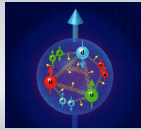
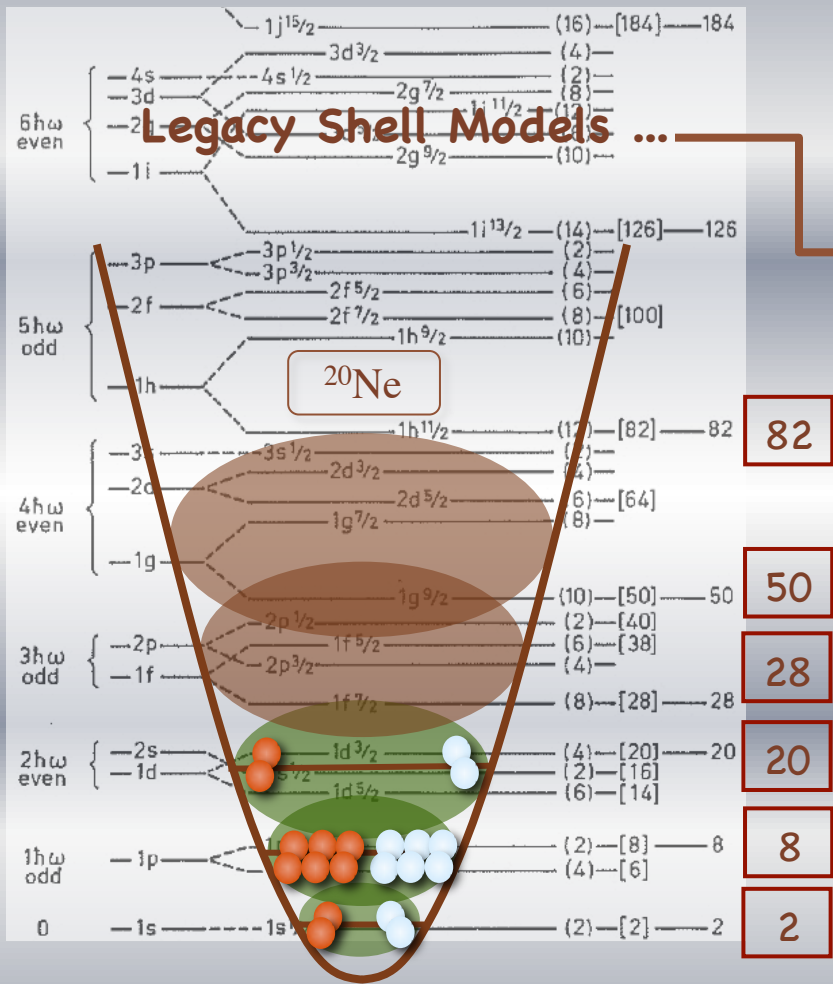
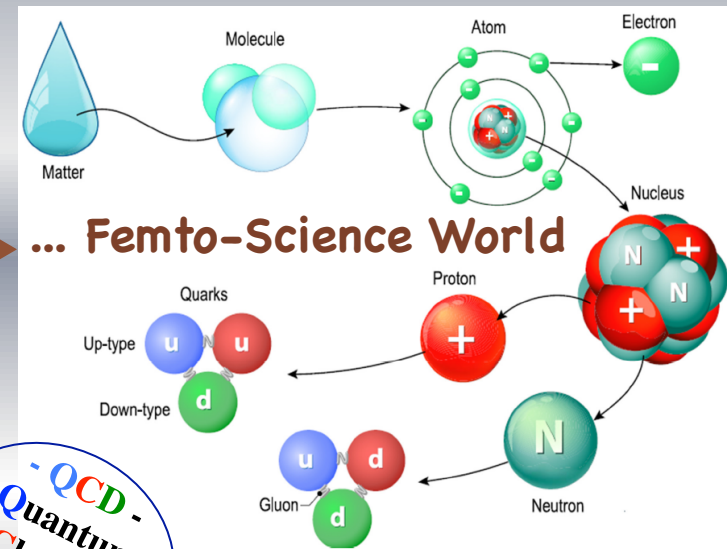


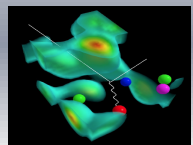
Paving the way to understanding Nuclear Structure from Strong QCD



21st Century Cross Over



**-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 LSM, HPC & QCD meet!

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

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

Shell Model

No-Core

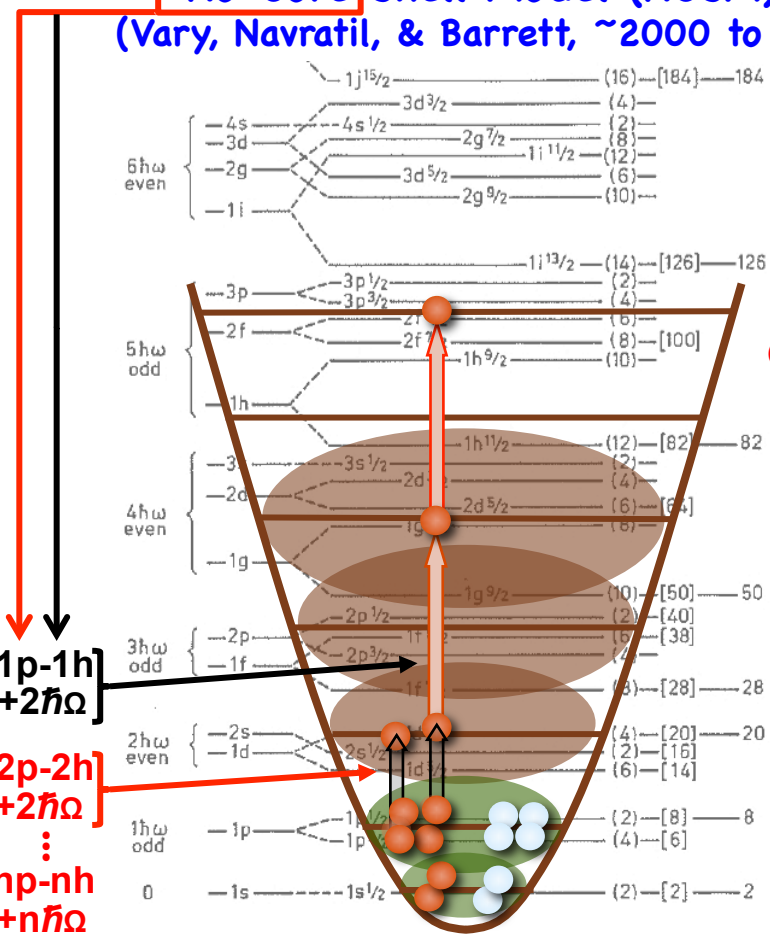
Collective Model

No-Core Shell Model (NCSM)*

(Vary, Navratil, & Barrett, ~2000 to present)

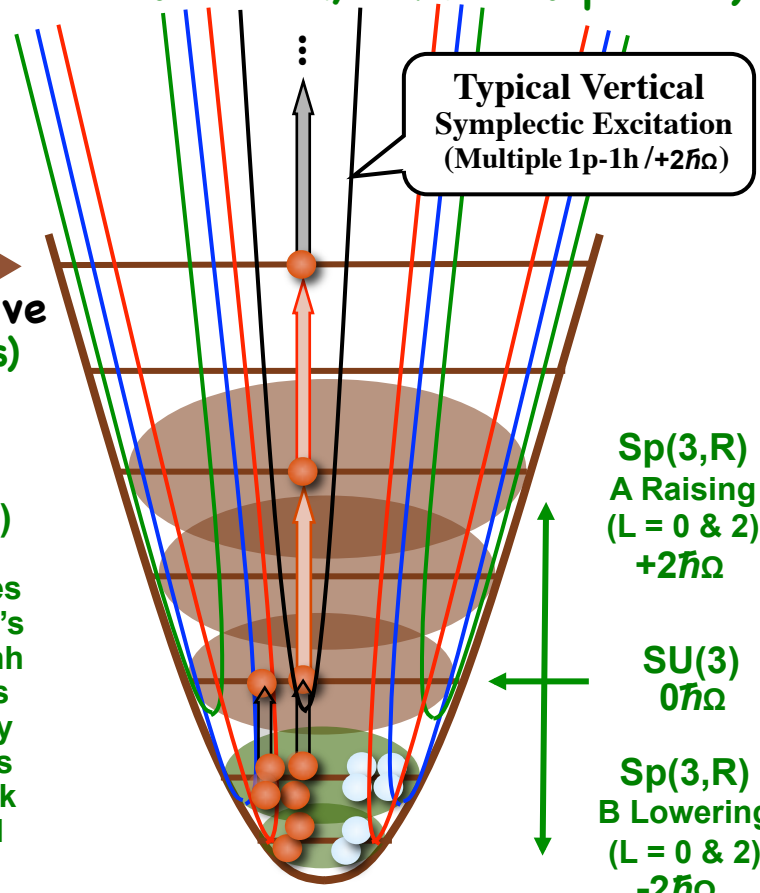
Symplectic Shell Model (Sp-NCSM)*

(Rowe & Rosensteel, ~1980s to present)



Reorganize Shell-Model Space
Cluster & Collective (Natural Subspaces)

- Symmetry Adapted Basis (Special Features)
- Canonical & unitary
 - Organized by shapes
 - Quadratic in x's & p's
 - Band-heads → np-nh
 - Spurious free bands
 - Captures collectivity
 - No effective charges
 - Algebraic framework
 - Deformation natural
 - Field theory linkage

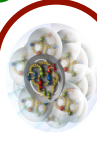


Typical Vertical Symplectic Excitation (Multiple 1p-1h / +2ħΩ)

- Sp(3,R) A Raising (L = 0 & 2) +2ħΩ
- SU(3) 0ħΩ
- Sp(3,R) B Lowering (L = 0 & 2) -2ħΩ

*Realistic interaction (local or not; NN, NNN, ...)
• In principle, exact solutions, up to N_{max} cutoff
• Successful descriptions to date through ^{16}O

