

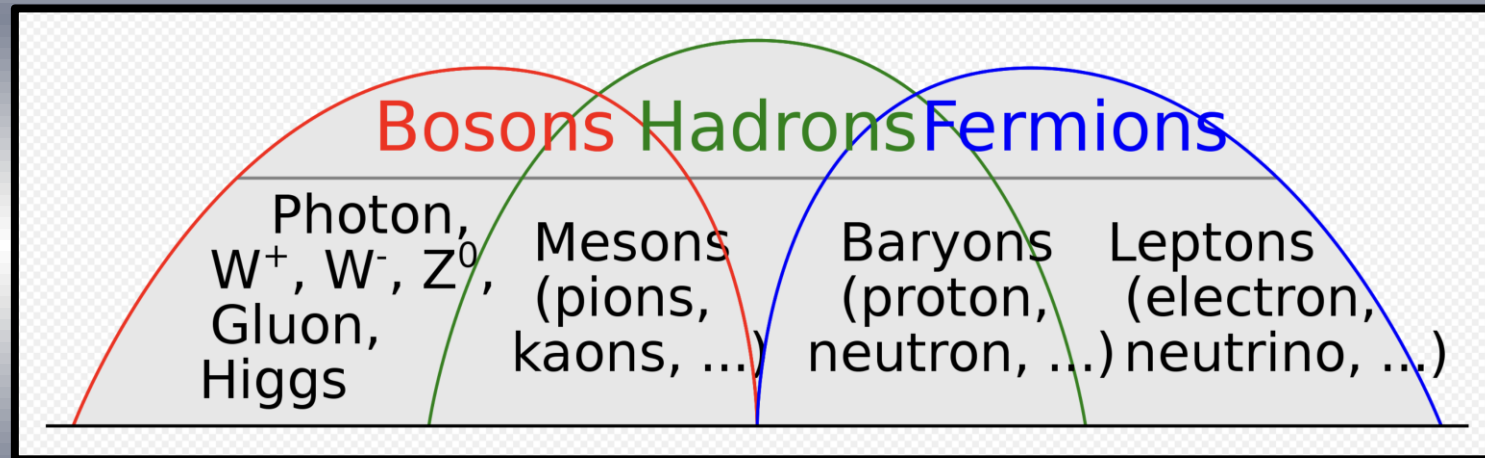
Forging a Path for Understanding Nuclear Structure from Strong QCD

(JLab 2019: 'Particle Picture') ← (Seville 2022: 'Field Focus')

Jerry P Draayer (Louisiana State U) & David S Kekejian (U North Carolina)

(Lessons learned from Low-energy NP) & (Learning from Medium/High-energy NP)

Mr. Wikipedia: Subatomic World



Bosons (integer spin – Pauli blocking OFF) form one of the **two fundamental classes of subatomic particles**, the other being **Fermions** (half-integer spin – Pauli blocking ON). **All subatomic particles must be one or the other**. Composite particles (**Hadrons**) may fall into either class depending on their composition.

PI Team: Jerry P. Draayer, Kristina D. Launey, Alexis Mercenne / Tomas Dytrych, Feng Pan / David S. Kekejian

U.S. NSF & DOE & LSU Sponsored Research

- Abstract -

The focus of our program – and hence this paper – is to recast lessons learned over the last half of the 20th Century regarding the structure of atomic nuclei (primarily a particle-based picture) into a forward leaning 21st Century (field-theory-based framework) in anticipation that this will encourage the establishment of a natural bridge between the low-energy and medium-to-high energy nuclear physics communities. This has been and continues to be enabled by two major developments, the first technical (high-end computational facilities of the 90s) and the other analytical (underpinned by the so-called ‘no-core’ *ab initio* – from first principles – shell-model theories). Early successes of the latter rest upon a realization that special symmetries and the associated algebraic methods that this enables are much better than previously anticipated. Consequently, this presentation includes a few-slide dive into some key group theory concepts, plus showing some early results that expose ‘simplicity within complexity’ in atomic nuclei that has until now it seems been under appreciated!

Next Slide (same as) Final Slide – Captures Key Message

Status of our hunt for **Symplicity within Complexity*** in nuclear matter!

(*Charge received from Eugene Wigner, 1st year as Assistant Professor at LSU, S-1974)



Symplectic Effective Field Theory for Nuclear Structure Studies

(David Kekejian, Thesis Research @ LSU 10/21 & Currently Post Doc, UNC)

Generic (Scalar) Field Theory

Quantum (Scalar) Field Theory

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \varphi)(\partial^\mu \varphi) + \frac{1}{2} m^2 \varphi^2 \xrightarrow{\text{canonical quantization}} H = \sum_k E_k (b_k^+ b_k^- + \frac{1}{2})$$

$$\varphi(r, t) = \frac{1}{\sqrt{V}} \sum_k b_k^- \frac{1}{\sqrt{|2k^0|}} e^{-ik^\mu x_\mu} + \frac{1}{\sqrt{V}} \sum_k b_k^+ \frac{1}{\sqrt{|2k^0|}} e^{ik^\mu x_\mu}$$

$$\mathcal{L}^{(n)} = \frac{\alpha^n}{2(n+1)!} (\partial_\mu \varphi \partial^\mu \varphi^* + m^2 \varphi \varphi^*)^{n+1}$$

$$\mathcal{H}^{(n)} = \frac{\alpha^n}{2(n+1)!} (\dot{\varphi} \dot{\varphi}^* - \varphi' \cdot \varphi'^* + m^2 \varphi \varphi^*)^n ((2n+1) \dot{\varphi} \dot{\varphi}^* + \varphi' \cdot \varphi'^* - m^2 \varphi \varphi^*)$$

$$H^{(n)} \sim \left(\frac{\alpha}{V} \hbar \Omega\right)^n \times (g^2 Q \cdot Q)^n, (K \cdot K)^n, (gQ \cdot K)^n, (gK \cdot Q)^n \quad \text{Where: } \frac{\alpha}{V} \hbar \Omega = \frac{\beta^2}{8N_\sigma} \quad g = \frac{m^2}{\hbar^2 \omega^2}$$

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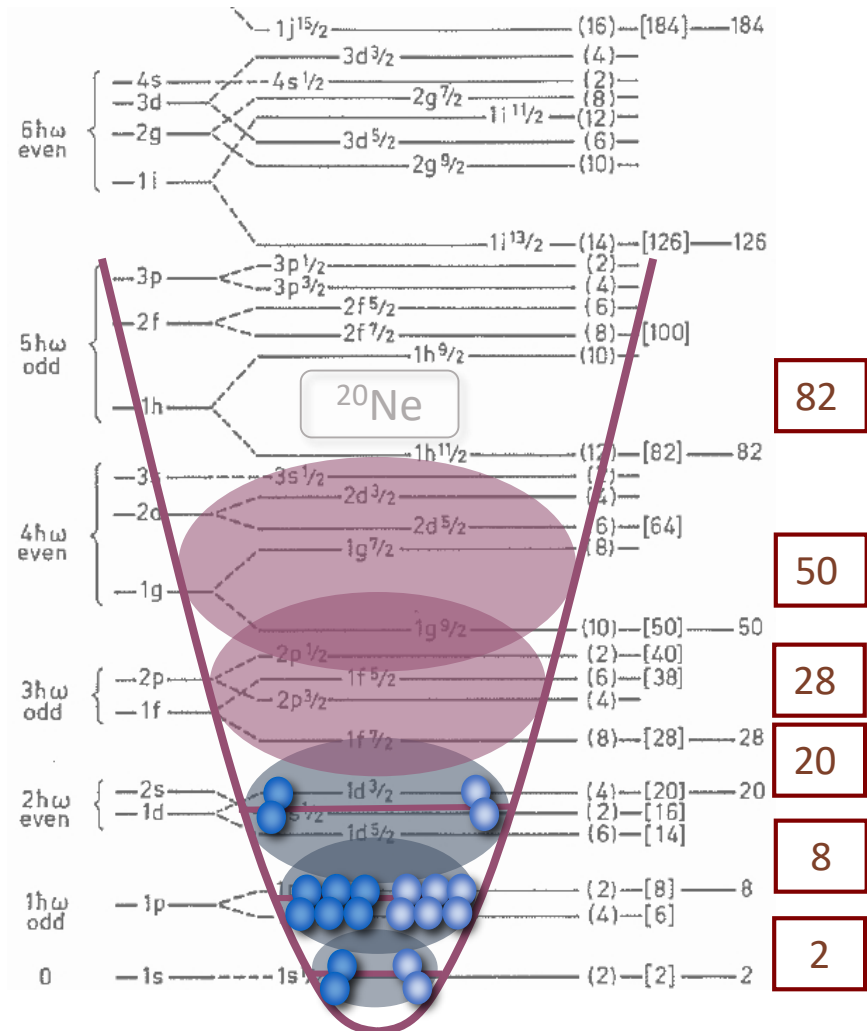
(DOI: 10.1103/PhysRevC.106.014304)

