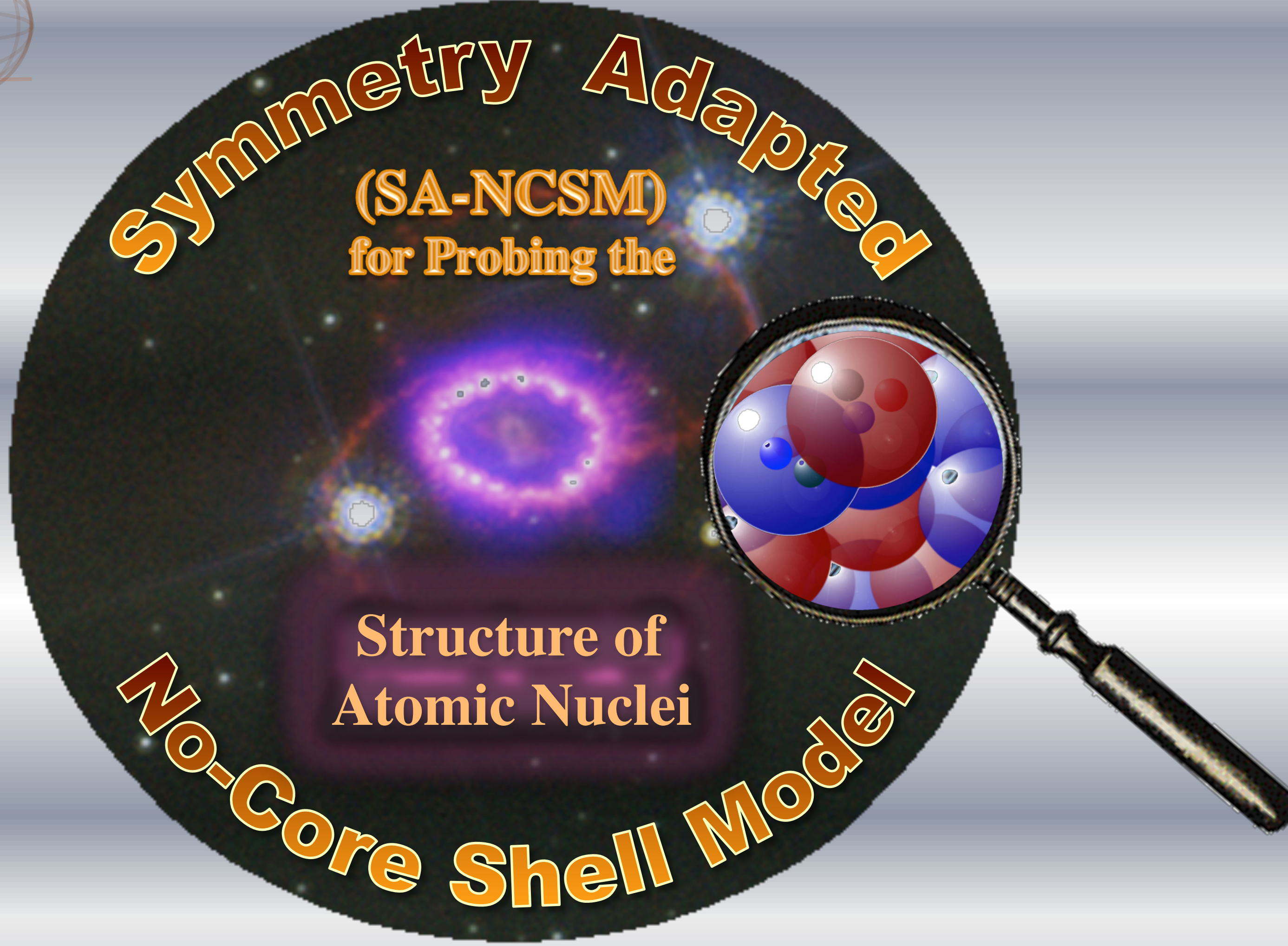
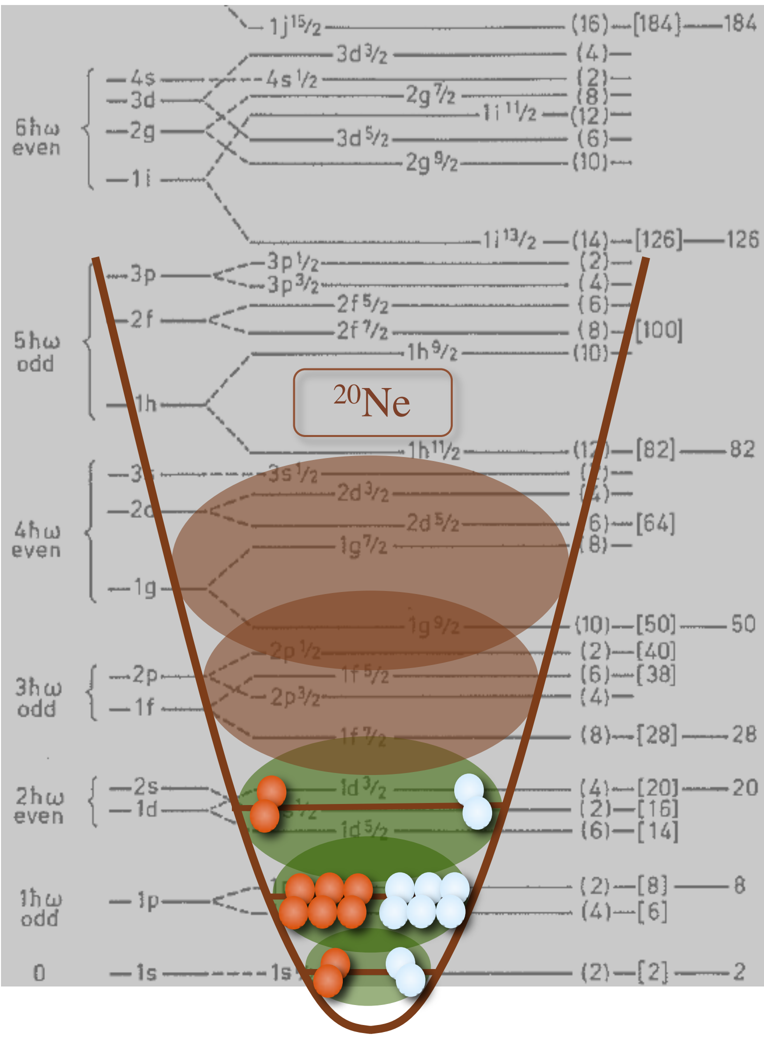


PIs: Jerry P. Draayer, Kristina D. Launey, Tomas Dytrych; Post-Doc Alexis Mercenne
Graduate Students: Alison C. Dreyfuss, Robert Baker, Grigor Sargsyan & David S. Kekejian

U.S. NSF & DOE plus LSU & SURA Sponsored Research

… before < 2000 > after …

Legacy Shell Model …

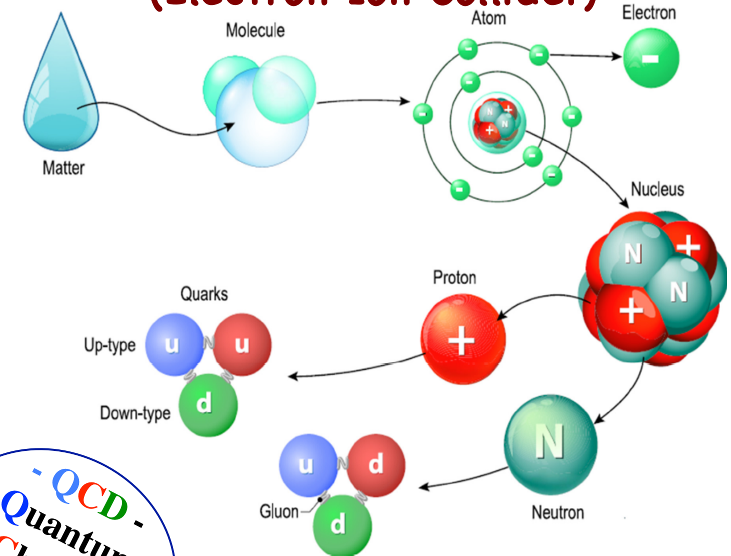


82
50
28
20
8
2

21st Century
Walk Over

… Femto-Science World

NAS Report – 08/18 (Electron Ion Collider)



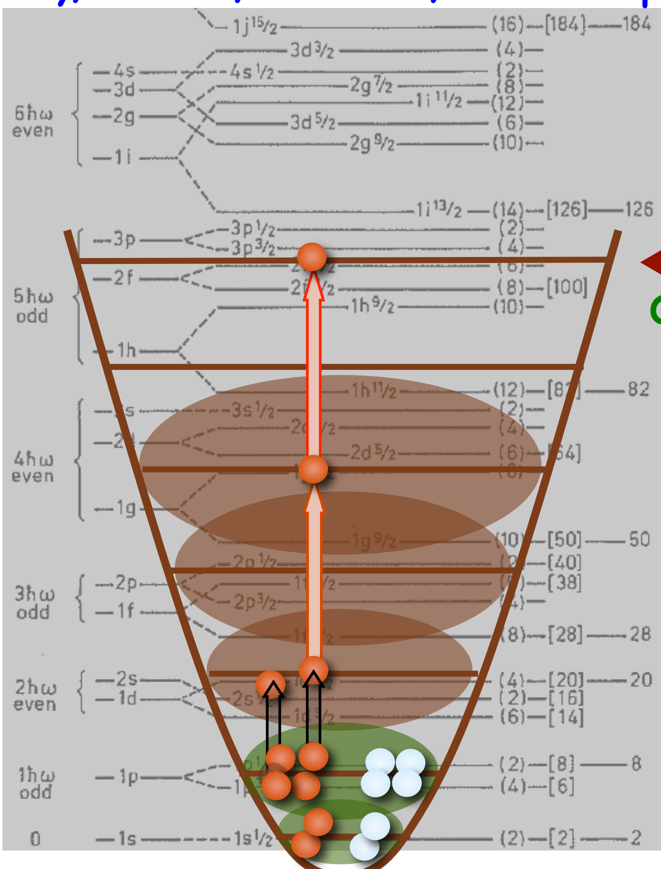
- QCD -
Quantum
Chromo
Dynamics

Two forces – strong color force and the electromagnetic force – are responsible for holding the fundamental pieces – quarks & gluons plus electrons together …

Where HPC, XYZ-NCSM & LE-QCD (χEFT) converge!