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



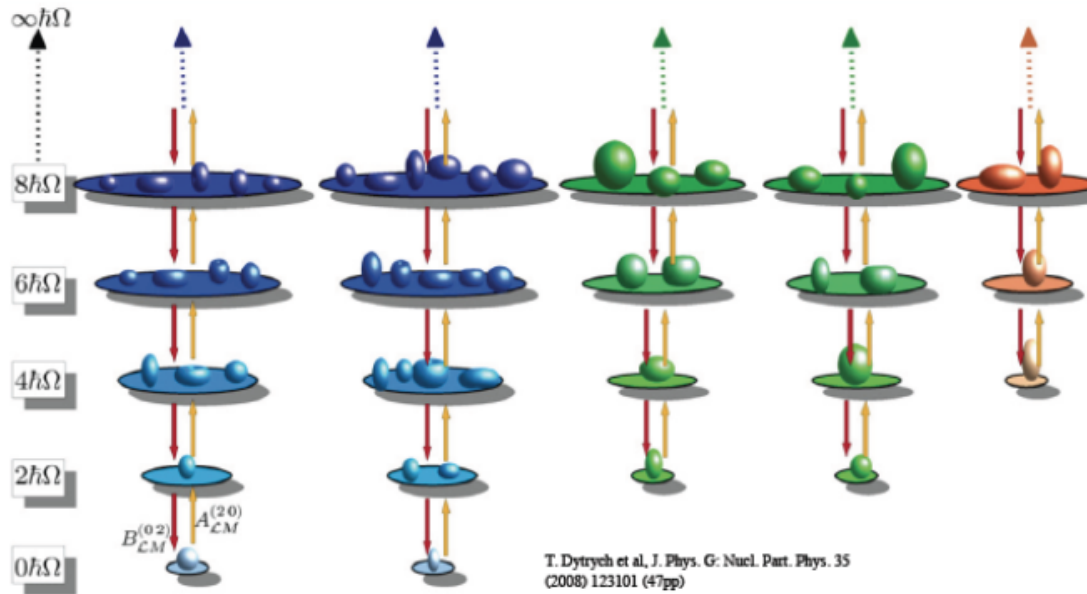
Symplectic Symmetry / Algebra

Realized by 21 generators of the $Sp(3,R)$ symplectic algebra - all distinct quadratic forms in coordinates (q_i) and momenta (p_i)



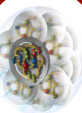
$$Q_{ij} = \sum_n^A q_{in}q_{jn} \quad K_{ij} = \sum_n^A p_{in}p_{jn} \quad L_{ij} = \sum_n^A (q_{in}p_{jn} - q_{jn}p_{in}) \quad S_{ij} = \sum_n^A (q_{in}p_{jn} + p_{in}q_{jn})$$

Quadrupole Moment "Tensor" (6) **Kinetic Energy "Tensor" (6)** **Orbital Angular Operator (3)** **Deformation Flow "Circulation / Vorticity" (6)**

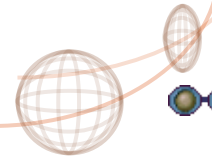


Every configuration is labeled by the $SU(3)$ (λ, μ) quantum numbers of the Elliott Model (1958), which in turn defines the shape of the so-called "band head" configuration.)

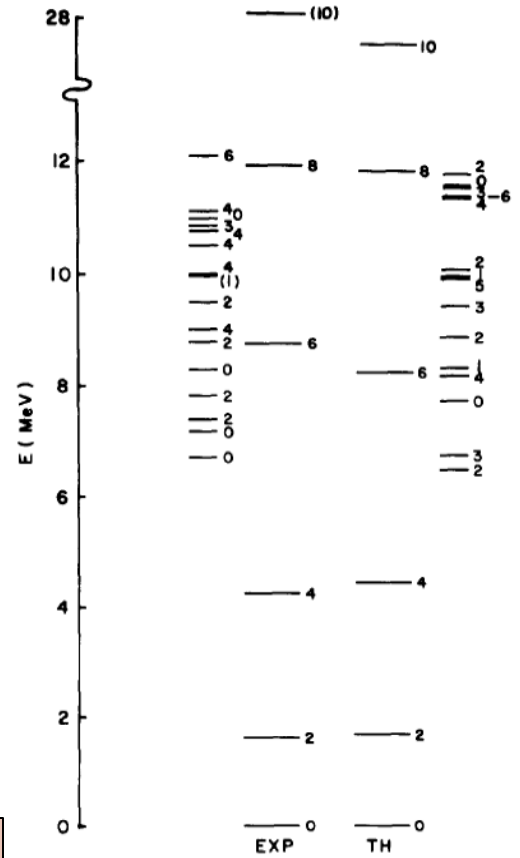
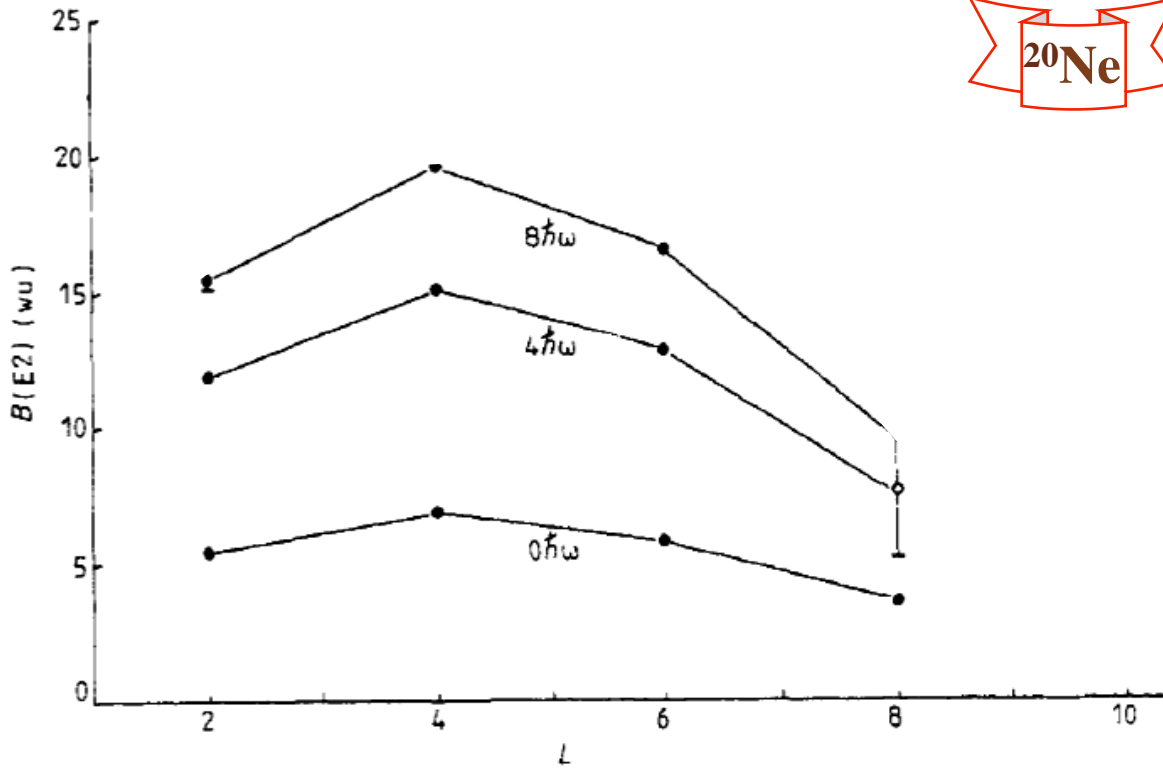
David Kekejian - Graduate Student (JPD#20) from Armenian



Simple (Early Shell Model) Picture



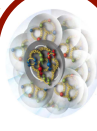
²⁰Ne



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

G. Rosensteel and D.J. Rowe - 1977

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



'Symmetry Adapted' NCSM Campaign

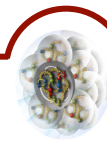
Timeline: 5 (2002-06) + 5 (2007-2011) + 5 (2012-16)

Goal -

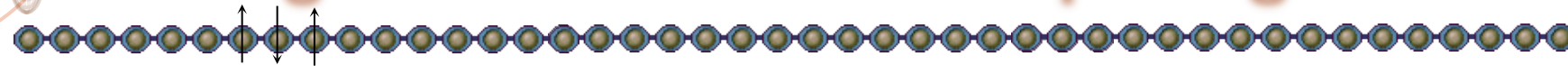
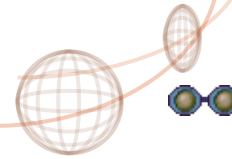
Reproduce and predict properties of heavy as well as light nuclei, starting with and building upon QCD/EFT informed and inspired interactions ...

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 (partial) 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 (ab initio) 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 Models

NCSM

Coupled Cluster Theory

Monte Carlo Methods

.....

NSF
Frontera } (TACC)
Stampede }
Blue Waters (NCSA)
... upgrades ...

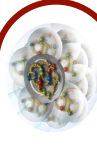
***21st Century**
- Ab Initio -
Nuclear Physics

HPC Era ...

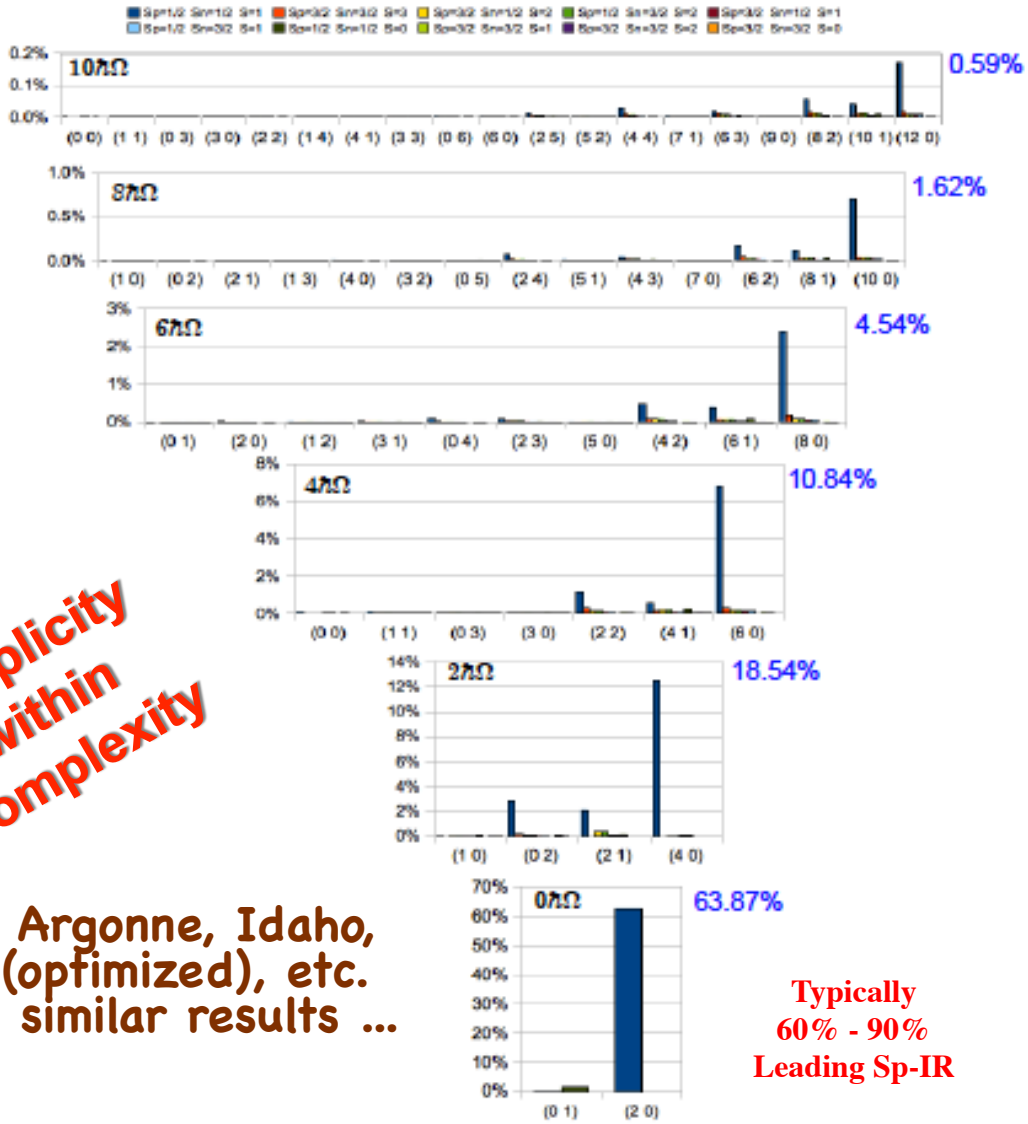
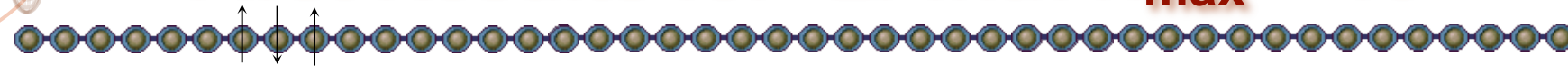
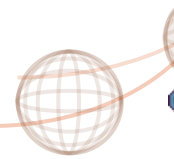
DOE
NERSC-X (Berkeley)
Summit (Oak Ridge)
Aurora (Argonne)
... upgrades ...