Kekejian (Thesis), Draayer & Mokeev, Roberts

Conclusion: Symplectic Symmetry emerges naturally from a quantum effective Field Theory!



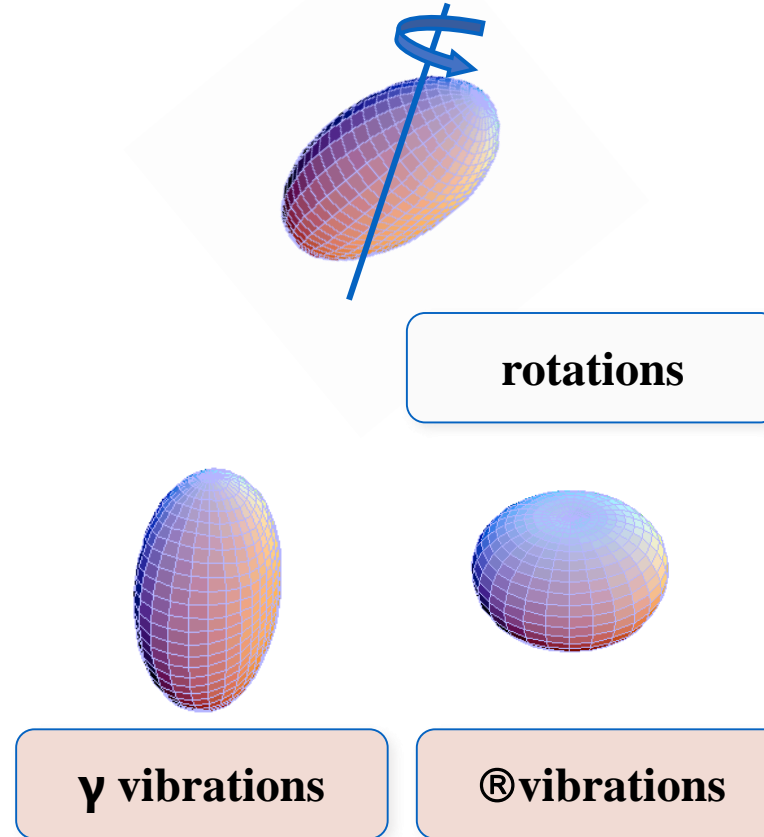
Shell Model



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

Collective Model

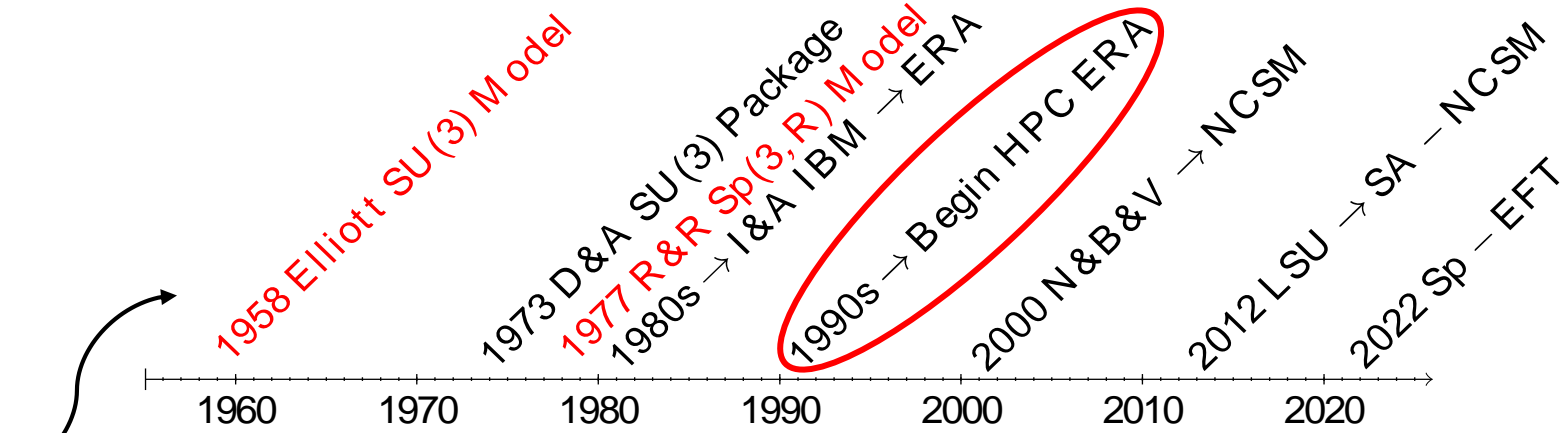
A.N. Bohr, B.R. Mottelson & J. Rainwater ('50s)
 "... for the discovery of the connection between collective motion and particle motion in atomic nuclei and the development of the theory of the structure of the atomic nucleus based on this connection ..."
(1975 Nobel Prize)



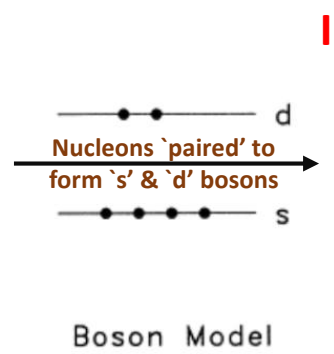
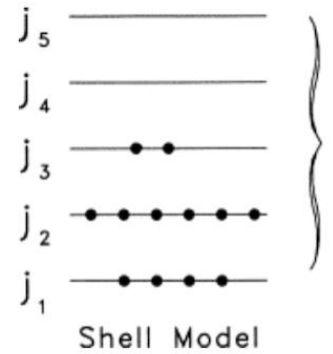
Shell Model (Particle Picture) versus (Field Focused) Dynamics

Caricature of an Evolving Nuclear Structure Landscape

- 50s** Structureless Point Particles (proton & neutrons)
- 60s** 3D Harmonic Oscillator 'Box' (rotations & vibrations)
- 70s** Various Algebraic Theories (Fermion & Boson)
- 80s** Phenomenological versus Realistic Interactions
- 90s** **Supercomputers enabled a Transformational Change**
- 00s** Open (No-Core) Models with 'ab initio' Interactions
- 10s** Algebraic theories extended via non-compact structures
- 20s** Inter-nucleon Fields drive Nuclear Structure



Shell Model Approach
(Elliott & Harvey plus Rowe & Rosensteel ...)
Has both **fermion** and field theory features.



