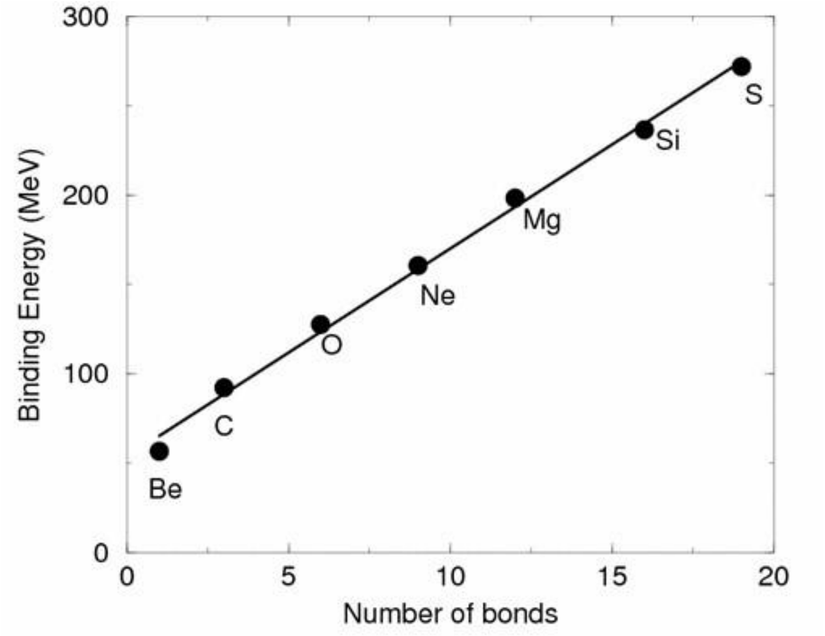
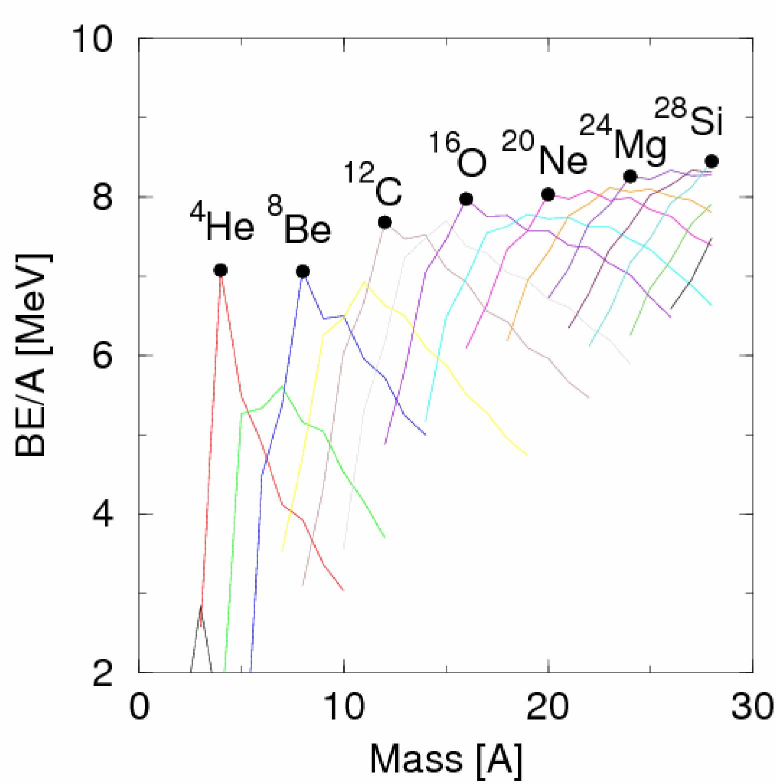
Outline

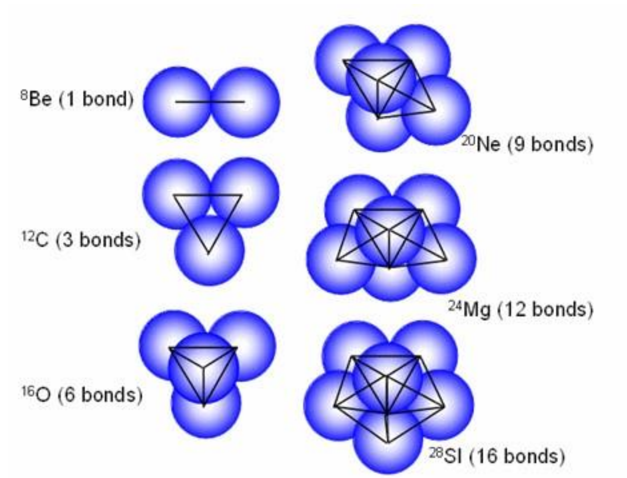
- Phenomenon of α clustering
- Spectrum of ^{12}C and famous Hoyle state
- Low-lying spectra of ^{12}C within Symmetry-adapted NCSM

Alpha clustering

- large binding energy of ^{4}**He**
- first excited state at 20.2 MeV (close to S_p, S_n)
- light α-conjugate nuclei energetically favoured
- cluster structure usually not pronounced in ground states





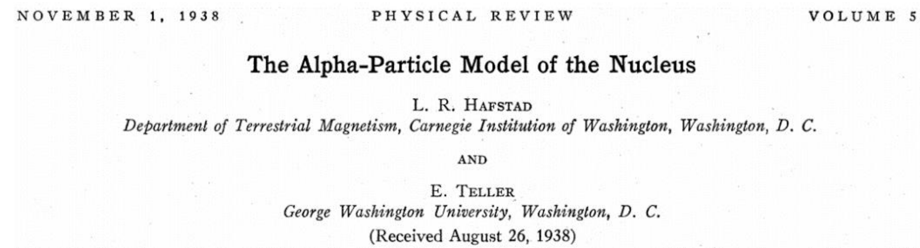


http://www.scholarpedia.org/article/Clusters_in_nuclei

First α cluster models

Cluster models: nucleus is a system of (diluted?) α particles

1938
Hafstad and *Teller* proposed α particle model as complementary to liquid drop and independent particle models

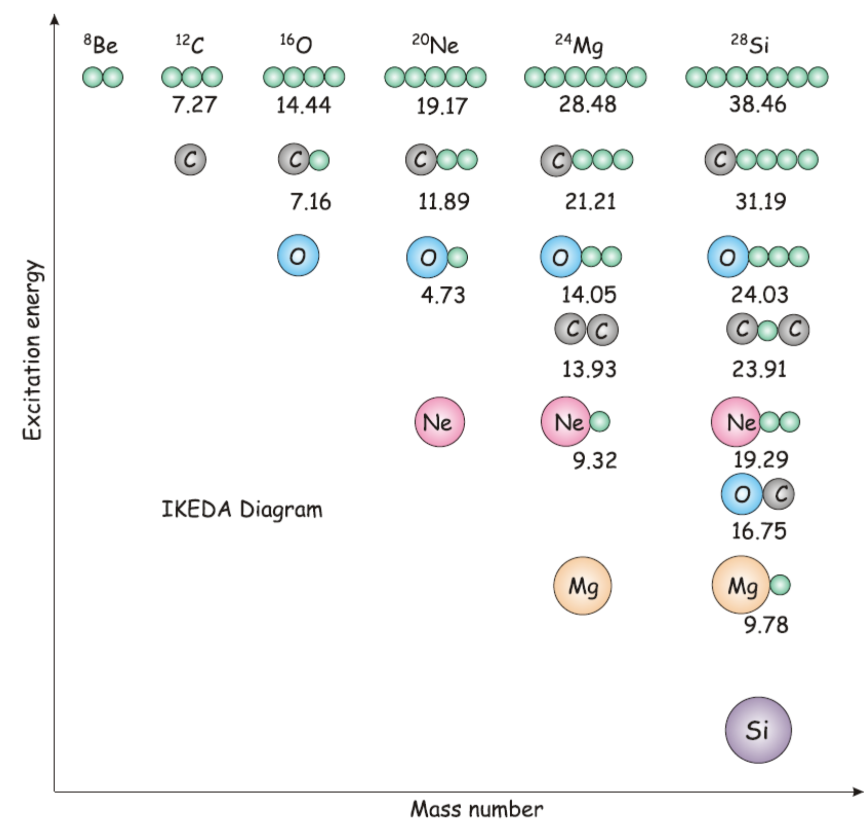

NOVEMBER 1, 1938 PHYSICAL REVIEW VOLUME 54

The Alpha-Particle Model of the Nucleus

L. R. Hafstad
Department of Terrestrial Magnetism, Carnegie Institution of Washington, Washington, D. C.
AND
E. Teller
George Washington University, Washington, D. C.
(Received August 26, 1938)

1956
Morinaga interpreted some excited states of nuclei as linear chains of α particles

M. Freer, H.O.U. Fynbo / Progress in Particle and Nuclear Physics 78 (2014) 1–23



1968
Ikeda, Tagikawa, Horiuchi

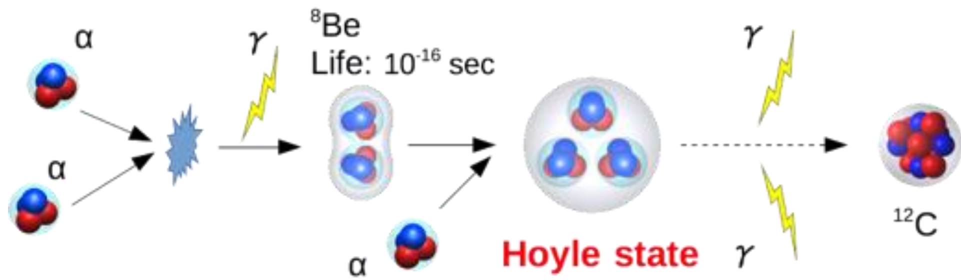
The Ikeda diagram

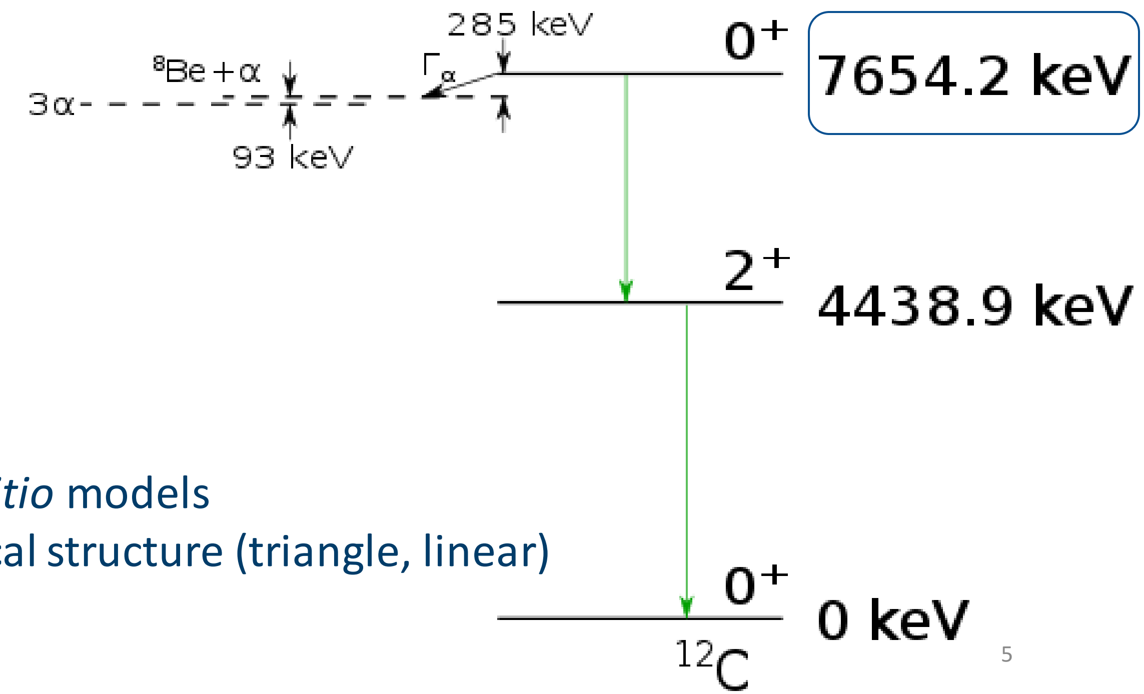
close to the cluster decay threshold energy nuclei can undergo structural changes