Shell Model No-Core Collective Model

No-Core Shell Model (NCSM)*
(Vary, Navratil, & Barrett, ~2000 to present)



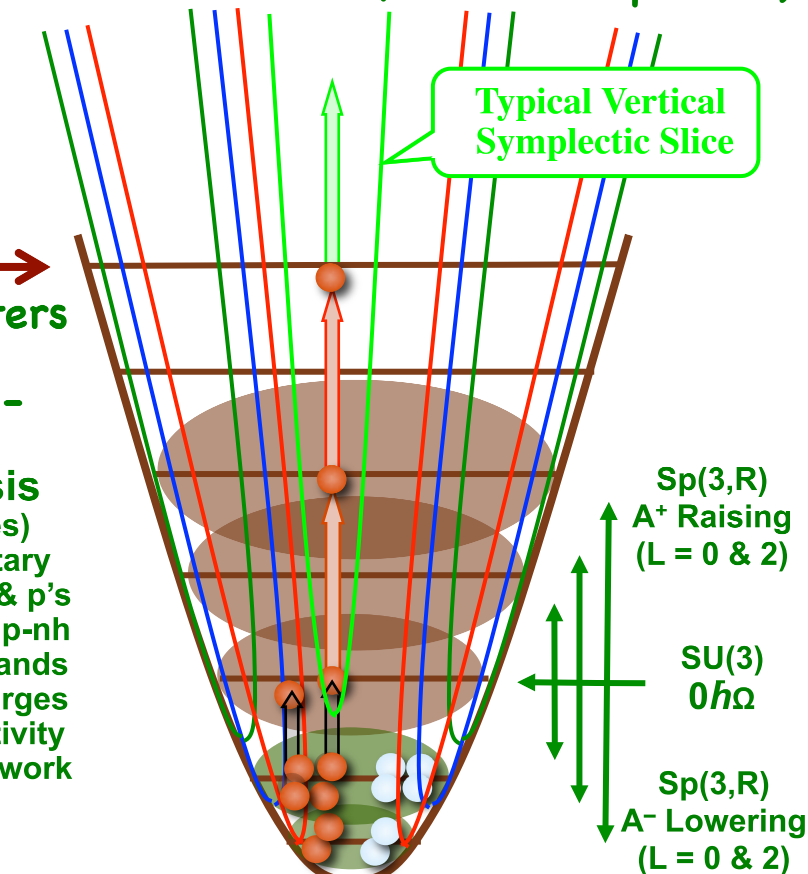
Reorganize Shell-Model Space

Collective/Clusters Subspaces

Symmetry Adapted Basis
(Special Features)

- Canonical & Unitary
- Quadratic in x's & p's
- Band-heads ➔ np-nh
- Spurious Free Bands
- No Effective Charges
- Captures Collectivity
- Algebraic Framework

Symplectic Model (Sp-NCSM)*
(Rowe & Rosensteel, ~1980s to present)

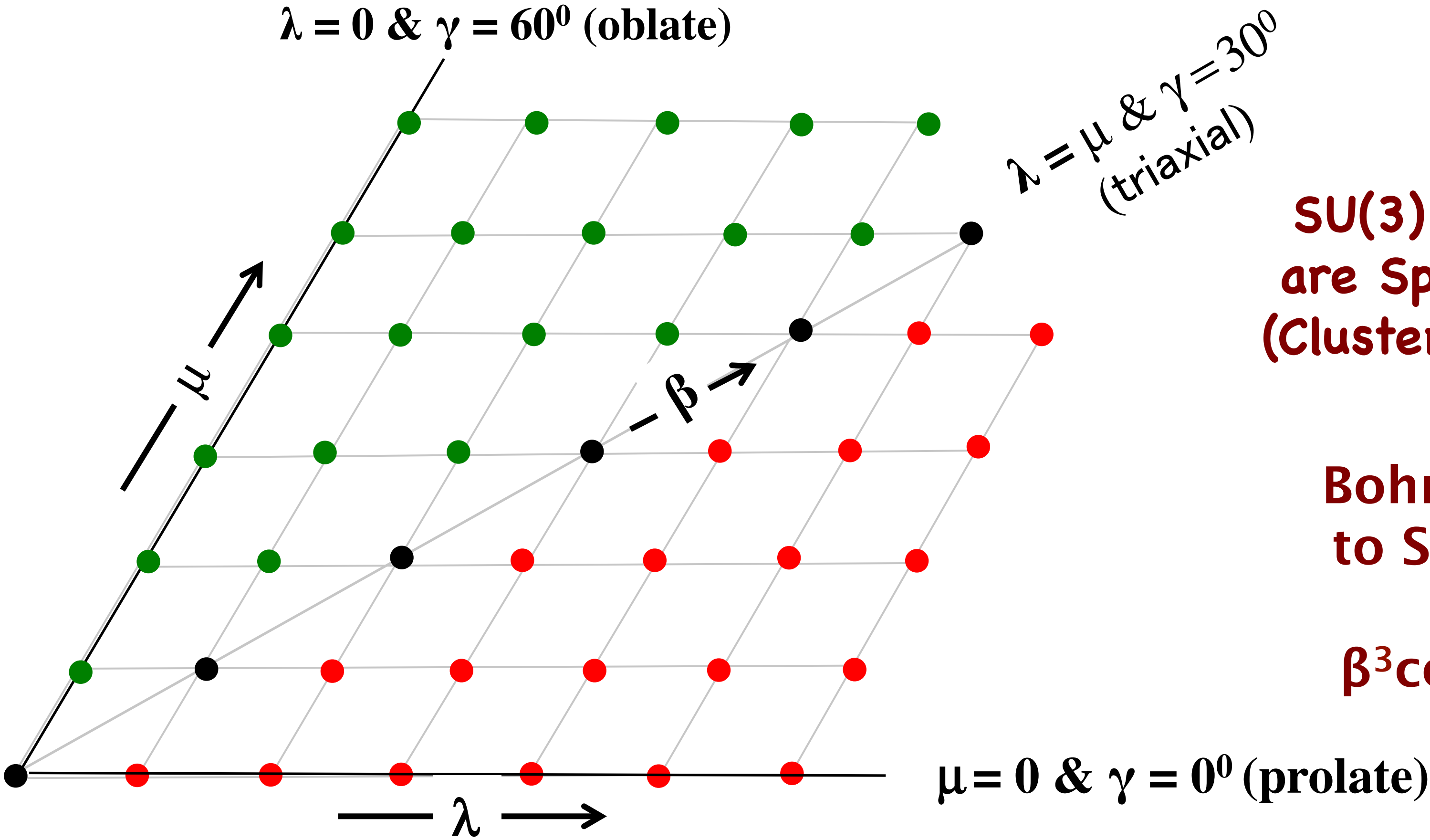


*Realistic interaction (local or not; NN, NNN, …)
- *In principle*, exact solutions, up to N_{max}
- Successful description up through ^{16}O

*Sound & Simple algebraic underpinning
- Elliott SU(3) if no symplectic modes
- Sp(3,R) add monopole & quadrupole

Spatial Plateau

U(Ω) -> SU(3) Lattice versus Bohr-Mottelson Picture (β,γ)



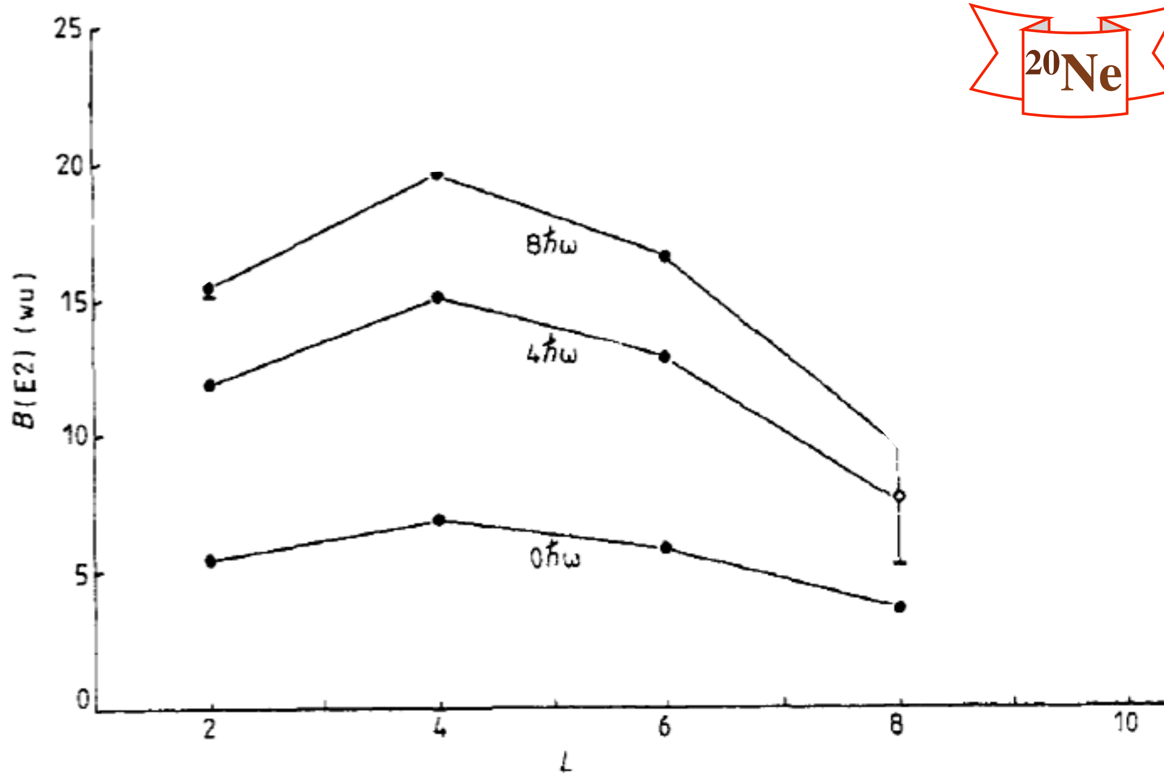
SU(3) Irrep (λ,μ) are Sp(3,R) Irreps (Cluster Bandheads)