Collective Models

NCSM
Sp-NCSM Sp(3,R)
SA-NCSM SU(3)
.....



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



Simplicity within Complexity

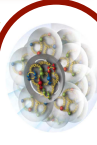
*Bonn, Argonne, Idaho, N3LO (optimized), etc. ... yield similar results ...

Typically 60% - 90% Leading Sp-IR

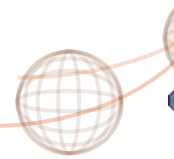
... Proof of Principle ...
 > 99% of Physics In < 1% of the "reorganized" space

JISP16* bare interaction in $N_{\text{max}} = 10$ space with $\hbar\Omega = 20$ MeV

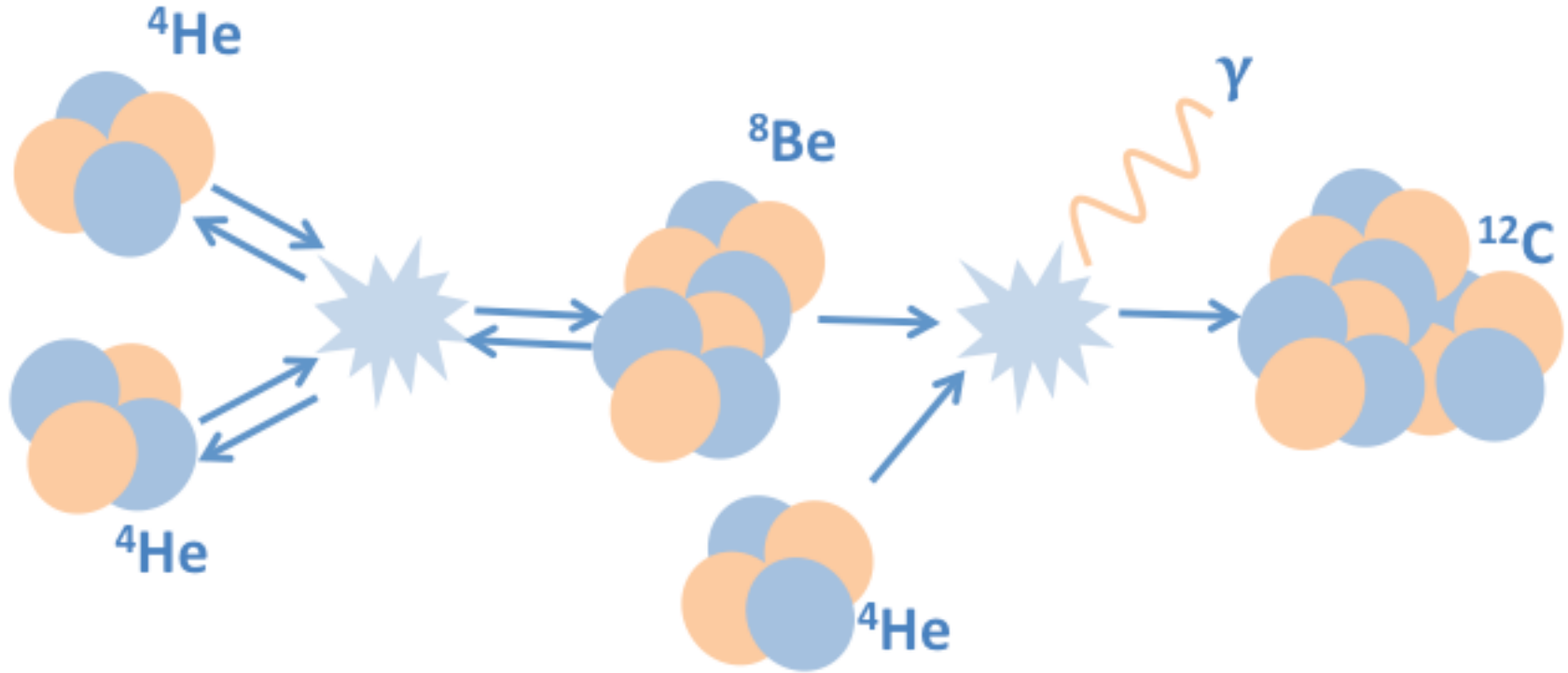
... Team Work ...
 Many "helps" along the way ... e.g., James Vary making his NCSM available to us, Mark Caprio (ND) visiting LSU on a sabbatical, along with quality input from Anna Hayes of LANL, various collaborators from Bulgaria, China, Mexico, and so on. Also to NSF for a PetaApps award, and DOE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



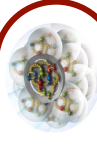
Pushing NC-Shell / Cluster Connection



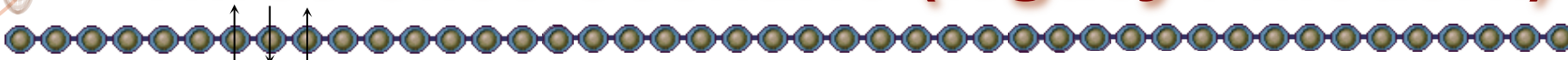
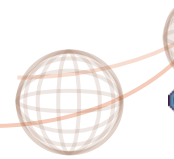
Creation of ^{12}C in hot stars



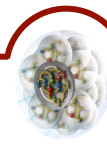
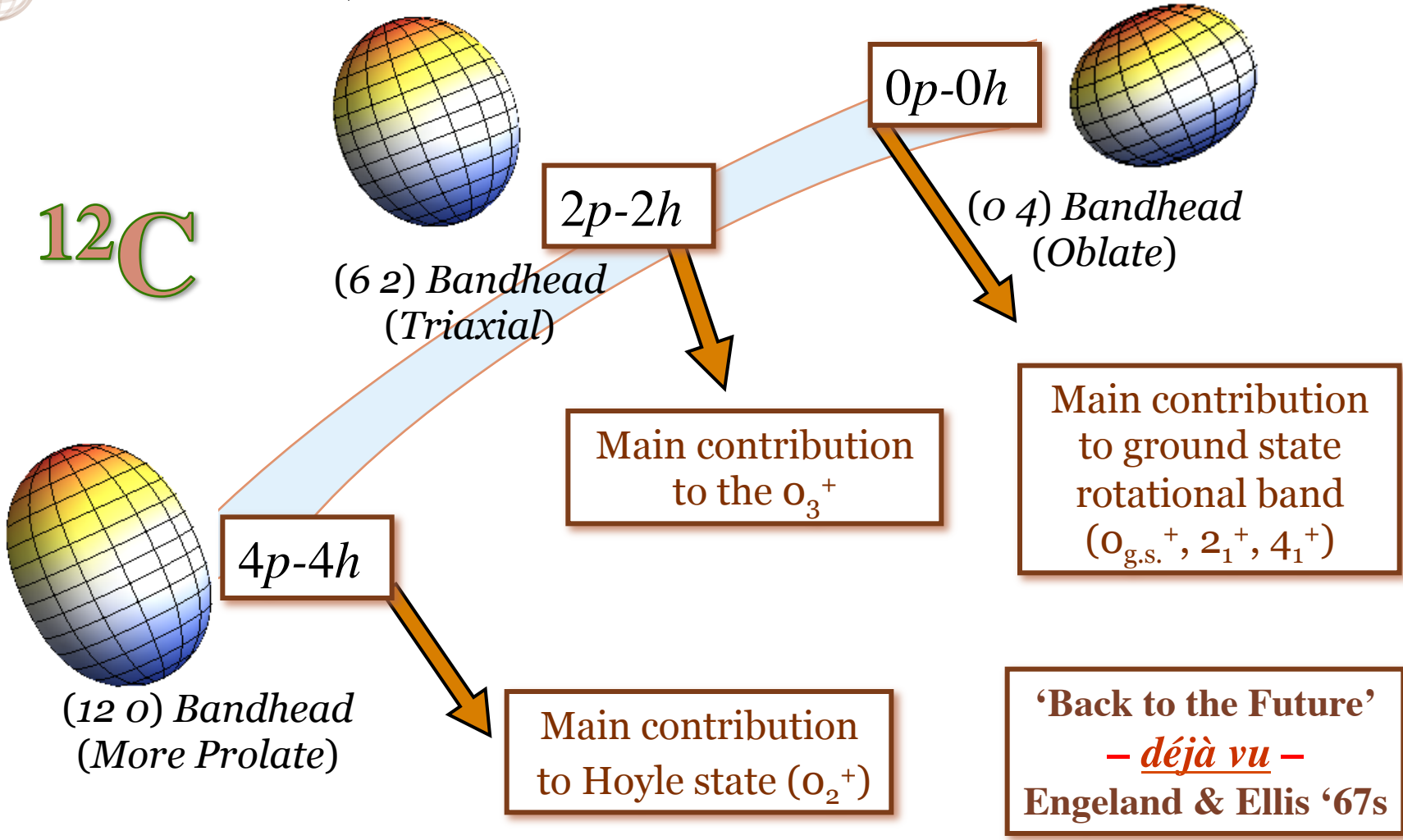
... The elusive Hoyle state ...