Interacting Boson Model
(Iachello & Arima plus Many IBM Disciples ...)
Has both **boson** and field theory features.

non-compact		Symmetry Platforms		compact only	
Blue 'Basis States' Elliott SU(3); R&R Fermion Model	$Sp(3,R)$ (non-compact)	U(6) (pairing modes) & SU(3) (rotor modes) \supset SO(3) (3D-rotations)	}	Red 'Basis States' IBM: Interacting Boson Model	
	\supset SU(3) (3D-oscillator)				
	\supset SO(3) (3D-rotations)				



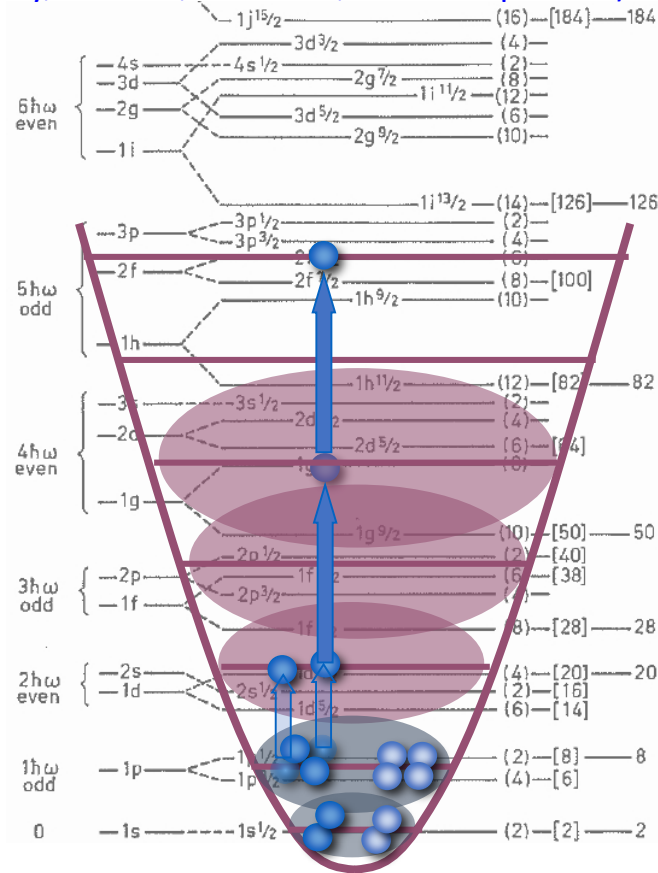
Shell Model

Advances

Collective Model

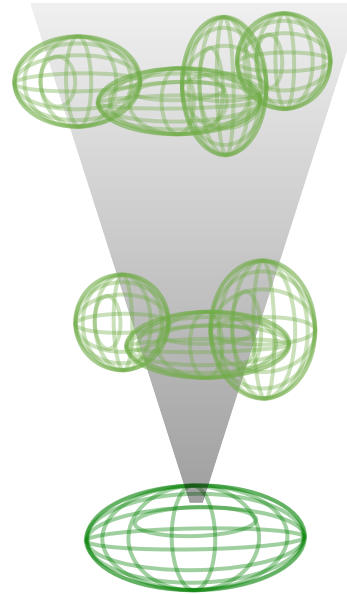
No-Core Shell Model (NCSM)*

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



*Realistic interaction (local or not; NN, NNN,...)

- In principle, exact solutions, up to N_{\max}
- Successful description up through ^{16}O



Symplectic Model – NCSpM*

(Rowe & Rosensteel ~1980s to Present)

- $Sp(3,R)$ group structure
- $SU(3)$ - symmetry adapted basis
- Schematic interactions

Typical Vertical
Symplectic Slice

(monopole/quadrupole
excitations, including
 $2p2h, 4p4h, \dots$)

$0\hbar\Omega$ Elliott's $SU(3)$

- *Multi-shell generalization of Elliott Model
- No spurious center-of-mass motion
- Fully microscopic, equals NCSM if all symplectic slices included
- Reproduces rotational bands & $B(E2)$ rates without effective charge

'Symmetry Adapted' / SA-NCSM Campaign

Timeline: 5 (2002-06) + 5 (2007-2011) + 5 (2012-20XX)

Goal –

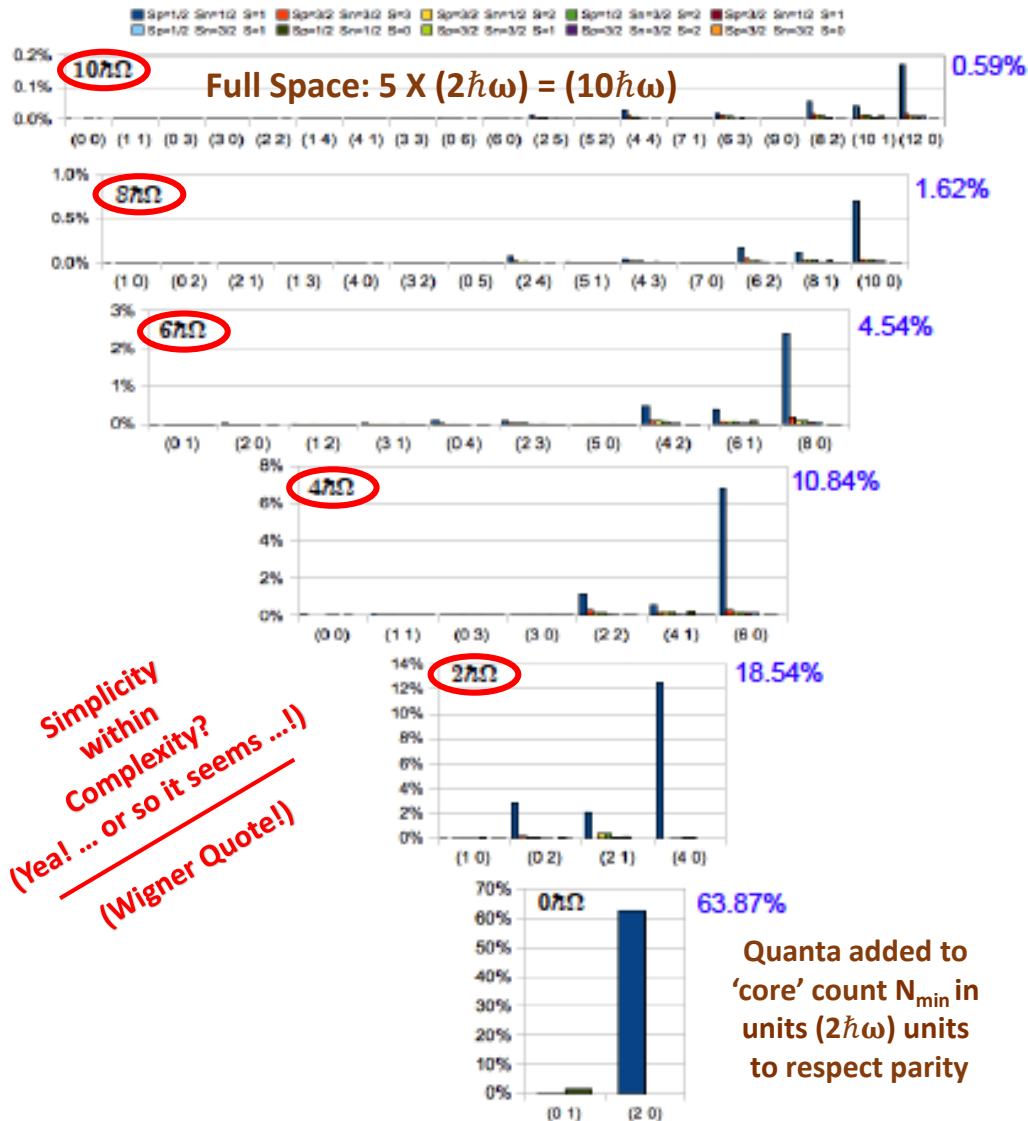
Reproduce and predict properties of heavy as well as light nuclei, starting with and building upon QCD/EFT informed and inspired interactions ...