→ cluster structure expected in excited states of nuclei (g.s. in ^{8}**Be**)

Most famous cluster state in nuclei: The Hoyle state

- $J^{\pi} = 0^{+}$ state at 7.65 MeV in ^{12}**C**
- proposed in 1950 by F. Hoyle in order to explain production of carbon in nucleosynthesis: $\mathbf{^{4}He + {}^{4}He \leftrightarrow {}^{8}Be,\ {}^{8}Be + {}^{4}He \leftrightarrow {}^{12}C^{*}}$





- interesting for nuclear structure
  models for its cluster structure
- a big challenge for nuclear *ab-initio* models
- open questions about geometrical structure (triangle, linear)

Emergence of clusters from mean-field

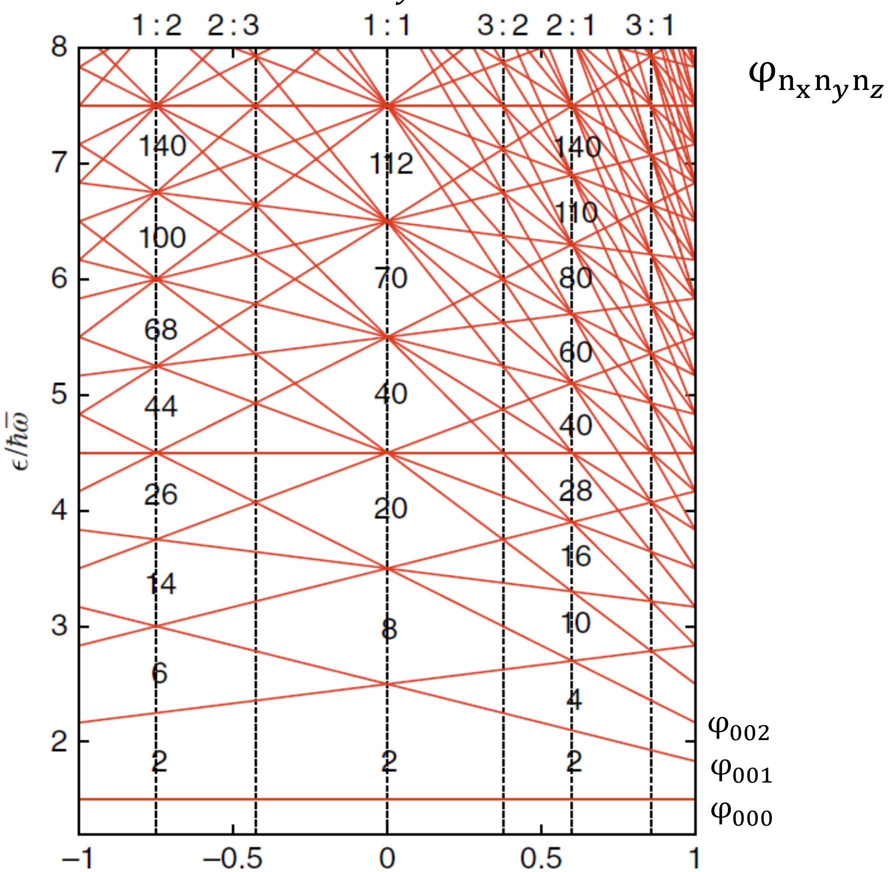
- How can clusters arise from an independent particle motion (i.e. shell model)?

textbook example of a simple mean-field model of deformed nucleus → axially symmetric ($\omega_x = \omega_y$) HO

$$V = \frac{m}{2}\left(\omega_x x^2 + \omega_y y^2 + \omega_z z^2\right) \qquad \varepsilon(\mathrm{n_x}, \mathrm{n_y}, \mathrm{n_z})/\hbar\bar{\omega} = \mathrm{n_x} + \mathrm{n_y} + \mathrm{n_z} + \frac{3}{2} - \frac{1}{3}\delta(2\mathrm{n_z} - \mathrm{n_x} - \mathrm{n_y})$$

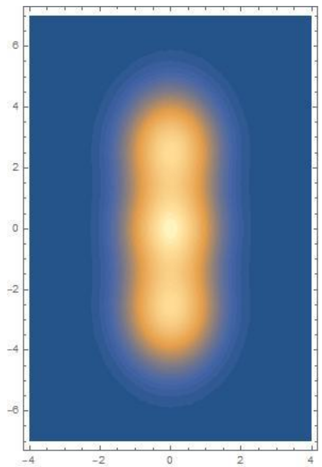
$$\bar{\omega} = \frac{1}{3}(\omega_x + \omega_y + \omega_z)$$

$\omega_x (= \omega_y) : \omega_z$

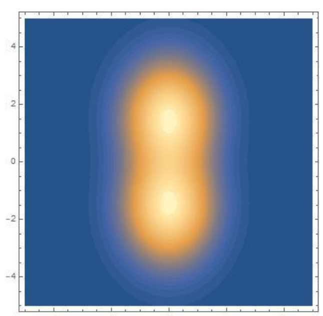


deformation $\delta = \frac{\omega_x - \omega_z}{\bar{\omega}}$

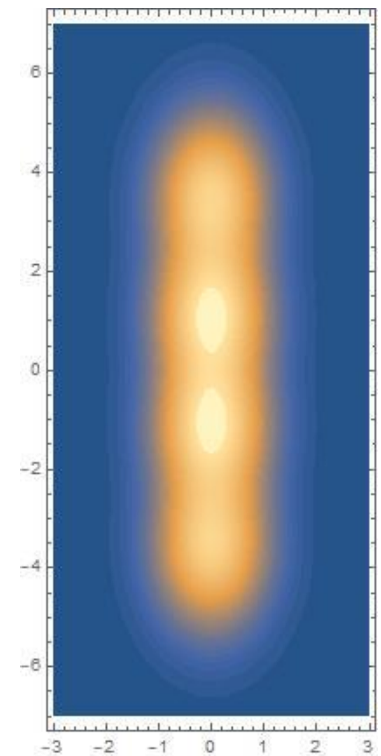
V.Zelevinsky: Physics of Atomic Nuclei



$|\varphi_{000}|^2 + |\varphi_{001}|^2 + |\varphi_{002}|^2$



$|\varphi_{000}|^2 + |\varphi_{001}|^2$



$|\varphi_{000}|^2 + |\varphi_{001}|^2 + |\varphi_{002}|^2 + |\varphi_{003}|^2$

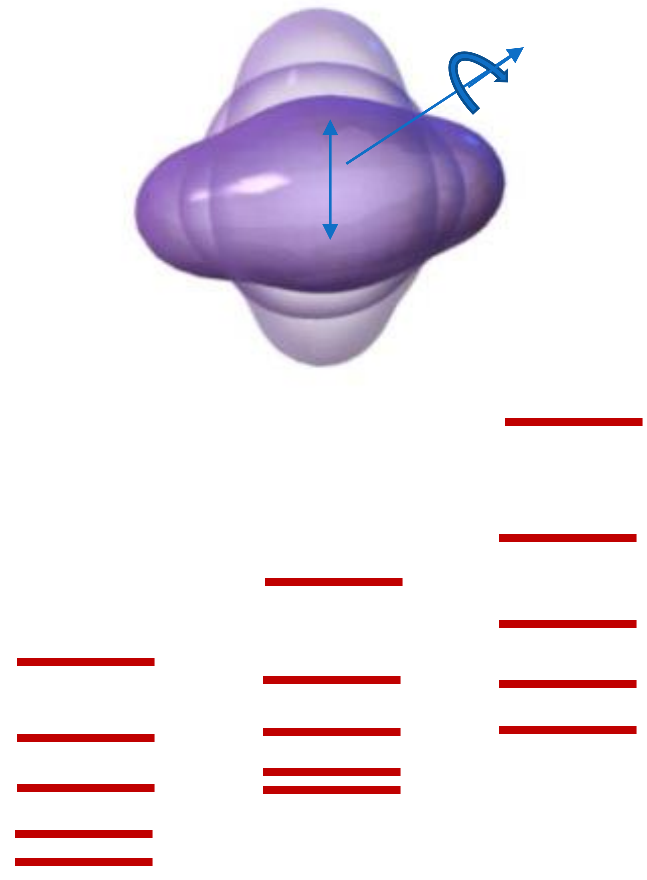
Is nucleus spherical, deformed, rotating or (and) vibrating?

characteristic patterns (sequences of spins and parities) in nuclear spectra are related to shapes and basic (collective) excitations (rotations, vibrations ...)

spherical vibrator

rigid rotor

non-rigid (vibrating) rotor



Rotational-vibrational spectrum of ^{12}C?