Three Slice Scenario (legacy / modern)

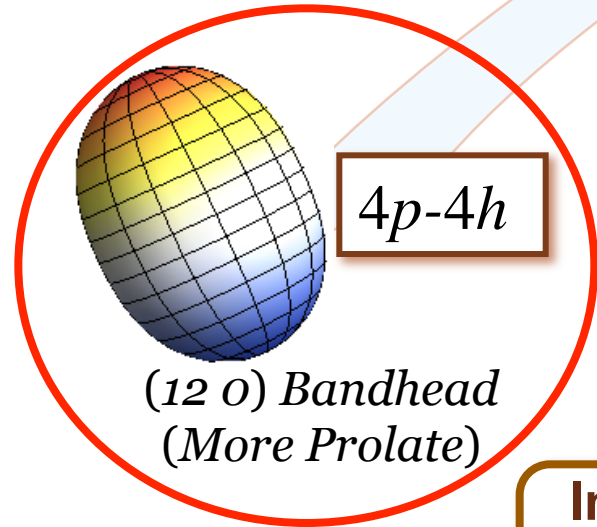
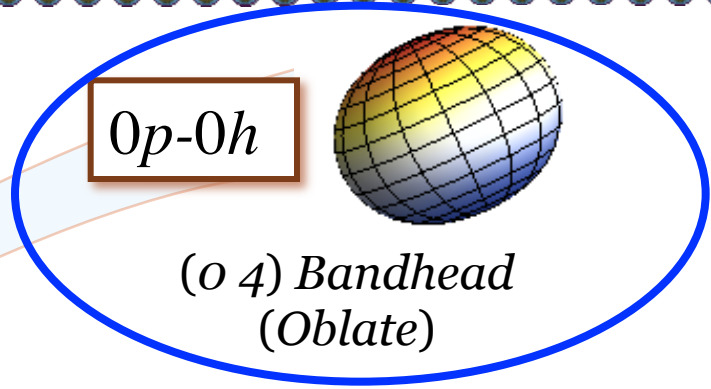
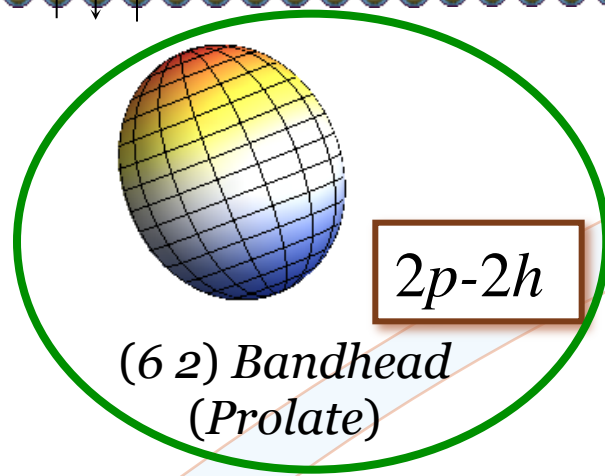


^{12}C

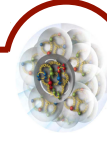
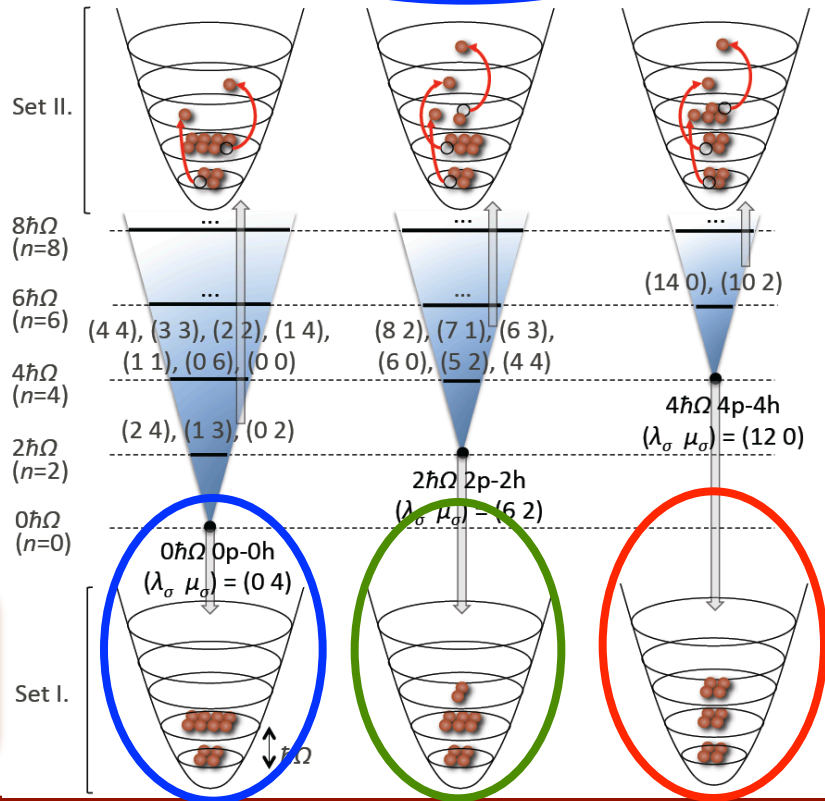


Choose Three Slices (NCSpM View)

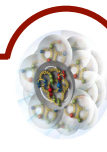
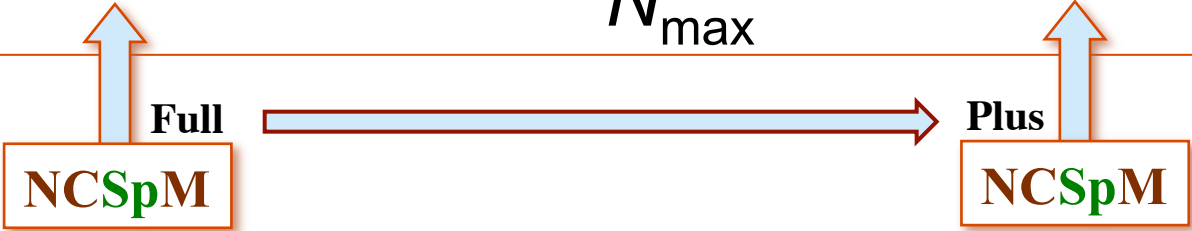
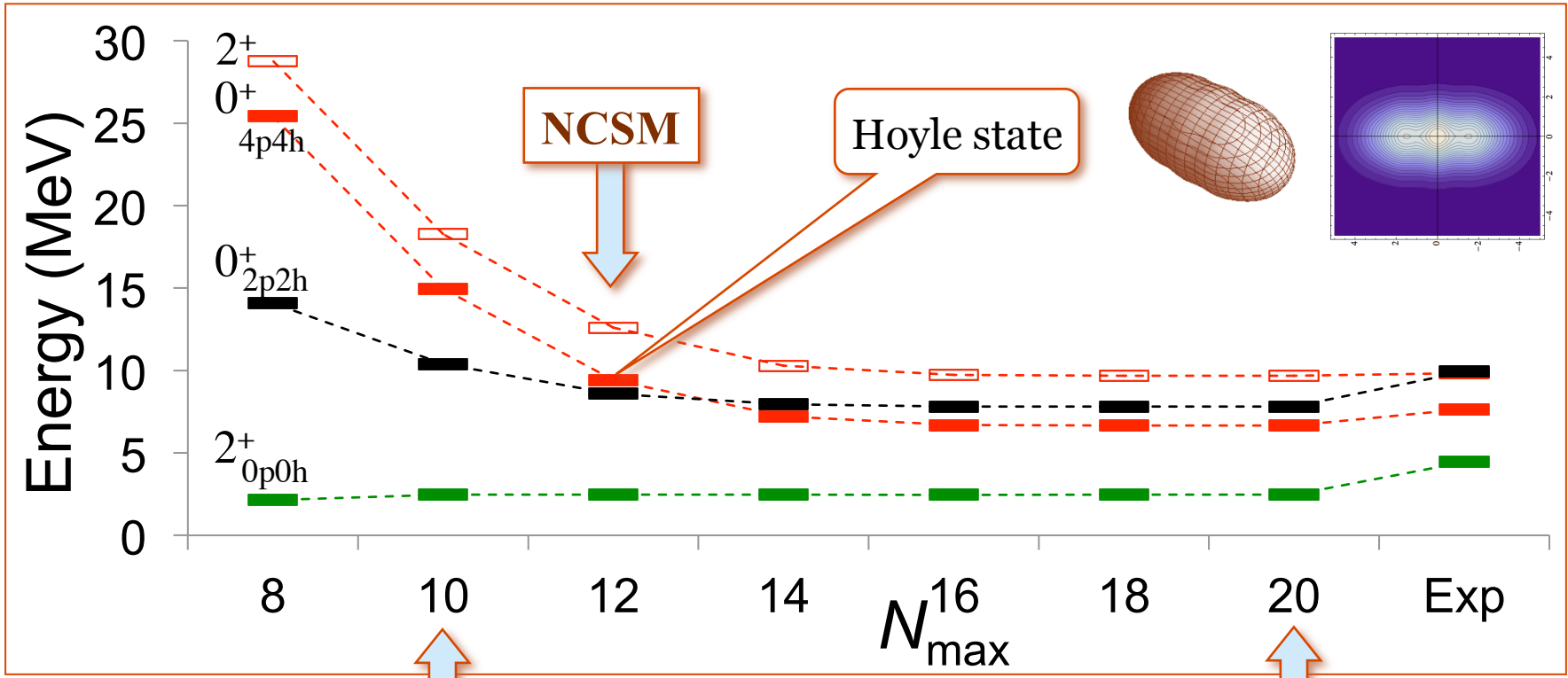
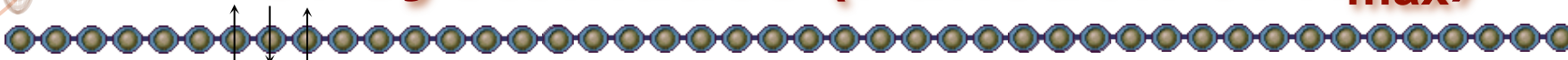
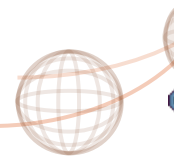
^{12}C