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 the space to physically relevant and tractable subspaces, etc.
 - Evaluate extensibility of theory and its characteristics by taking full advantage of 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 very important to understanding nuclei and nuclear systems
 - Ultimately develop a 'user-friendly' code (desktop version) for easy applications and teaching as well as training purposes
 - Extend the theory to nuclear reactions - coupling to continuum and apply the results to important astrophysical processes

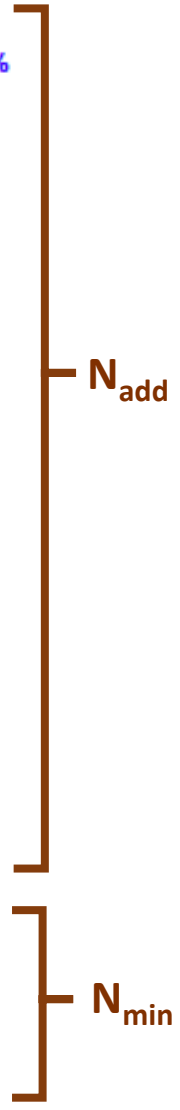


First Results for ${}^6\text{Li}$ with $N_{\text{add}} = 10$



Simplicity within Complexity? (Yea! ... or so it seems ...!) (Wigner Quote!)

Quanta added to 'core' count N_{min} units ($2\hbar\omega$) units to respect parity



... Proof of Principle ...

Answer: > 85% of Physics In < 1% of the "extended" space

JISP16 'bare' interaction in $N_{\text{add}} \Rightarrow 10$ 'space'; i.e., $5 \times (2\hbar\omega) = (10\hbar\omega)$ to N_{min} 'core'

*Bonn, Argonne, Idaho, N3LO (optimized), etc. ... all yield close results ... (only change at the 1-2% level)

... 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 (LANL) & various other 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!

Simply Add 3D-HO Quanta to 'core'!

Typically ... 75% -> 95% Leading Sp-IR

Many examples published, so ...

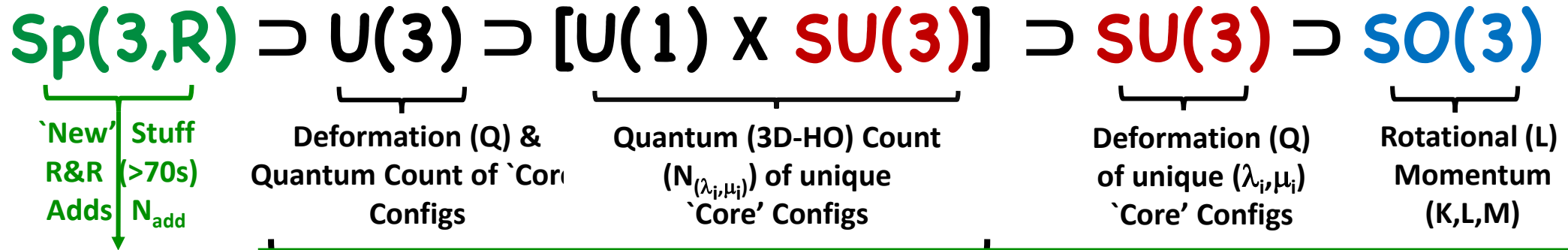
Why does it work?

The rest of the story follows ...

Hint: The Physics is in the Fields!



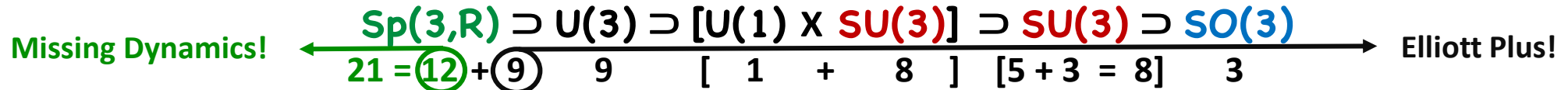
Symplectic Symmetry: The Dynamical Symmetry of 3D-HO



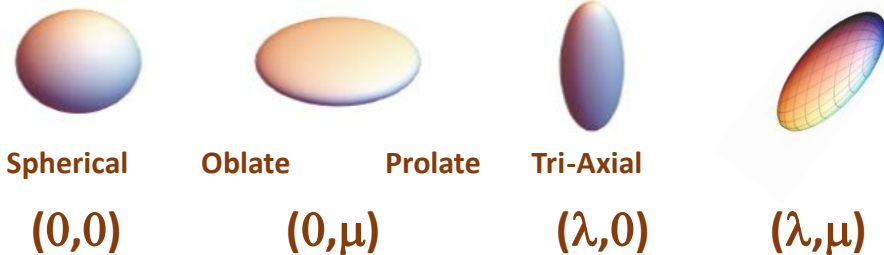
Non-compact Group ‘Extension’ of $U(3)$... adds multiple $[(\lambda, \mu) = (2, 0) / (2\hbar\omega)]$ 3D-HO excitations (N_{add}) to the initial ‘core’ configuration(s) count (N_{min}) for total ‘field’ count: $N_{tot} = N_{add} + N_{min}$ (Quanta).

In principle, N_{add} can run from 0 to infinity (∞), but practically, as shown on previous slide, results converge at ~ 10 , which sets the scale of the extension; i.e., ~ 200 MeV [$10 \times (2\hbar\omega)$] energy units.

Digging deeper into the group structure: Number of ‘generators’ of the respective groups listed above follows:



Elipsoidal Shapes as related to (λ, μ) values



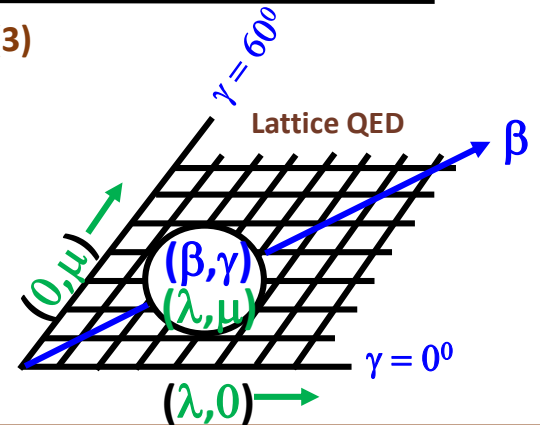
Mapping 3-D Rotor to $SU(3)$

(β, γ) Bohr-Mottelson

(λ, μ) Elliott (1958)

$\beta^2 \sim C_2$
(2nd Order $SU(3)$ Invariant)

$\beta^3 \cos(3\gamma) \sim C_3$
(3rd Order $SU(3)$ Invariant)



Symplectic Symmetry: Spectrum Generating Algebra (3D-HO)

The 21 generators of $Sp(3,R)$ - characterized on the last slide in terms of their group/subgroup properties - can be recast in terms of 'field operators/tensors' built from distinct quadratic forms in the coordinates (q_i) and momenta (p_i) of the system:

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

Quadrupole (Shape) 'Tensor' (6)	Kinetic Energy 'Tensor' (6)	Orbital Angular Momentum Operator (3)	Internal Dynamics 'Circulation' / 'Vorticity' (6)
------------------------------------	--------------------------------	--	--