- Algebraic Cluster Model: „triatomic like“ structure similar to H_3^+ molecule
  → rotations and vibrations of 3α system arranged in equilateral triangle

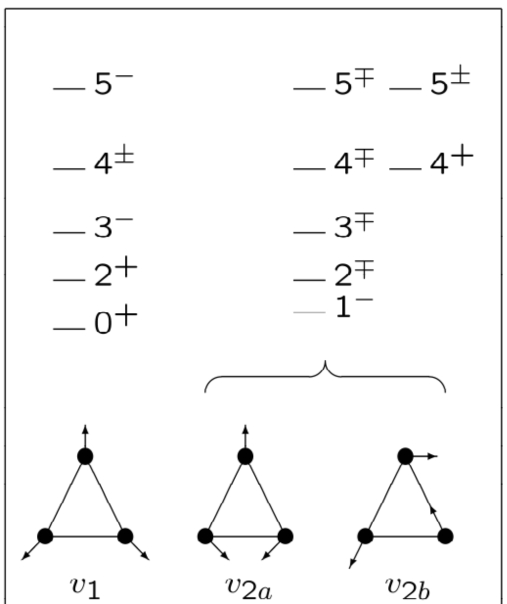
- boson model (2 vector bosons + 1 auxiliary scalar), no fermionic structure of α particles
- spectrum generating algebra U(7)

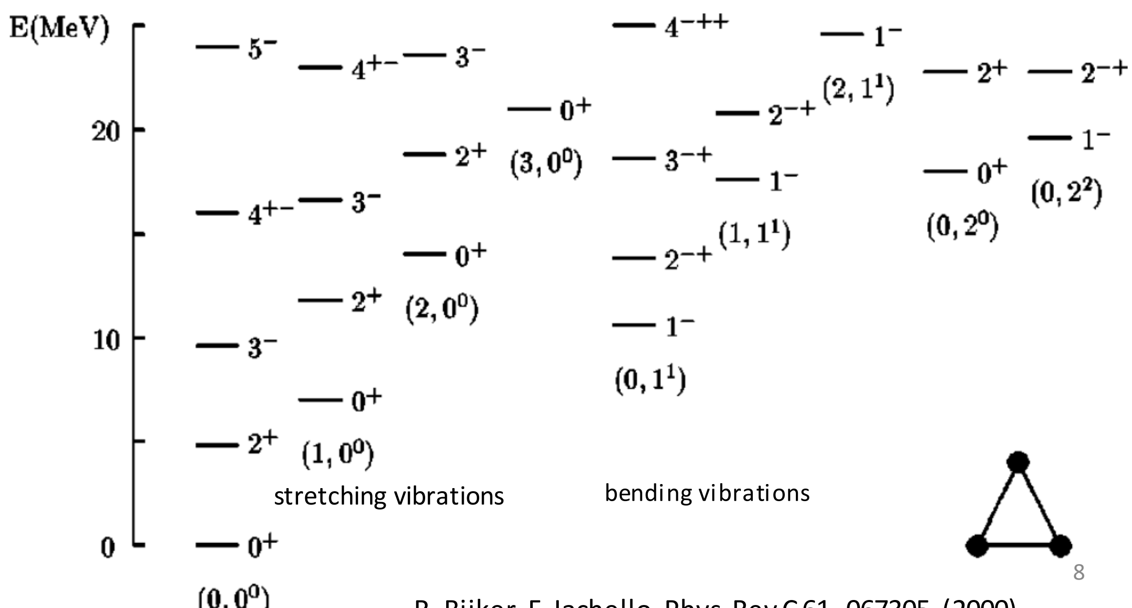
- **band structure of the spectrum: fingerprints of geometric configurations**

$$E(v_1, v_2, l, L, K, M) = E_0 + Av_1 + Bv_2 + CL(L+1) + D(K \pm 2l)^2$$

vibrations *rotations*

- Hoyle state: vibrational (stretching) breathing vibration
- lowest 1^- state: bending vibration





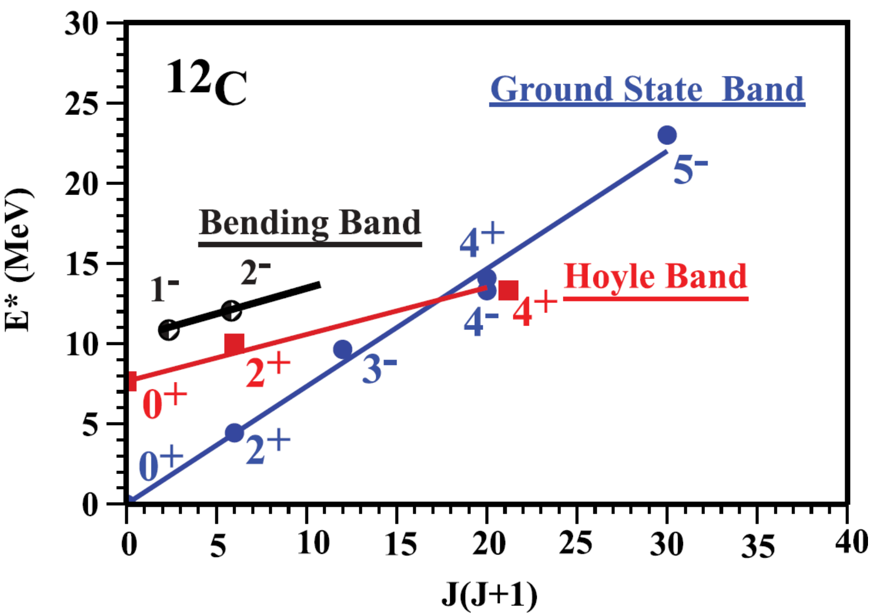
R. Bijker, F. Iachello, Phys. Rev C 61, 067305 (2000).

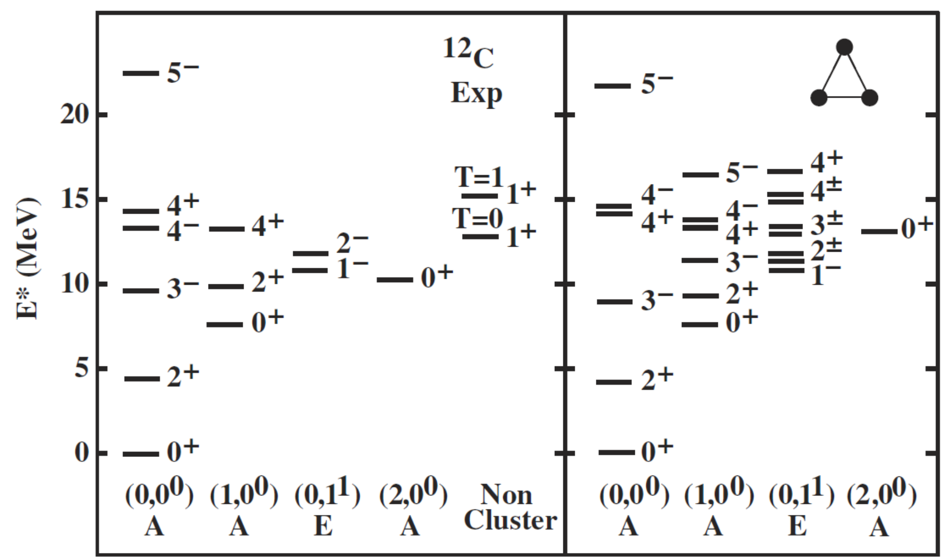
Rotational-vibrational spectrum of ^{12}C?

- observed sequence of low-lying states fits *J(J+1)* rotational pattern

$$E_{rot}=\frac{\hbar^2 J(J+1)}{2I}$$

- ACM (with anharmonicities and vibrational dependence of moment of inertia) describes all cluster states bellow 15 MeV (and many more)
- prediction for ground state band and Hoyle band
- $J^{\pi}=5^-$ state and doublet $4^+\ 4^-$ identified via **$^{12}C(^4He,3\alpha)\ ^4He$** reaction fit *J(J+1)* law
- signature of D_{3h} symmetry in nuclei

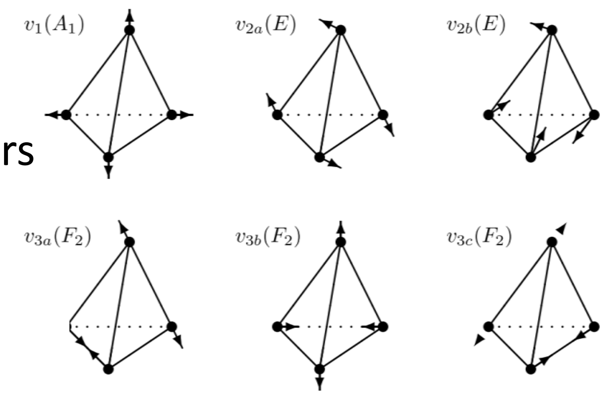




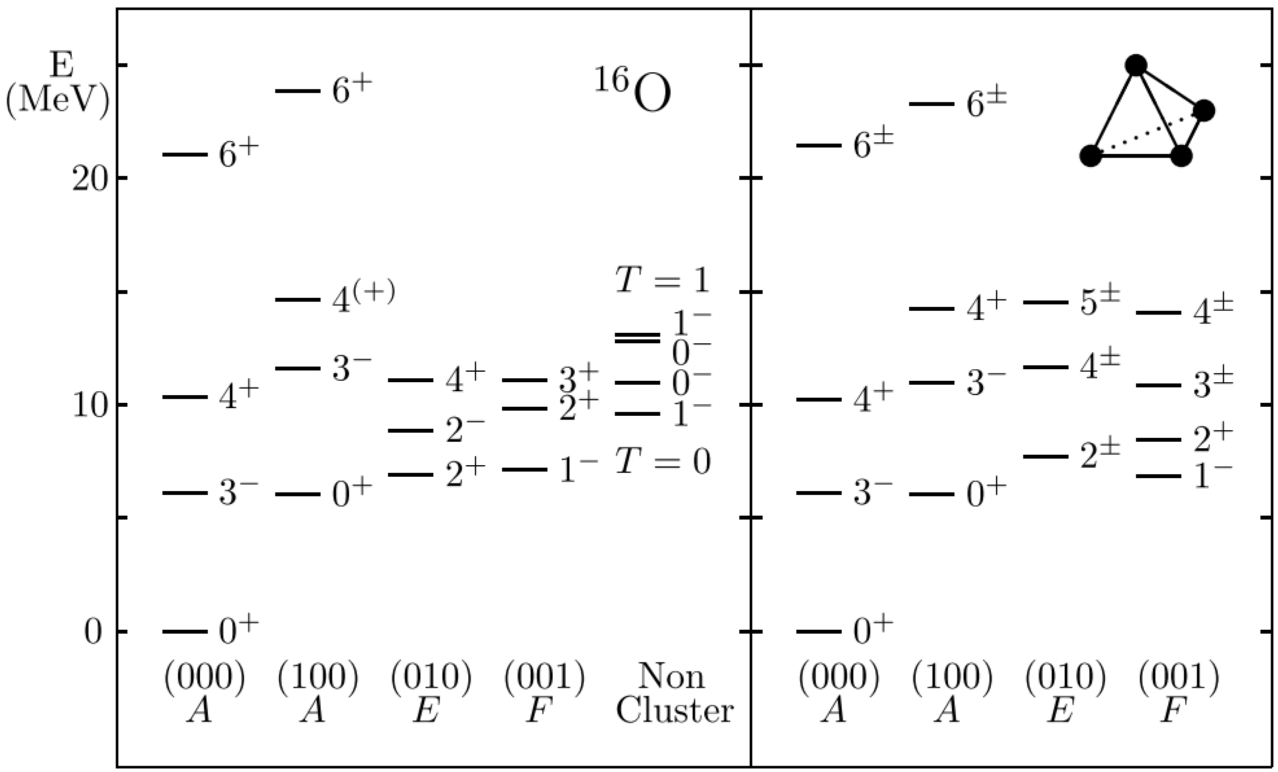
Marin-Lambarri D J *et al,* Phys. Rev. Lett. **113**, 012502 (2014).