Bohr-Mottelson to SU(3) map …

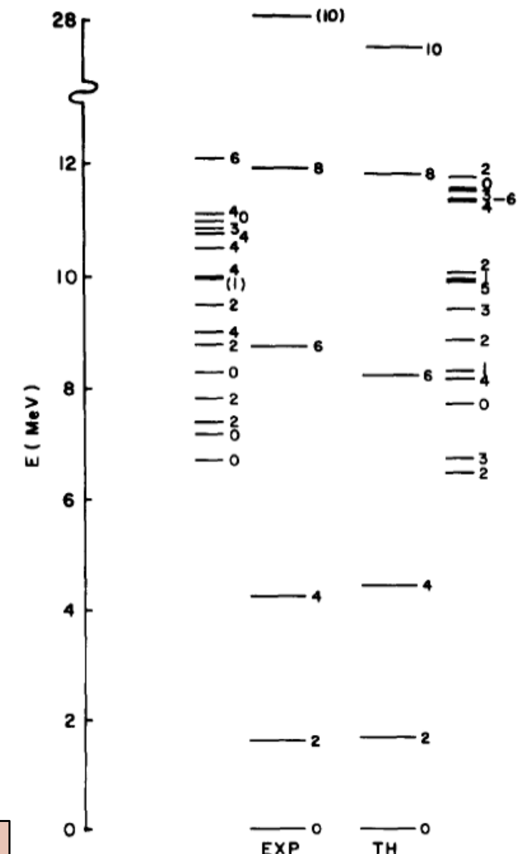
$\beta^2 \sim C_2$

$\beta^3 \cos(3\gamma) \sim C_3$

Simple (Sp-NCSM) Picture



^{20}Ne

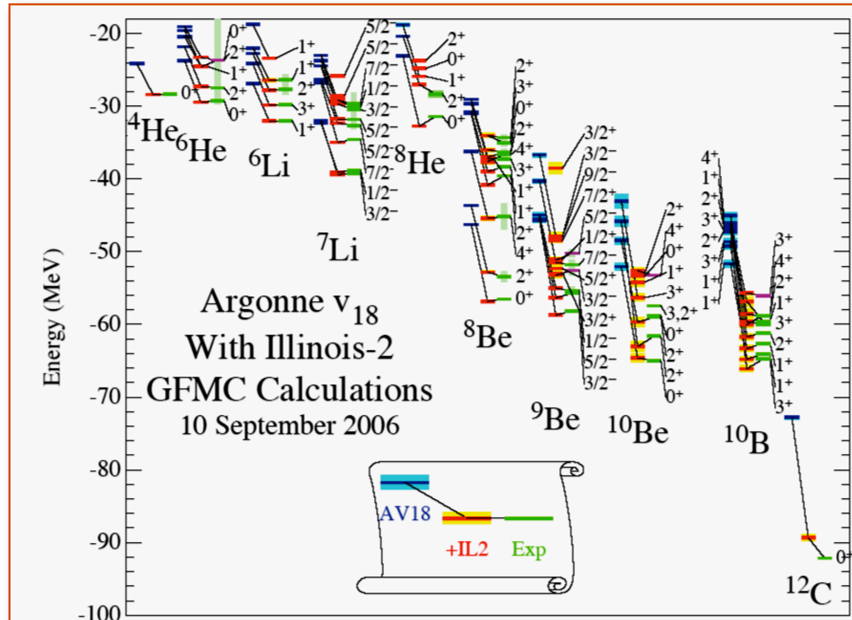


$$H = \hbar\omega H_0 + b_2 Q\cdot Q + b_3 (Q\times Q)\cdot Q + b_4 (Q\cdot Q)^2 \boxed{+\sum_j \varepsilon_j n_j + G_0 P}$$

G. Rosensteel and D.J. Rowe – 1977

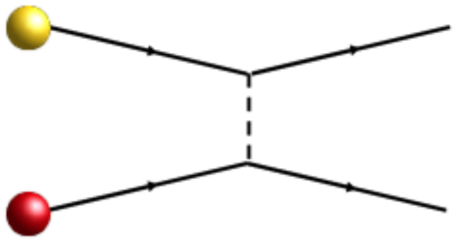
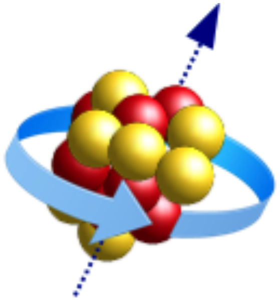
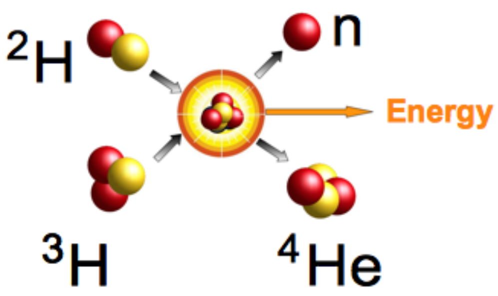
J.P. Draayer, K.J. Weeks, G. Rosensteel – 1984

… Contemporary Interpretation …



- Variational & Green's Function Monte Carlo (VMC/GFMC): A≤12, local interactions
- Coupled-cluster Theory (CCT): near closed-shell nuclei (^{4}He, ^{16}O, ^{40}Ca); space truncation
- No-core Shell Model: A≤16, space truncation - binomial space growth is model's Achilles' Heal
- No-Core Symplectic Model (first results, major investment time/effort required - think smart!)

… Contemporary Interpretation …

Strong Interaction	Many-body Dynamics	Nuclear Reactions
		
		
realistic interaction & nuclear potentials	nuclear properties & collective phenomena	reaction dynamics & nuclear cross-sections

‘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

High Performance Computing Era*

Shell Model

NCSM

Coupled Cluster Theory

Monte Carlo Methods

....

HPC Era . . .

DOE

NERSC-X (Berkeley)
Summit (Oak Ridge)
Aurora(Argonne)
... upgrades ...

NSF

Stampede, Wrangler (TACC)
Blue Waters (NCSA)
... upgrades ...

Collective Model

NCSM

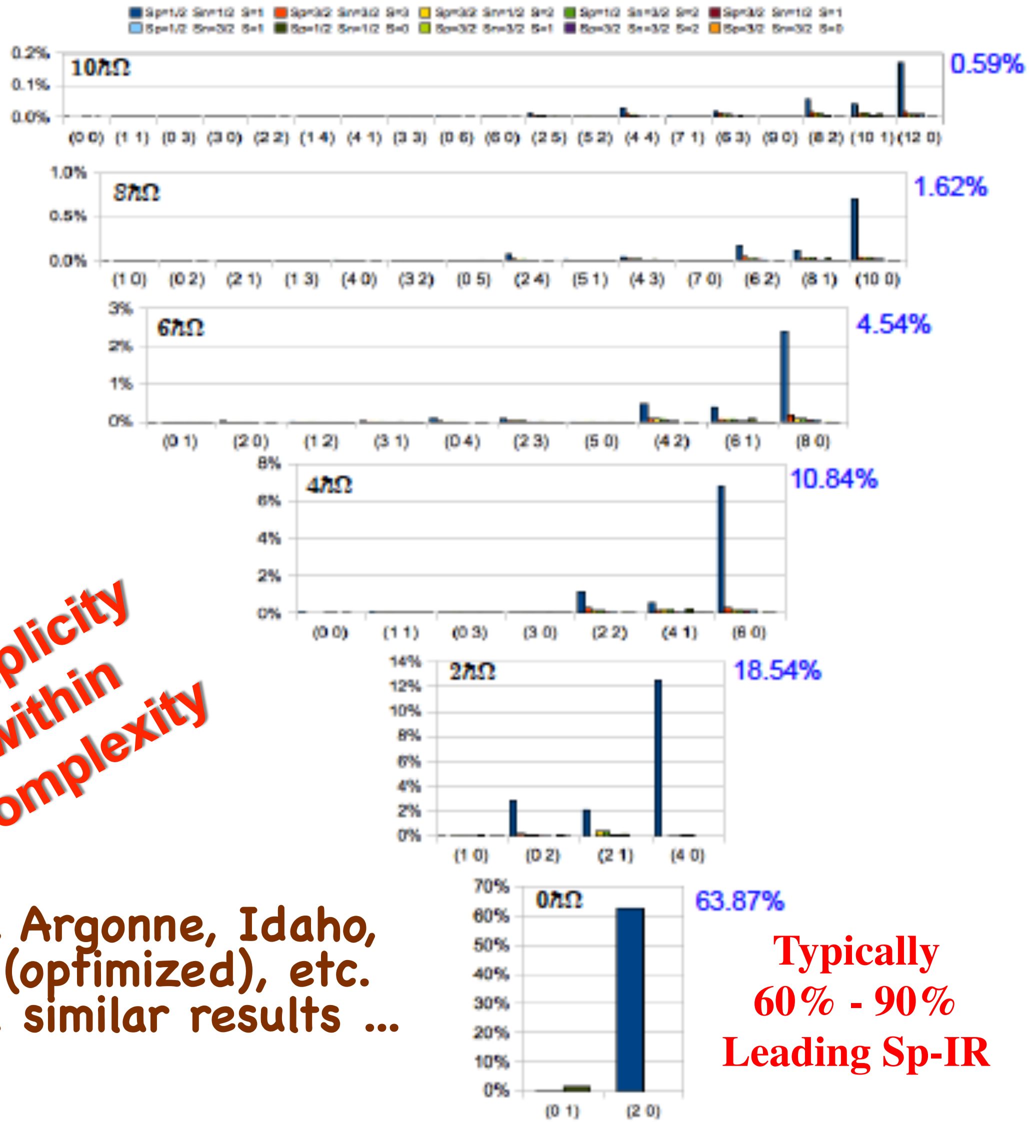
Sp-NCSM — Sp(3,R)

SA-NCSM — SU(3)

....