Important observations: **First** of all, note that these 'field tensors/operators' are 'particle neutral' since the sum runs over all particles, signaling a shift in focus from 'particles' to the 'field' (single frequency) through which particles 'communicate' with one another. **Second**, the 'isotropy of space' means the field can only be represented in terms of 'rotational scalars'. And **Third**, this suggests that an understanding the 'field dynamics' of such a system may be simpler than heretofore appreciated; specifically, it depend upon the size of the set of 'rotational scalars' that one can construct, which is a relatively small number - 5 total of operator rank 4 or less. Specifically, there are 2 rank 2 tensors (L^2 and C_2), and as well 2 rank 3 tensors [C_3 and $X_3 = (LxQxL)^0$], plus 1 rank 4 tensor ($X_4 = [(LxQ)x(QxL)]^0$). Of these, 3 are group invariants: [L^2 for $SO(3)$] and the 2 invariants of $SU(3)$ [C_2 and C_3] augmented by 2 special non-invariant scalars (X_3 and X_4) that split states in an IR of $SU(3)$, but do not break $SU(3)$ symmetry. To illustrate the simplicity and beauty of exploiting such a framework, the Hamiltonian for a 3D-HO Triaxial Rotor follows:

$$H_{(\text{triaxial rotor})} = a_1(L_1)^2 + a_2(L_2)^2 + a_3(L_3)^2 \Leftrightarrow (L_1)^2/2I_1 + (L_2)^2/2I_2 + (L_3)^2/2I_3 \Rightarrow b_1(L^2) + b_2(X_3) + b_3(X_4)$$

(Leschber & Draayer, [https://doi.org/10.1016/0370-2693\(87\)90829-X](https://doi.org/10.1016/0370-2693(87)90829-X))

where the $a_i = 1/[2I_i]$ are moments of inertia of a triaxial rotor along it's i-th symmetry axes, with the 1-to-1 mapping between the a's and b's and analytic results for matrix elements of X_3 and X_4 all known.



Symplectic Symmetry: Independent Rotational Scalars (3D-HO)

If H is a subgroup of G ($G \supset H$), finding the independent H scalars one that one can build from the generators of G is a well-defined group theoretical problem; namely, establishing the **Integrity Basis (IB)** for the ($G \supset H$) structure. In our case, G is $U(3)$ and H is $SO(3)$, and the **IB** is well-known. Also, due to the group commutation properties, all such scalars can be expressed in terms of a subset of scalars, the so-called generators of the **IB**. For the case of $SU(3) \supset SO(3)$ the result of such an analysis, given in terms of their tensorial rank (number of generators involved), is as follows:

*Tensorial Rank of Rotational Scalars in $U(3) \supset SU(3)$ Reduction

Rank 1 Tensors: N [total number of oscillator quanta]

Rank 2 Tensors: L^2 [angular momentum squared: $(L \times L)^0$]

C_2 [2nd order invariant of $SU(3)$]

N^2 [2nd order N]

Rank 3 Tensors: C_3 [3rd order invariant of $SU(3)$]

X_3 {3rd order **non-invariant*** $SU(3)$ scalar: $(L \times Q \times L)^0$ }

$(N \times L^2)$

$(N \times C_2)$

N^3 [3rd order N]

Rank 4 Tensors: X_4 {4th order **non-invariant*** $SU(3)$ scalar: $[(L \times Q) \times (Q \times L)]^0$ }

$L^2 \times L^2 = (L^2)^2$ (square of L^2)

$C_2 \times C_2 = (C_2)^2$ (square of C_2)

$L^2 \times C_2 =$ Product of L^2 & C_2

$(N^2 \times L^2)$

$(N^2 \times C_2)$

$(N \times X_3)$

N^4 [4th order N]

*Nuclear Physics A439 (1985) 61-85

(Draayer & Rosensteel)

*Identifying subgroup scalars [$SO(3)$ in our case], within a larger group [$U(3)$ for us] is best done in two steps with the first being the establishment of the so-called **Integrity Basis** for this group-subgroup system, from which all others can be given as polynomials of the **IB** set. The results given in the table to the left lists all such tensorial forms - up to and including rank 4 terms - **5** 'tensors' if powers of N are excluded; **17** if included!

[Note: If limited to no more than rank 3 tensors, the count drops to **5** 'tensors' (X_4 dropped) but with this the ability to reproduce stable triaxial shapes is lost. The latter suggests that our EFT friends might need to assess the importance of including 4th order terms in their analyses to gain even better (i.e., 'ab initio') results for next generation nuclear physics studies!]



Simple Question: How do Nucleons `talk' to one another? *



Old School: Shell Model approach: $\mathcal{H} | \Psi \rangle = E | \Psi \rangle$, find 'matrix solution' if this can be achieved.

- Last half of 20th Century – Robust collection of methodologies proffered but usually computationally challenged,
- Early 21st Century – Open systems (NCSM & SA-NCSM) – yields reasonable results – inclusive of 'ab initio' input,
- The dominance of deformation across nuclides uncovered within the $Sp(3,R) \supset U(3) \supset SU(3) \supset SO(3)$ framework!

New School: Field Theory approach: $\mathcal{H} | \Psi \rangle = E | \Psi \rangle$, with a $U(3) \supset SO(3)$ expansion of \mathcal{H} .

- The dominance of deformation means \mathcal{H} is dominated by a very small number (5) of low-order scalar invariants,
- These low-order scalar invariants are ubiquitous, with analytic results for their matrix elements all well-known,
- This suggests (to me anyway) that an 'ab initio' Chiral-EFT linkage might be simpler than previously anticipated,
- Also, with Chiral-EFT 'low-energy constants' in play, alignment with IB expansion coefficients seems to be likely,
- Not all invariants are of the $Sp(3,R)$ type, mixing will occur (e.g., for pairing modes) so mode-mixing is required,
- The latter is a 'work-in-progress', and a very necessary part of the symplectic picture - we'll keep you posted,
- Never lose sight of the fact that the goal is to 'build-a-bridge' between the low-energy & medium-energy NP,
- Generally, never minimize the importance of symmetry - exposing 'simplicity within complexity' is sound science!

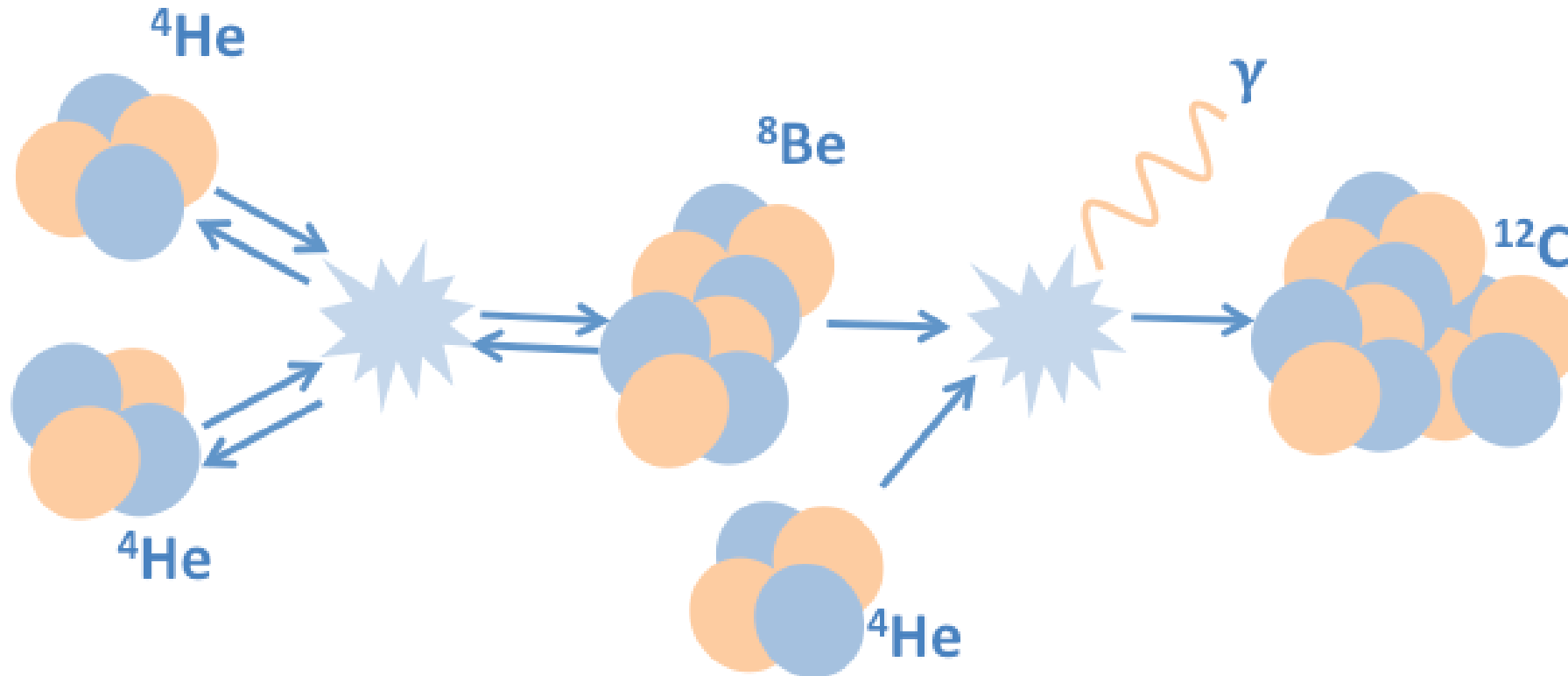
***I will now show results from some more `recent examples' applying the SA-NCSM - (Slides #10-#17)
and then I will close out with some additional remarks regarding `bridge building' - (Slides #19-#20)**