Tetrahedral symmetry of ^{16}O?

- interpretation of low-lying states in ^{16}O within ACM
  → rotations and vibrations of 4α particles located in corners of tetrahedron



R. Bijker, F. Iachello / Nuclear Physics A 957 (2017) 154–176



Realistic NN interactions

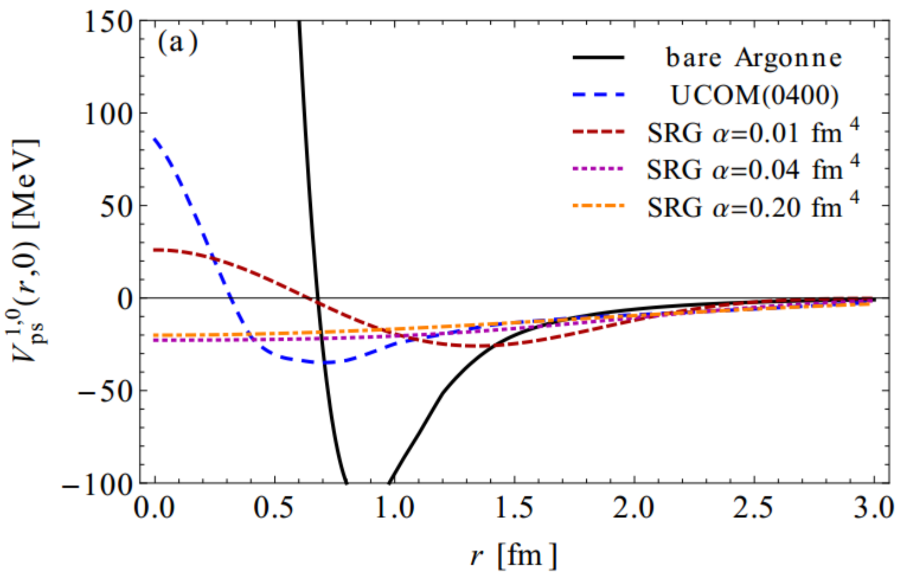
- derivation of inter-nucleon interaction from fundamental theory – QCD not available
- „realistic“ NN potentials -

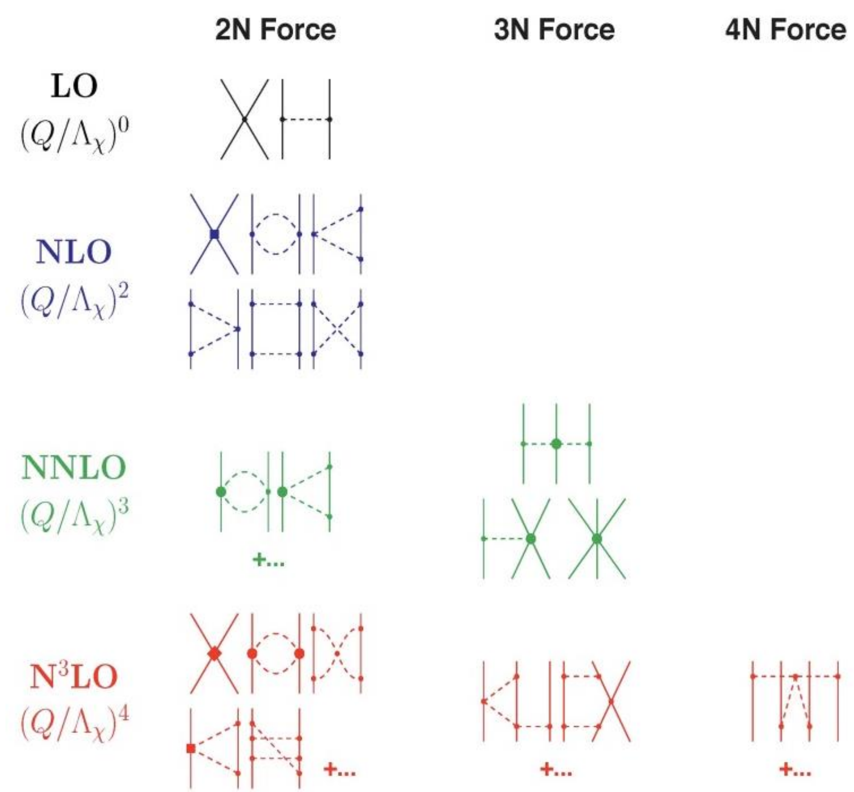
reproduce NN scattering data (phase shifts) up 300 MeV.
existence of phase-shift equivalent potentials
non-local forces (dependence on impulses)
existence of effective many-body forces

- *Chiral perturbation theory*- links low-energy nuclear physics to QCD

degrees of freedom: nucleons and pions
hierarchy of relevant diagrams, 3-, 4- ...body forces
short distance physics not resolved, but captured in short range couplings fitted to *NN* scattering data and A=3,4 nuclei

Feldmeier et al. arXiv:1407.4325

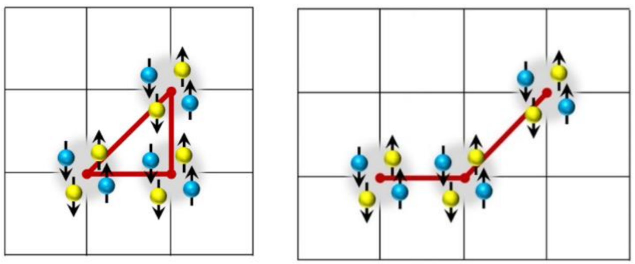




Lattice calculations of ^{12}C and ^{16}O

- *Ab-initio* lattice calculation within *chiral effective field theory*
- first (succesful) *ab-initio* calculation of the Hoyle state

^{12}C: ground state dominated by triangular configuration
Hoyle state bent-arm (obtuse triangle) configuration



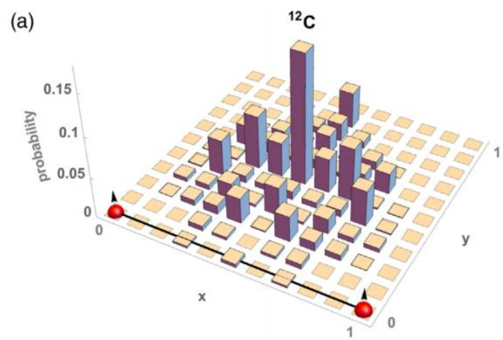


TABLE II. Lattice and experimental results for the energies of the low-lying even-parity states of ^{12}C, in units of MeV.

	0_1^+	$2_1^+(E^+)$	0_2^+	$2_2^+(E^+)$
LO	$-96(2)$	$-94(2)$	$-89(2)$	$-88(2)$
NLO	$-77(3)$	$-74(3)$	$-72(3)$	$-70(3)$
NNLO	$-92(3)$	$-89(3)$	$-85(3)$	$-83(3)$
Expt.	-92.16	-87.72	-84.51	$-82.6(1)$ [8,10] $-81.1(3)$ [9] $-82.32(6)$ [11]

E. Epelbaum et al, Phys. Rev. Lett. 109, 252501 (2012)
S. Elhatisari et al, Phys. Rev. Lett. 119, 222505 (2017)

^{16}O : ground state tetrahedral structure
first excited state squarelike with rotational 2^+ excitation

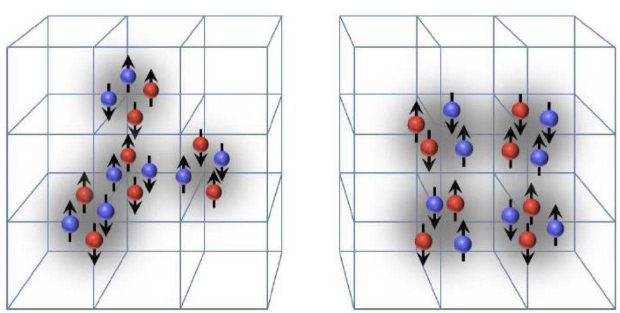


TABLE I. NLEFT results and experimental (Expt.) values for the lowest even-parity states of ^{16}O (in MeV). The errors are one-standard-deviation estimates which include both statistical Monte Carlo errors and uncertainties due to the extrapolation $N_t \to \infty$. The notation is identical to that of Ref. [21].

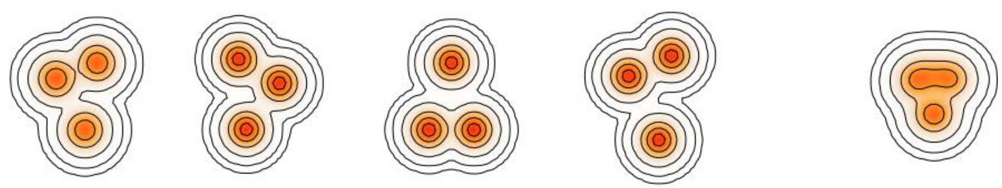
J_n^p	LO (2N)	NNLO (2N)	$+3N$	$+4N_{\rm eff}$	Expt.
0_1^+	$-147.3(5)$	$-121.4(5)$	$-138.8(5)$	$-131.3(5)$	-127.62
0_2^+	$-145(2)$	$-116(2)$	$-136(2)$	$-123(2)$	-121.57
2_1^+	$-145(2)$	$-116(2)$	$-136(2)$	$-123(2)$	-120.70

E. Epelbaum et al, Phys. Rev. Lett. 112, 102501 (2014)

Fermionic molecular dynamics

- microscopic model based on realistic UCOM interaction
- fermionic structure: nucleons represented by Gaussian wave packets
- fluster and non-cluster configurations
- parameters are determined variationally: similar to Hartree-Fock in Gaussian single-particle basis: variety of shapes (symmetry breaking of the Hamiltonian)
- configuration mixing of mean-field states (Generator Coordinate Method)

PRL **98,** 032501 (2007) PHYSICAL REVIEW LETTERS week ending 19 JANUARY 2007



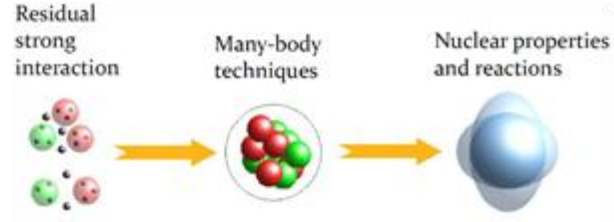
$|\langle 1|0_1^+\rangle| = 0.30$ $|\langle 2|0_1^+\rangle| = 0.25$ $|\langle 3|0_1^+\rangle| = 0.15$ $|\langle 4|0_1^+\rangle| = 0.08$ $|\langle 5|0_1^+\rangle| = 0.94$

$|\langle 1|0_2^+\rangle| = 0.72$ $|\langle 2|0_2^+\rangle| = 0.71$ $|\langle 3|0_2^+\rangle| = 0.61$ $|\langle 4|0_2^+\rangle| = 0.61$ $|\langle 5|0_2^+\rangle| = 0.04$

FIG. 2 (color online). Intrinsic one-body densities of the four FMD states which contribute most to the Hoyle state and their respective amplitudes for the ground state (0_1^+) and the Hoyle state (0_2^+). The fifth state, obtained by variation after projection on angular momentum, is the leading component in the ground state. Note that the FMD states are not orthogonal.