*21st Century
– *Ab Initio* –
Nuclear Physics

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



Simplicity within Complexity

*Bonn, Argonne, Idaho, N3LO (optimized), etc. … yield similar results …

… Proof of Principle …

\> 99% of Physics
In < 1% of the
"reorganized" space

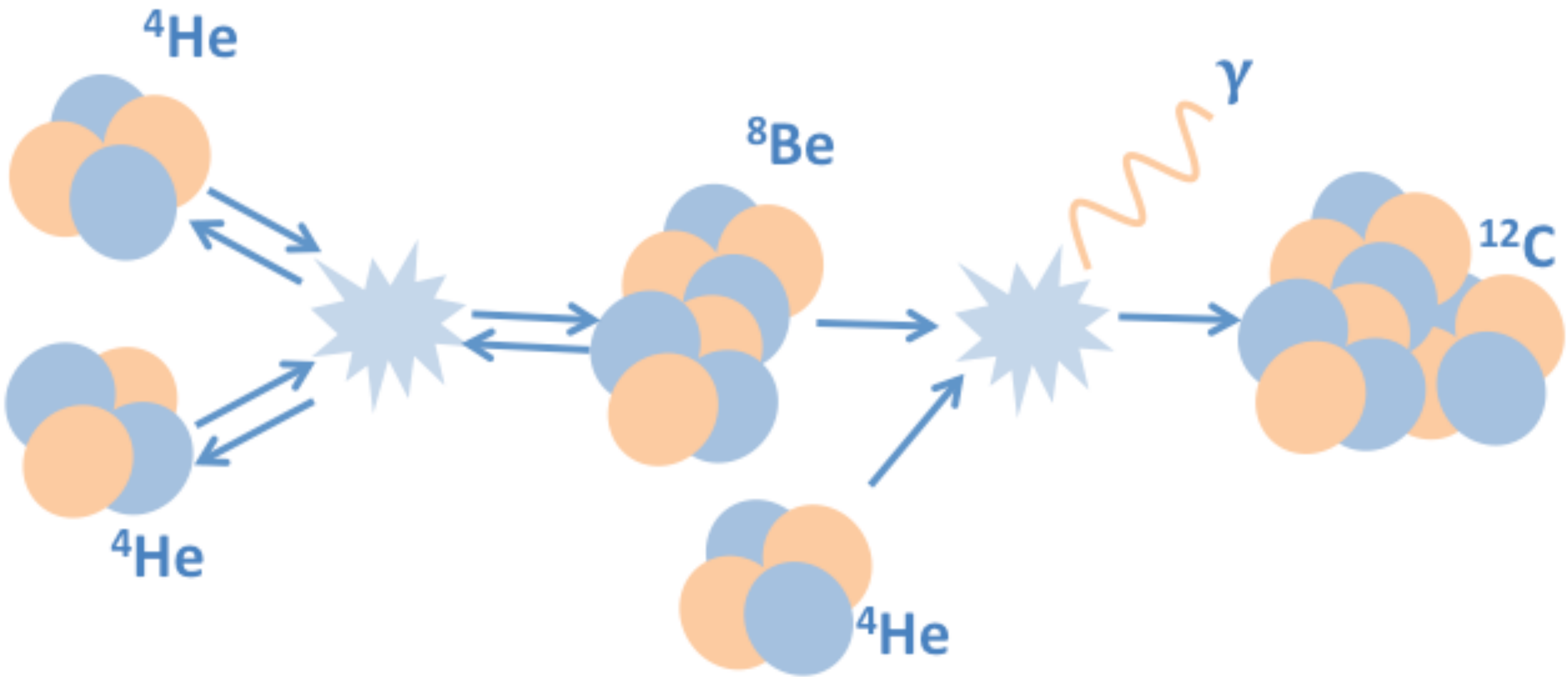
JISP16* bare interaction in Nmax = 10 space with $\hbar\Omega$ = 20 MeV

… Team Work …

Many "helps" along the way … e.g., James Vary making his NCSM available to us, Mark Caprio (ND) visiting LSU on a sabbatical, along with quality input from Anna Hayes of LANL, various 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!

Pushing NC-Shell / Cluster Connection

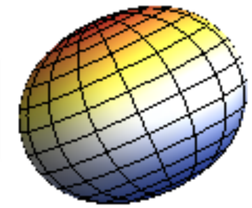
Creation of ^{12}C in hot stars



... The elusive Hoyle state ...

Three Slice Scenario (legacy / modern)

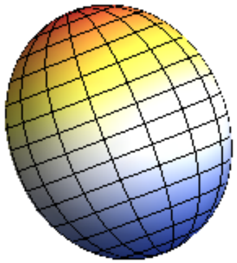
^{12}C



0*p*-0*h*

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

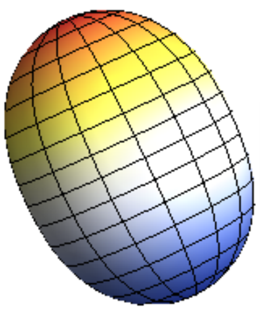
Main contribution
to ground state
rotational band
($0_{g.s.}^{+}$, 2_1^{+}, 4_1^{+})



2*p*-2*h*

(6 2) *Bandhead*
(*Triaxial*)

Main contribution
to the 0_3^{+}



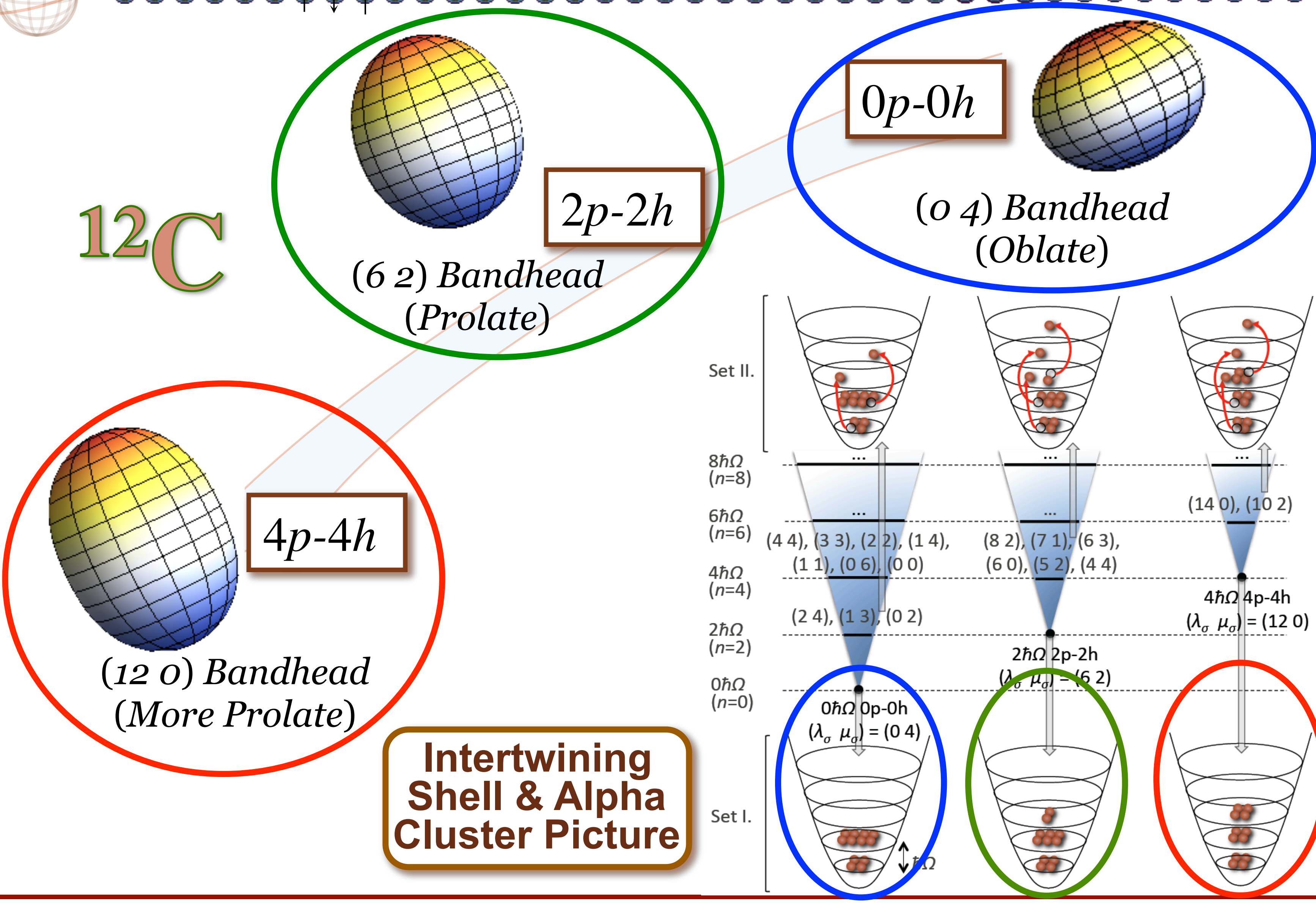
4*p*-4*h*

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

Main contribution
to Hoyle state (0_2^{+})