**Intertwining
Shell & Alpha
Cluster Picture**

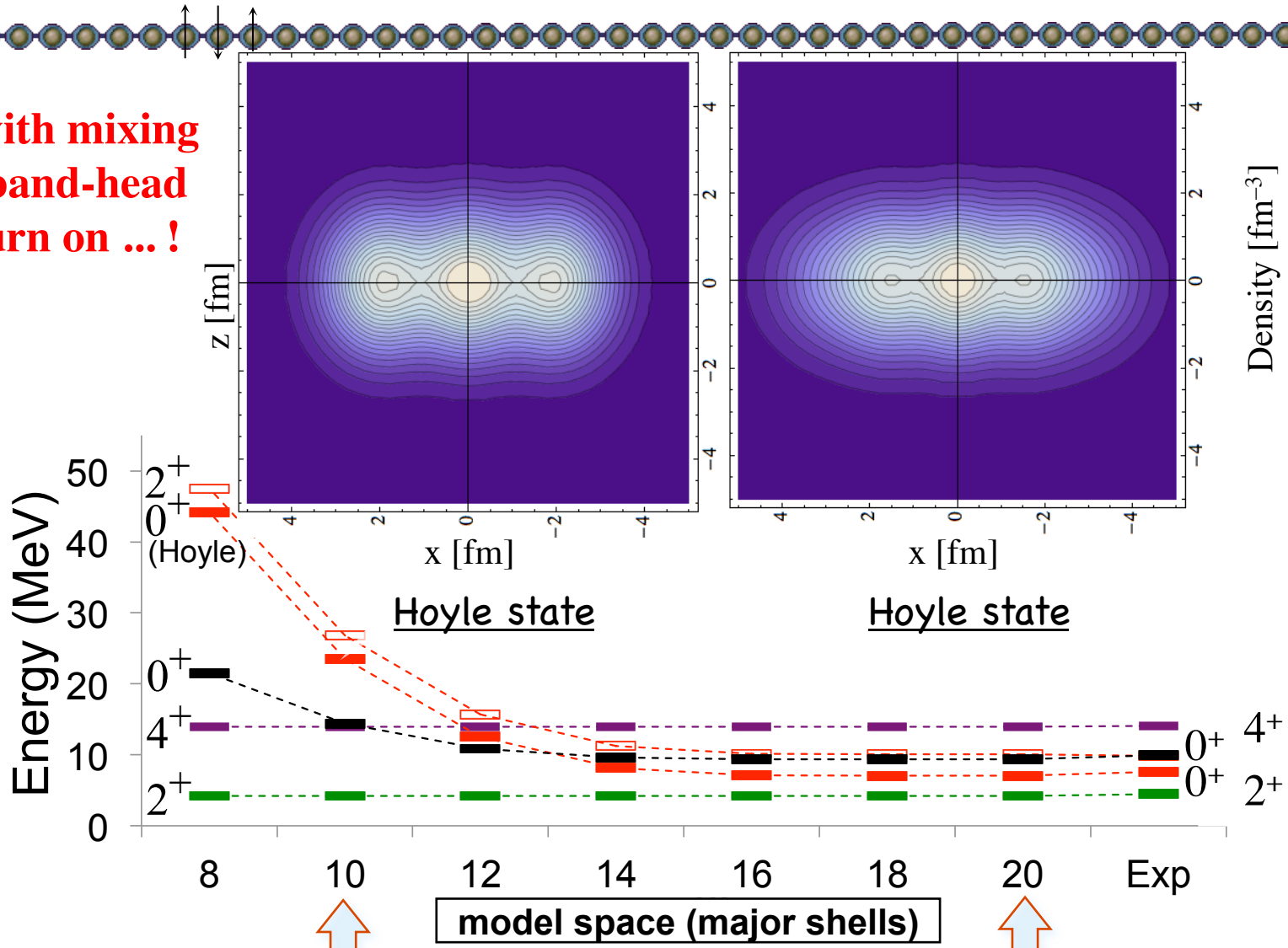


^{12}C : Systematics (Function of N_{max})



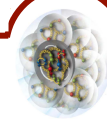
Formation of Clusters!

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

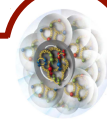
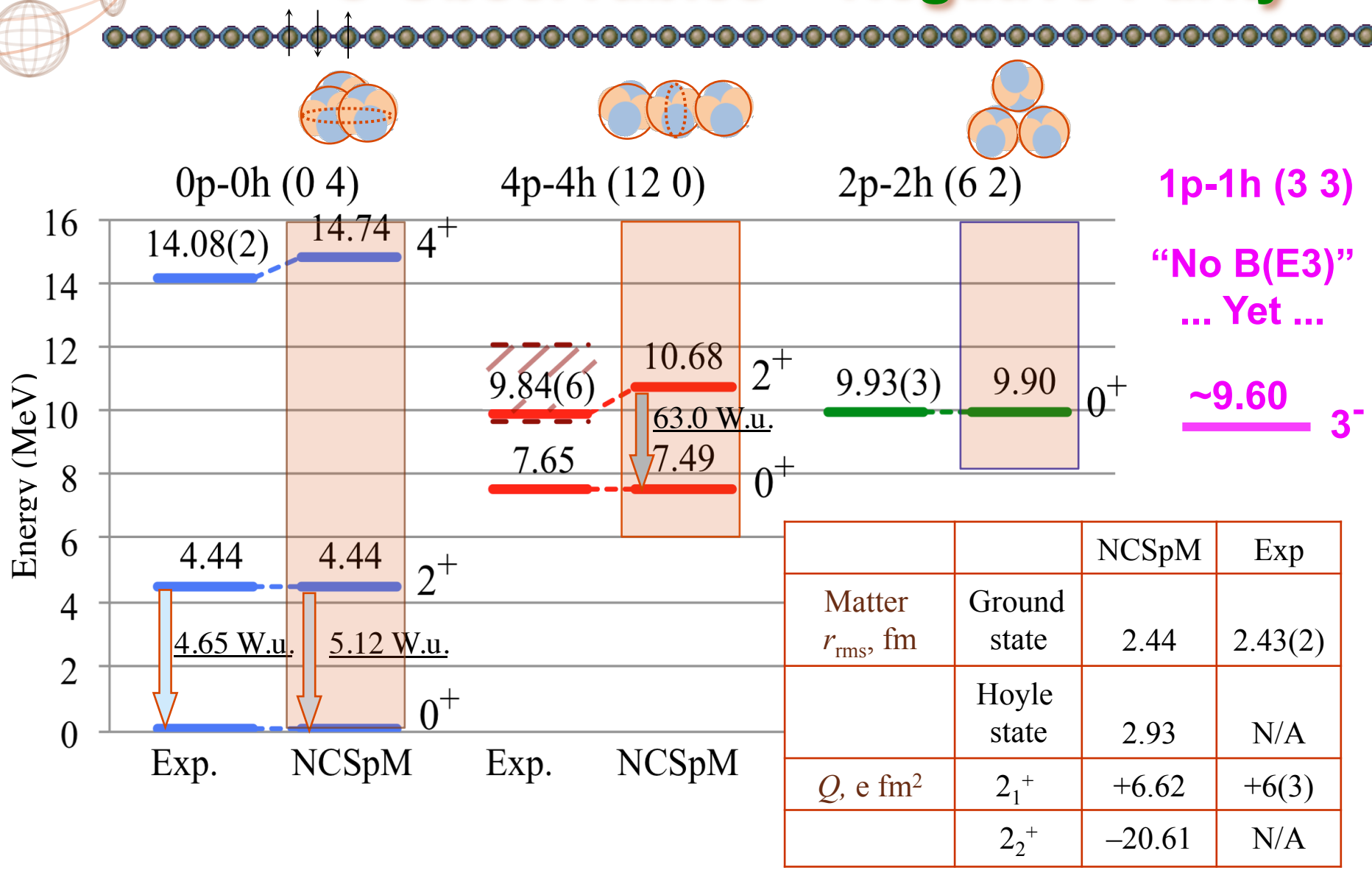


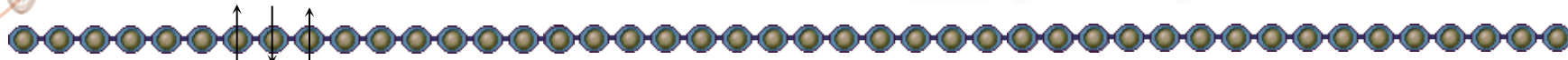
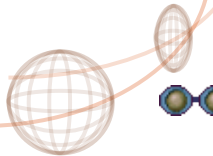
Standard ab initio NCSM

*(NCSpM & Band Mixing)



¹²C Observables – Negative Parity





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

Review

Symmetry-guided large-scale shell-model theory

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Collectivity

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 $Sp(3, \mathbb{R})$ 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 ${}^6\text{Li}$, ${}^8\text{B}$, ${}^8\text{Be}$, ${}^{12}\text{C}$, and ${}^{16}\text{O}$, and *sd*-shell nuclei exemplified by ${}^{20}\text{Ne}$, based on first-principle explorations; through the Hoyle state in ${}^{12}\text{C}$ 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 $Sp(3, \mathbb{R})$, 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.

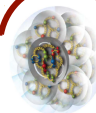
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... Also ...