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 or $\hbar\omega$)

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

sources of uncertainty

- convergence of observables due to the finite basis expansion
- NN+(NNN) interaction

Complexity of the interaction is traded against the simplicity of the basis!

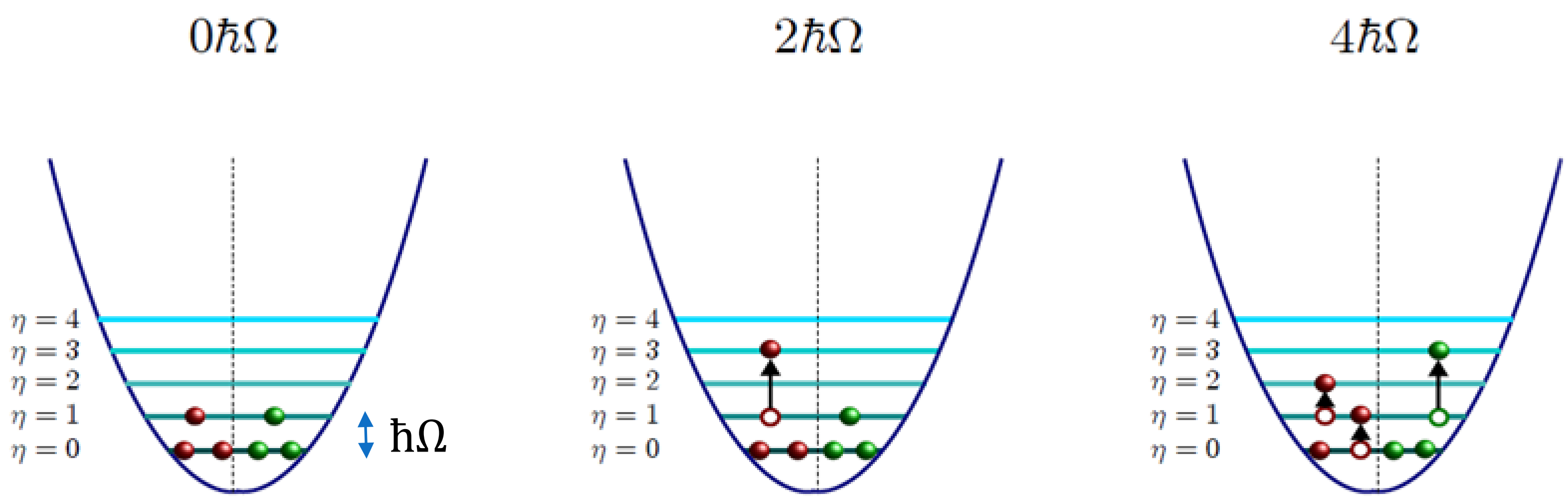
NCSM essentials

- basis construction $\rightarrow$ A nucleons moving independently in spherical 3D HO potential

- configuration mixing due to the „residual“ interaction (NN+NNN)

- many-body problem transformed to symmetric eigenvalue problem

$$\boxed{\begin{aligned} \sum_{k'} H_{kk'} c_{k'} &= E c_k \\ H_{kk'} &= \langle \psi_k | H | \psi_{k'} \rangle \end{aligned}}$$



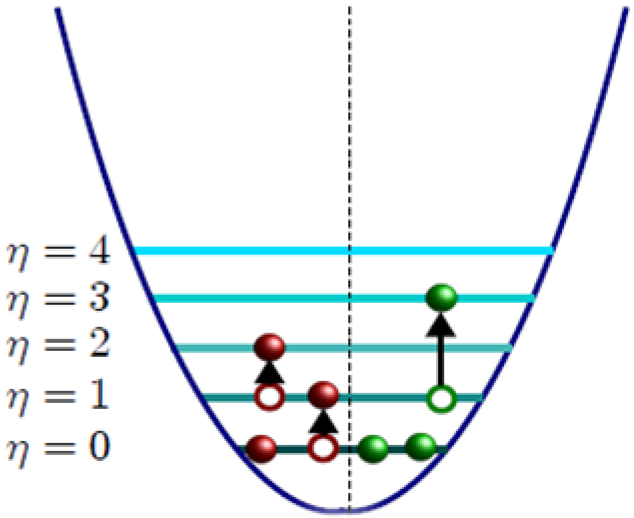
^{6}Li

NCSM dimensions

- dimension of space grows rapidly for heavier systems → combinatorial scale explosion

- 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 for spin ½ particle

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



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

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

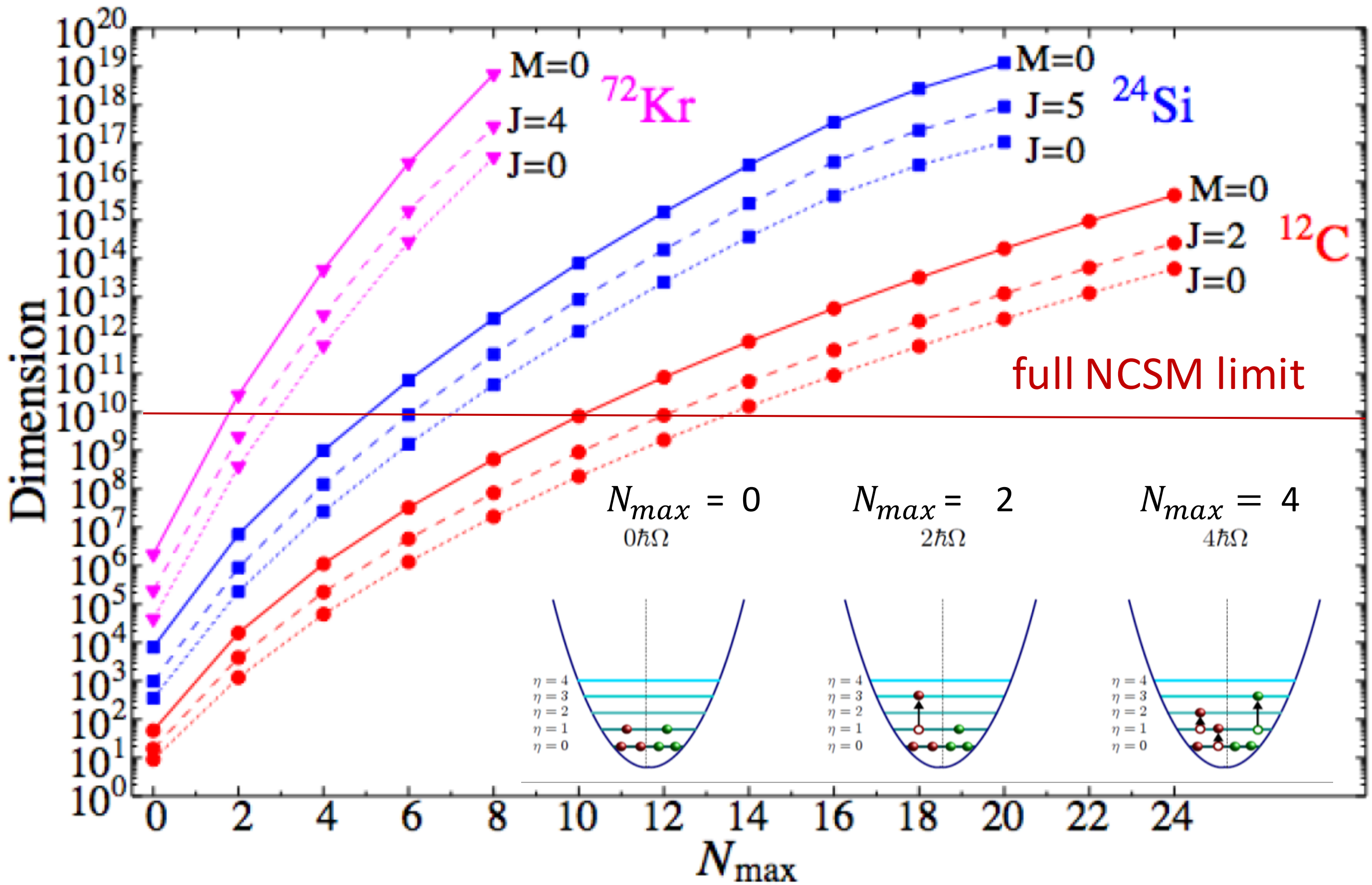
	^{12}C	^{16}O
$\eta_{max}=1$	1120^2	1^2
$\eta_{max}=2$	$38\,760^2$	$125\,970^2$
$\eta_{max}=6$	$28\,530\,983\,404^2$	$13\,288\,305\,520\,413^2$
$\eta_{max}=8$	$1\,713\,562\,300\,450^2$	$3\,202\,280\,747\,619\,525^2$

