Unraveling Mysteries of the Strong Interaction

'Top Down' versus 'Bottom Up' Considerations

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NSF REU and now Grad. Stud.

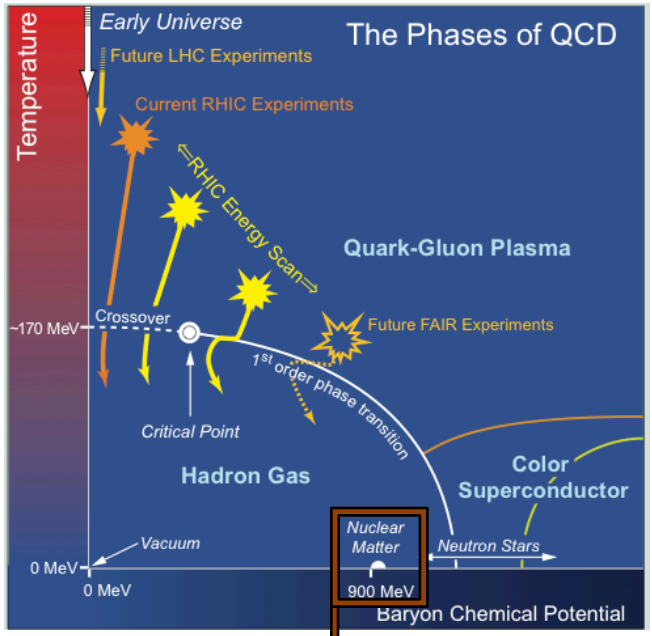
NSF PetaApps & DOE EPSCoR Supported Collaboration

Principals: James P. Vary (Iowa State) and Umit V. Catalyurek (Ohio State)

In the beginning…

… Overarching Framework …

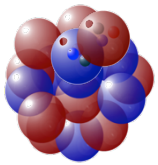
… quarks and gluons …



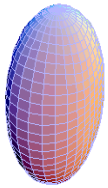
… ab initio vision …

Fundamental Principles

Many-body Dynamics

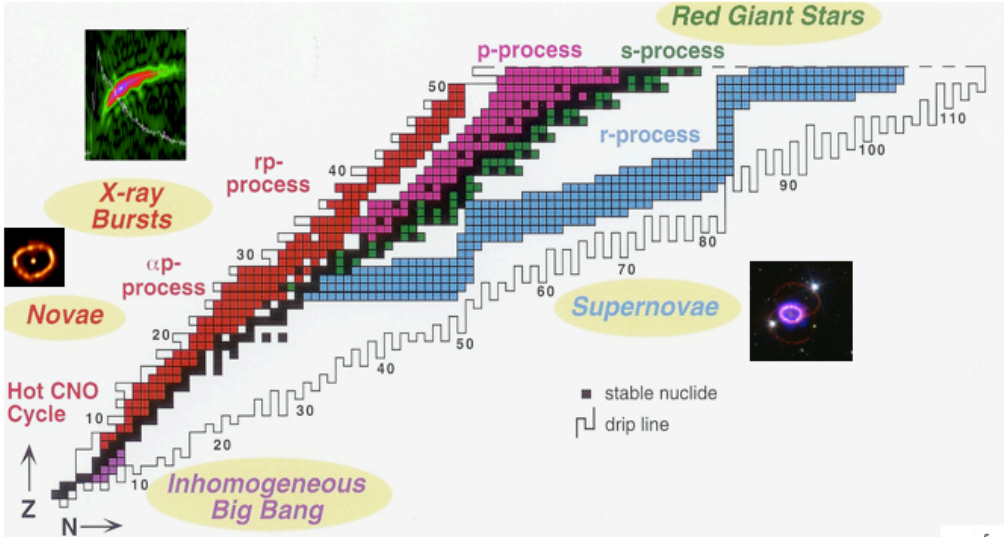


Collective Properties



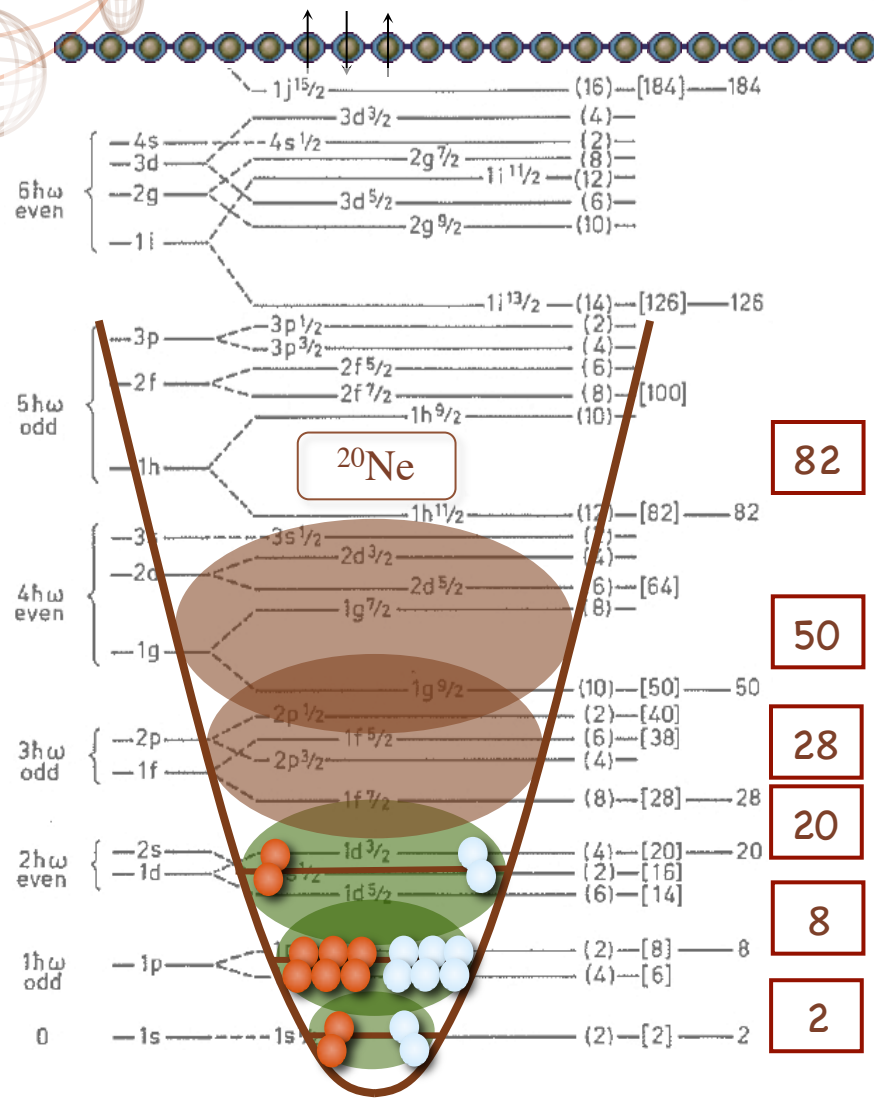
… FACTS …

- Quark masses < ~2% total mass of nucleons
- Magnetization does Not track charge distribution
- Only about 1/3 of spin of a nucleon is from quarks …



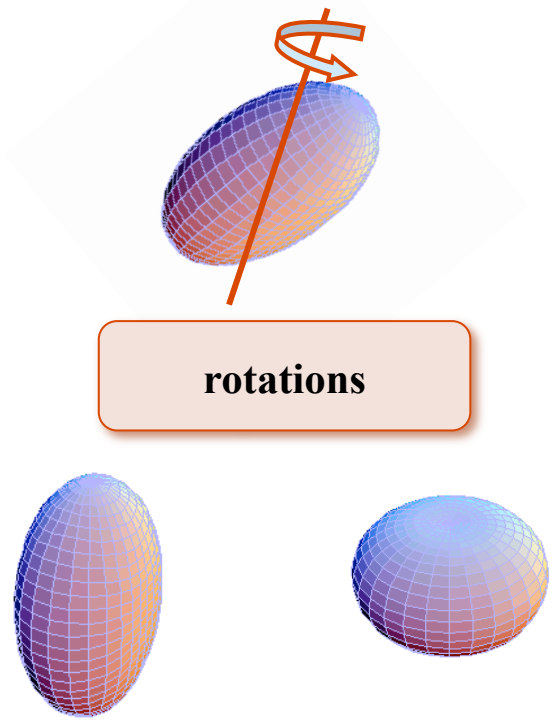
… quarks & gluons to nucleons & nuclei …

Shell Model Pillars Collective Model

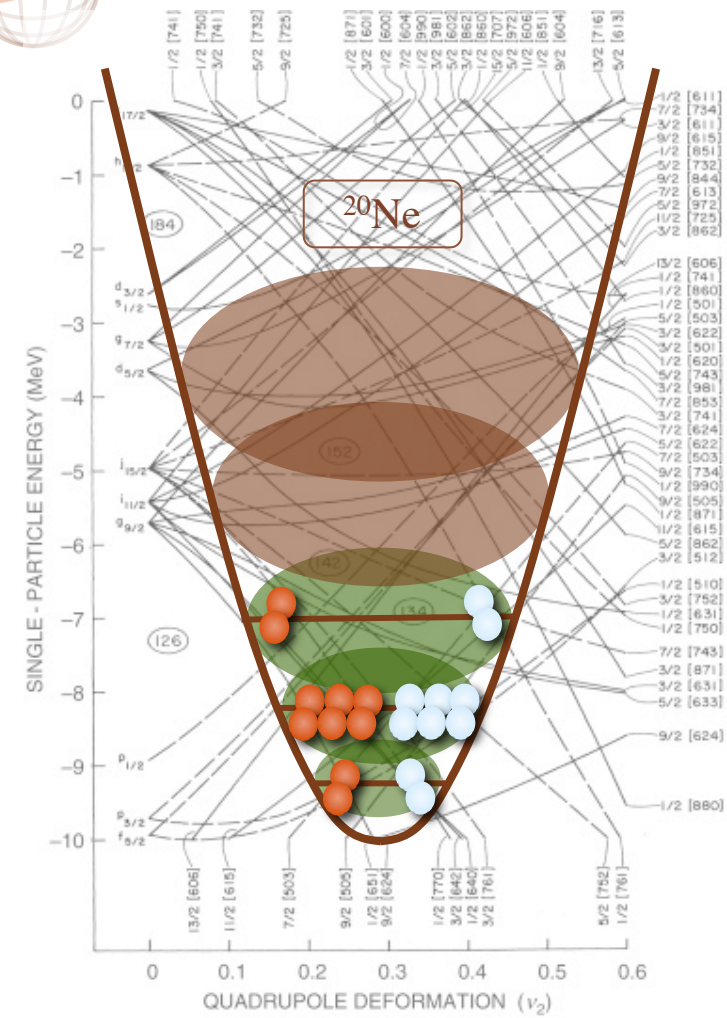


Maria Goeppert-Mayer & J. Hans D. Jensen (~'50)
"…for their discoveries concerning nuclear shell structure …" (1963 Nobel Prize)

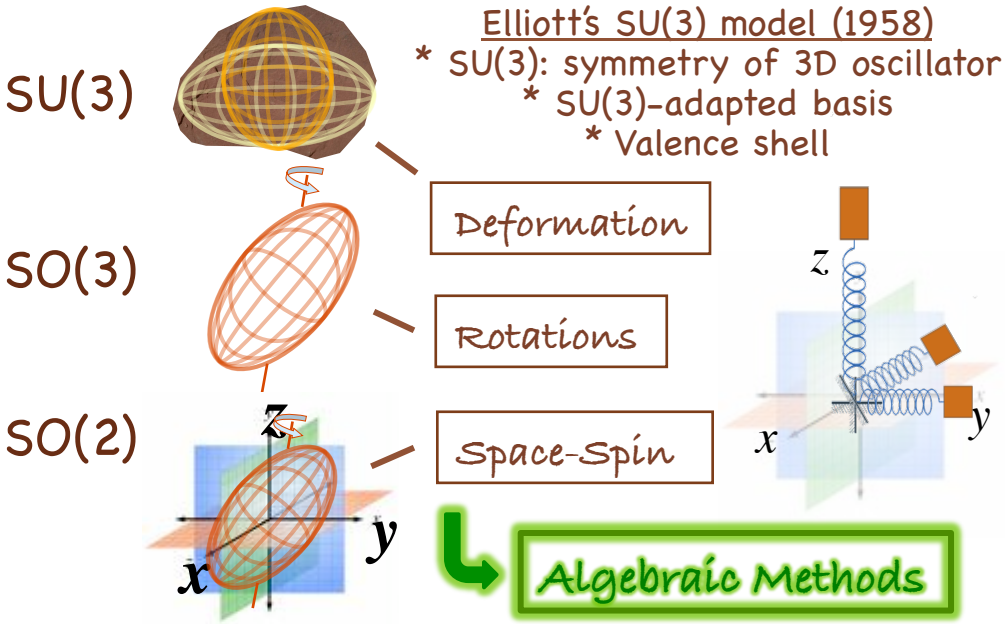
A.N. Bohr, B.R. Mottelson & J. Rainwater ('50s)
"… for the discovery of the connection between collective motion and particle motion in atomic nuclei and the development of the theory of the structure of the atomic nucleus based on this connection …" (1975 Nobel Prize)



Shell Model Successors Collective Model



Nilsson model
*independent particles
*deformation <-> mean field

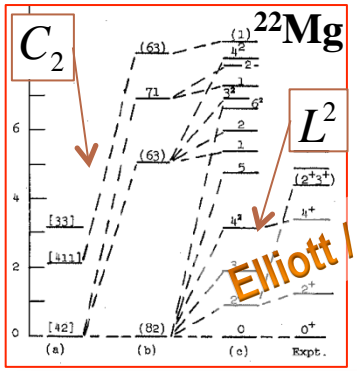


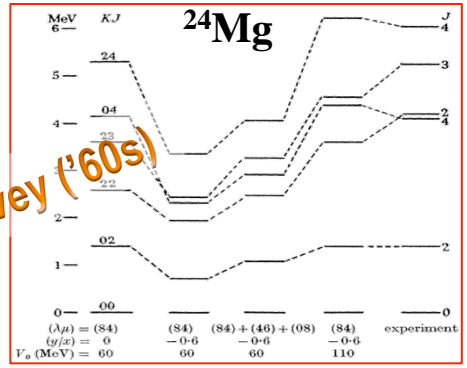
Elliott's SU(3) model (1958)
* SU(3): symmetry of 3D oscillator
* SU(3)-adapted basis
* Valence shell

Algebraic Methods

$$H = H_{HO} - \chi/2\, Q \cdot Q$$

Gaussian Central Force





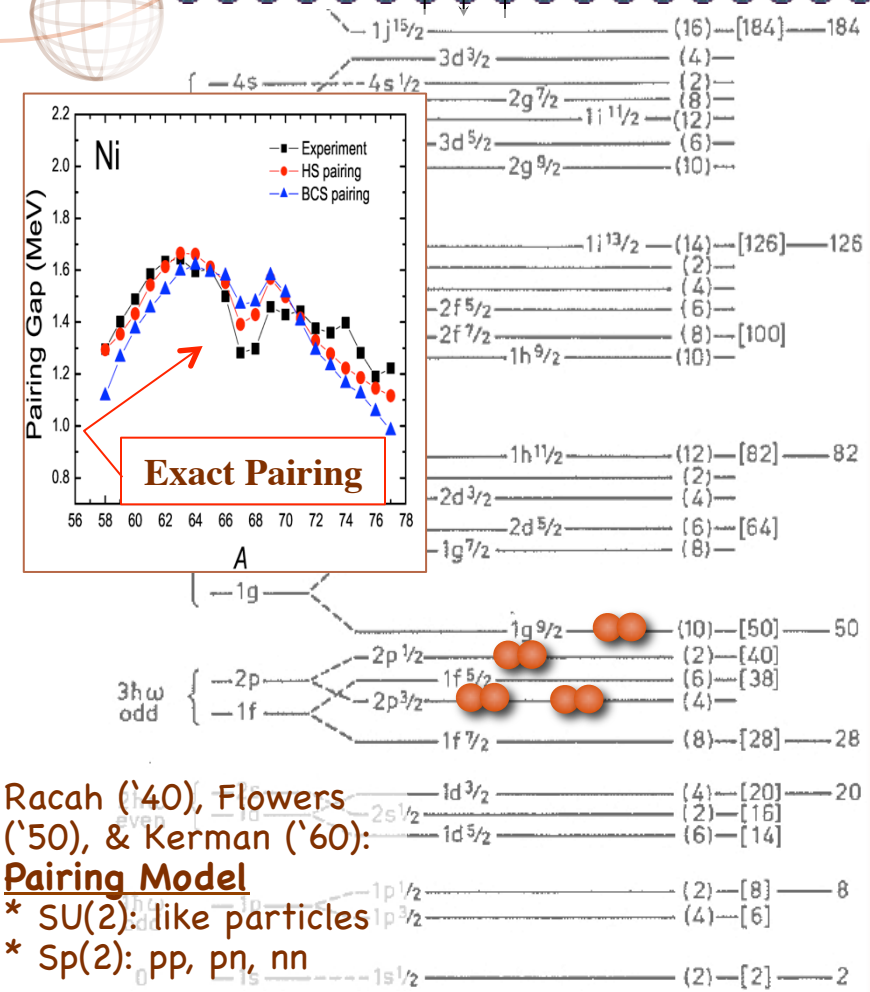
Elliott / Harvey ('60s)