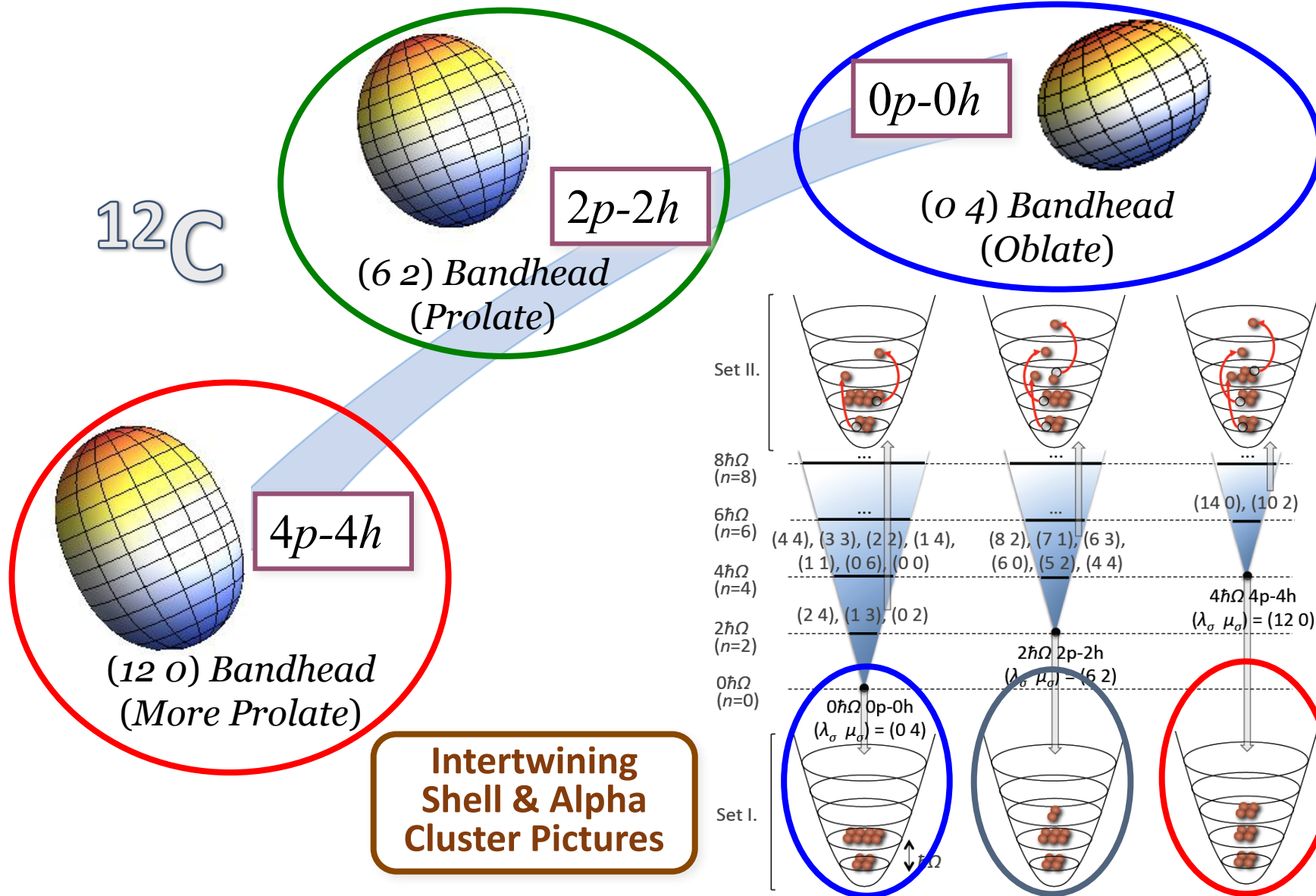
Back to the Future: Recent Examples and Bridge Building

Creation of ^{12}C in Hot Stars / Nucleosyntheses

... The Elusive Hoyle State ...