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

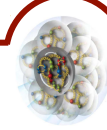
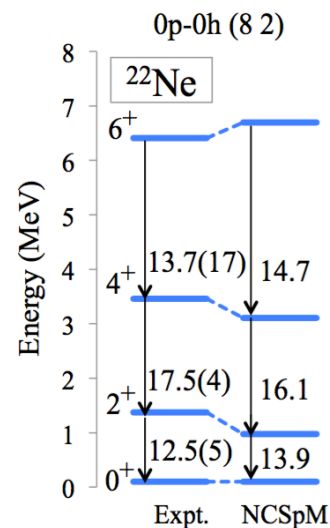
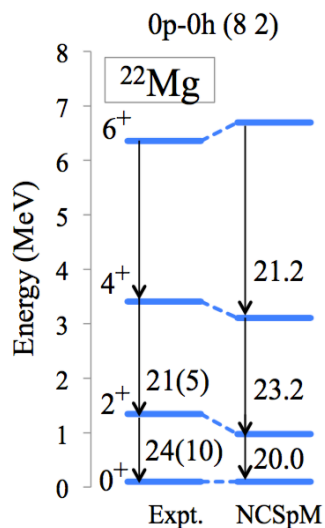
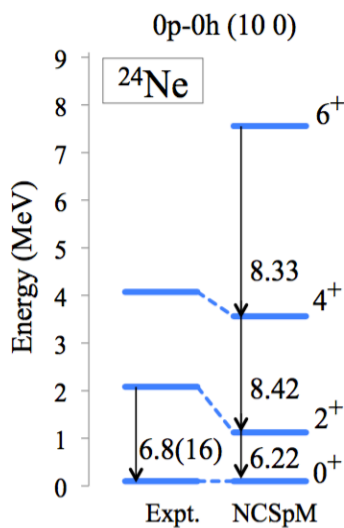
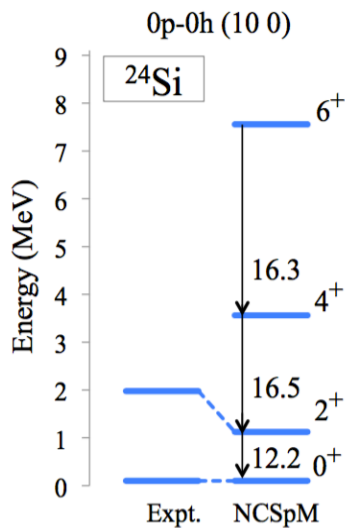
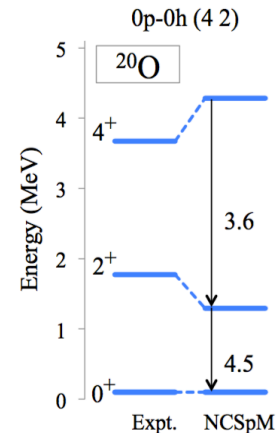
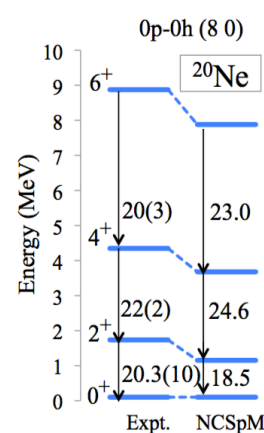
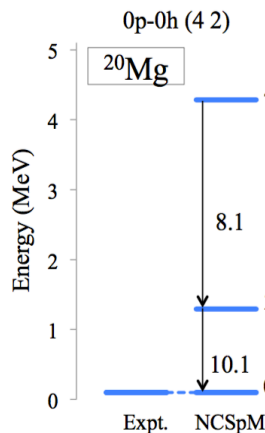
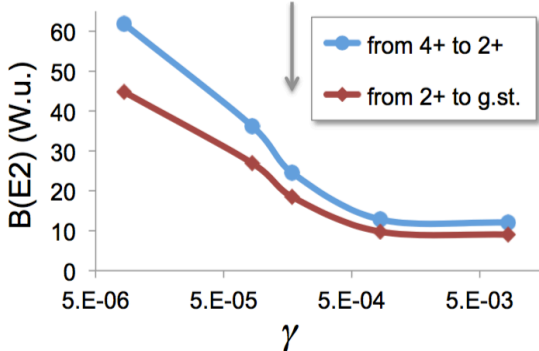
&

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

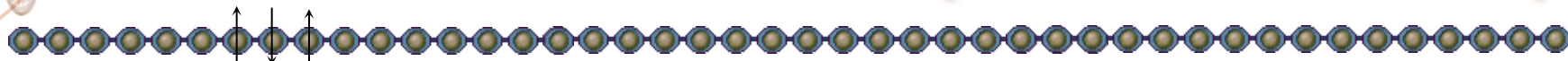
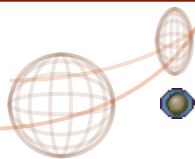


Medium Mass Nuclei (Gregory Tobin / REU)

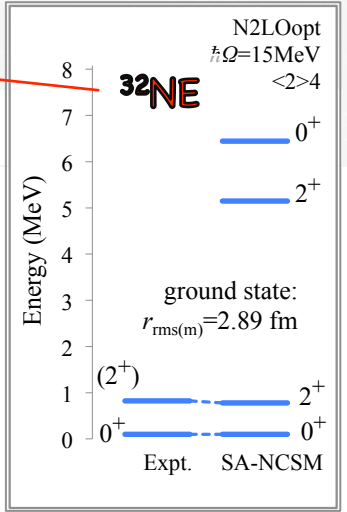
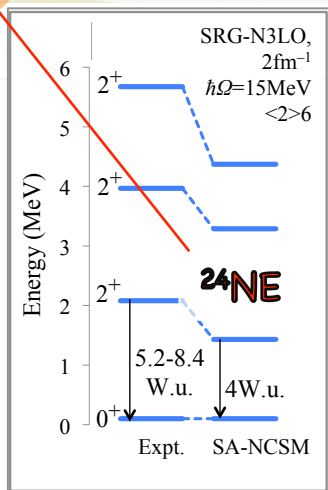
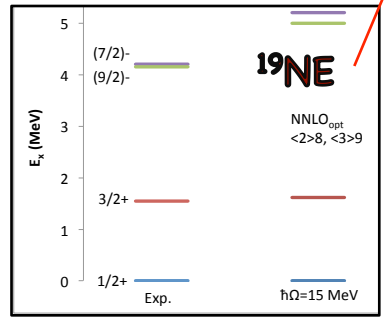
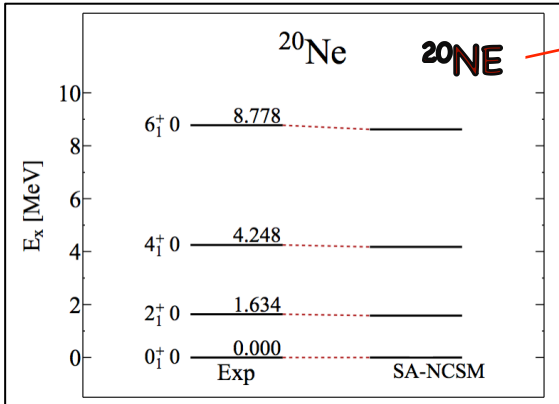
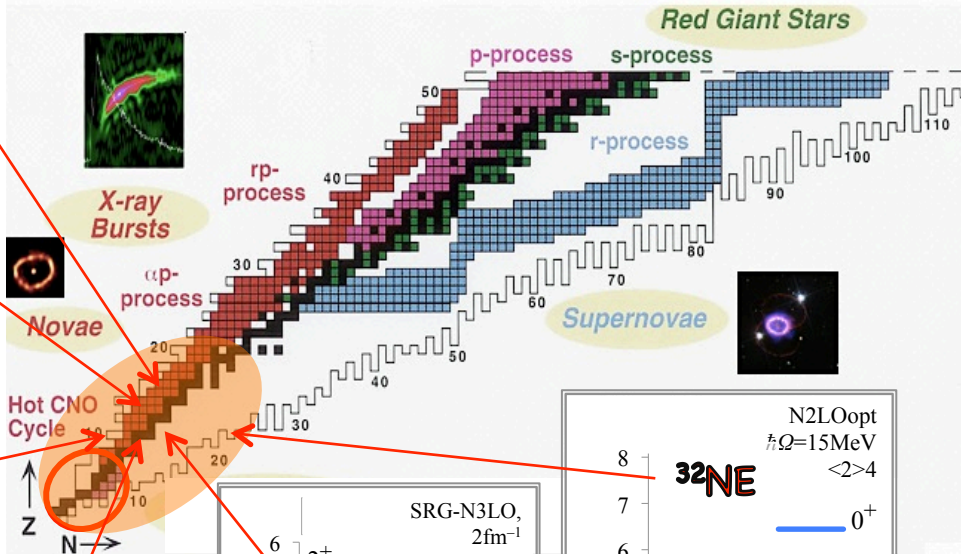
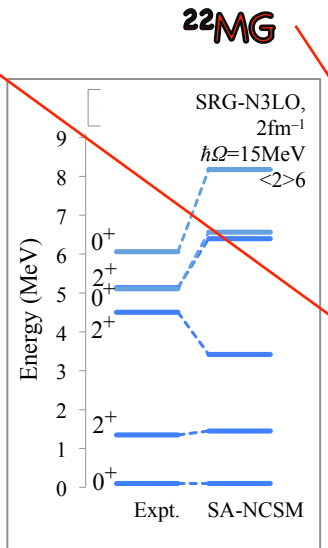
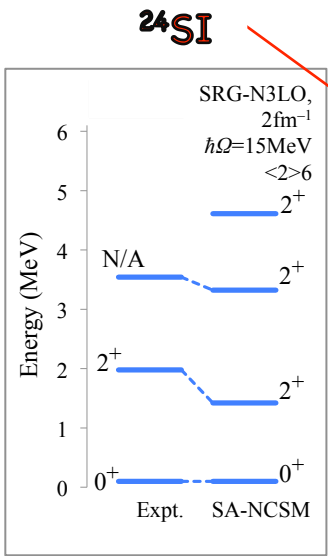
Ne-20: grey arrow is gamma used



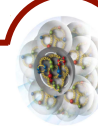
Further sd-shell Results (Robert Baker / GS)



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

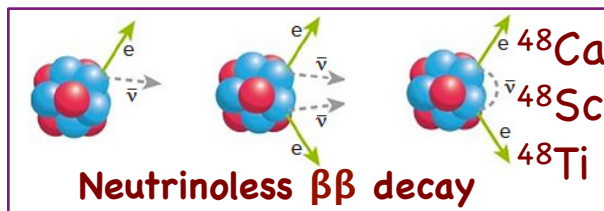


Ab initio description (converged selected spaces) (NNLO_{opt}, $\hbar\Omega=15\text{ MeV}$, 13 HO shells)



Plus fp-shell Results (Grigor Sargsyan / GS)

^{48}Ca



^{48}Ti

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

8 shells, N2LOopt

0^+

SA-NCSM (selected): 602,493

Complete model space: 24,694,678,414

2^+

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

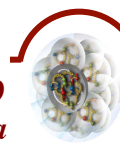
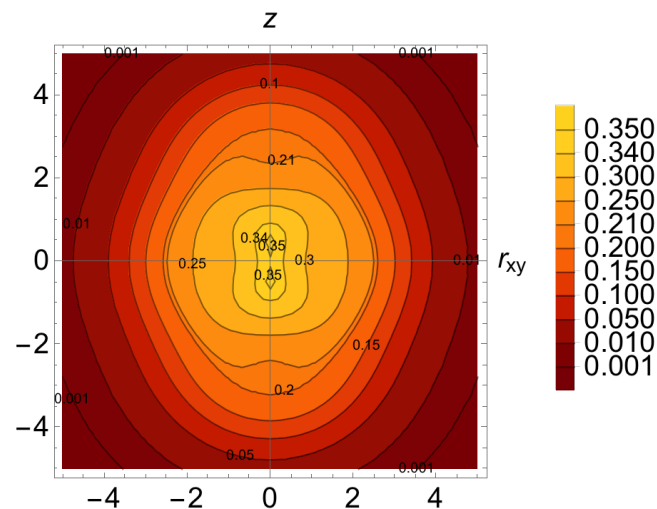
Complete model space: 113,920,316,658