Dominance of a few most deformed configurations

Extensions

Shell Model
+ pairing correlations

Collective Model
+ pairing correlations



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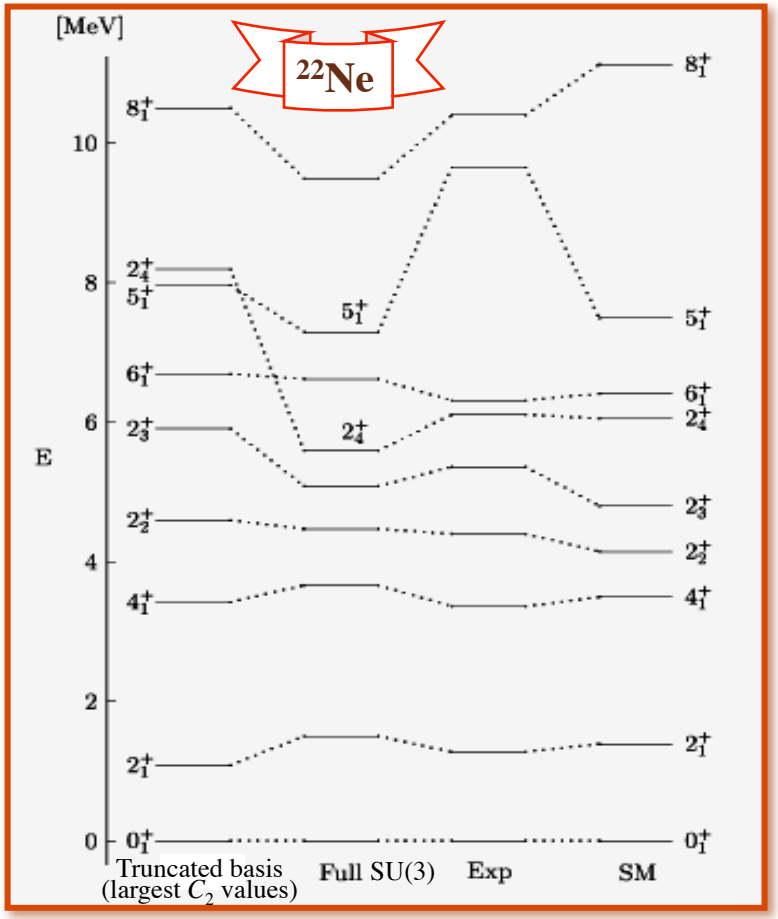


Racah ('40), Flowers ('50), & Kerman ('60):
Pairing Model
* SU(2): like particles
* Sp(2): pp, pn, nn

Guan, Pan, et al. ('12)
Exact Pairing
*spherical/deformed mean field
*exact solutions to standard pairing

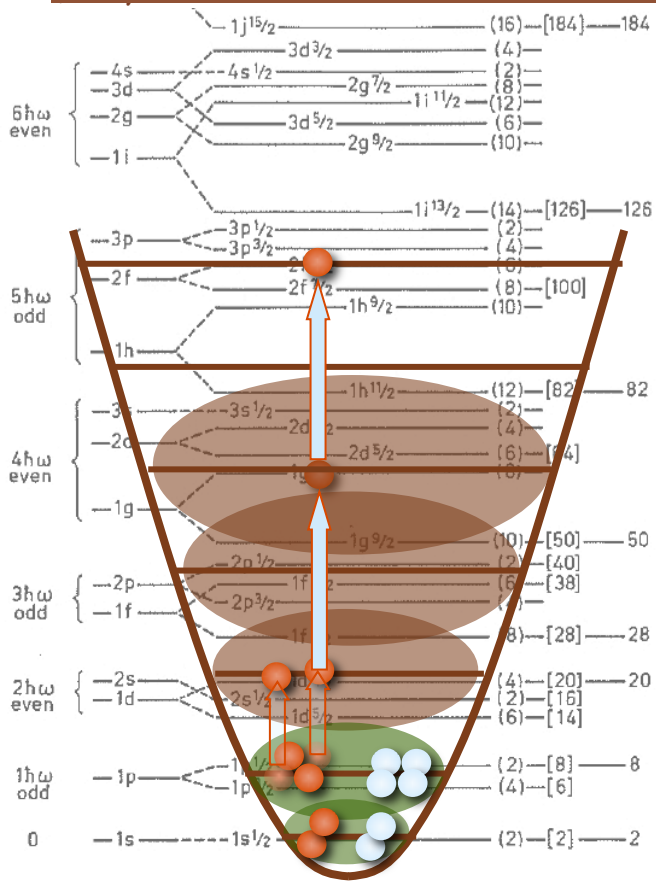
C.E. Vargas, J.G. Hirsch, et al. ('01)

$$H = H_{s.p.} - \frac{1}{2}\chi Q\cdot Q - \boxed{G_\pi H_{pair,\pi} - G_\nu H_{pair,\nu}} + aK_J^2 + bJ^2 + A_{sym}C_2$$

Shell Model Advances Collective Model

No-Core Shell Model (NCSM)

(Vary, Navratil, Barrett, … Maris … ~2000 - Present)



*Realistic interaction (local/nonlocal; NN, NNN,…)

- In principle, exact solutions
- Successful description up through O-16

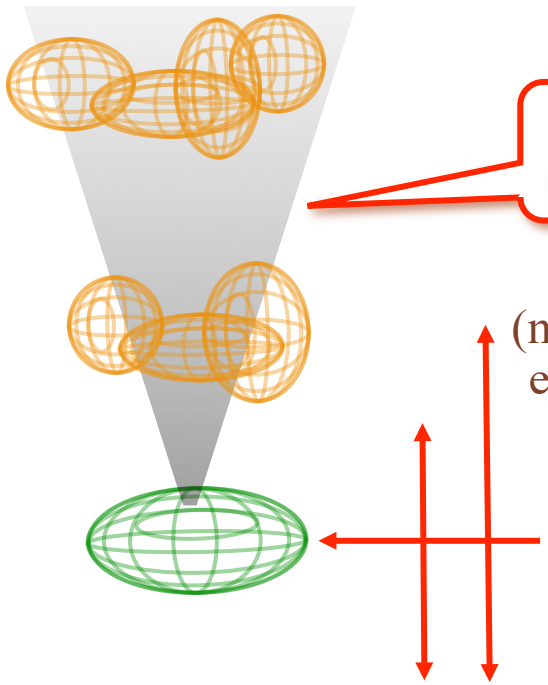
Symplectic Model – NCSpM

(Rowe & Rosensteel, ~1980s)

*Sp(3,R): natural symmetry of nuclei

*Sp(3,R)-adapted basis

*Schematic interactions

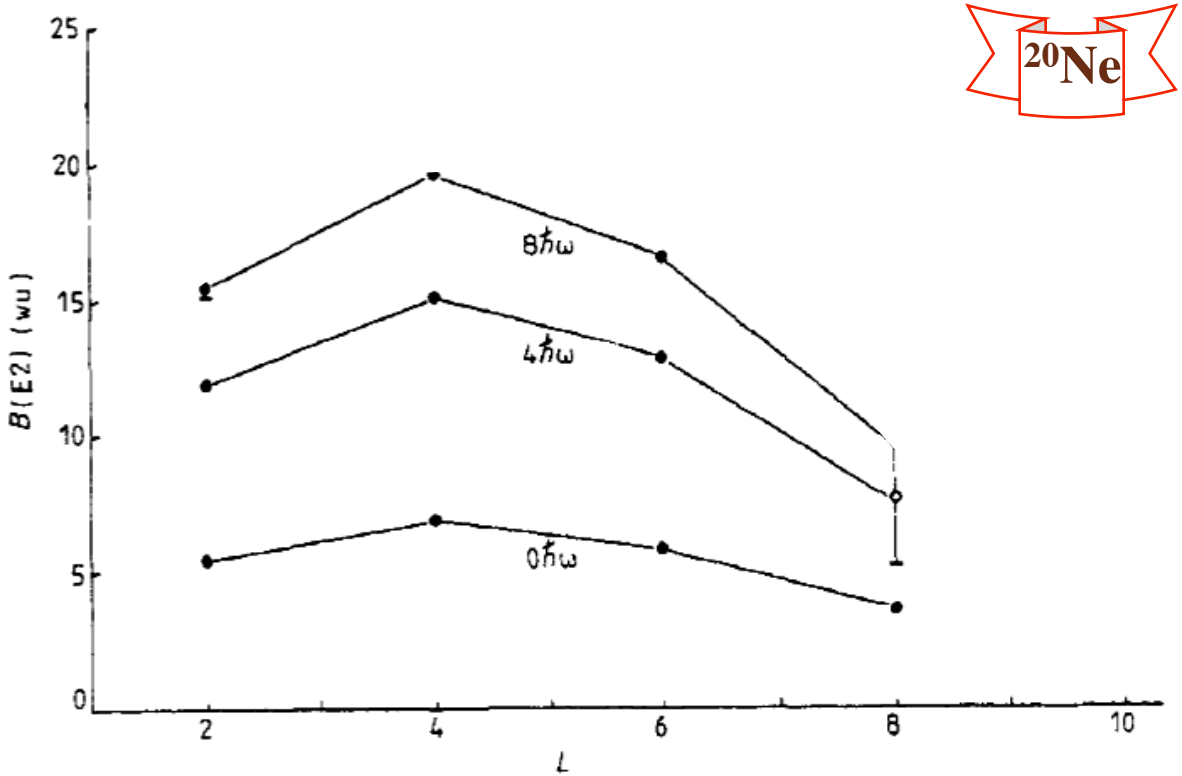


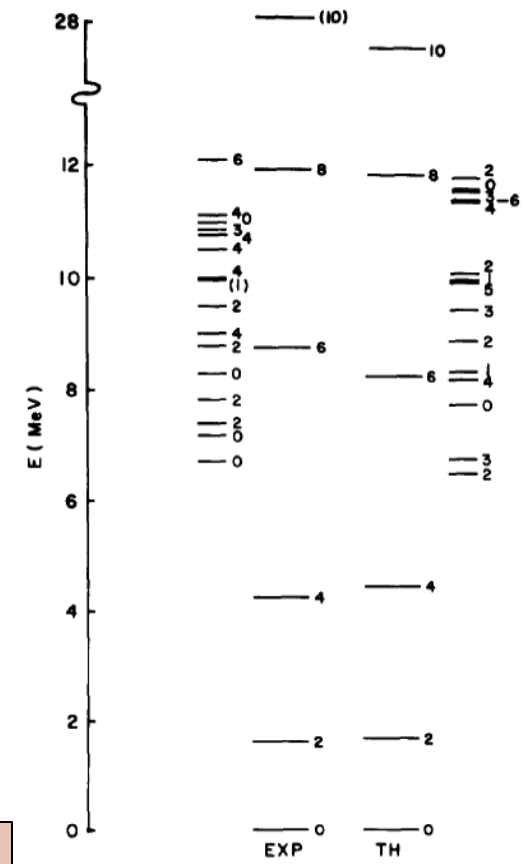
*Manage spurious center-of-mass motion

*Fully microscopic & equals NCSM if all symplectic slices included

*Reproduce rotational bands & transition rates without effective charge

Symplectic Model





$$H = \hbar\omega H_0 + b_2 Q\cdot Q + b_3 (Q\times Q)\cdot Q + b_4 (Q\cdot Q)^2 + \sum_j \varepsilon_j n_j + G_0 P$$

G. Rosensteel and D.J. Rowe – 1977

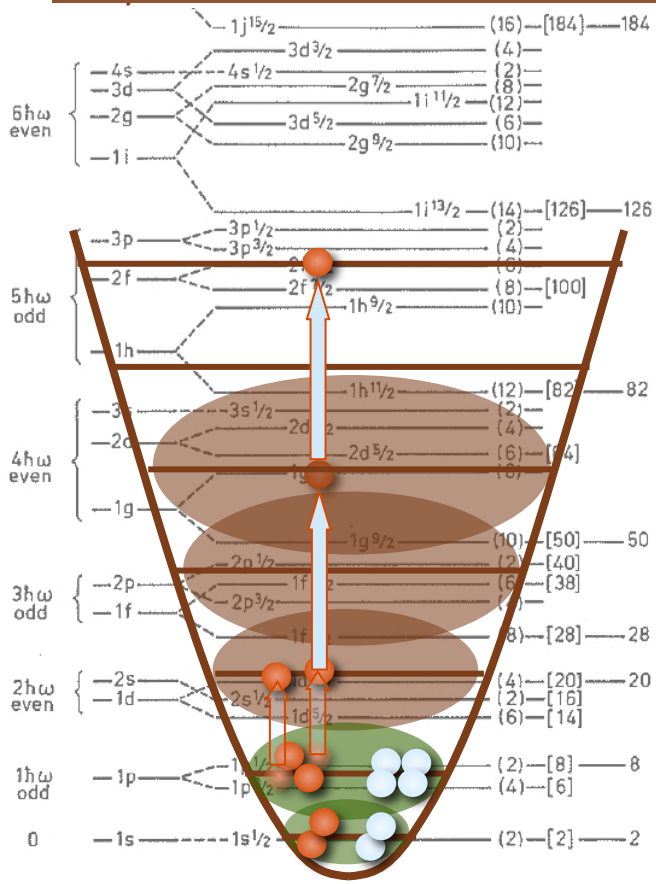
J.P. Draayer, K.J. Weeks, G. Rosensteel – 1984

NCSM — Next Generation — SA-NCSM

– Ab Initio –

No-Core Shell Model (NCSM)

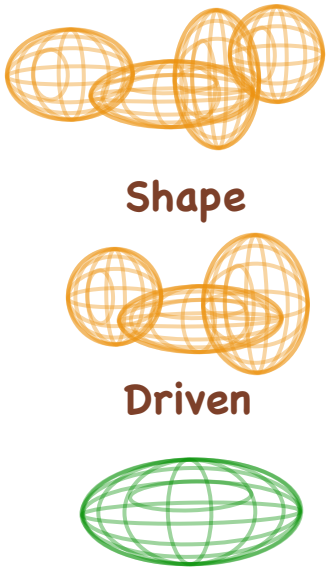
(Vary, Navratil, Barrett, … Maris … ~2000-Present)

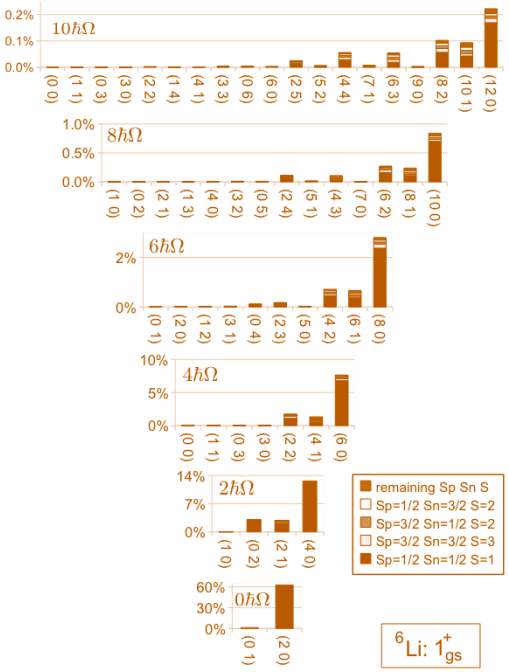


Symmetry Adapted NCSM (SA-NCSM)