NCSM model spaces

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

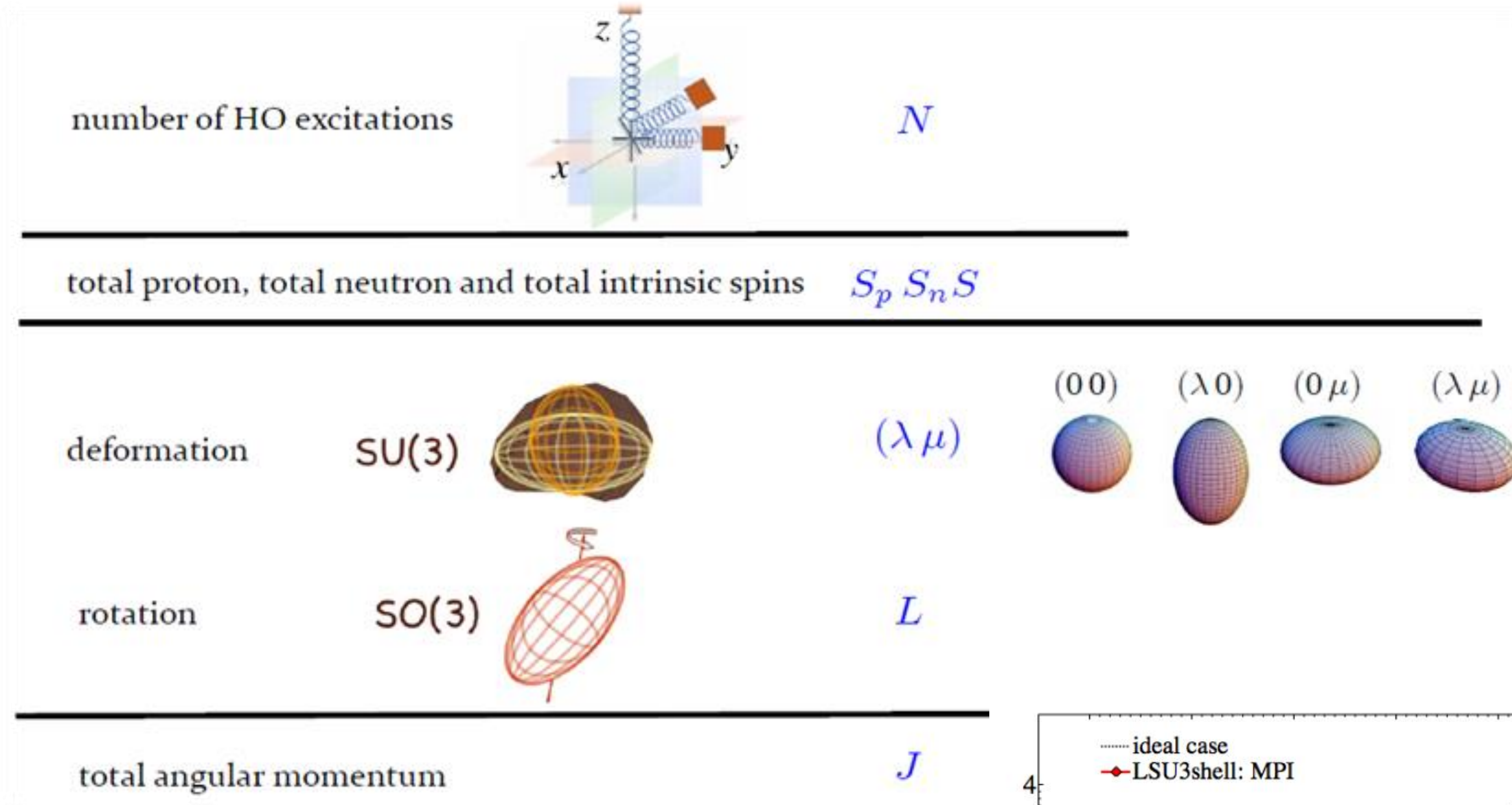
  - large dimension of matrices
- **J-scheme** + few orders od magnitude reduction

  - involved calculation of m.e., more dense matrices
- **Symmetry-adapted basis → SA-NCSM**



Symmetry-adapted NCSM

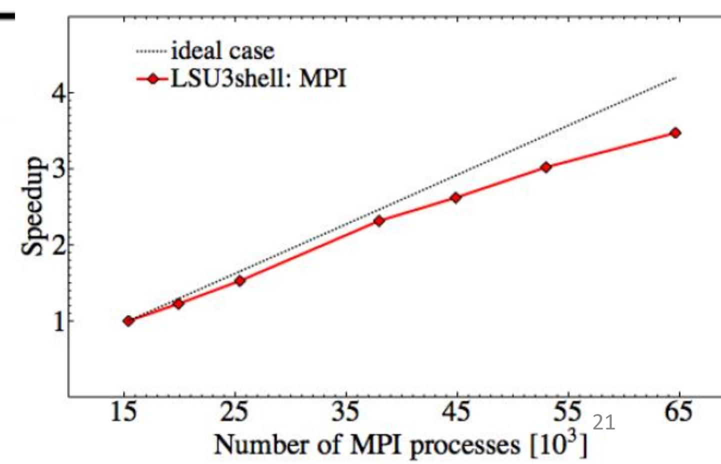
organization of NCMS basis into physically relevant subspaces → truncation



- **LSU3Shell** – MPI/OpenMP implementation of SA-NCSM

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

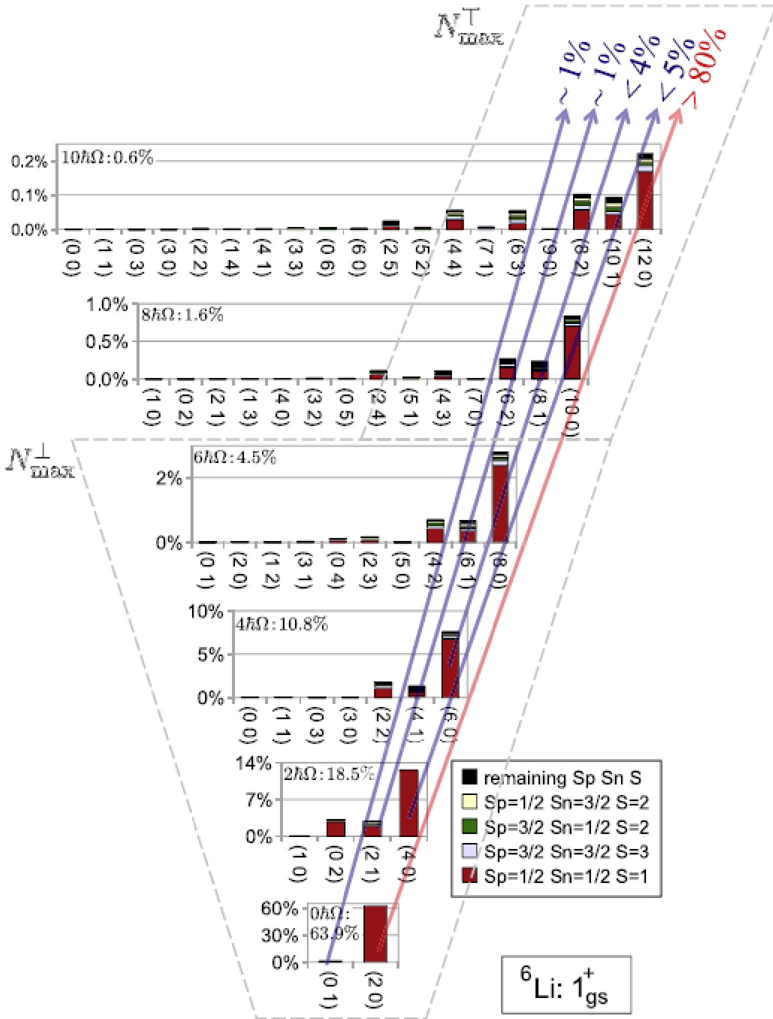
- highly nontrivial calculation of matrix elements 95% of runtime!

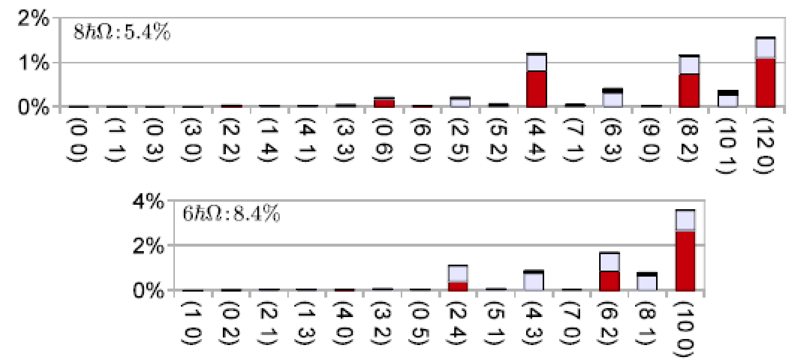


Symmetry-adapted NCSM

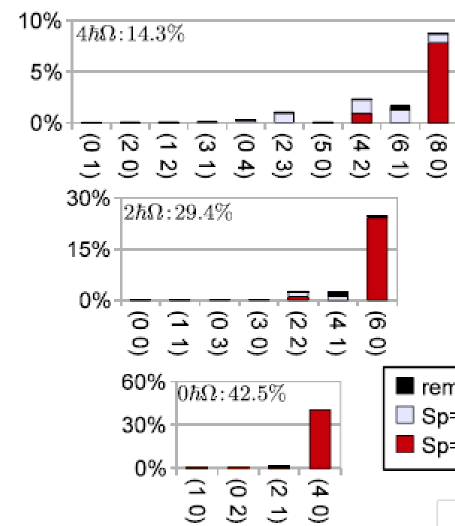
- decomposition of NCSM model space → dominant components in the w.f. → truncation
- simple patterns in the structure of low-lying states of light nuclei

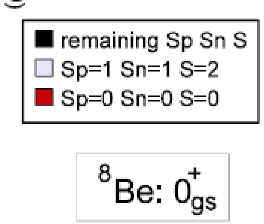
dominance **large deformation** (λμ) = (20) (40) (60) (80)…, **low spins** $S_p\ S_n\ S = \frac{1}{2}\ \frac{1}{2}\ 1$ ….





deformed prolate components with cluster structure





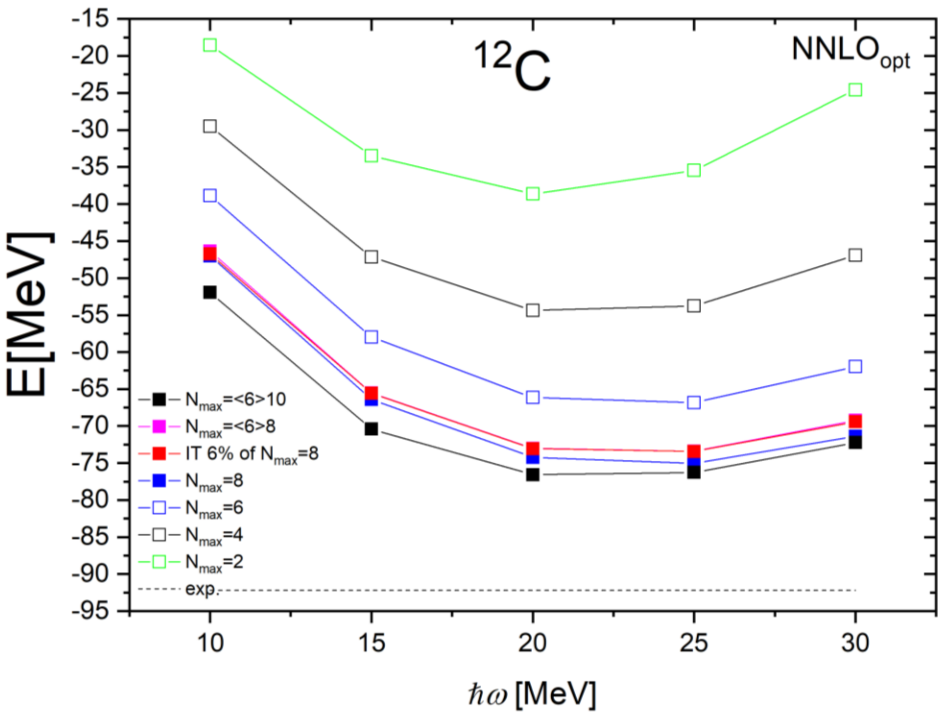
K.D. Launey et al., Progress in Particle and Nuclear Physics 89 (2016)