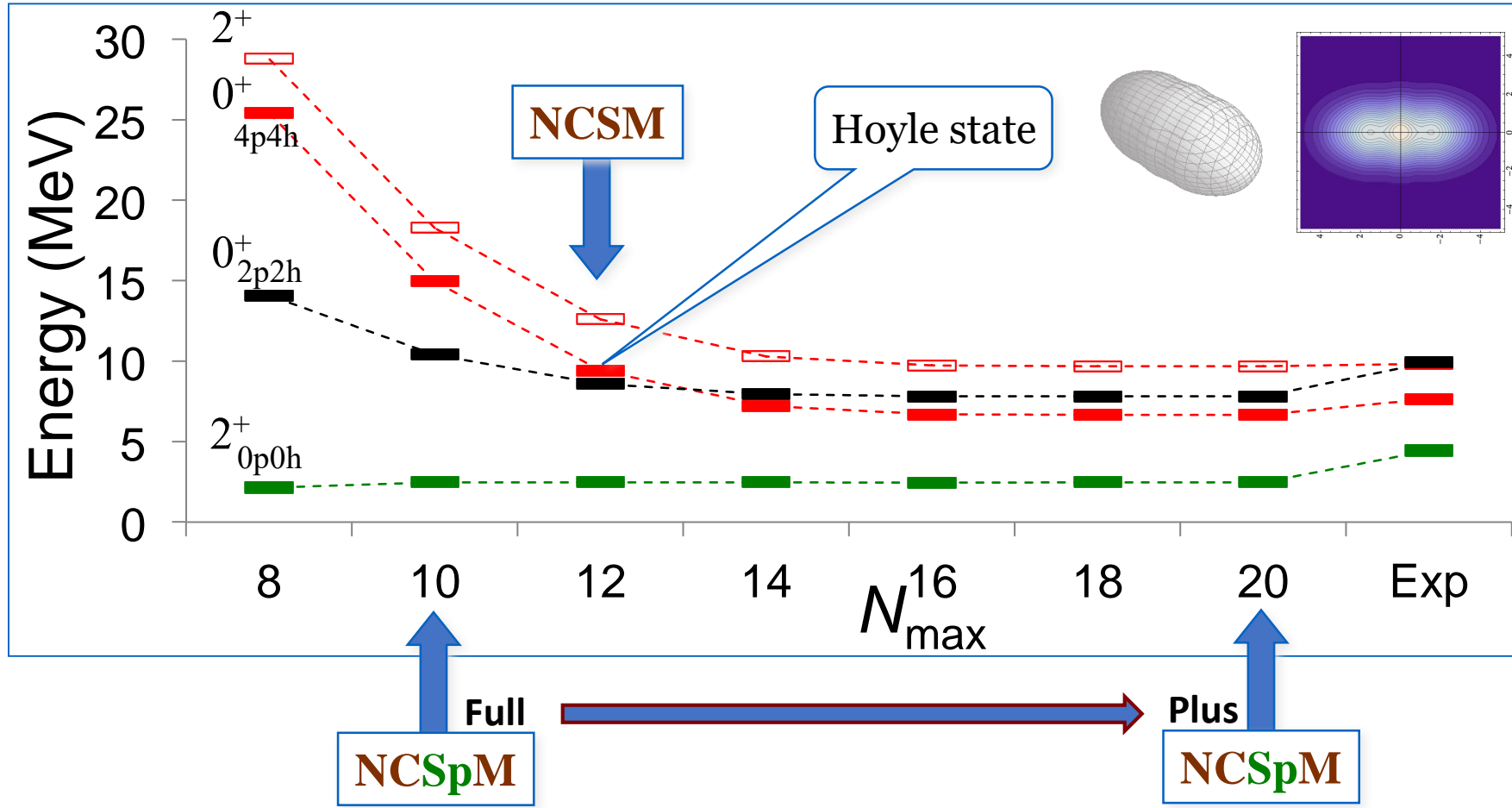


Three Primary 'Slices' within a NCSpM Description



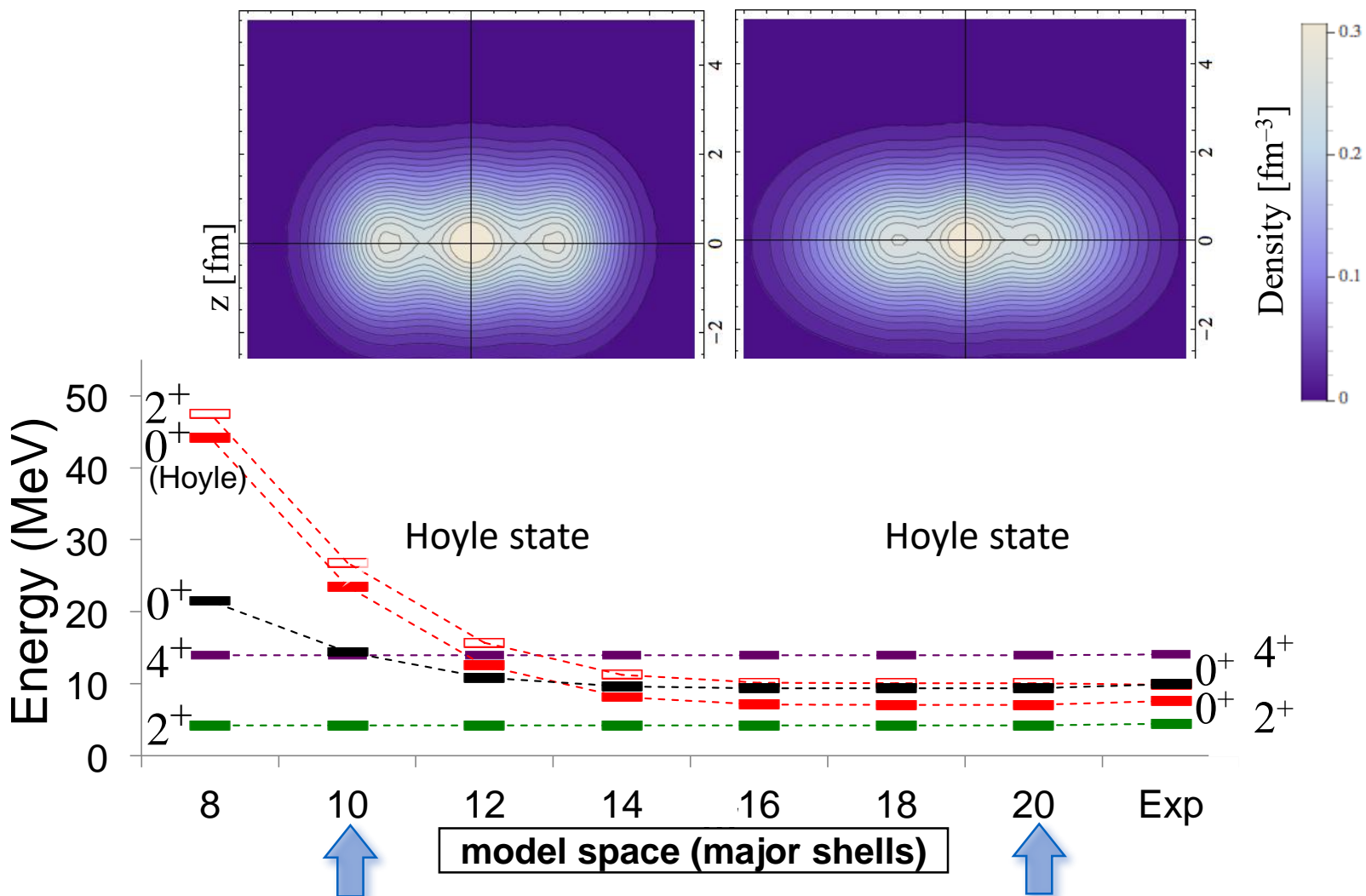
^{12}C Systematics as a Function of N_{add}

(N_{add} = Total Number of Excitations above Ground State)



^{12}C - Cluster Formations

(Now with mixing at the band-head level turned on ... !)