^{48}Ti , $Q(2^+)$ [$e \text{ fm}^2$]

Experiment -17.7

8 shells -19.3

(no effective charges)



Nucleosynthesis: Type I X-Ray Burst

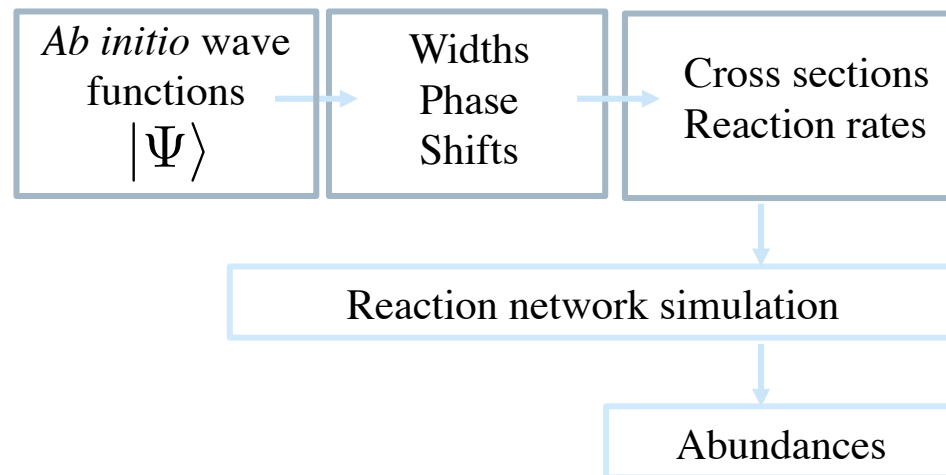
TABLE 2

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

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

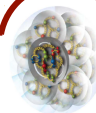
Simulations for XRB are sensitive to certain reaction rates

- $^{23}\text{Al}(p,\gamma)^{24}\text{Si}$
- improve rate precision to improve simulations

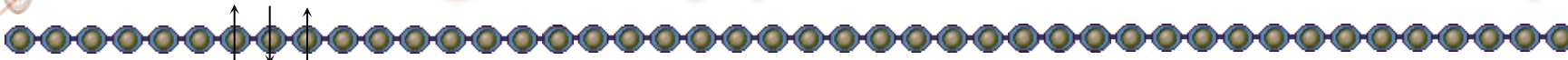
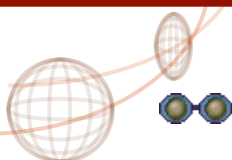


^a Up (U) or down (D) variation that has the largest impact

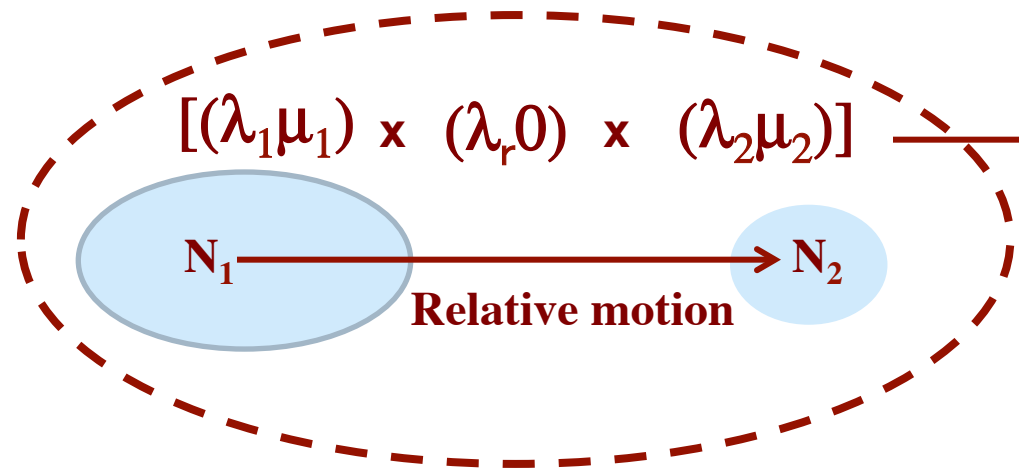
^b $M_{LC}^{(i)}$ in units of 10^{38} ergs/s



Scattering Theory (Alexis Mercenne / PDoc)

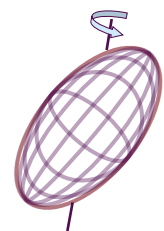


SA-NCSM + RGM



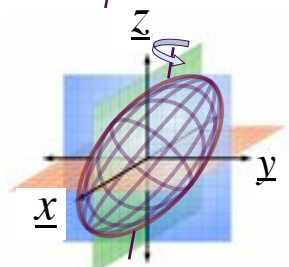
Deformation

L



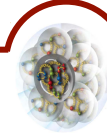
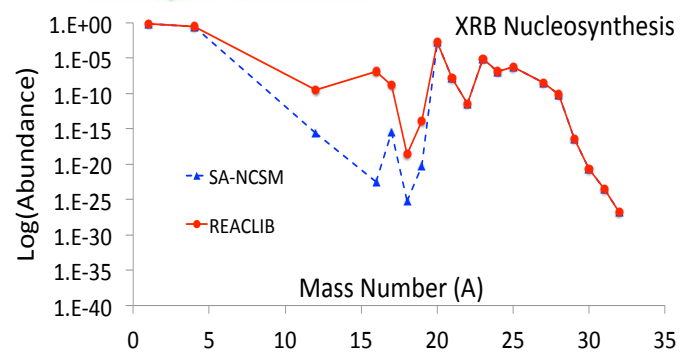
Rotations

M

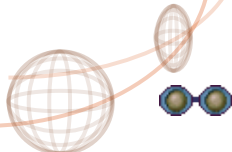


Spatial Orientation

- 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



Members of the LSU Nuclear Theory Group



Grigor Sargysyan



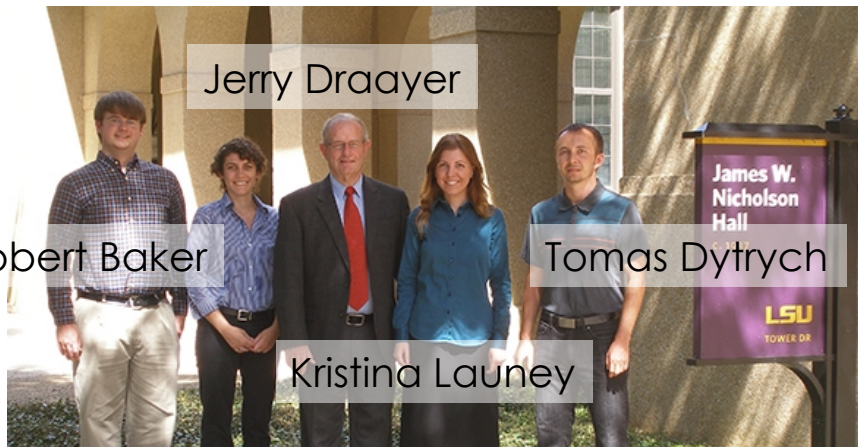
Alexis Mercenne



Charlie Barker



Alison C. Dreyfuss
Thesis Defense - 2019/10/25
(Headed to NNSA / LLNL - Regular Staff Appointment)



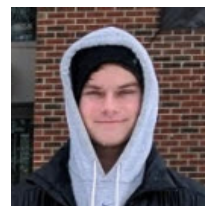
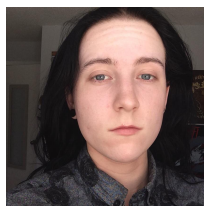
Jerry Draayer

Robert Baker

Tomas Dytrych

Kristina Launey

Charlee Amason Dustin Wleczyk



Jutta Escher

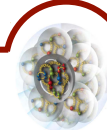


David Kekejian



U.S. DEPARTMENT OF
ENERGY

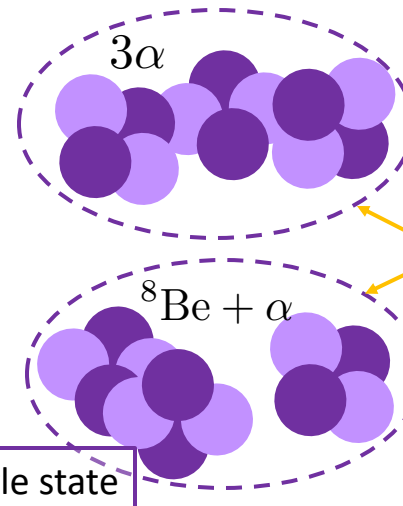
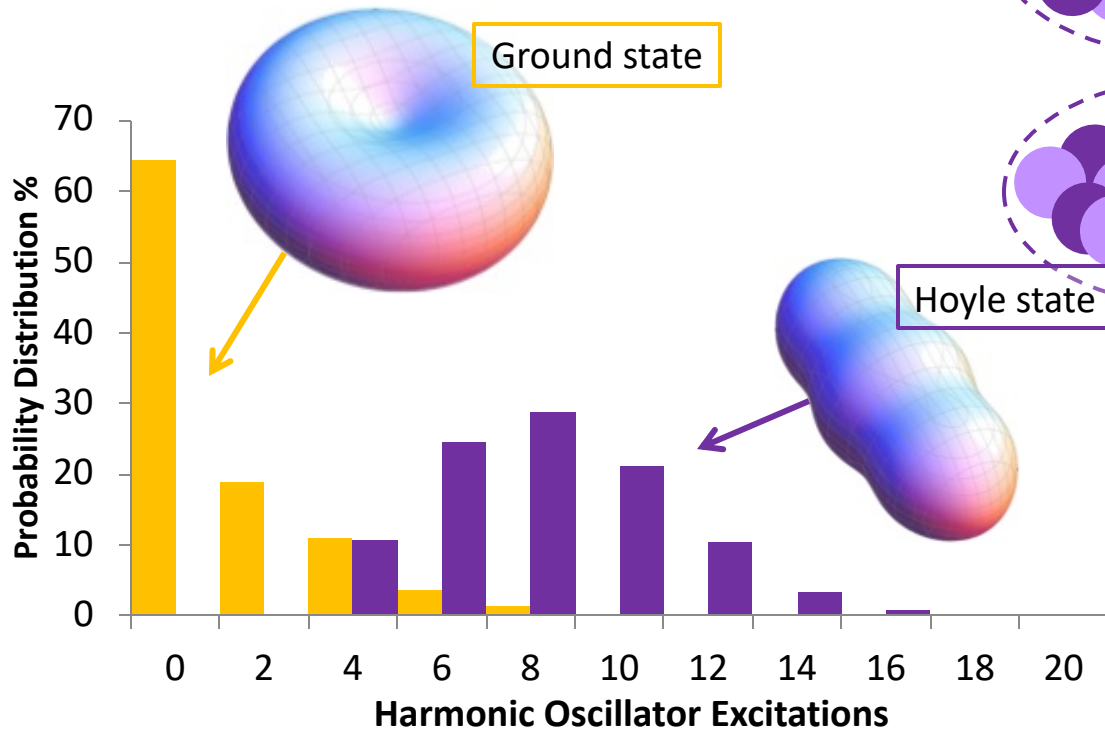
Office of
Science