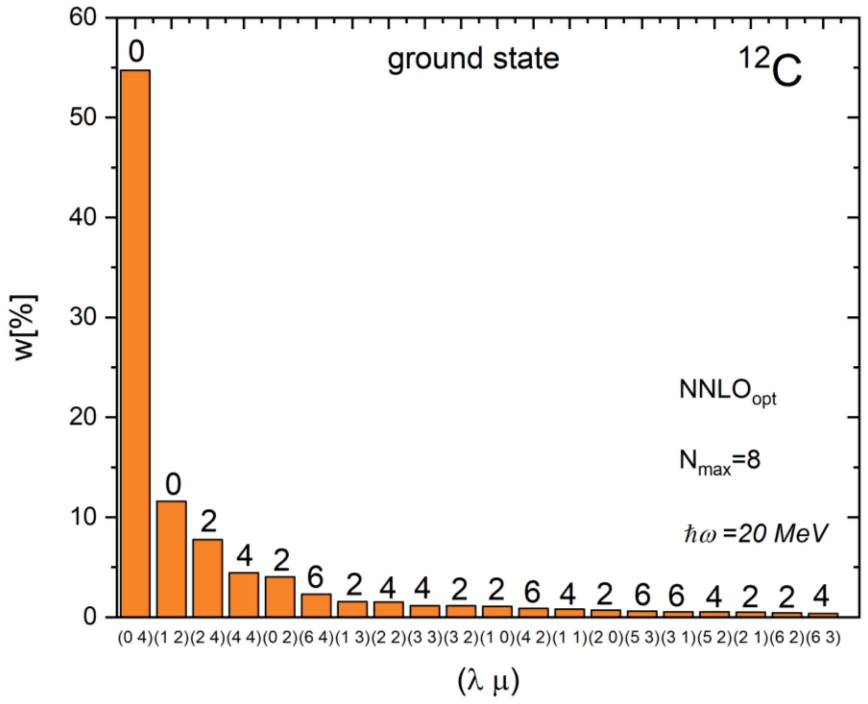
Ground state of ^{12}C within SA-NCSM

- dominant component: 45-55 %, N=0 (λ=0 μ=4) S_p =0 S_n =0 S =0 → oblate shape

Typical dimensions for g.s. calculation:

m. sp.	2	4	6	8	8 (IT)	<6>8	<6>10
dim.	12 x 10^2	54 x 10^3	12 x 10^5	19 x 10^6	1 x 10^6	6 x 10^6	27 x 10^6



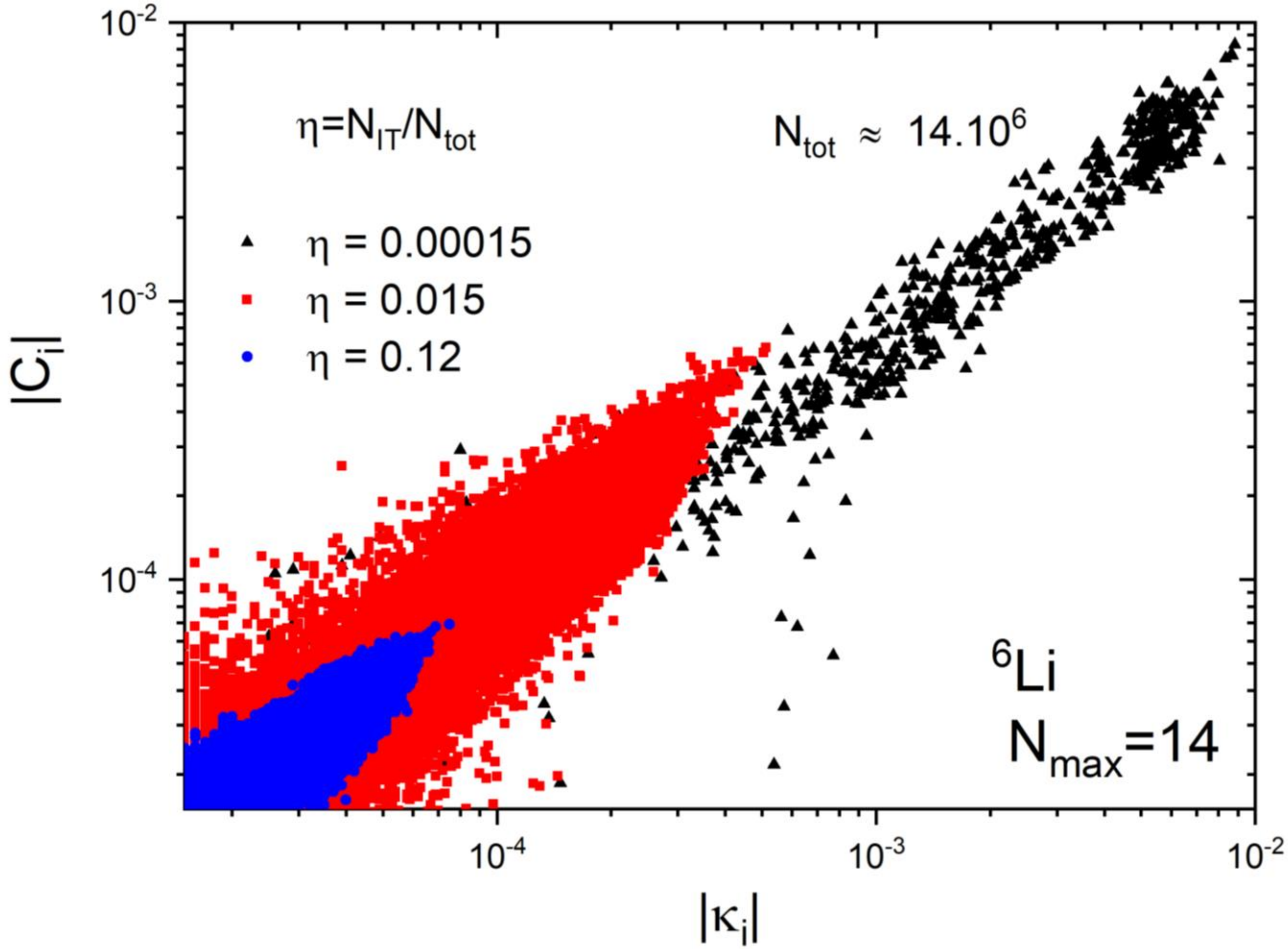


SA-NCSM with importance truncation

- How to measure importance of a basis state?
  estimate from many-body perturbation theory

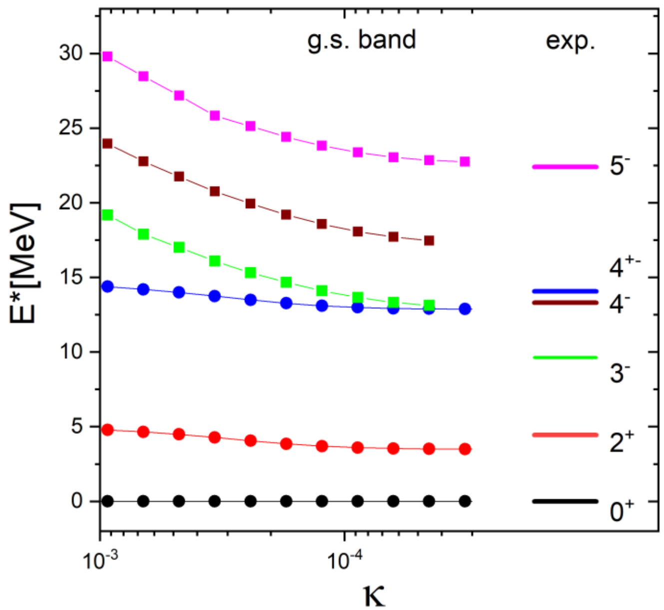
Importance measure parameter

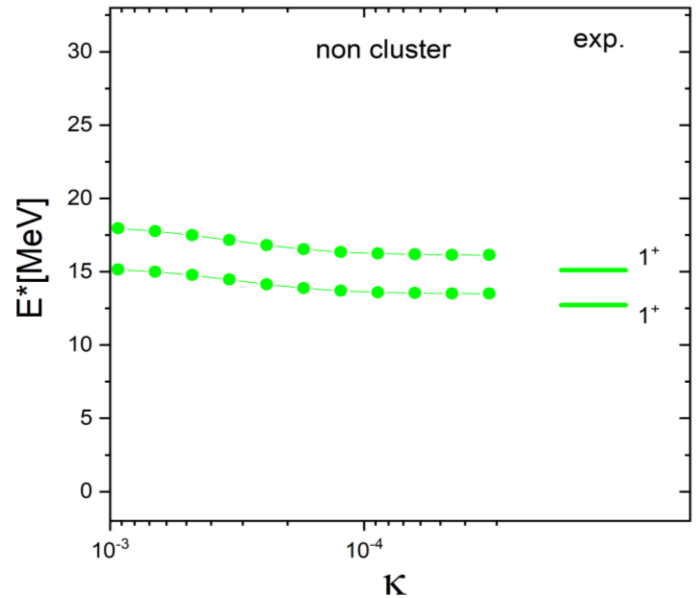
$$\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\mathrm{ref}} \rangle}{\epsilon_\nu - \epsilon_{\mathrm{ref}}}$$