(Dytrych … ~2007-Present)

- **Stage I:** SU(3)-adapted basis – a multi-shell Elliott model – **SA-NCSM**
- **Stage II:** Sp(3,R)-adapted basis – NCSpM

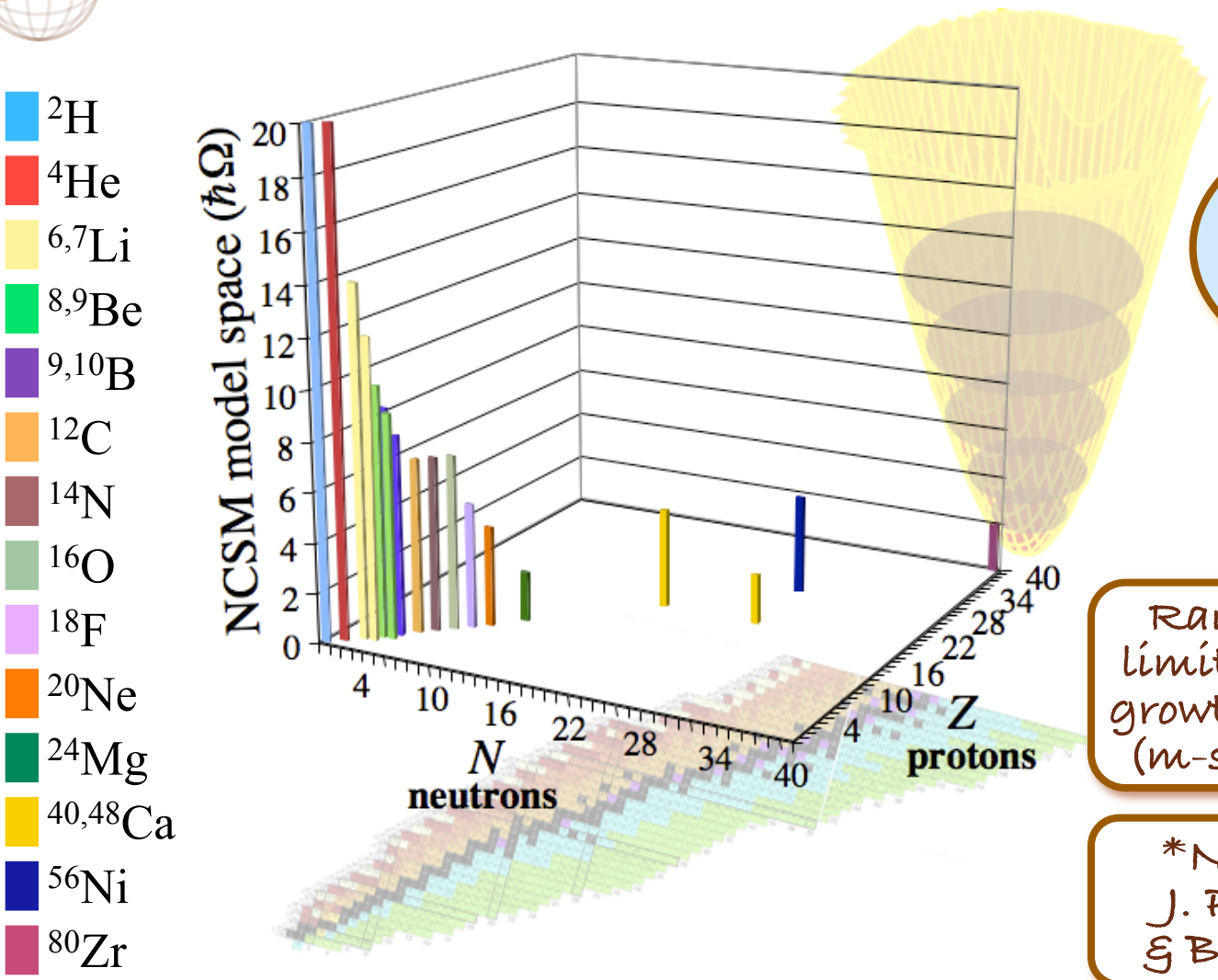




- Realistic interaction (local/nonlocal; NN, NNN,…)
- In principle, exact solutions
- Successful description up through O-16

Ab initio evidence for symmetry patterns

NCSM* / Applicability

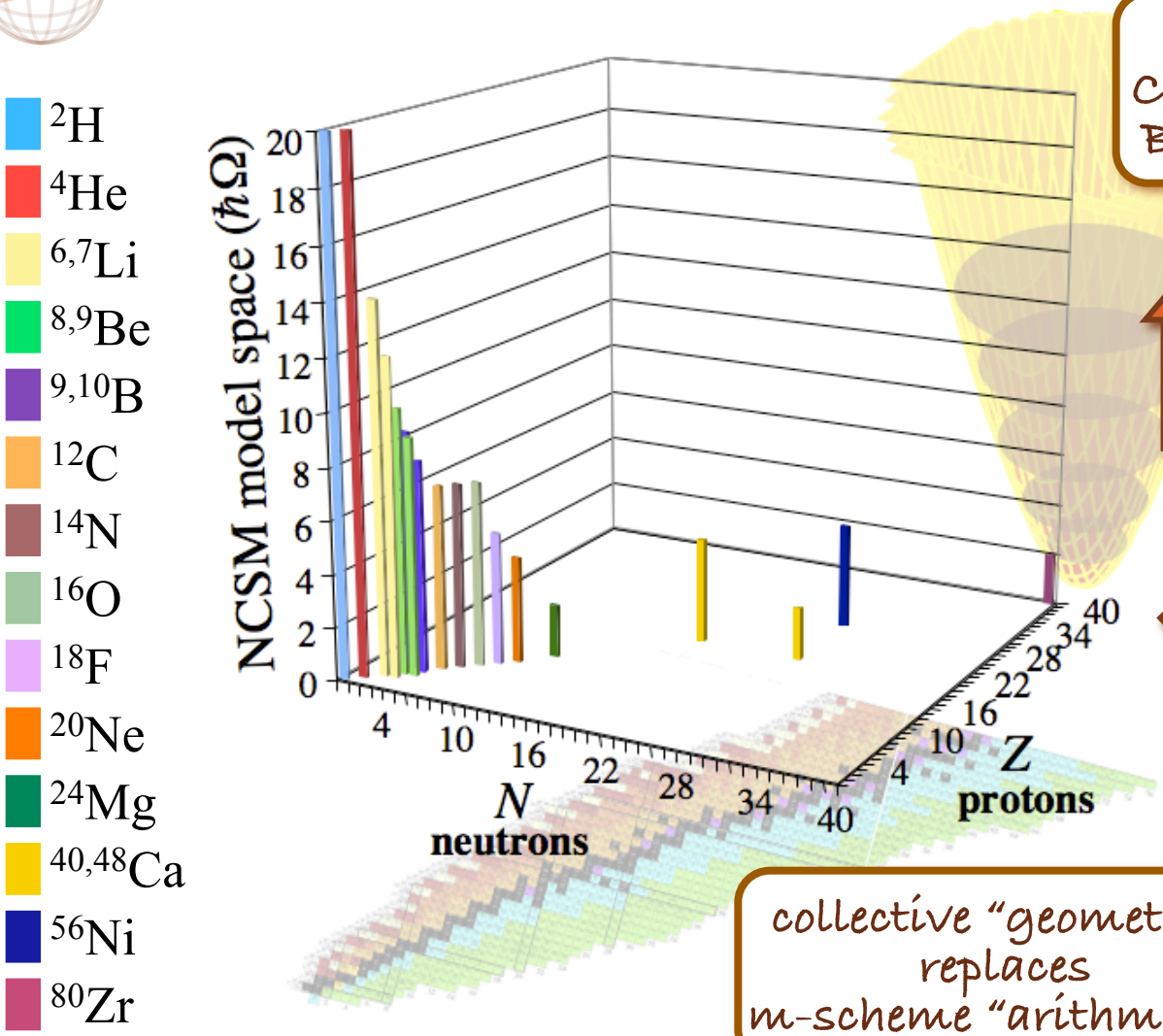


HPC
"WALL"
$\sim 10^{10}$

Range of applicability limited by combinatorial growth in # of basis states (m-scheme "arithmetic")

*No-Core Shell Model
J. P. Vary, P. Navratil & B. R. Barrett ~ 2000

SA-NCSM / Extended Applicability



Highly deformed modes, Cluster-like configurations, B(E2) w/o effective charges

'higher' spaces

'heavier' nuclei

... enables ...

collective "geometry" replaces m-scheme "arithmetic"

Symmetry NCSM Adapted

'Symmetry Adapted' NCSM Campaign

Timeline: 5 (2002-06) + 5 (2007-2011) + 5 (2012-16)

Goal –

Reproduce and predict properties of heavy as well as light nuclei, starting with and building upon QCD/EFT informed and inspired interactions …

Plan –

- ✓ Exploit existing capabilities to evaluate probability of success and level of effort required to develop a full-blown symmetry adapted NCSM
- ✓ Develop a symmetry adapted no-core shell model code that capitalizes on exact and approximate symmetries of nuclei (SA-NCSM)
  - Exploit existing NCSM technology to prove efficacy of method, revealing (or not) any inherent limitations
  - Explore need (or not) for renormalization, winnowing space to physically relevant and tractable subspaces
  - Evaluate extensibility of theory and its characteristics vis-à-vis current/emerging computational resources
- ✓ Study the emergence of collective phenomena, tracking their evolution to and from fundamental features of the interaction
  - Apply the theory to study of extreme processes known to be important to understanding nuclei and nuclear systems
  - Develop a user friendly desktop version of code for simple applications as well as educational and training purposes
  - Extend theory to include coupling to the continuum, and apply to the result to the study of nuclear reactions

SA-NCSM Development Tracks (current focus)

Part 1: Code Development (Tomas Dytrych led Team)

Work in progress. A first-generation code has been assembled (second-generation under construction) and used to carryout various independent analyses checking at each step to ensure reproducibility of NCSM "full-space" results. A laptop version also exists, but with limited reach due to processor and memory limitations. ^{6}Li examples (^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg available too).

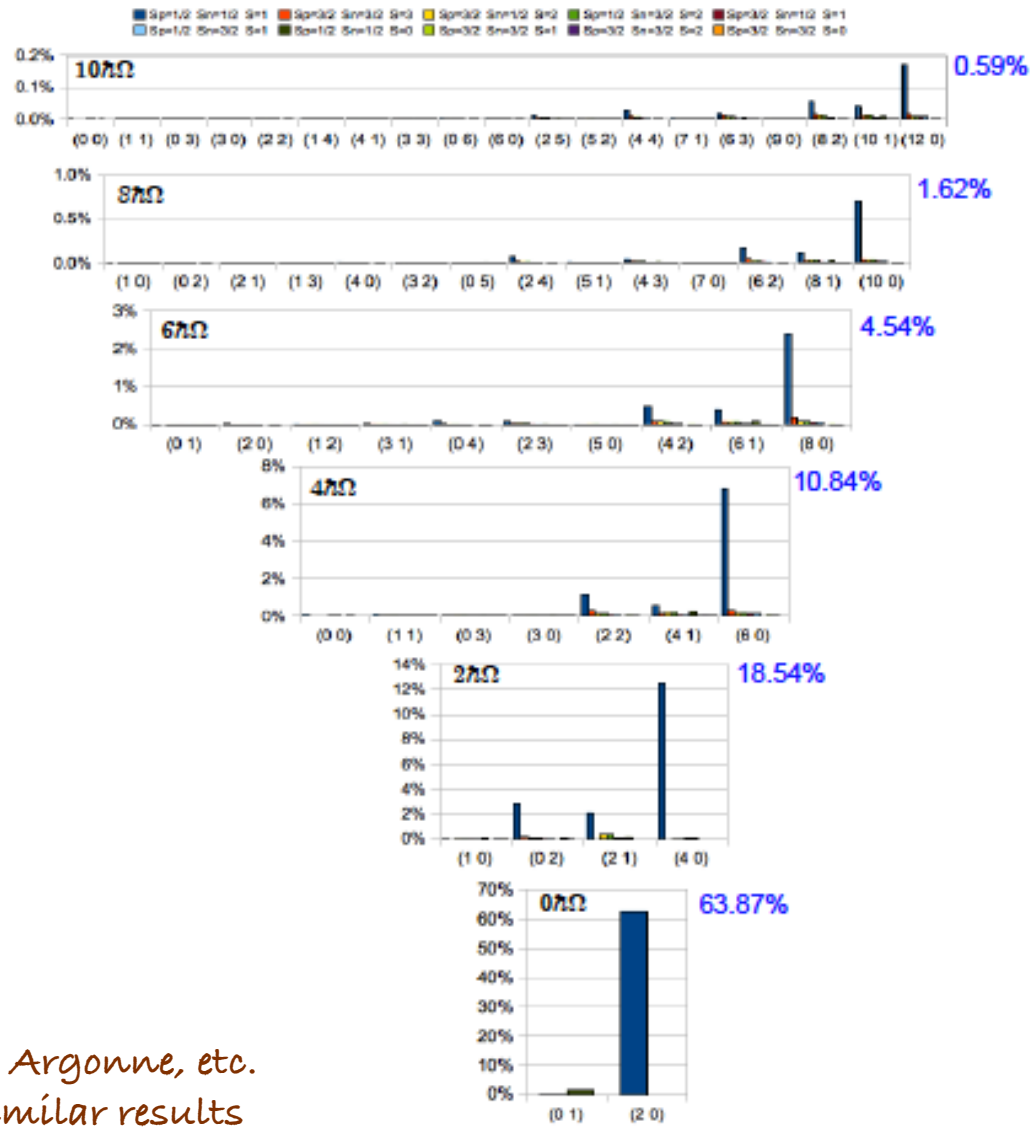
Tomas Dytrych

Part 2: Model Interaction (Kristina Launey led Team)

Also work in progress. Some early surprising results, which I will share below (unpublished). We believe this shows promise for building the bridge between QCD inspired interactions and simpler and more familiar phenomenological forms that have been used to reproduce experimental results in subspaces of the full model space - subject to various specific interpretation(s).

Kristina Launey

Results for ^{6}Li with $N_{max} = 10$



JISP16* bare interaction in Nmax = 10 space with $\hbar\Omega = 20$ MeV

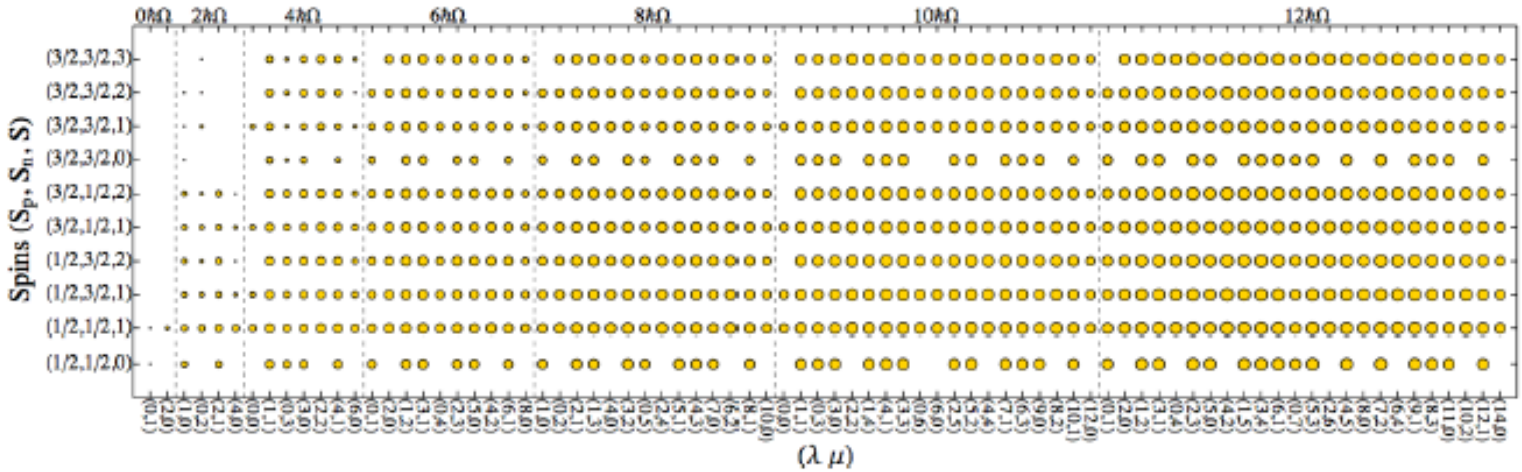
… Team Work …

Many "helps" along the way … e.g., James Vary making his NCSM available to us, Mark Caprio (ND) visiting LSU on his sabbatical last year, as well as quality input from Anna Hayes (LANL), collaborators from Bulgaria, China, Mexico, and so on. Also to NSF for a PetaApps award, and DOE for an EPSCoR grant, plus SURA for release time and financial assistance with postdoc team!