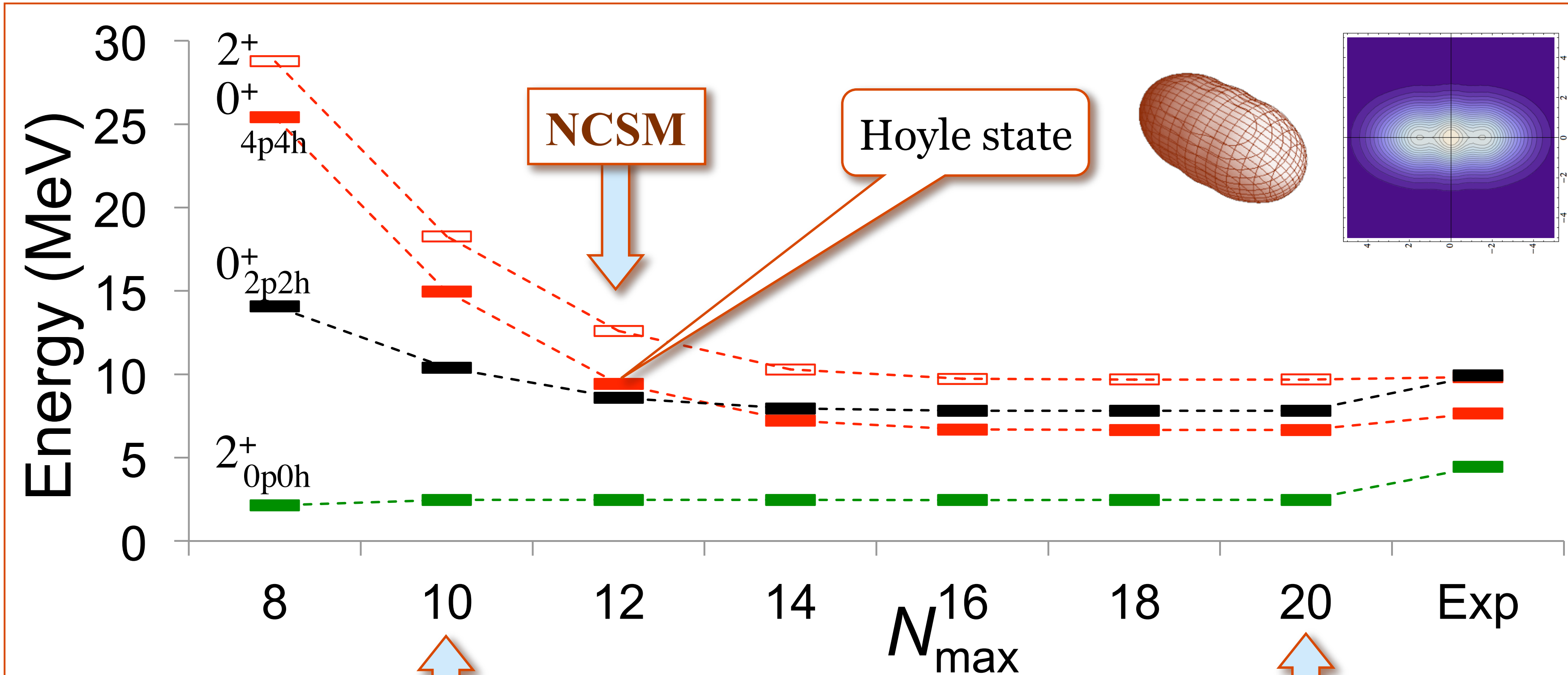
'Back to the Future'
– *déjà vu* –
Engeland & Ellis '67s

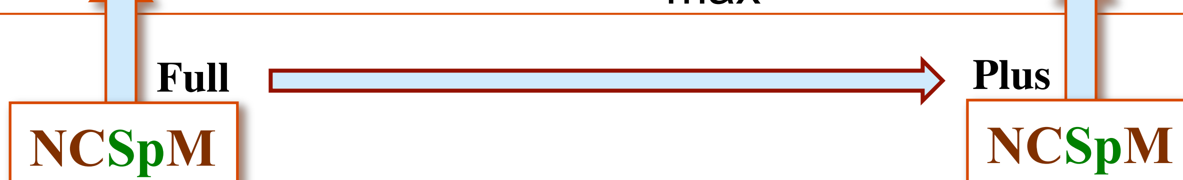
Choose Three Slices (NCSpM View)



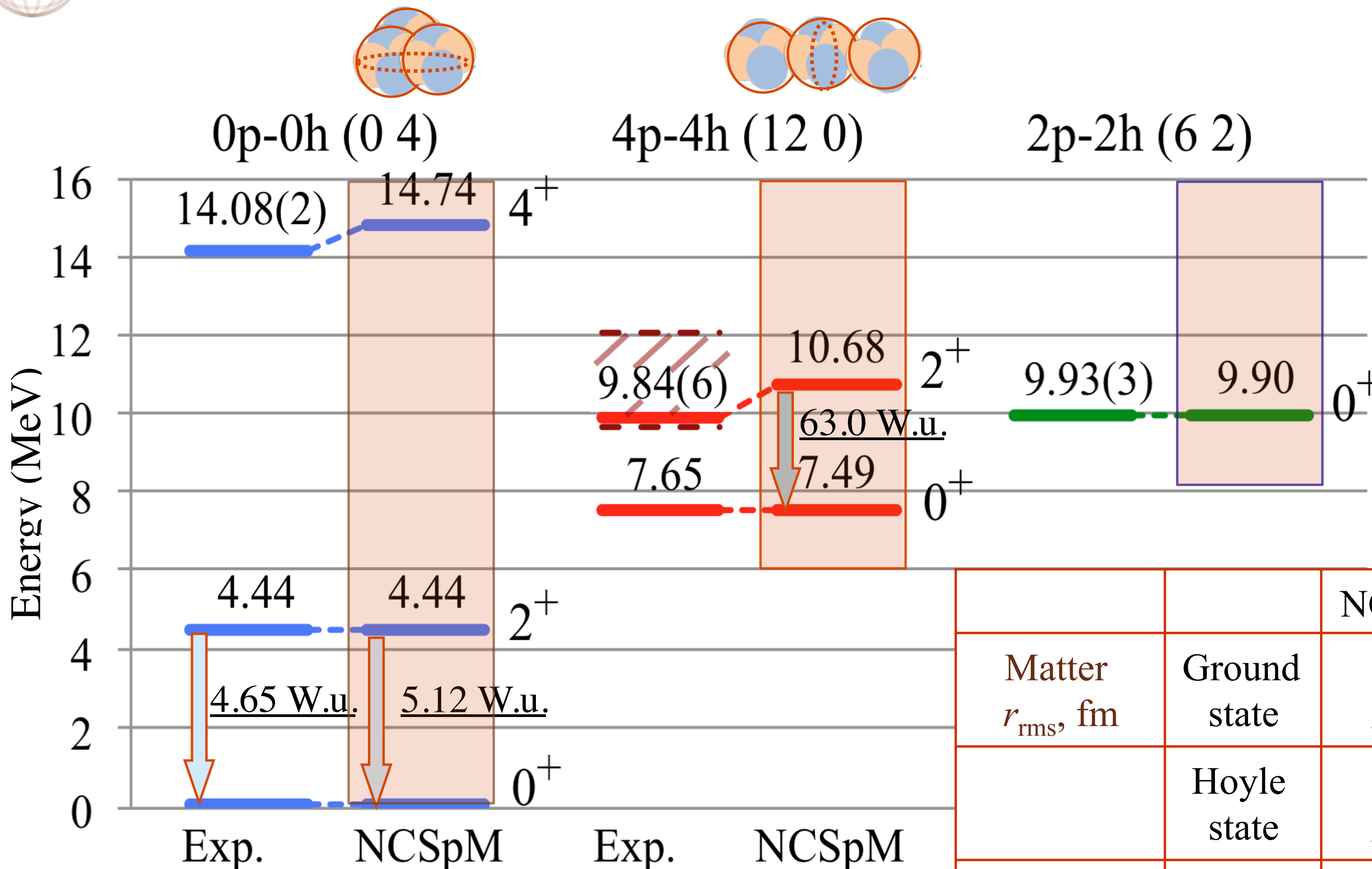
Intertwining Shell & Alpha Cluster Picture

^{12}C: Systematics (Function of N_{max})





^{12}C Observables – Negative Parity



1p-1h (3 3)

"No B(E3)"
... Yet ...