Exemplary Output - LSU Nuclear Theory Team

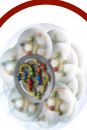
The elusive Hoyle state in ^{12}C

NCSpM wave functions



10.847	$1^-; 0$
10.3	$(0^+); 0$
9.87	$2^+; 0$
9.641	$3^-; 0$
7.654	$0^+; 0$
4.4398	$2^+; 0$
	$0^+; 0$

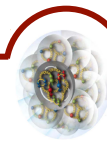
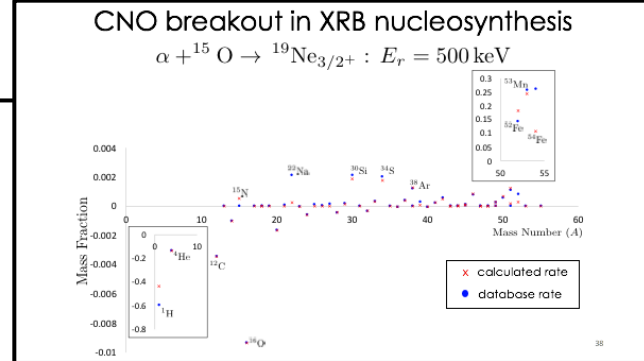
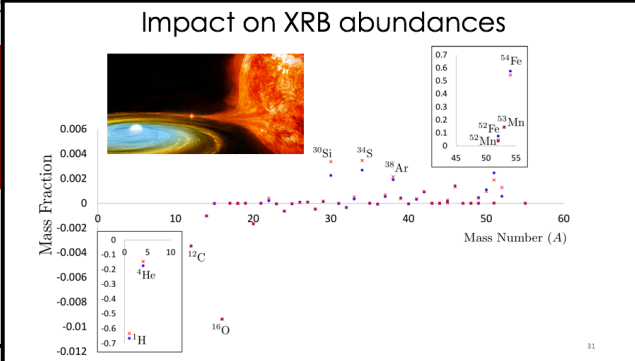
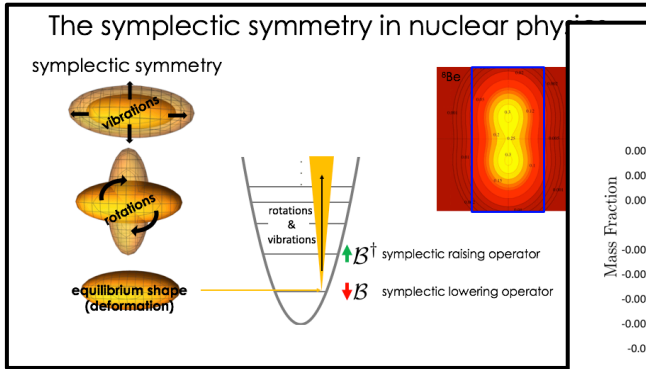
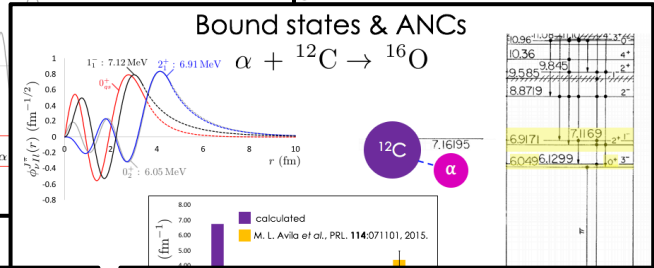
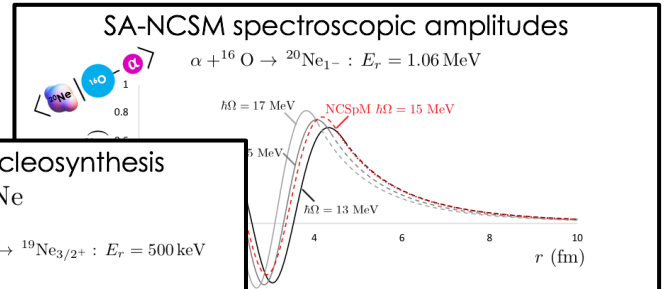
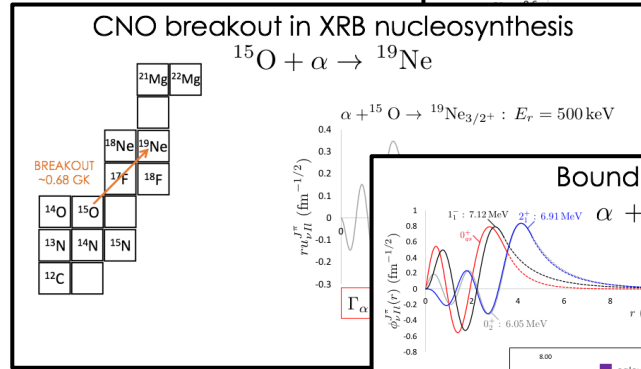
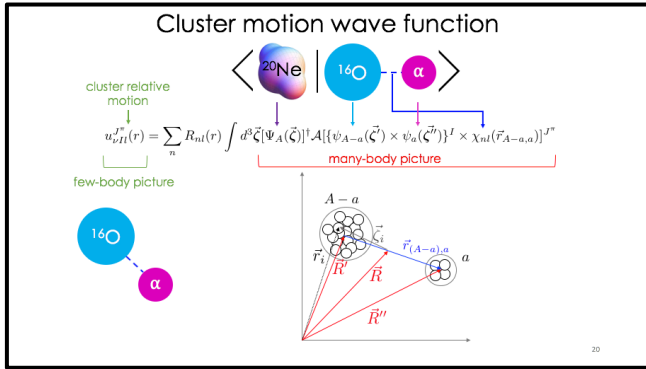
^{12}C 33



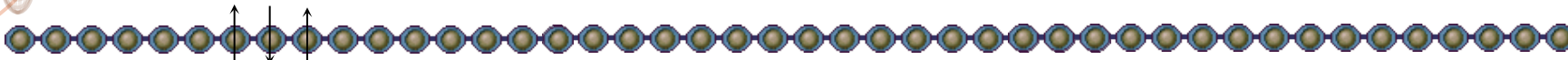
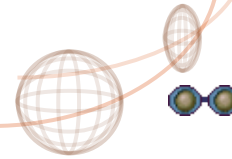
Exemplary Output - LSU Nuclear Theory Team

Conclusions

A simple framework...



Future Considerations / Tasks



Task #1:

SA-NCSM -> Deformation -> DSA-NCSM

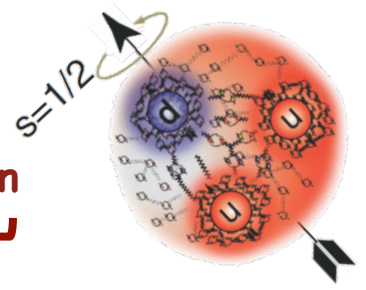
- Canonical & Unitary Transformation
- Algebraic Structure Unchanged
 - $L \rightarrow L(\text{deformed}) + S(\text{circulation})$

"Many-particle Nilsson Model"

Task #2:

Jefferson Lab 12GeV Era

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



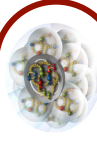
"Femtography of Nucleon"

"Normal Concept" versus "Pseudo Concept"

Task #3:

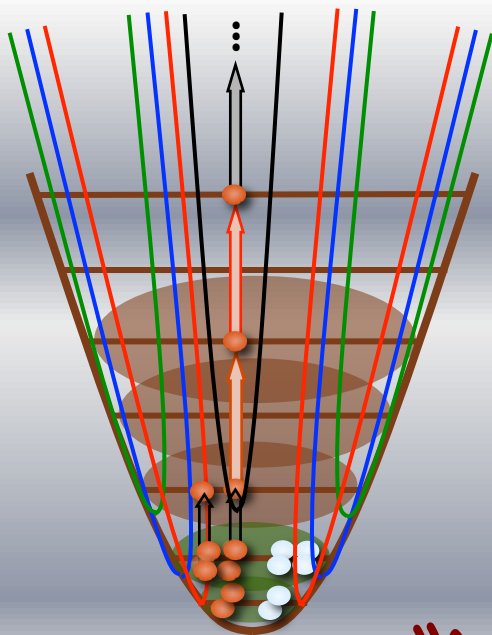
$$\bar{L} + \bar{S} = \bar{J} = \tilde{L} + \tilde{S}$$

"Collusion within & among Nucleons"

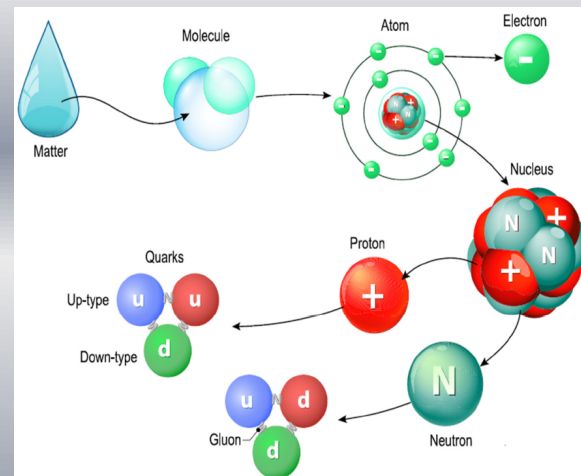
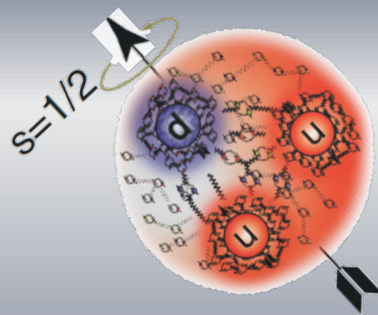




Discovering Simplicity within Complexity



... GRAZIE ...



... "Are Nucleons Deformed?" ...