*N3LO, Argonne, etc. yield similar results

Complete Space for ^{6}Li / N_{max} = 12

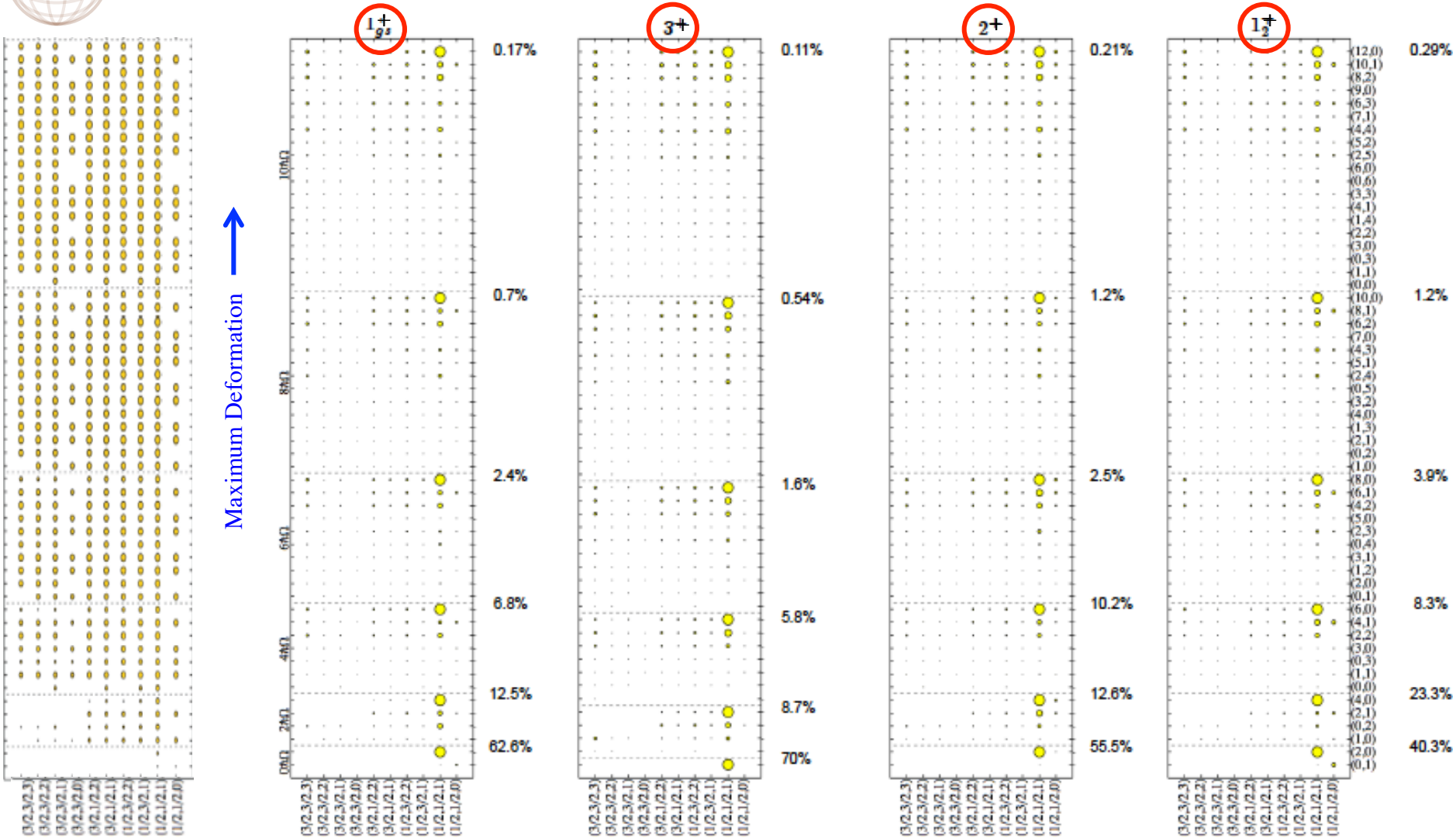
Example: ^{6}Li and N_{max} = 12 – Complete Configuration Space [$\log_{10}$(dimension)]



- $N\hbar\Omega$ space: direct sum of subspaces [O] of states carrying the same $(\lambda\ \mu)$ and $S_p S_n S$
- c.m. spurious states can be removed from each subspace exactly

- SU(3)-scheme allows truncations according to
  (1) maximal number of total HO quanta Nmax
  (2) intrinsic spins $S_p\ S_n\ S$
  (3) deformations $(\lambda\ \mu)$
- Realistic interactions: enormous mixing of different $S_p S_n S\ (\lambda\ \mu)$ subspaces
- Coherent mixing of $N\hbar\Omega\ S_p S_n S\ (\lambda\ \mu)$ subspaces due to a persistent Sp(3,R) symmetry

Distributions for ^{6}Li / N_{max} = 10

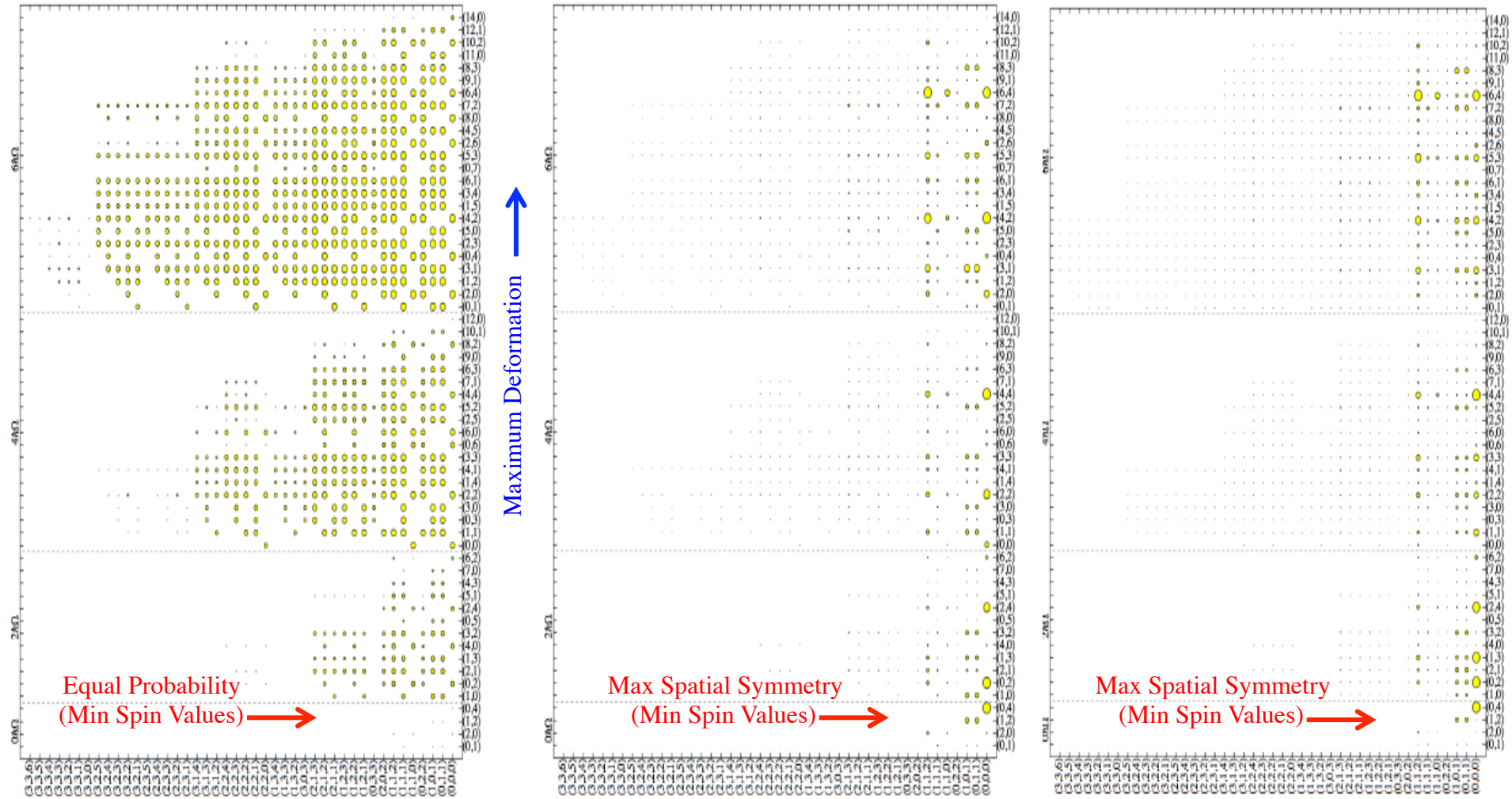


Distributions for ^{12}C / $N_{max} = 6$

All

$J = 0^+$

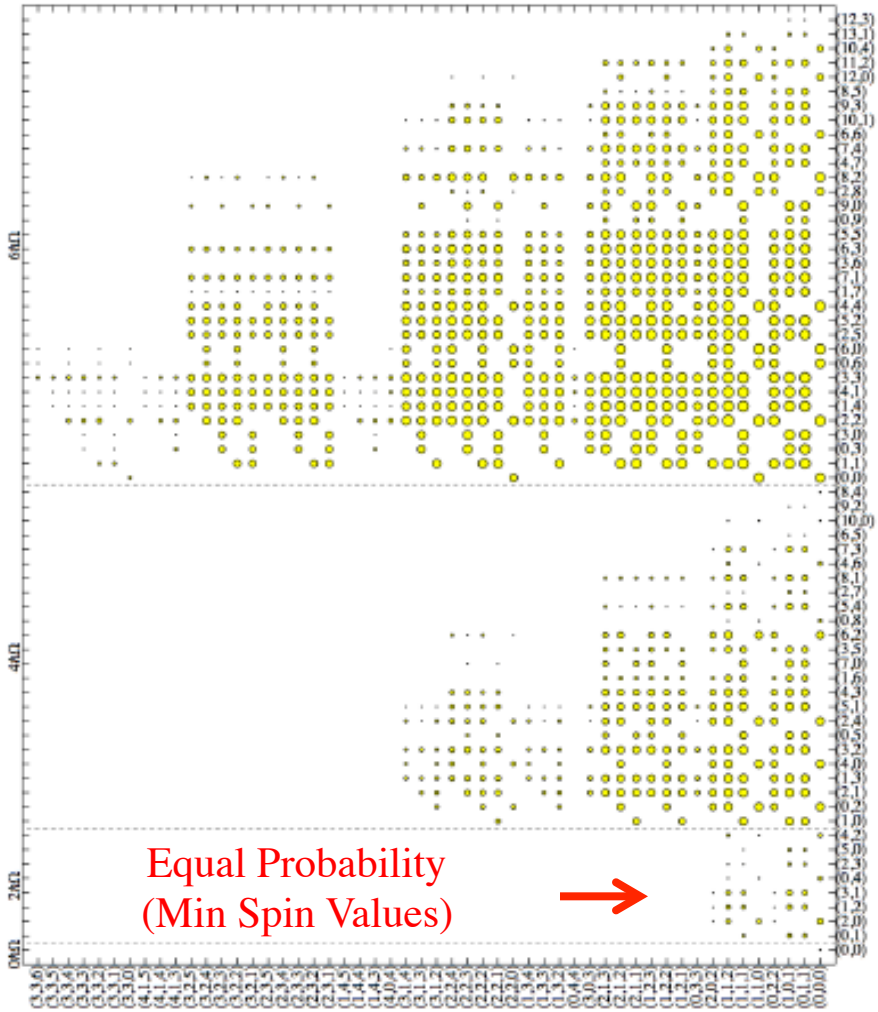
$J = 2^+$



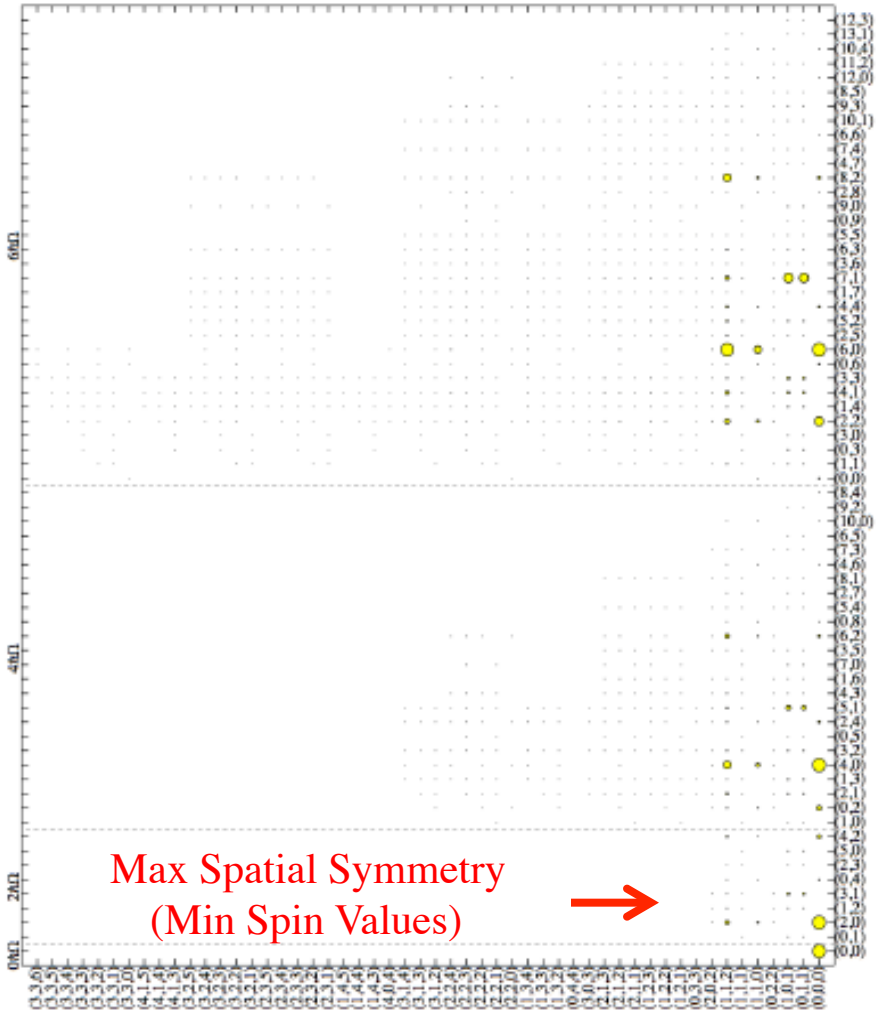
Distributions for ^{16}O / $N_{max} = 6$