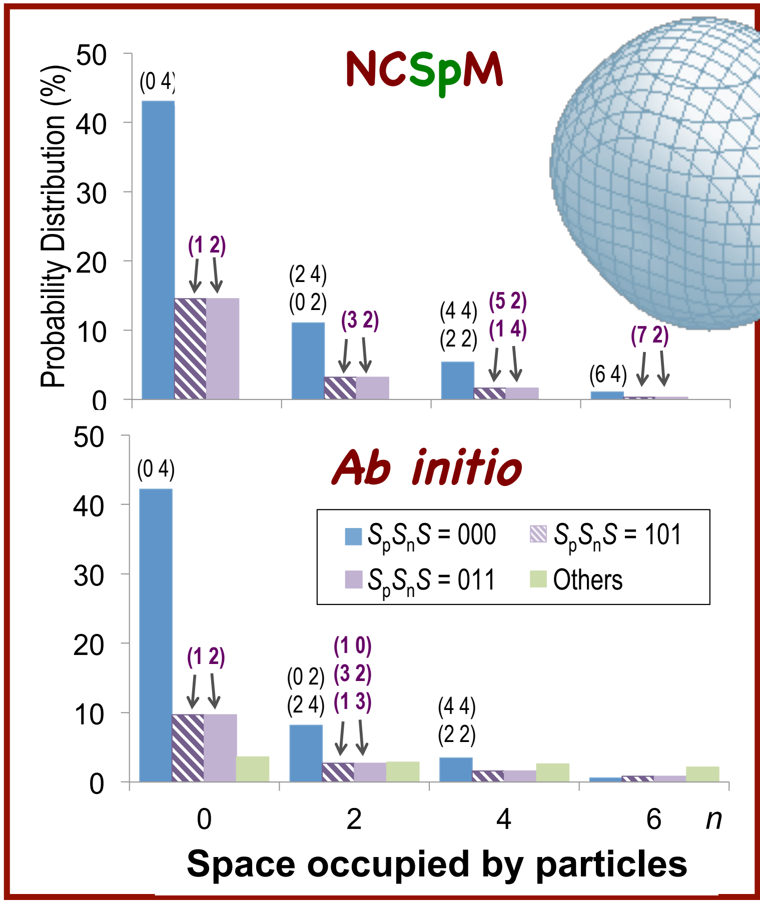
~9.60 **3⁻**

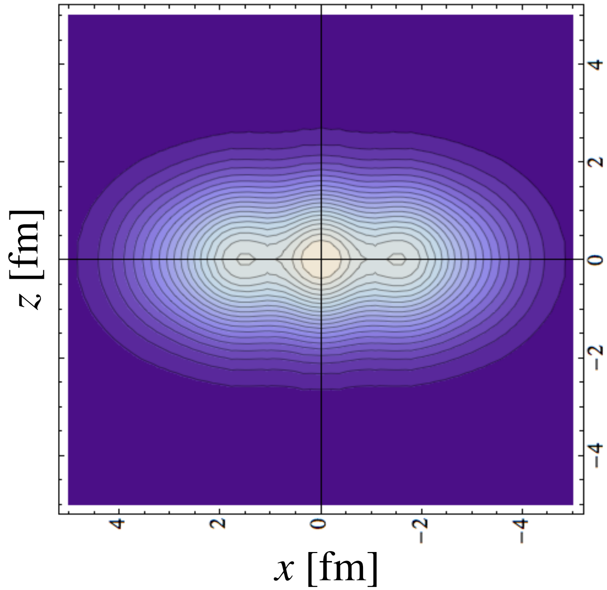
		NCSpM	Exp
Matter r_{rms}, fm	Ground state	2.44	2.43(2)
	Hoyle state	2.93	N/A
Q, e fm^2	2_1^+	+6.62	+6(3)
	2_2^+	–20.61	N/A

Formation of Clusters!

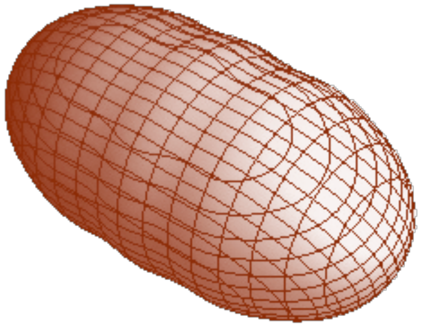
Ground state

Agrees with first-principle results in smaller spaces

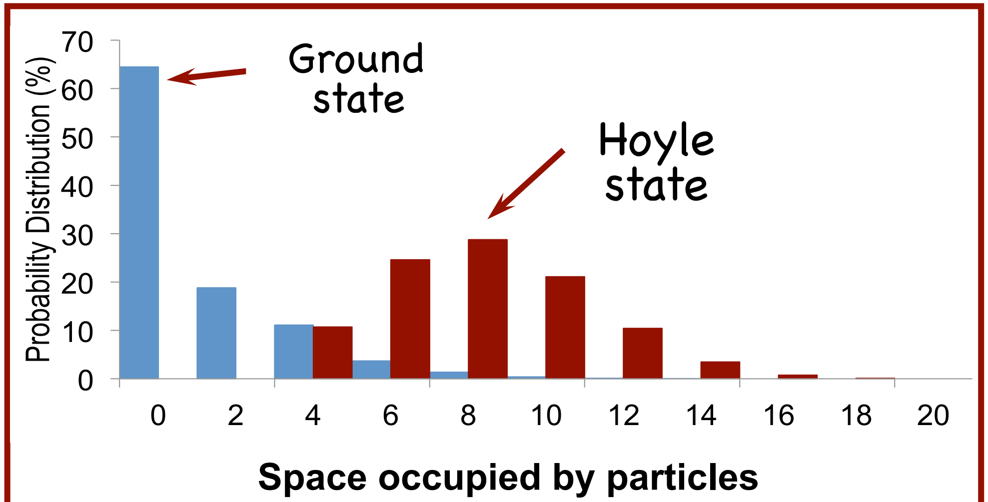




Hoyle state

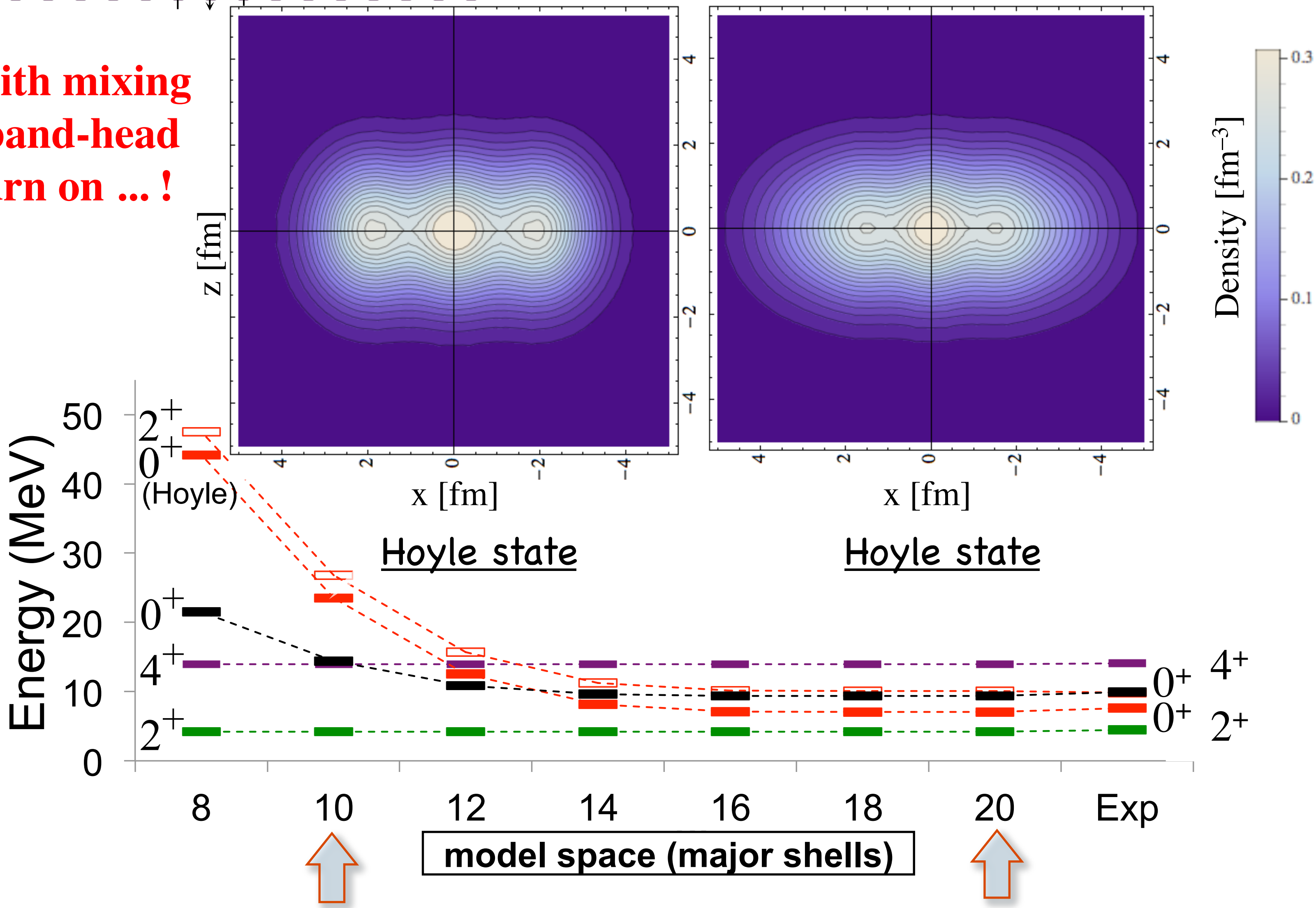


Needs at least 18–20 shells



Formation of Clusters!

*Now with mixing at the band-head level turn on ... !



Standard ab initio NCSM

*(NCSpM & Band Mixing)

Review Article – PPNP 89 (2016) 101-136

Progress in Particle and Nuclear Physics 89 (2016) 101–136

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Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

ELSEVIER

Review

Symmetry-guided large-scale shell-model theory

CrossMark

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Clusters
Hoyle state
Orderly patterns in nuclei from first principles

ABSTRACT

In this review, we present a symmetry-guided strategy that utilizes exact as well as partial symmetries for enabling a deeper understanding of and advancing *ab initio* studies for determining the microscopic structure of atomic nuclei. These symmetries expose physically relevant degrees of freedom that, for large-scale calculations with QCD-inspired interactions, allow the model space size to be reduced through a very structured selection of the basis states to physically relevant subspaces. This can guide explorations of simple patterns in nuclei and how they emerge from first principles, as well as extensions of the theory beyond current limitations toward heavier nuclei and larger model spaces. This is illustrated for the *ab initio* symmetry-adapted no-core shell model (SA-NCSM) and two significant underlying symmetries, the symplectic Sp(3, ℝ) group and its deformation-related SU(3) subgroup. We review the broad scope of nuclei, where these symmetries have been found to play a key role—from the light *p*-shell systems, such as ^{6}Li, ^{8}B, ^{8}Be, ^{12}C, and ^{16}O, and *sd*-shell nuclei exemplified by ^{20}Ne, based on first-principle explorations; through the Hoyle state in ^{12}C and enhanced collectivity in intermediate-mass nuclei, within a no-core shell-model perspective; up to strongly deformed species of the rare-earth and actinide regions, as investigated in earlier studies. A complementary picture, driven by symmetries dual to Sp(3, ℝ), is also discussed. We briefly review symmetry-guided techniques that prove useful in various nuclear-theory models, such as Elliott model, *ab initio* SA-NCSM, symplectic model, pseudo-SU(3) and pseudo-symplectic models, *ab initio* hyperspherical harmonics method, *ab initio* lattice effective field theory, exact pairing-plus-shell model approaches, and cluster models, including the resonating-group method. Important implications of these approaches that have deepened our understanding of emergent phenomena in nuclei, such as enhanced collectivity, giant resonances, pairing, halo, and clustering, are discussed, with a focus on emergent patterns in the framework of the *ab initio* SA-NCSM with no *a priori* assumptions.