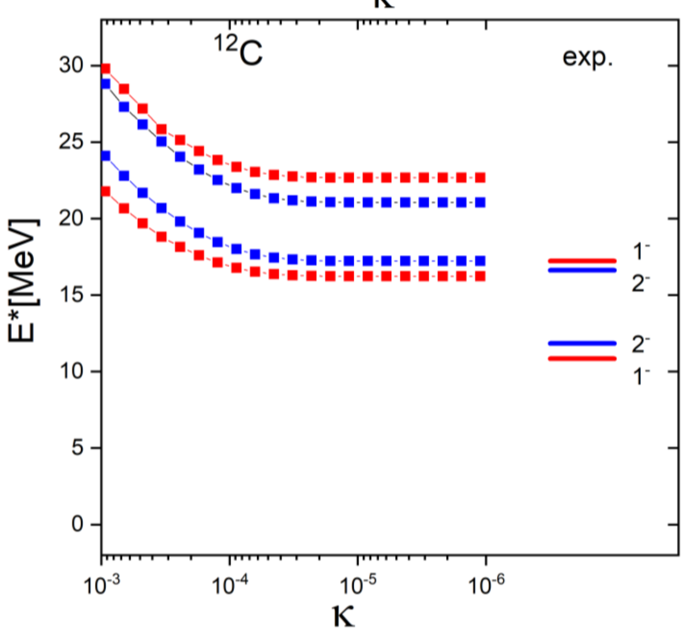


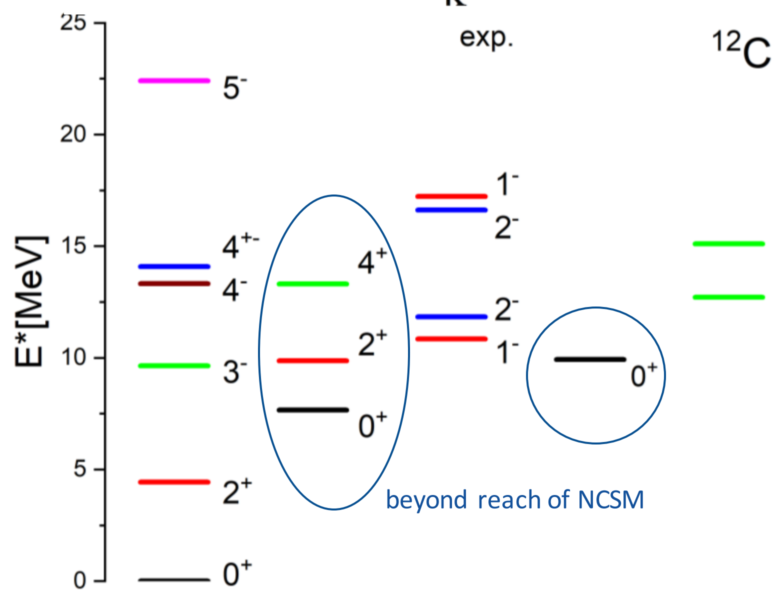
^{12}C spectrum within SA-NCSM

reasonable description of the ground state band and non-cluster states



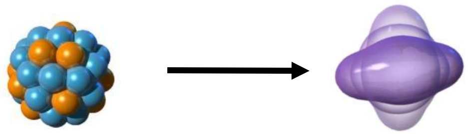


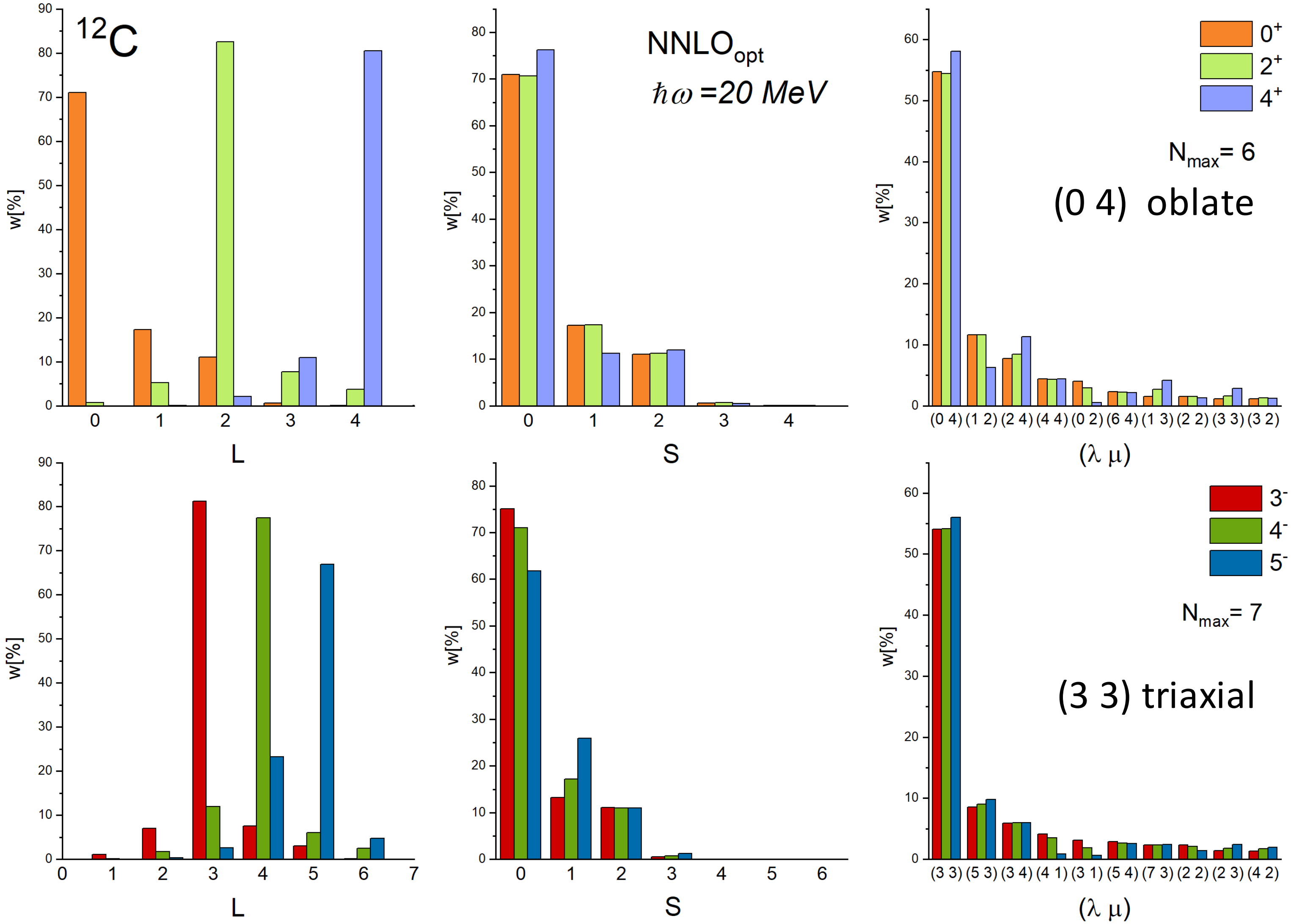




^{12}C ground state band within SA-NCSM

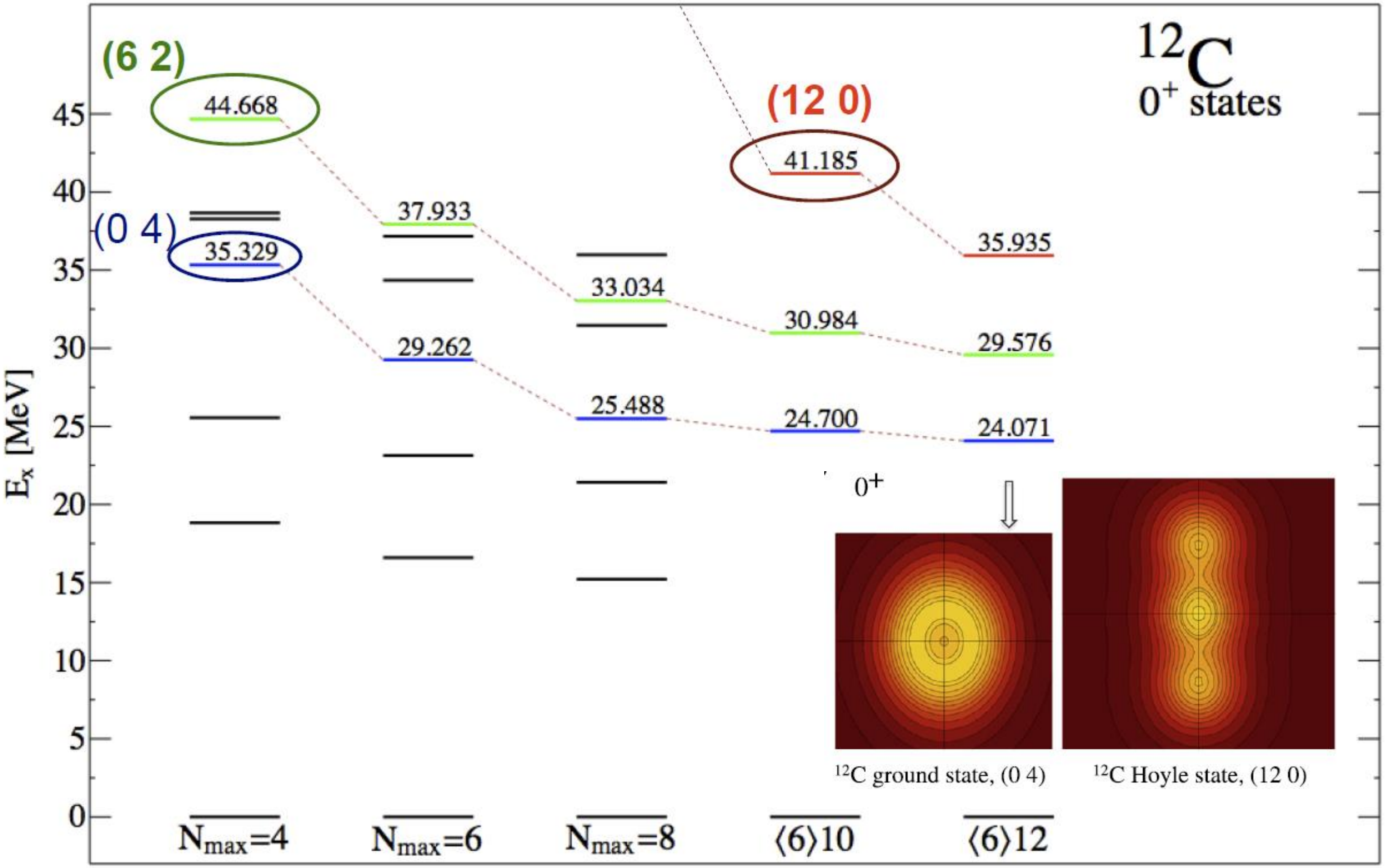
- ab-initio description of the ground state band in ^{12}C
  LS coupling scheme **J=L+S**





Where is the Hoyle state?

- prolate compoments of w.f. lower energy of specific high-lying 0^+ state, but much larger spaces are needed (N_{max}=20)



courtesy of T. Dytrych

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: $J^{\pi} = 0^{+}$ of ^{12}C in N_{max} = <6>10 space

- dim. ≈ 27.10^{6}
- runtime ≈ 45 min for calculation of Hamiltonian + diagonalization by using 9 460 nodes (≈ 302 720 cores)
- matrix storage: 23 TB in CRS format
- n.n.z el. 3 204 675 835 182

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Thank you!