All

$J = 0^+$

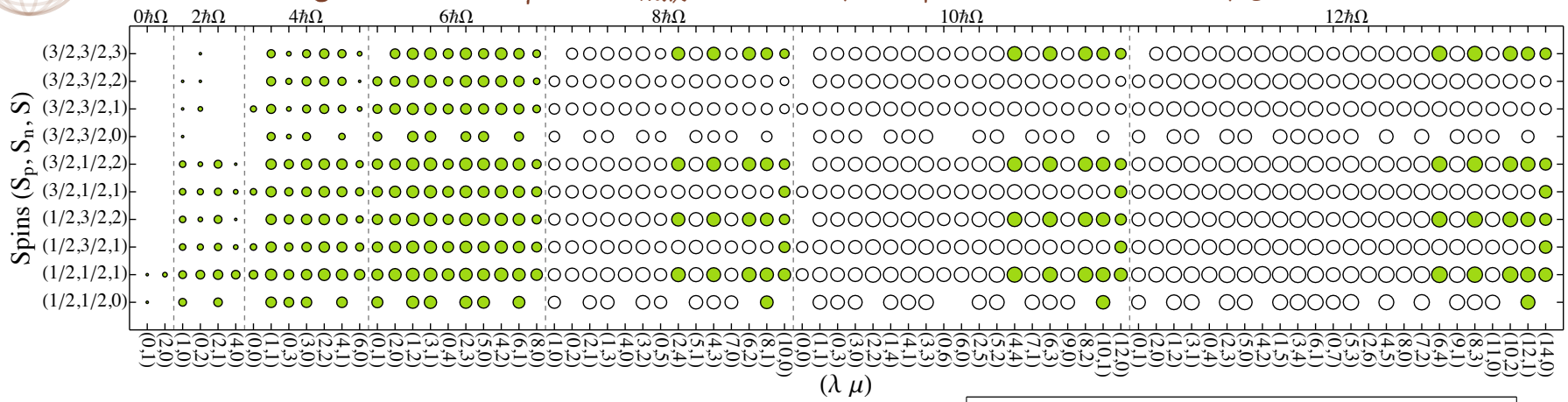


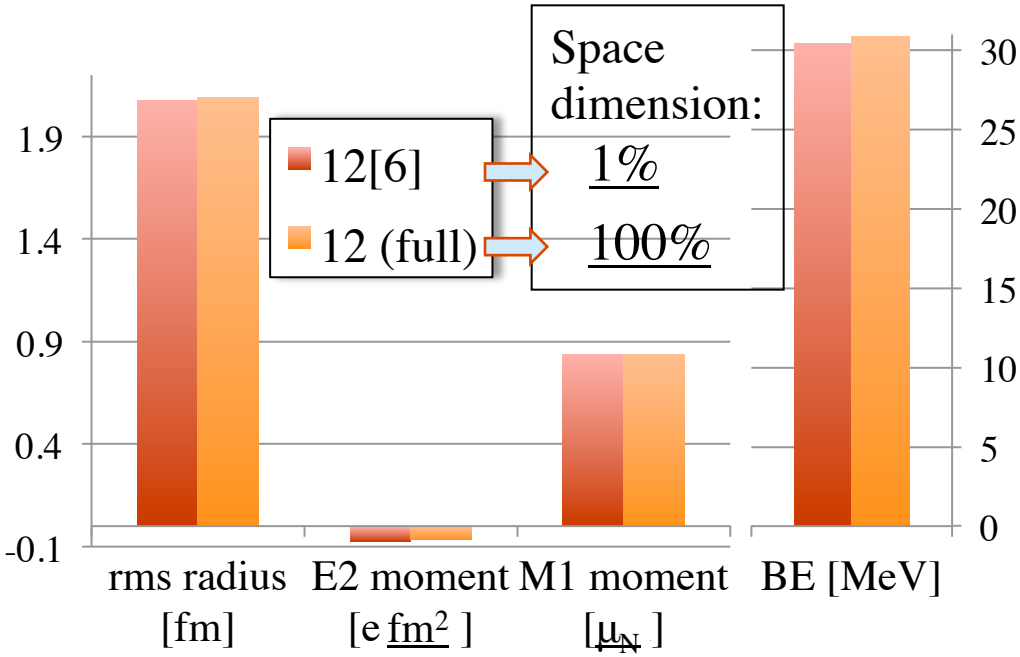
Maximum Deformation

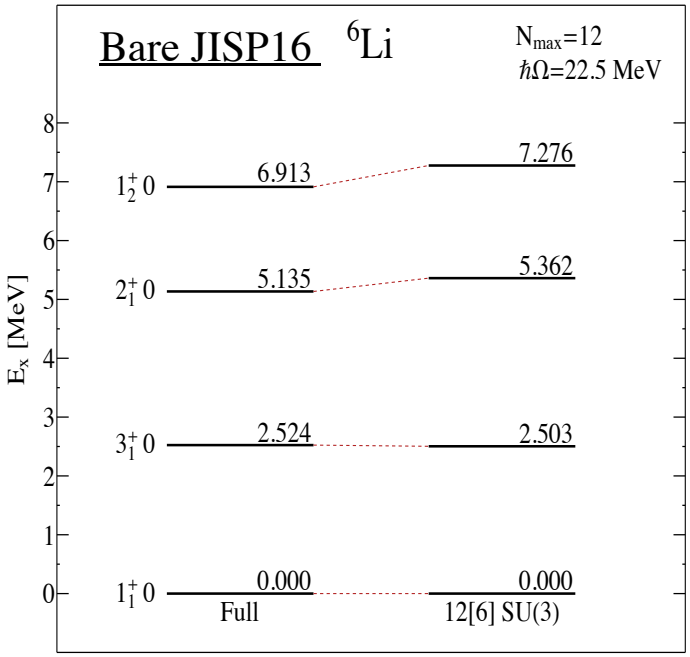


Efficacy of SA-NCSM: ^{6}Li

Winnowing the model space: N_{max}=12[6] (full up to 6ħΩ; selected configurations in 8-12 ħΩ)

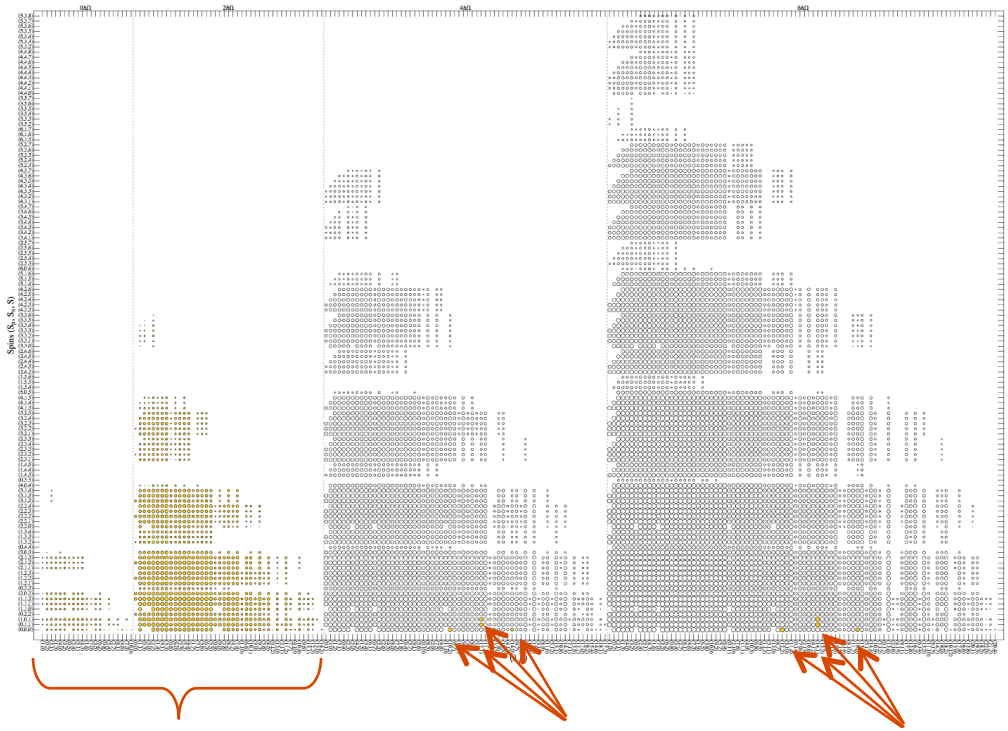






SA-NCSM: reaching sd-shell nuclei

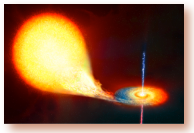
Winnowing the model space: $N_{max}=6$ [2]



Full
8×10^9

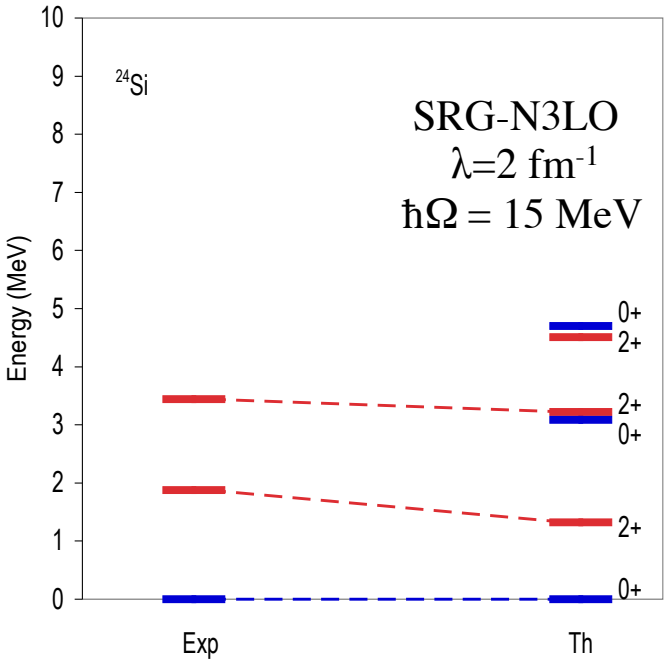
Selected
3×10^6

0.04% of full $N_{max}=6$ space

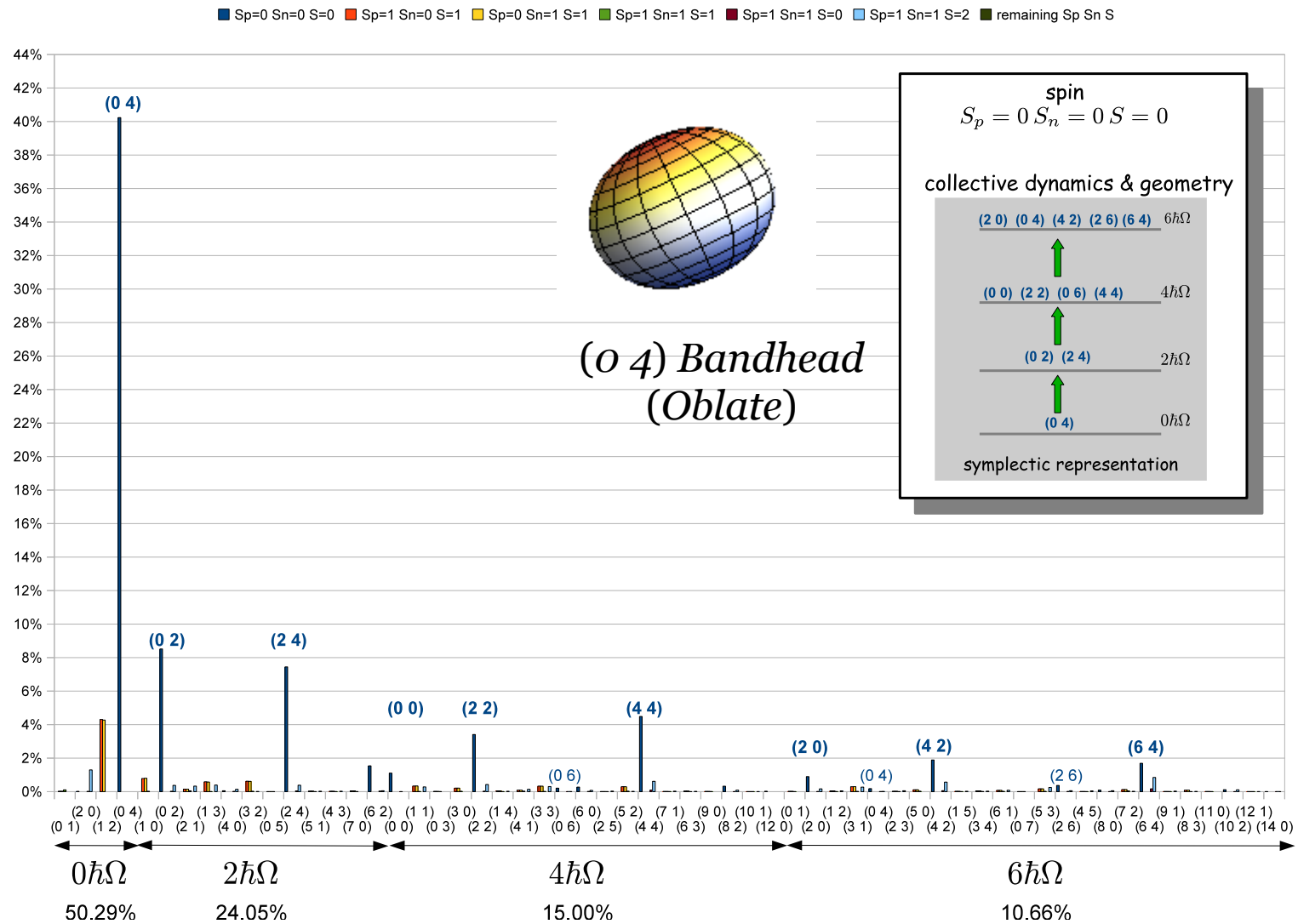


Novae and X-ray bursts

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

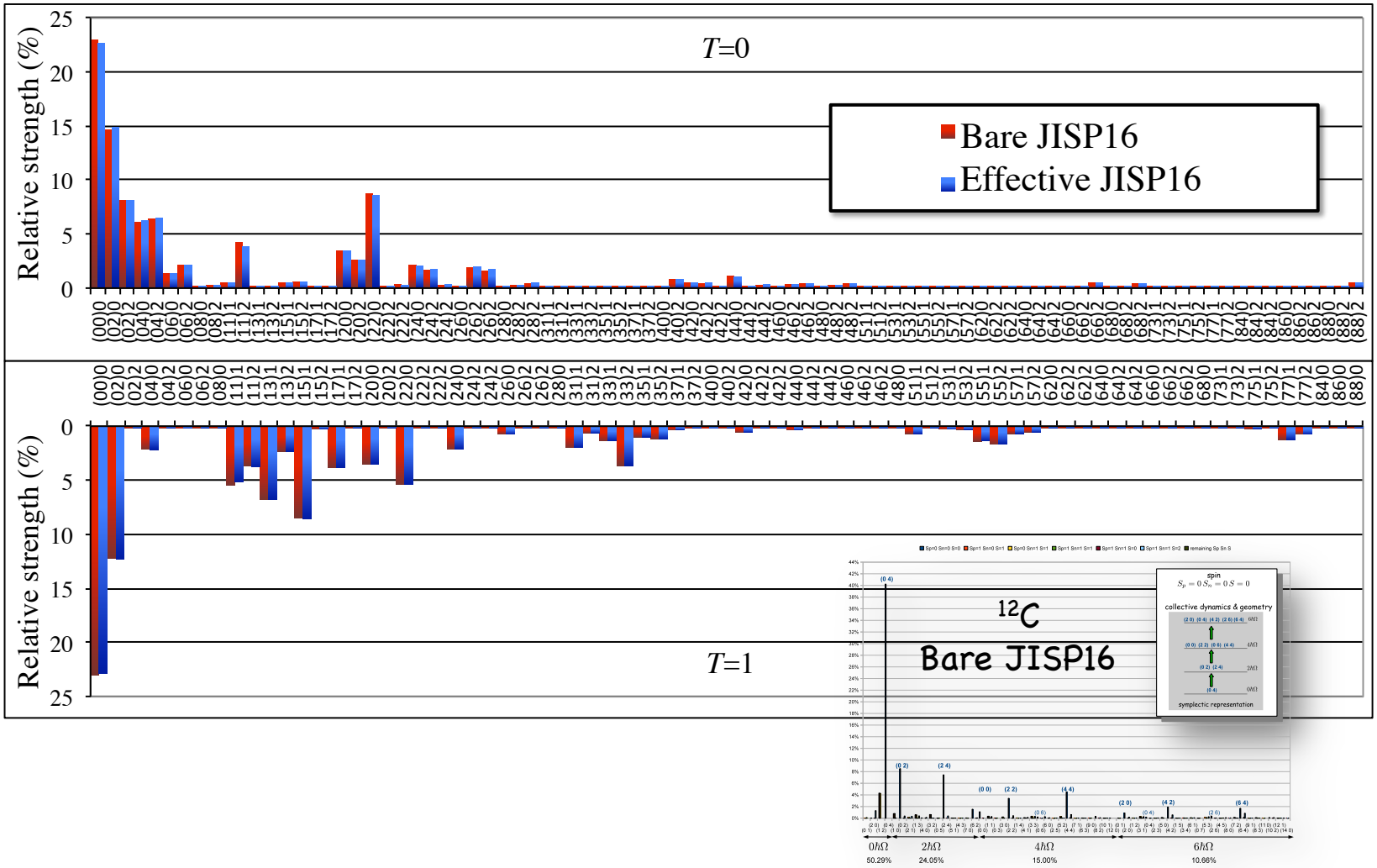


^{12}C: bareJISP16 (N_{max} = 6)