… Also …

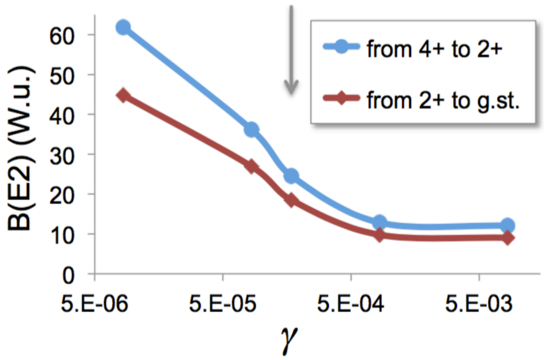
– Kristina Launey –
"State of the Art in Nuclear Cluster Physics"
(**SOTANCP3**)
Yokohama, Japan
May 26-30, 2014

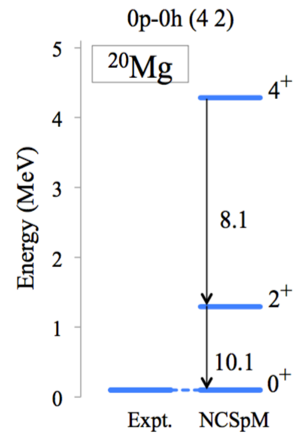
&

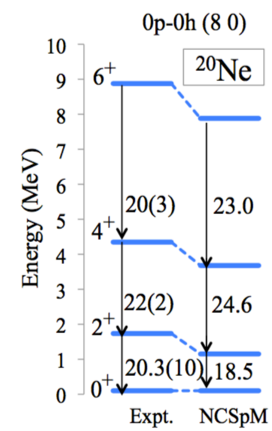
– Kristina Launey –
"State of the Art in Nuclear Cluster Physics"
(**SOTANCP4**)
Galveston, Texas, USA
May 13-18, 2018

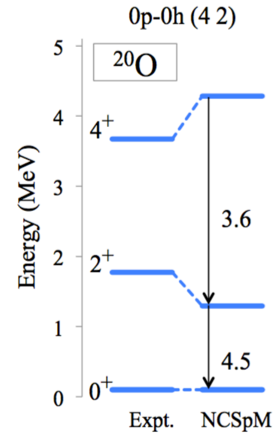
Medium Mass Nuclei (Gregory Tobin / REU)

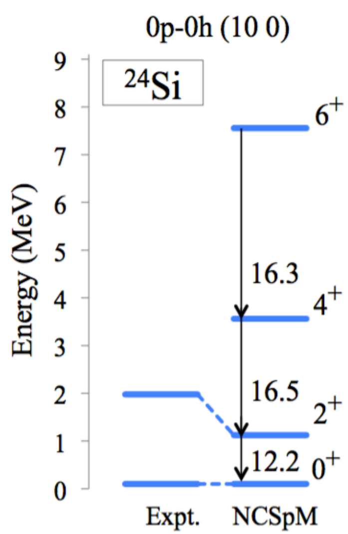
Ne-20: grey arrow is gamma used

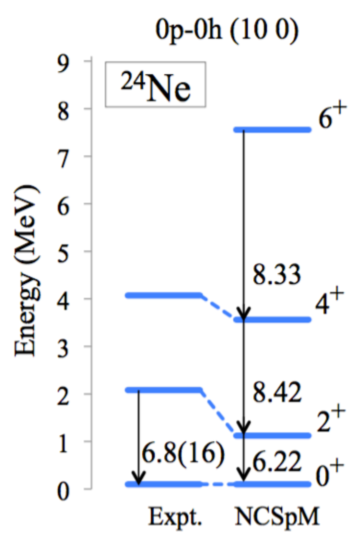


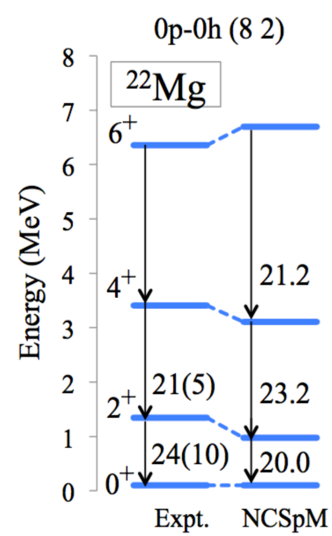


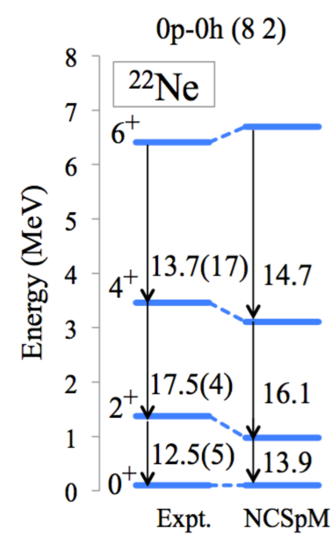








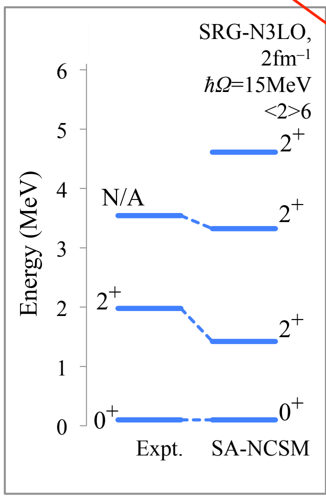




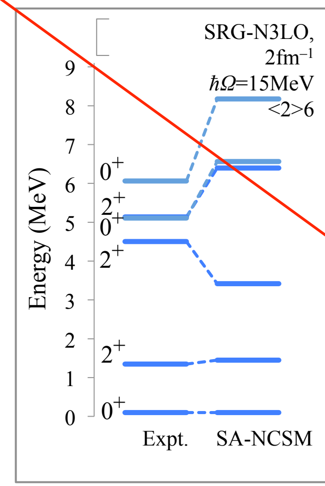
Further sd-shell Results (Robert Baker / GS)

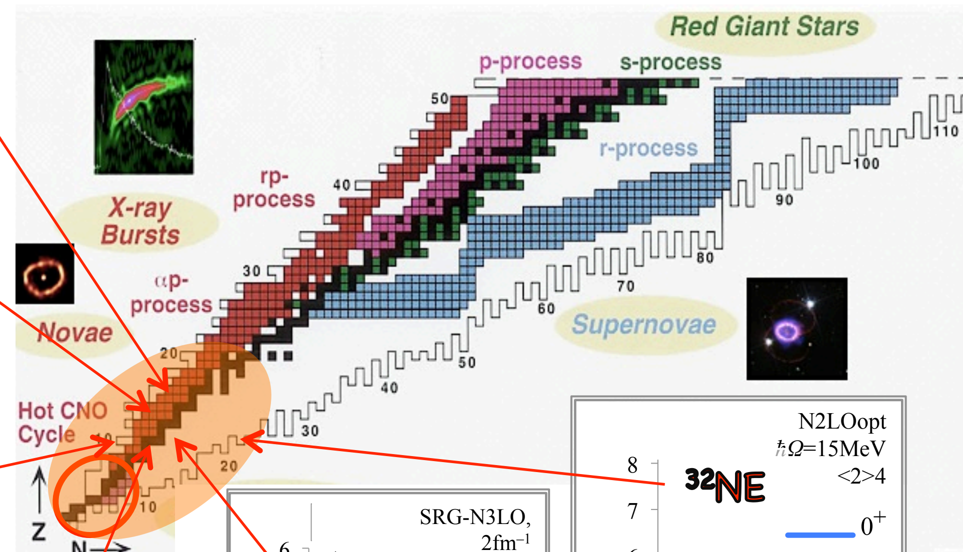
**Selected (pre-thesis) Examples
(Now onto Beta Decay)**

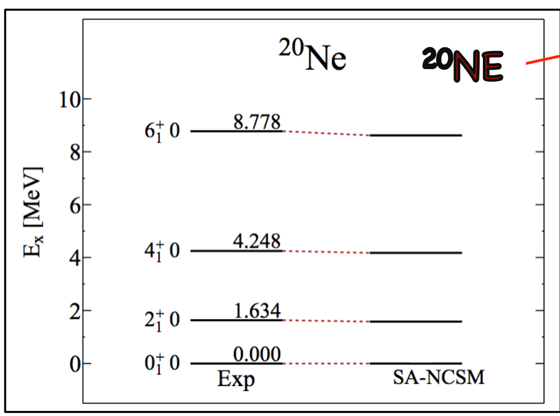
^{24}SI

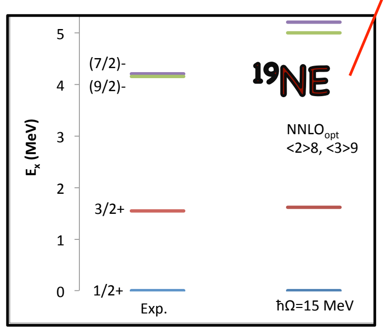


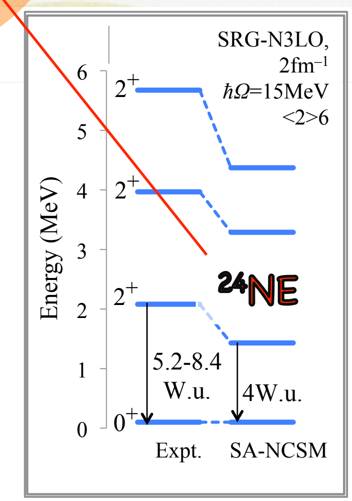
^{22}MG

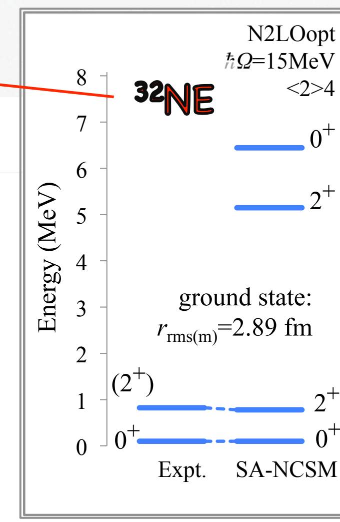






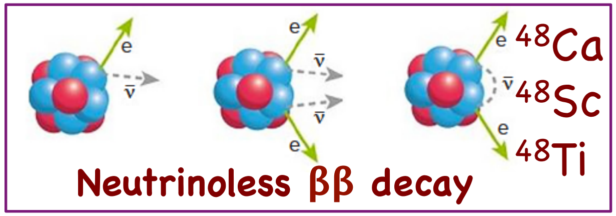






Ab initio description (converged selected spaces) (NNLO$_{opt}$, ħΩ=15 MeV, 13 HO shells)