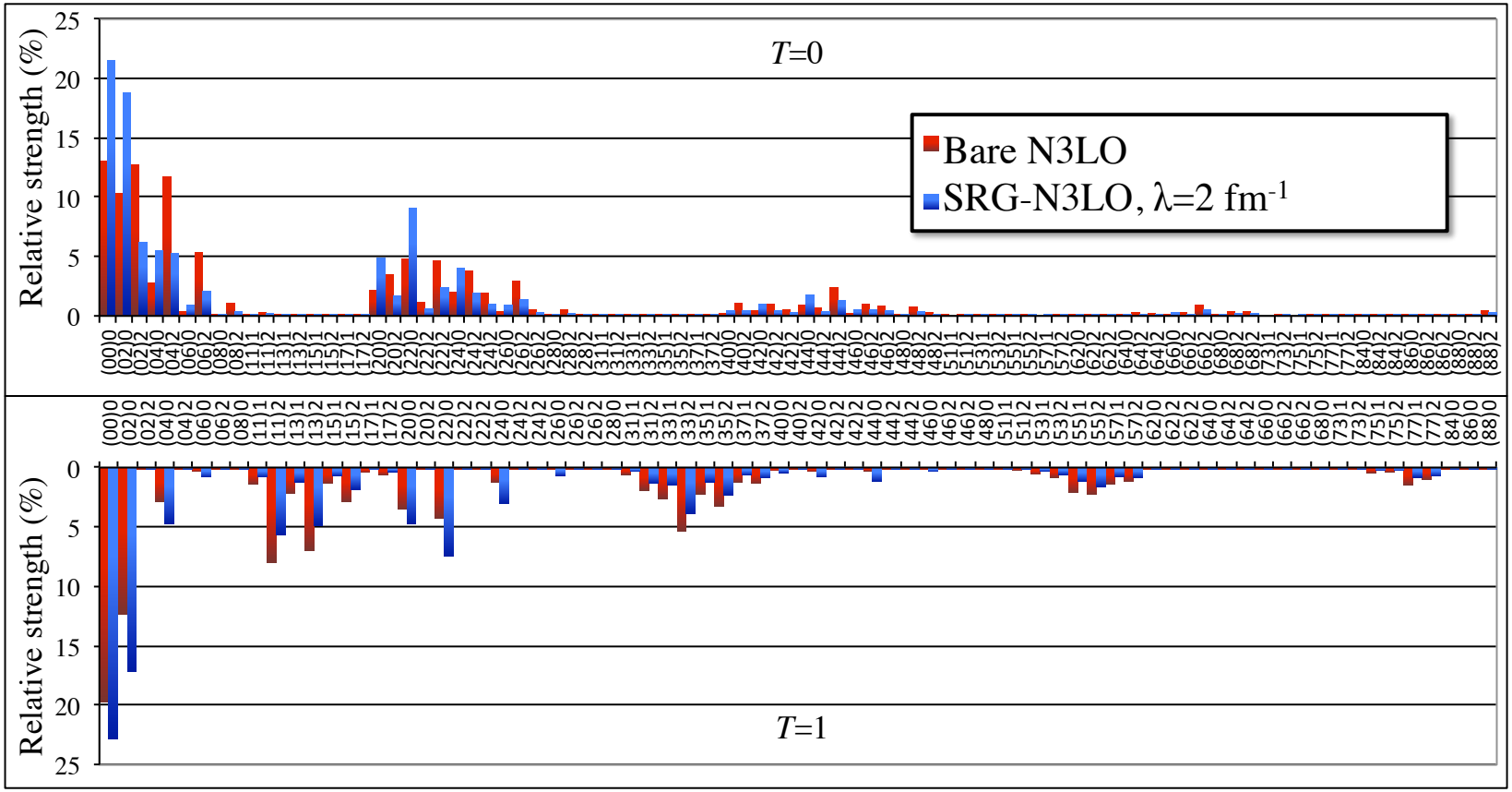
Nucleon-nucleon interaction: SU(3) Tensors

JISP16 (N_{max}= 6)
$\hbar\Omega$ = 15 MeV



Nucleon-nucleon interaction: SU(3) Tensors

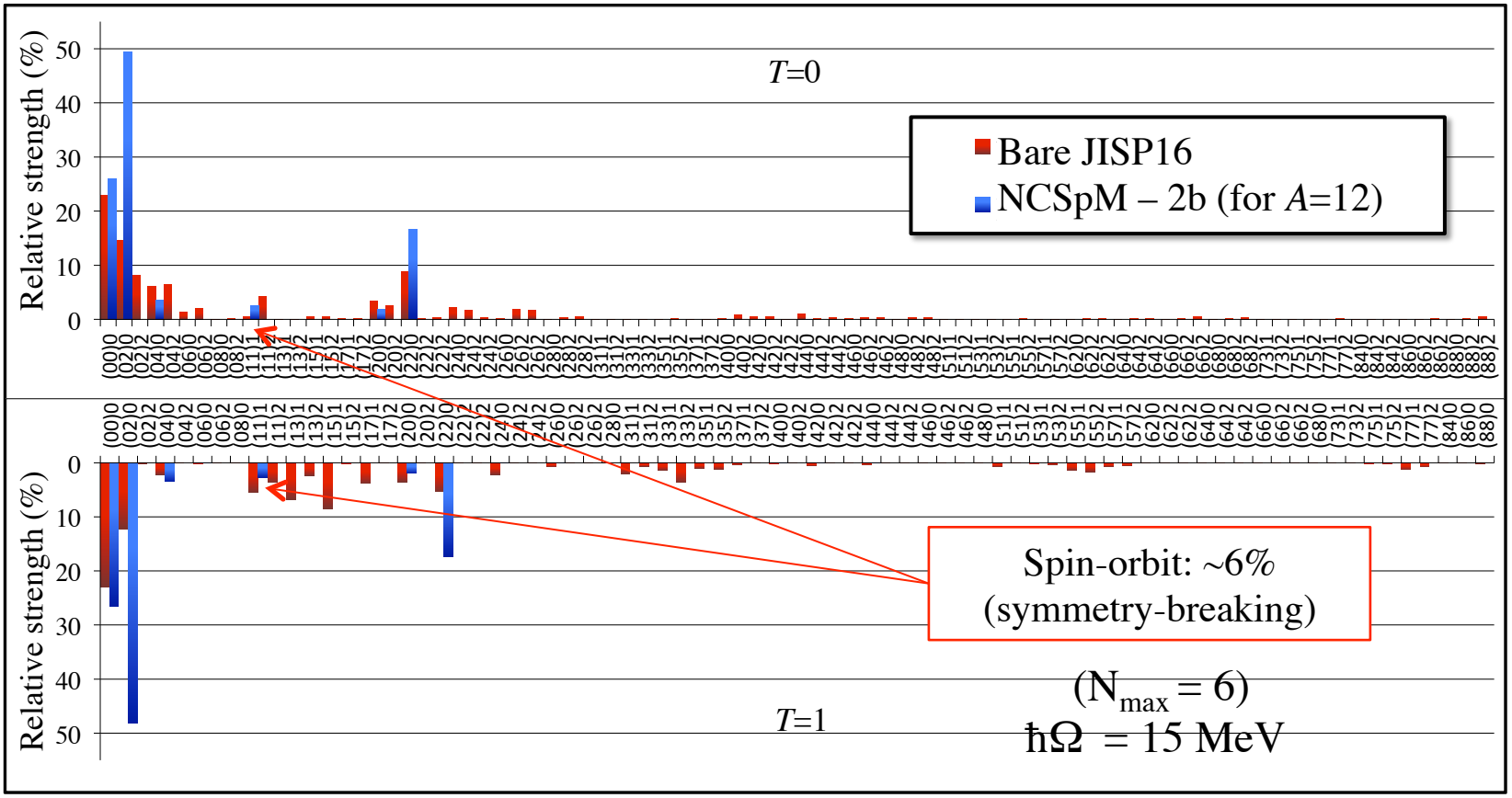
N3LO (N_{max}= 6)
$\hbar\Omega$ = 11 MeV



Nucleon-nucleon interaction: SU(3) Tensors

Proposed Interaction
(long-range central + l.s)

$$H_\gamma = \sum_i^A \left(\frac{p_i^2}{2m} + \frac{m\Omega^2 r_i^2}{2}\right) - \frac{\chi}{2}\frac{(e^{\gamma Q\cdot Q}-1)}{\gamma} - \frac{20}{A^{2/3}}\sum_i^A l_i.s_i$$

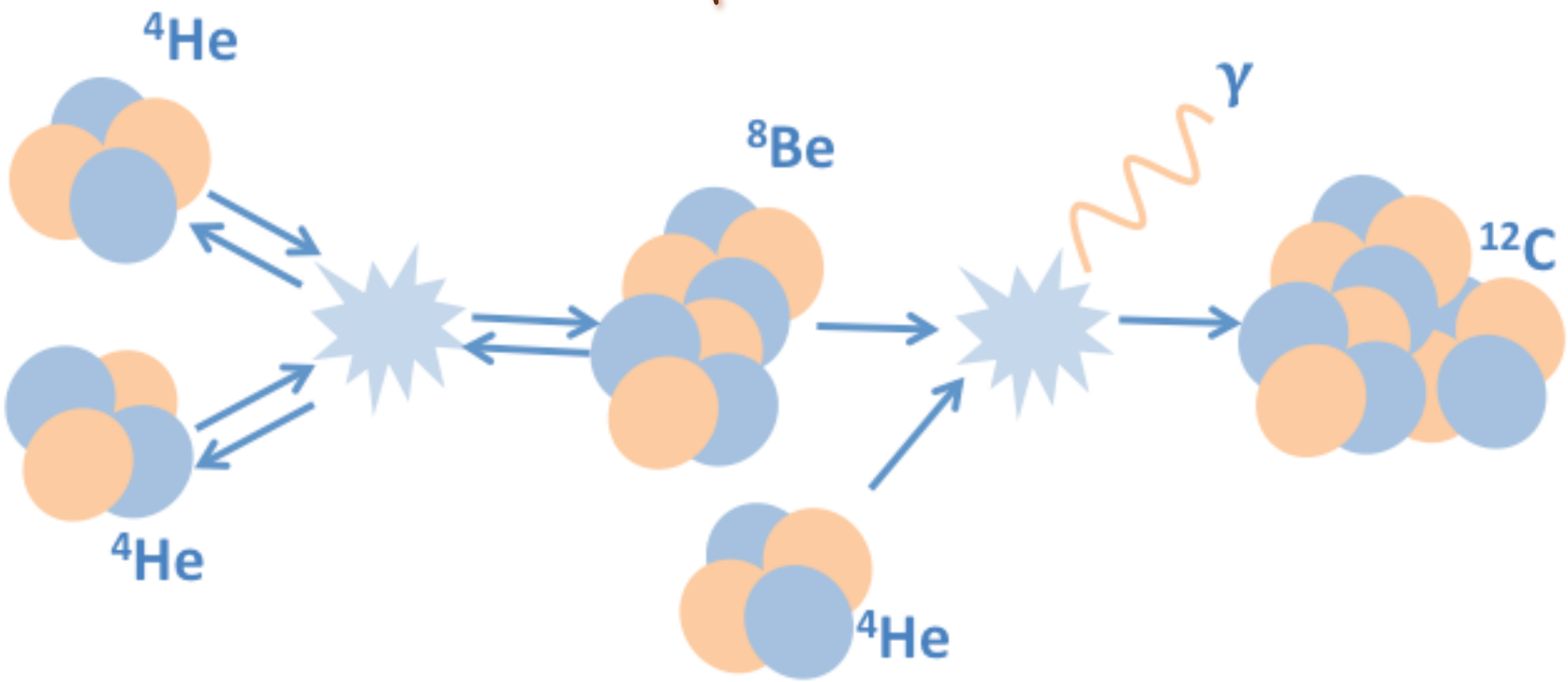


2-body: similar to JISP16, except (2 0) & (1 3)/(1 5)

3-body & 4-body: important to reproduce rotational band

Pushing the NC-Shell / Collective Connection

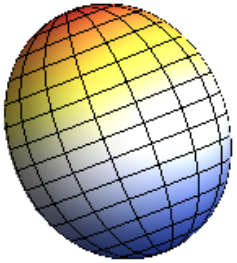
Creation of ^{12}C in hot stars



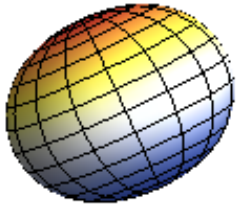
... The elusive Hoyle state ...

Choose Three Slices (ancient but current)

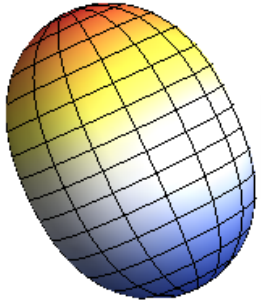
^{12}C



(6 2) *Bandhead*
(*Prolate*)



(0 4) *Bandhead*
(*Oblate*)



(12 0) *Bandhead*
(*More Prolate*)

0p-0h

2p-2h

4p-4h

Main contribution to the 0_3^+

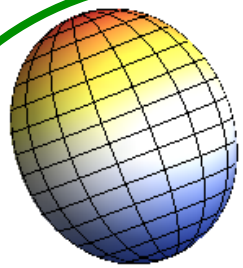
Main contribution to ground state rotational band ($0_{g.s.}^+$, 2_1^+, 4_1^+)

Main contribution to Hoyle state (0_2^+)

'Back to the Future'
– *déjà vu* –
Engeland & Ellis '67s

Choose Three Slices (modern picture)

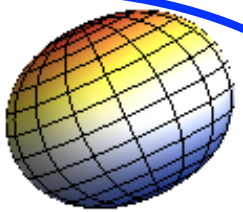
^{12}C



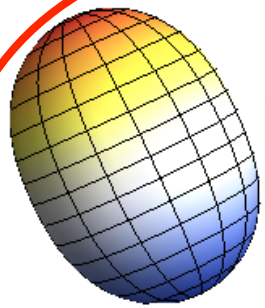
2p-2h

(6 2) Bandhead
(Prolate)

0p-0h

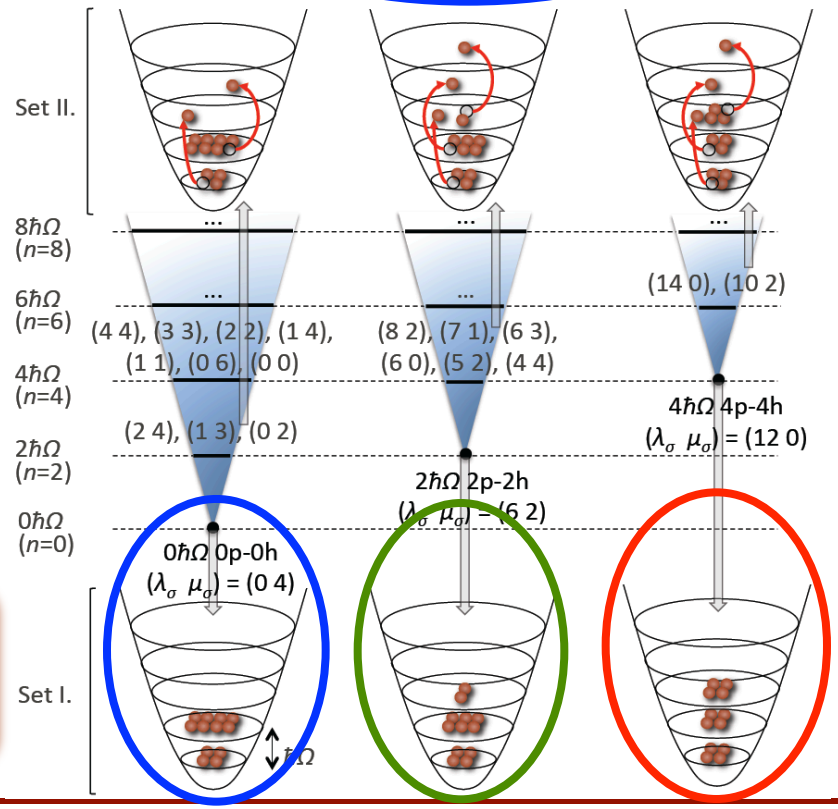


(0 4) Bandhead
(Oblate)



4p-4h

(12 0) Bandhead
(More Prolate)



Intertwining Shell & Alpha Cluster Picture

Proposed (LSU) Interaction ($-\frac{20}{A^{2/3}}\sum_i l_i.s_i$)

New! New!

Proposed Interaction*

$$H_\gamma = \sum_i^A \left(\frac{p_i^2}{2m} + \frac{m\Omega^2 r_i^2}{2}\right) - \frac{\chi}{2}\frac{(e^{\gamma Q\cdot Q}-1)}{\gamma}$$

$\gamma \to 0$

Limit yields Elliott Model (only $0\hbar\omega$ model space)

Choice means independent of the oscillator strength

One-parameter theory for collective & cluster modes

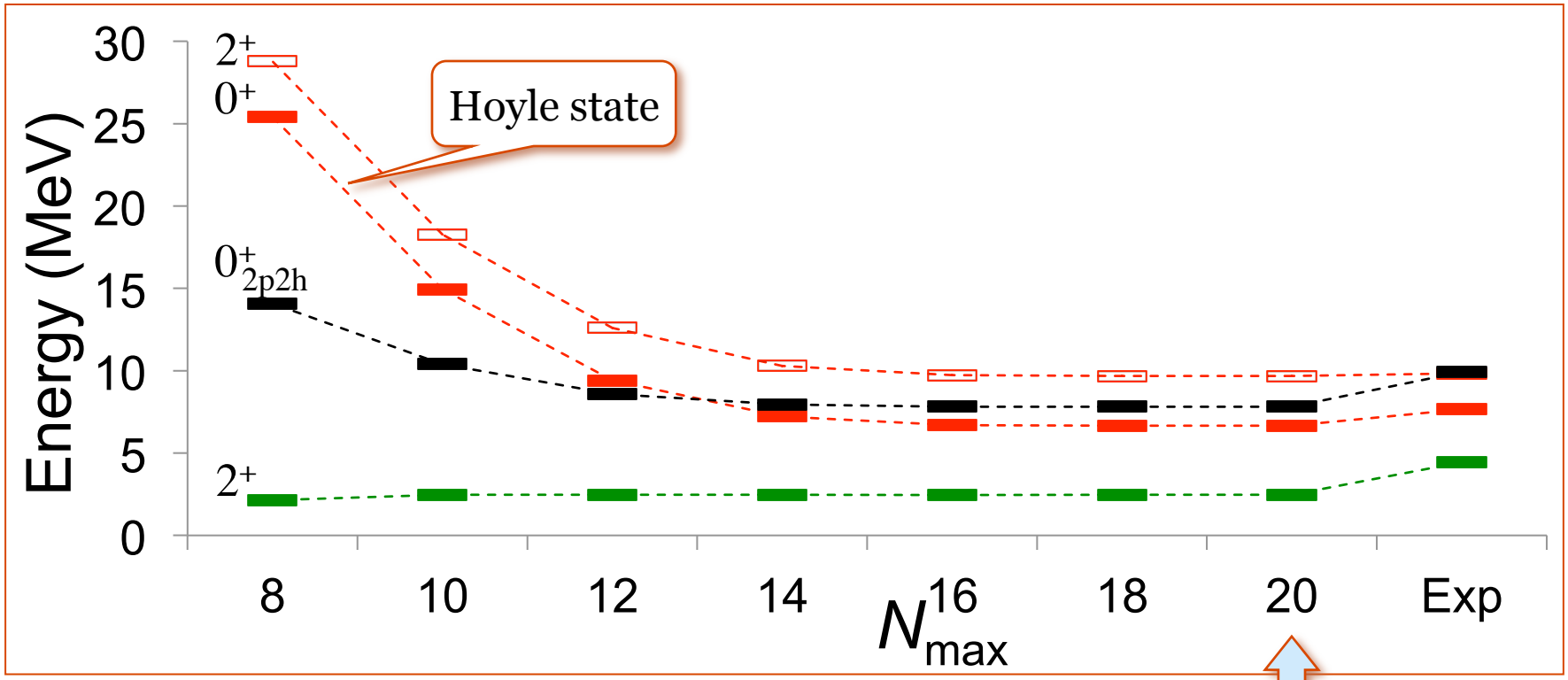
$$H = H_0 - \frac{\chi}{2} Q\bullet Q$$

$$\chi = \hbar\Omega / (4\sqrt{N_f N_i})$$

H_γ introduces simple, but important many-body interactions (three & four-body) that enter in a prescribed hierarchical way

*Note: For connoisseurs of algebraic methods, Q.Q has to be "centered" within each major oscillator shell (simple scalar operator) so it doesn't "overpower" structure imposed by H_0

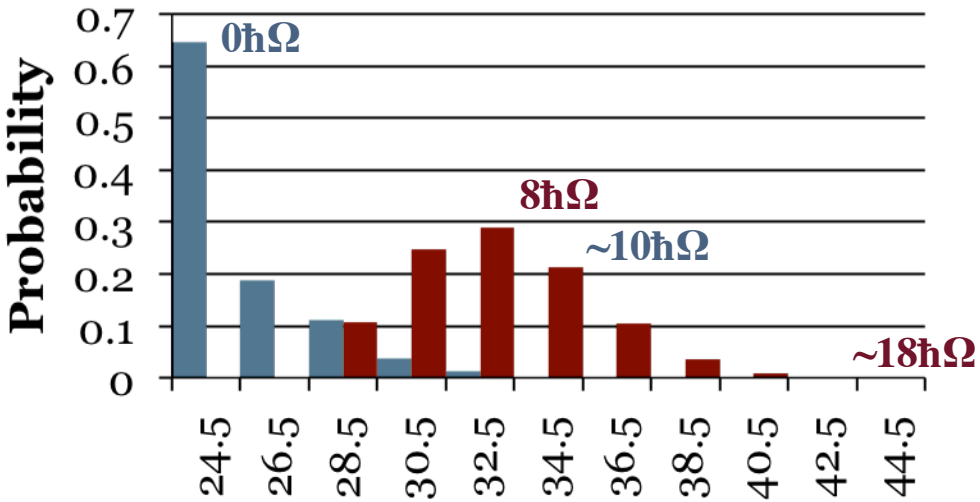
^{12}C Systematics



NCSpM

^{12}C: 0^+ Probability Distributions

- Ground 0_1 state peaks at $0\hbar\Omega$ extends to $\sim 10\hbar\Omega$
- Hoyle state peaks at $8\hbar\Omega$ and extends to $\sim 18\hbar\Omega$
- Ground state: compared to bare JISP16

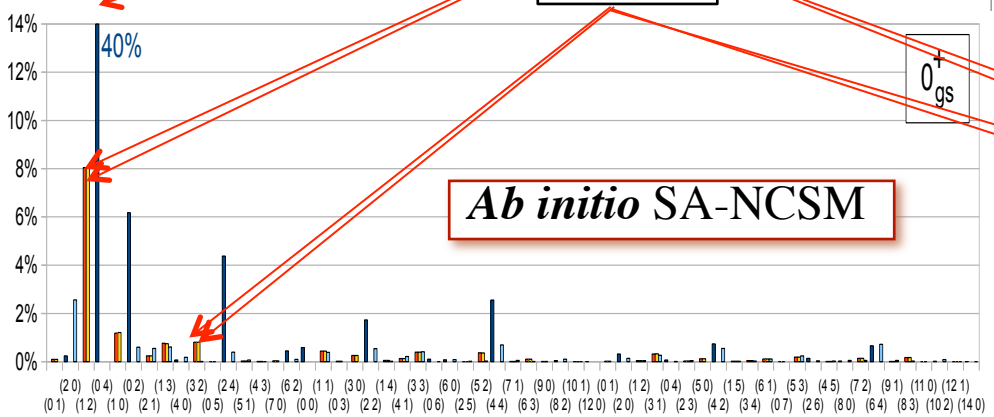


SA-NCSM (full N_{max} = 6)

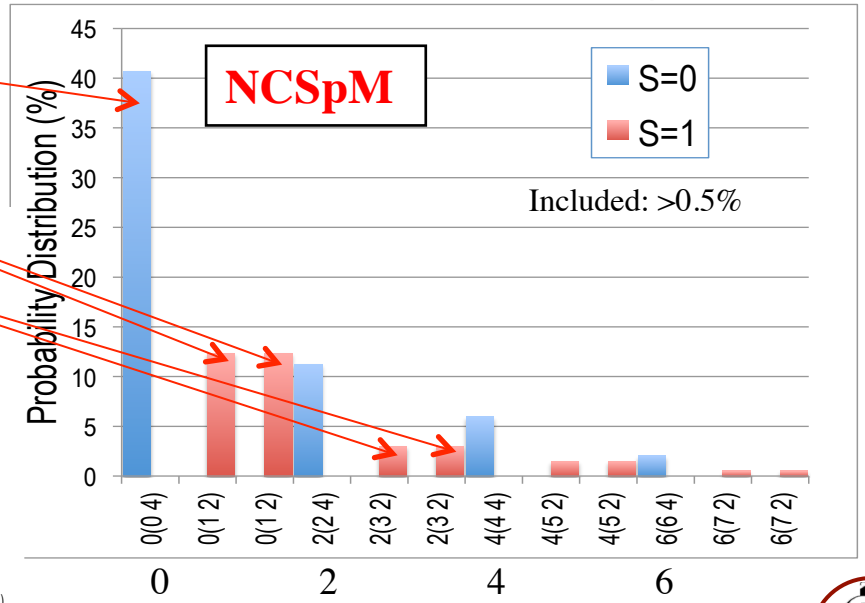
S=0 (0 4)

S=1 (1 2)

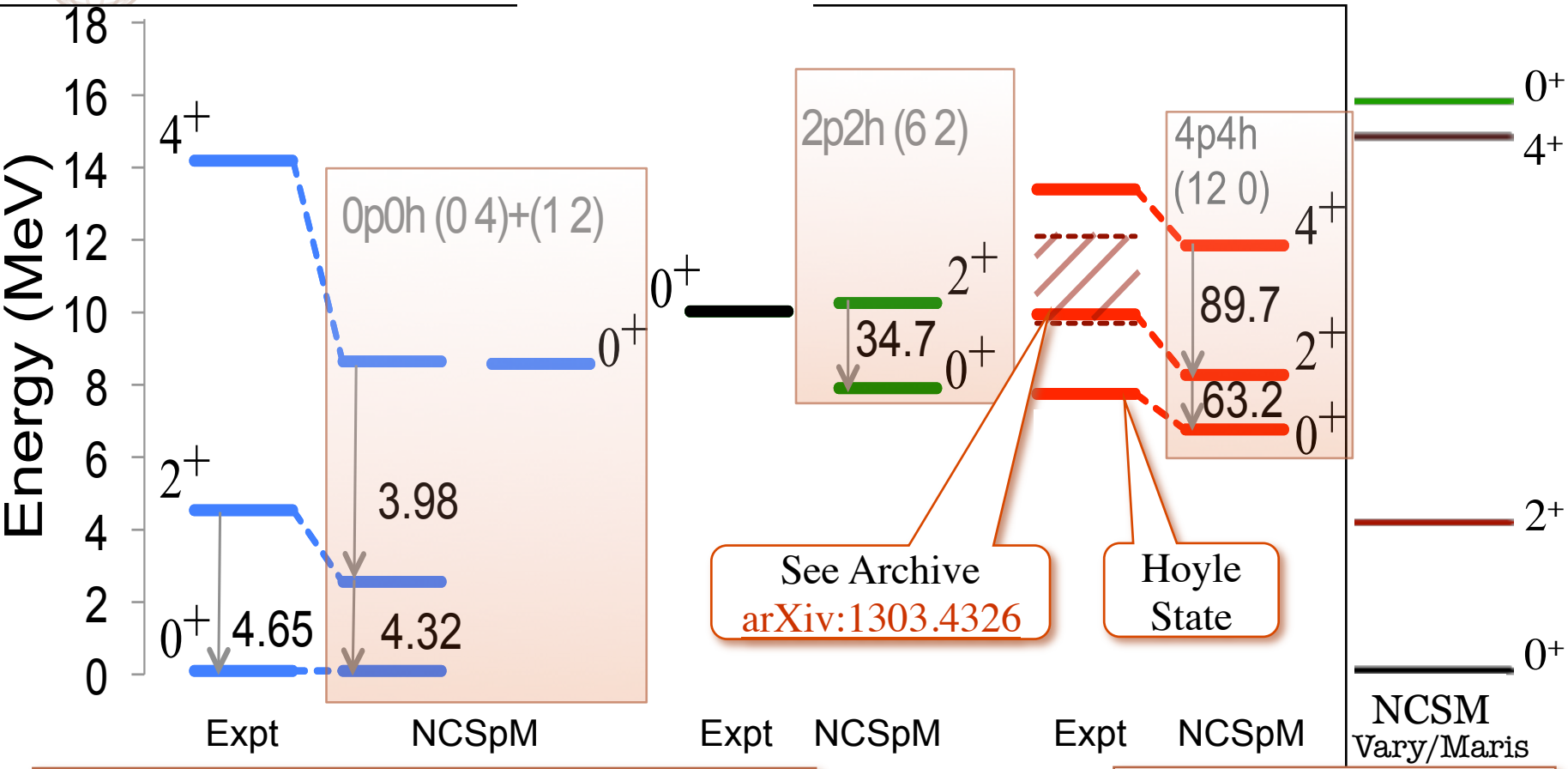
S=1 (3 2)



Ab initio SA-NCSM



^{12}C Spectrum + B(E2) [W.u.]