Plus fp-shell Results (Grigor Sargsyan / GS)



^{48}Ca

8 shells, N2LOopt

0^+

SA-NCSM (selected): 966,152

Complete model space: 3,162,511,819

2^+

SA-NCSM (selected): 3,055,554

Complete model space: ... 14,522,234,982

^{48}Ti

8 shells, N2LOopt

0^+

SA-NCSM (selected): 602,493

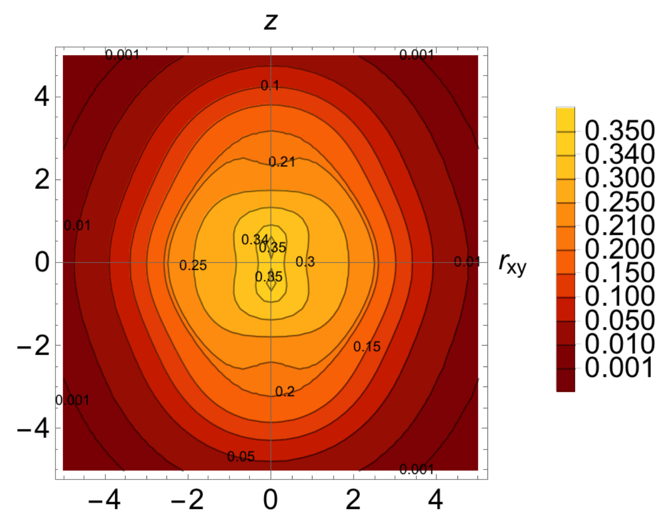
Complete model space: 24,694,678,414

2^+

SA-NCSM (selected): 1,178,834

Complete model space: 113,920,316,658

^{48}Ti, $Q(2^+)$ [e fm^2]	
Experiment	−17.7
8 shells	−19.3
(no effective charges)	



Reaction Theory (Alexis Mercenne / PDoc)

Nucleosynthesis: Type I X-Ray Burst

TABLE 2
REACTIONS THAT IMPACT THE BURST LIGHT CURVE
IN THE MULTI ZONE X-RAY BURST MODEL.

Rank	Reaction	Type[a]	Sensitivity[b]	Category
1	^{15}O$(\alpha,\gamma)^{19}$Ne	D	16	1
2	^{56}Ni$(\alpha,$p$)^{59}$Cu	U	6.4	1
3	^{59}Cu(p,$\gamma)^{60}$Zn	D	5.1	1
4	^{61}Ga(p,$\gamma)^{62}$Ge	D	3.7	1
5	^{22}Mg$(\alpha,$p$)^{25}$Al	D	2.3	1
6	^{14}O$(\alpha,$p$)^{17}$F	D	5.8	1
7	^{23}Al(p,$\gamma)^{24}$Si	D	4.6	1
8	^{18}Ne$(\alpha,$p$)^{21}$Na	U	1.8	1
9	^{63}Ga(p,$\gamma)^{64}$Ge	D	1.4	2
10	^{19}F(p,$\alpha)^{16}$O	U	1.3	2
11	^{12}C$(\alpha,\gamma)^{16}$O	U	2.1	2
12	^{26}Si$(\alpha,$p$)^{29}$P	U	1.8	2
13	^{17}F$(\alpha,$p$)^{20}$Ne	U	3.5	2
14	^{24}Mg$(\alpha,\gamma)^{28}$Si	U	1.2	2
15	^{57}Cu(p,$\gamma)^{58}$Zn	D	1.3	2
16	^{60}Zn$(\alpha,$p$)^{63}$Ga	U	1.1	2
17	^{17}F(p,$\gamma)^{18}$Ne	U	1.7	2
18	^{40}Sc(p,$\gamma)^{41}$Ti	D	1.1	2
19	^{48}Cr(p,$\gamma)^{49}$Mn	D	1.2	2

[a] Up (U) or down (D) variation that has the largest impact
[b] $M_{LC}^{(i)}$ in units of 10^{38}ergs/s

Simulations for XRB are sensitive to certain reaction rates

- ^{23}Al(p,γ)^{24}Si
- improve rate precision to improve simulations

Ab initio wave functions $|\Psi\rangle$ → Widths Phase Shifts → Cross sections Reaction rates

↓

Reaction network simulation

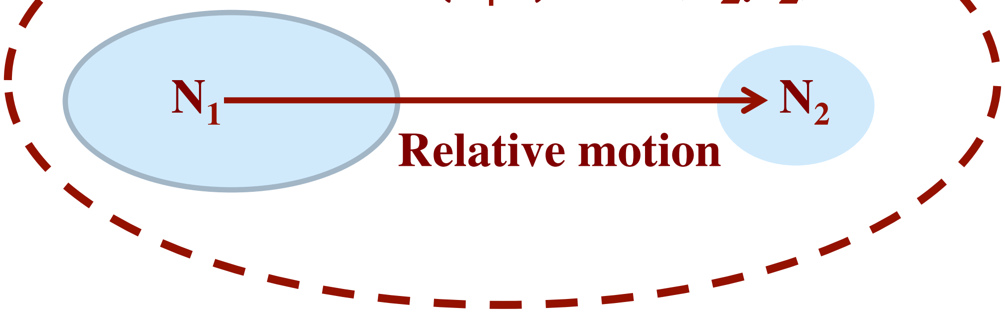
↓

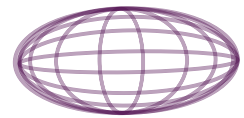
Abundances

Scattering Theory (Alexis Mercenne / PDoc)

SA-NCSM + RGM

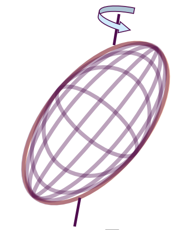
$[(\lambda_1\mu_1) \times (\lambda_r 0) \times (\lambda_2\mu_2)] \rightarrow (\lambda,\mu)$





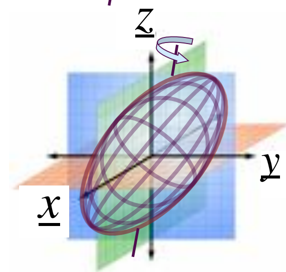
Deformation

L



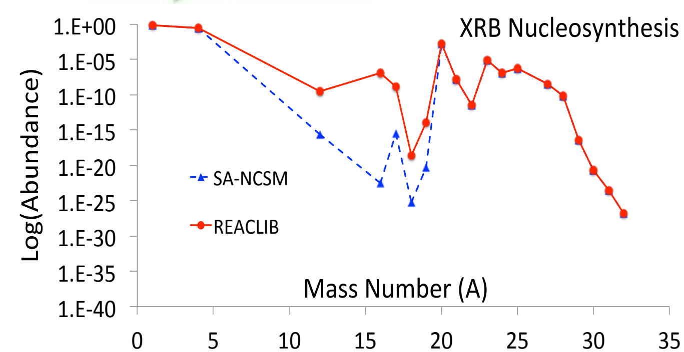
Rotations

M

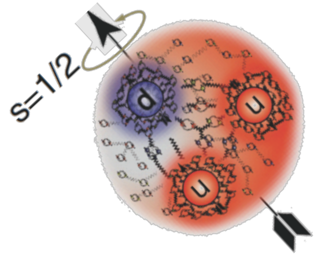


Spatial Orientation

- Deformation is the only relevant information
- All calculations prior to R-matrix use the SA basis/deformation, that is the SU(3) symmetry and corresponding Wigner-Eckart theorem:
  - Norm and Hamiltonian Kernel
  - CM treatment
  - Inversion of the Norm Kernel
- Dependence on orbital momentum (and partial waves) needed to compute cross section, which is introduced at the last step



Future Considerations



Jefferson Lab 12GeV Era

- Excited States of the Nucleon
- Electric Charge vs Magnetic Distribution
- Total Spin -> Angular Momentum plus Quark Spin

"Femtography of Nucleon"

"Normal Concept" versus "Pseudo Concept"

$$\bar{L} + \bar{S} = \bar{J} = \tilde{L} + \tilde{S}$$

"Collusion within & among Nucleons"

2^{nd} Decade (& Beyond) of 21^{st} 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 studying 3 & 4-particle correlations …)

- Push forward on the Sp-NCSM – Hybrid model $N^{plus}[N_{full}]$ (… including band-head symplectic symmetry mixing…)

- Continue SA-NCSM development & applications − laptop version (^{6}Li, ^{X}C, ^{X}O, ^{X}Ne, ^{X}Mg … odd-A, and greater A…)

Next Up ... Deformed Versions ... DSp-NCSM & DSA-NCSM

... Future is Golden ...

The End
&
A New Beginning

"Back to the Future"

... Déjà-vu ...

[Armed with many more tools; especially, simple symmetries and special (unique) collaborations!]