NCSpM:

Fixed:

$\hbar\Omega = 18$ MeV, $N_{max} = 20$

Adjusted:

$\gamma = -1.71\times10^{-4}$

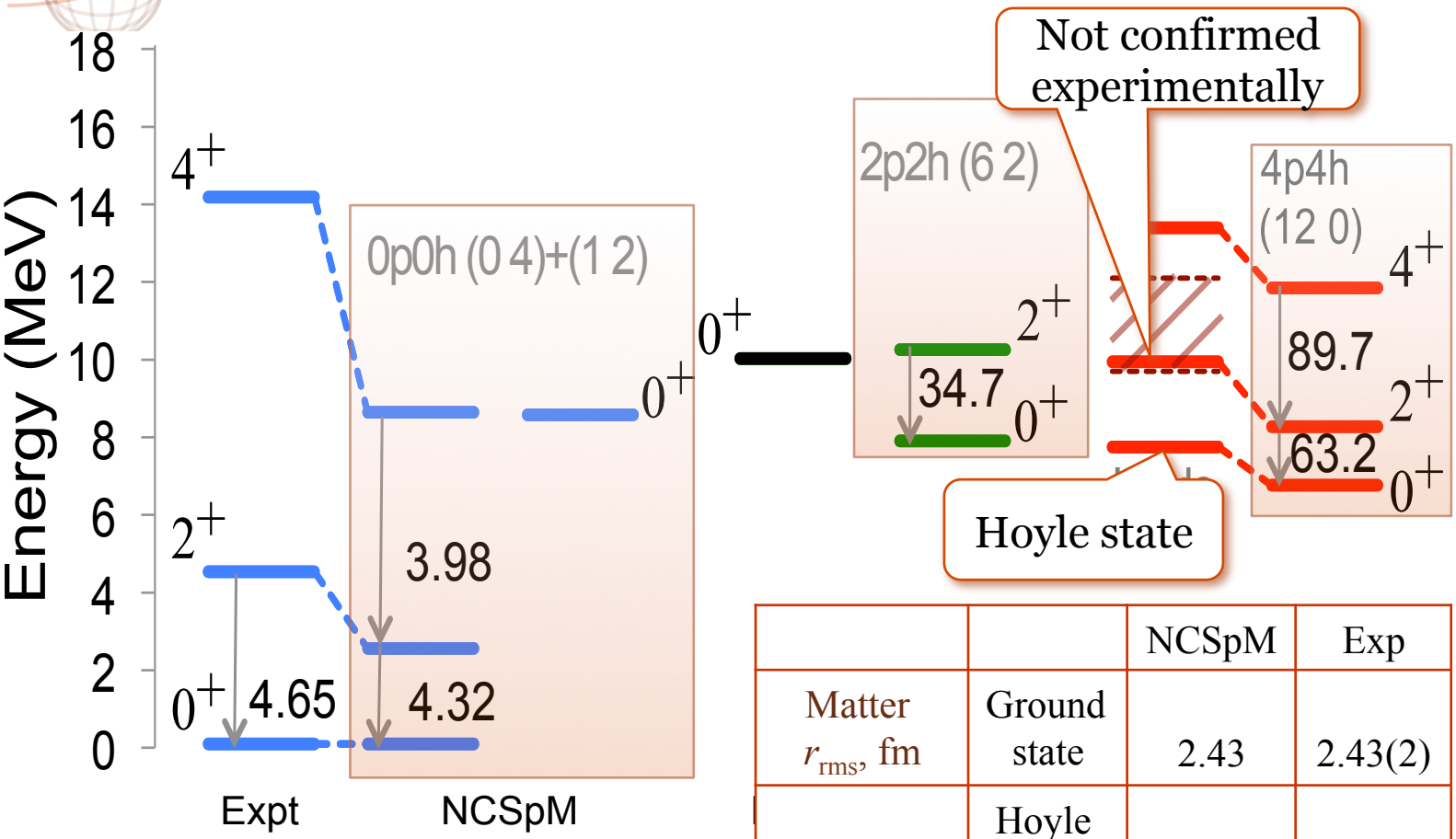
– PARAMETERS –

NCSM with JISP16:

Fixed:

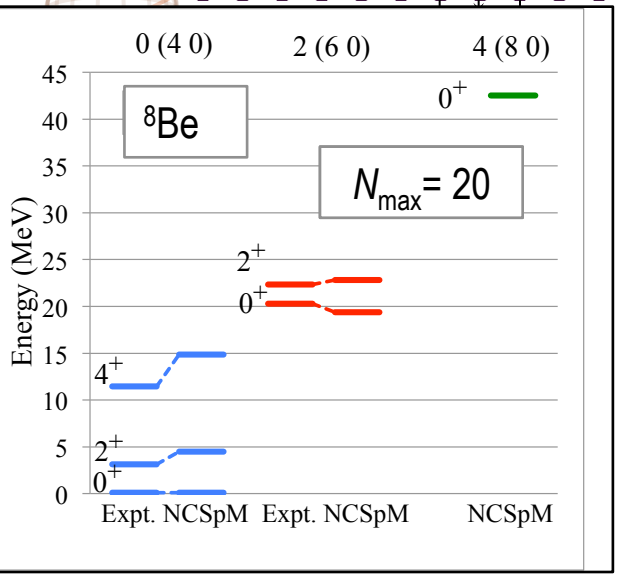
$\hbar\Omega = 15$ MeV, $N_{max} = 6$

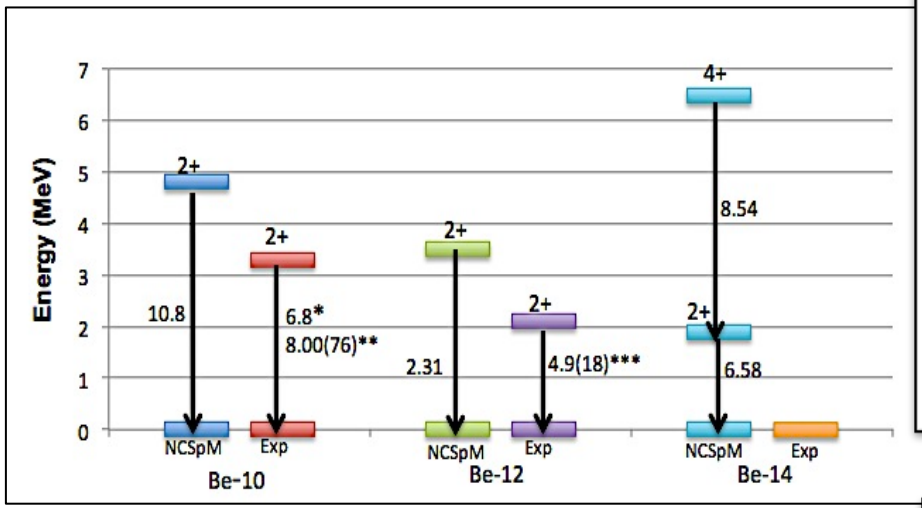
^{12}C Observables – cont'd

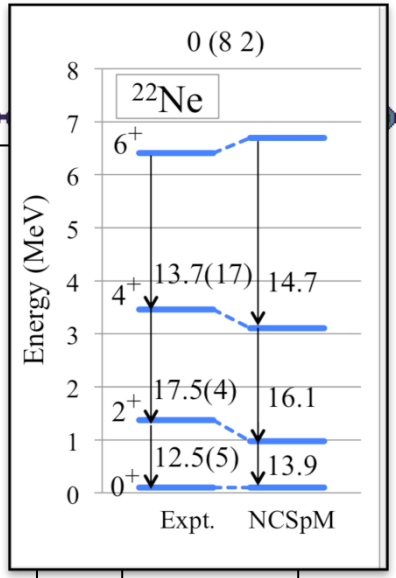


		NCSpM	Exp
Matter r_{rms}, fm	Ground state	2.43	2.43(2)
	Hoyle state	2.93	N/A
Q, e fm^2	2_1^+	+5.89	+6(3)
	2_2^+	–20.61	N/A

NCSpM for p- and sd-shell nuclei

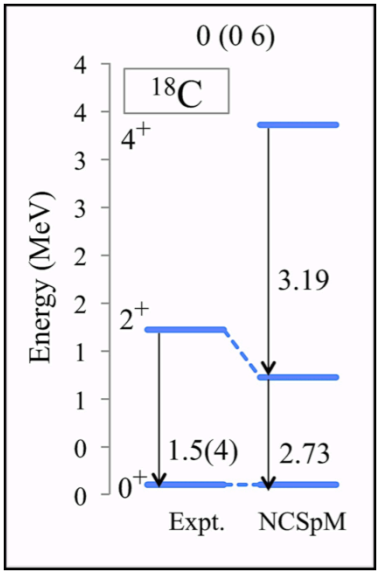




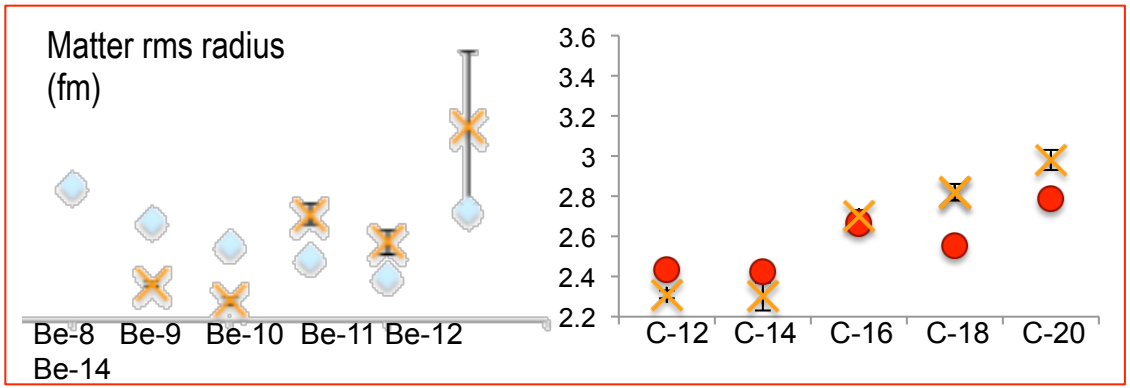


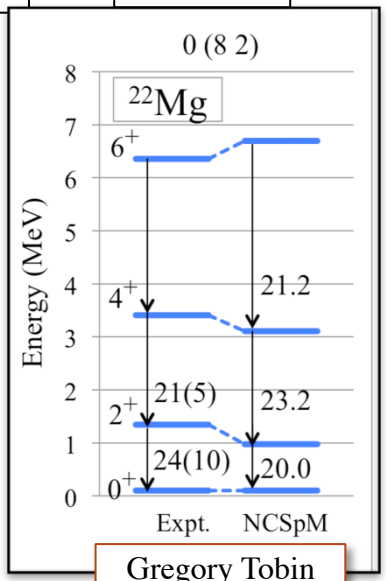
N_{max}= 12

Mia Ferriss (UG – LSU)



No parameter adjustment





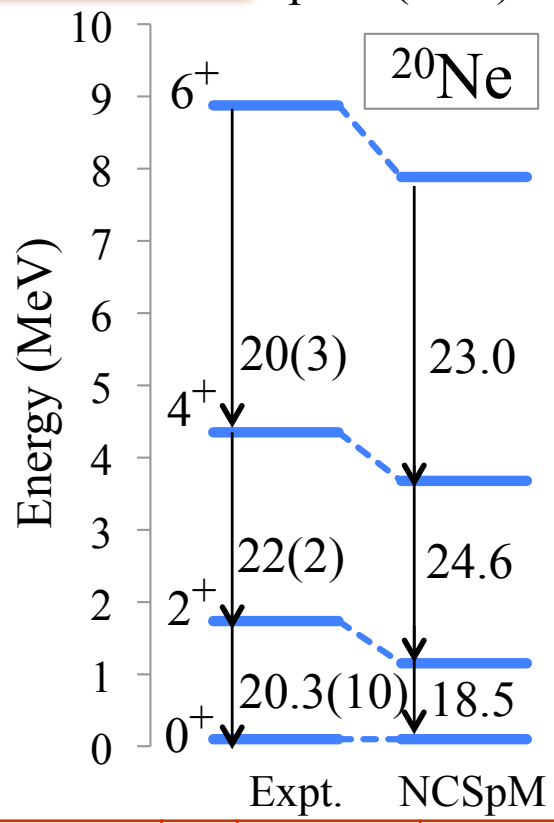
Gregory Tobin
(UG – LSU)

NCSpM for p- and sd-shell nuclei

$\hbar\Omega = 15$ MeV
$N_{max} = 12$

Gregory Tobin (LSU)

0p-0h (10 0)

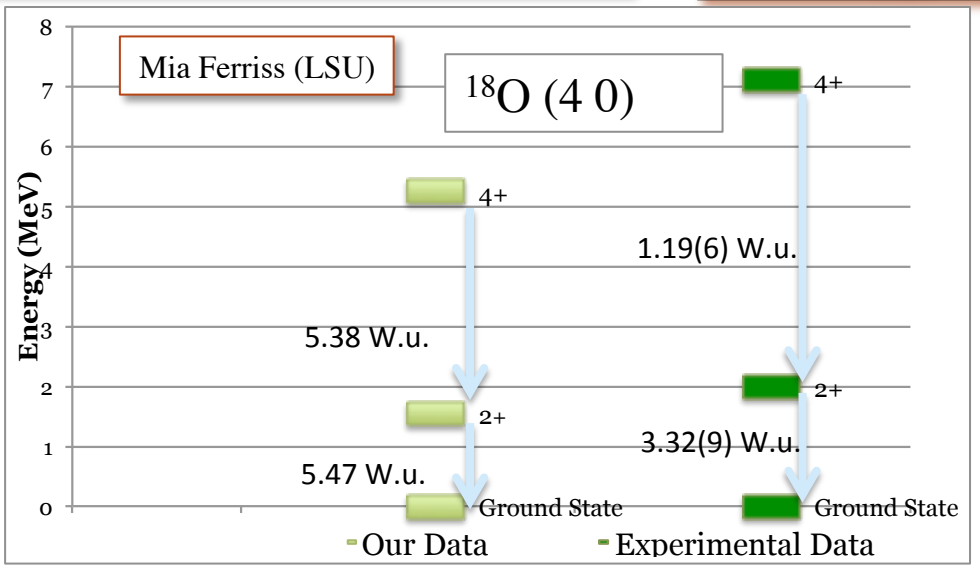


		NCSpM	Exp
Q, e fm^2	2^+	–15.7	–23 (3)

		$r_m(0^+_{gs})$	$Q_{2^+_1}$	$Q_{4^+_1}$	$Q_{6^+_1}$
^{20}Ne	Expt.	2.87(3)	−23(3)	–	–
	NCSpM	2.79	−15.69	−19.69	−21.05
^{22}Ne	Expt.	–	−17(3)	–	–
	NCSpM	2.82	−14.90	−19.22	−21.61
^{22}Mg	Expt.	2.89(6)	–	–	–
	NCSpM	2.82	−17.88	−23.07	−25.93
^{24}Ne	Expt.	2.79(13)	–	–	–
	NCSpM	2.94	−15.40	−19.48	−21.16
^{24}Si	Expt.	–	–	–	–
	NCSpM	2.94	−21.57	−27.27	−29.63
^{26}Mg	Expt.	2.93(12)	−13.5(20)	–	–
	NCSpM	2.95	−17.89	−23.14	−26.12
^{26}Si	Expt.	–	–	–	–
	NCSpM	2.95	−20.87	−26.99	−30.47

no parameter adjustment

$\hbar\Omega = 16$ MeV
$N_{max} = 20$



Themes

Background Information – (Complementary Methods)

- ✓ Shell Models
  - Maria Goeppert-Mayer & J. Hans D. Jensen (single-particle theory)
  - Nilsson Model (deformed mean field)
  - Pairing Modes (Kerman '60s, Hecht Sp(4) '70s and more; Exact Solutions)
  - **No-Core Shell Model – NCSM** (Vary, Navratil & Barrett ~'00s … Today & Tomorrow!)
- ✓ Collective Models
  - Niels Bohr & Ben Mottelson (dominance of deformation)
  - Elliott Model (algebraic realization of deformation & S(3) – '60s)
  - Symplectic Shell Model (Rowe & Rosensteel '70s & '80s]) Pairing Modes
  - **NC Symplectic Model – NCSpM** (Draayer & Collaborators, ~'05s … Today & Tomorrow!)

Dominant Structures – (Collaboration & Computers Essential)

- ✓ Copy-cat work (discovering symmetries within NCSM results)
- ✓ Stepping out (alternative approaches; e.g., SA-NCSM & NCSpM)
- ✓ Identifying "emergent properties" in QCD inspired interactions

Hoyle State Example – (Emergent Properties & Symmetries)

- ✓ Understanding light nuclei essential (focus on 0^+ states 1st)
- ✓ Identifying "emergent properties" in QCD inspired interactions
- ✓ Stretch goal – extending towards heavier nuclei – pseudo-symmetries

'Top Down' versus 'Bottom Up'

2nd Decade of 21st Century

- Robust stand- alone SA-NCSM code – publicly available (… tunable to available computational resources …)
- Designed to handle up to 3-body & 4-body interactions (… important for alpha-particle type correlations …)
- Push forward on the NCSpM – l.s term & pairing modes (… important for generating symmetry mixing…)
- Continue development with applications - laptop version (^{6}Li, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg … odd-A too & heavier …)

… Thanks for the invite / Best to James – Push On! …

The end is our future …