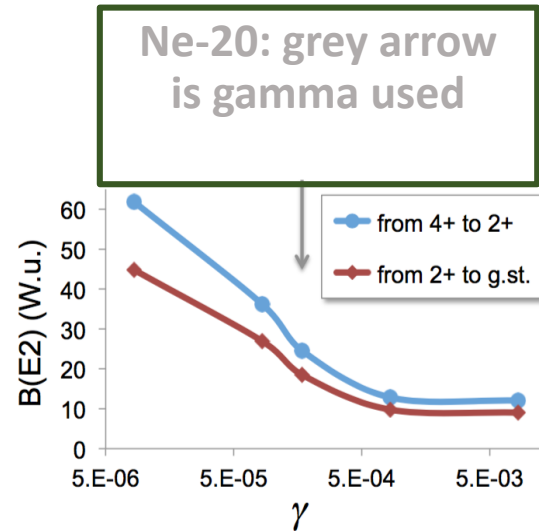


Standard ab initio NCSM

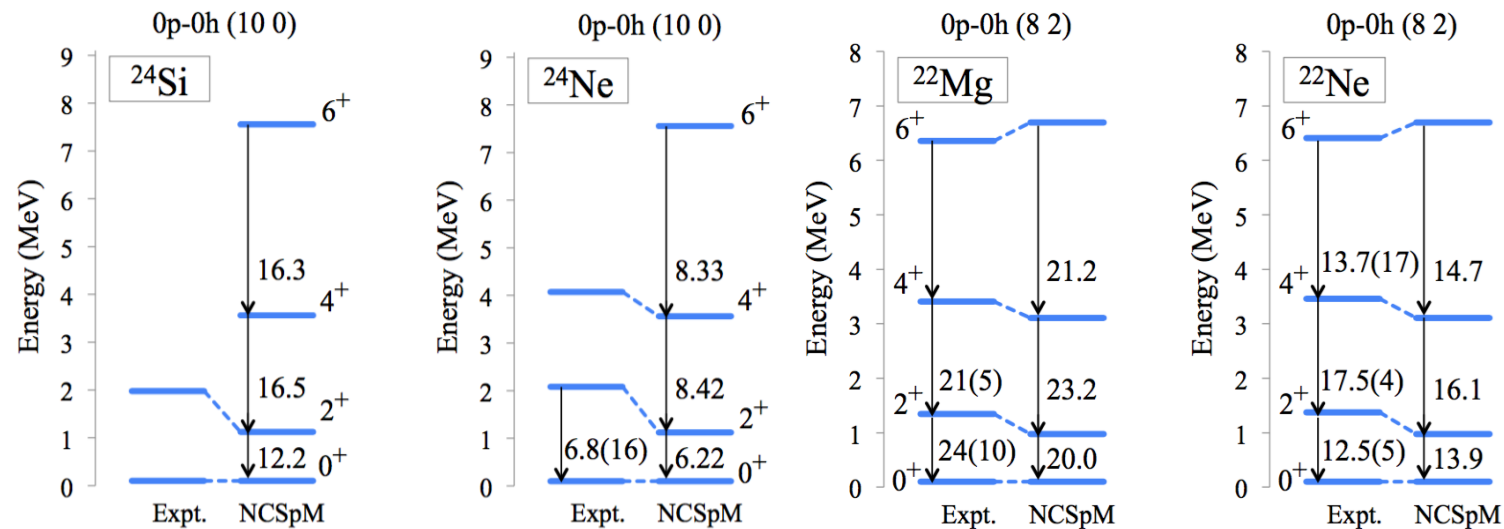
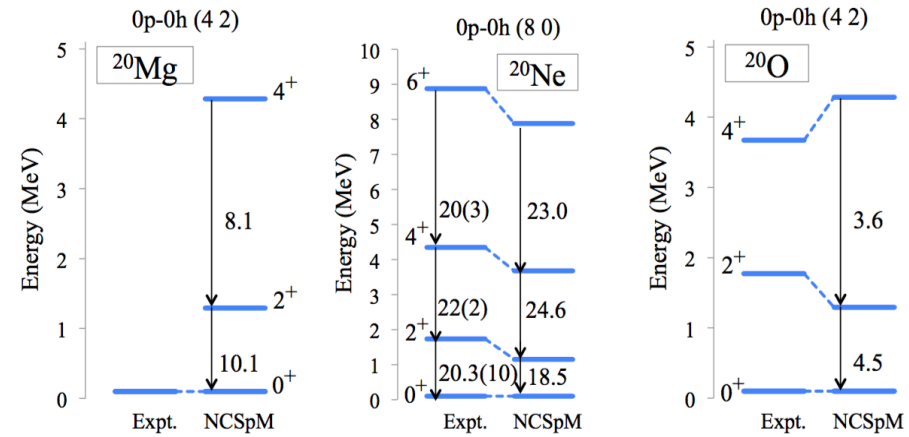
*(NCSpM & Band Mixing)



Medium Mass Nuclei (Gegory Tobin / REU Student)

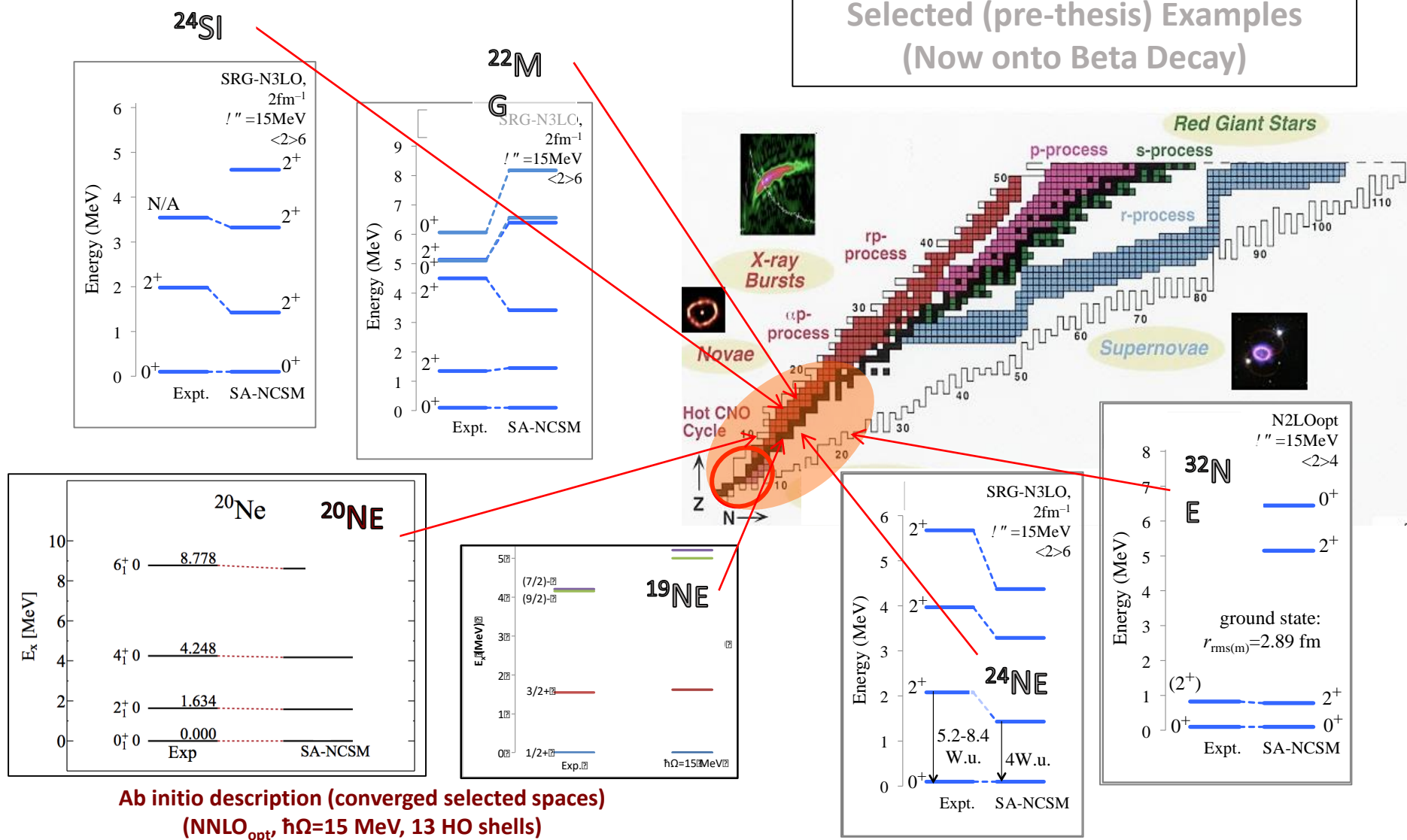


Almost "Laptop" Level Calculations!



Further sd-shell Results [Robert Baker – GS – Ohio U (Athens)]

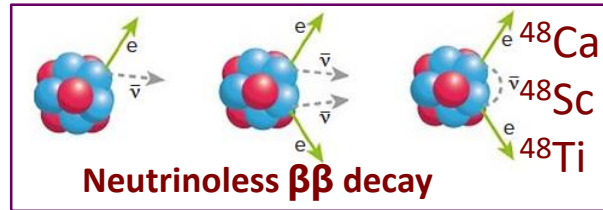
Selected (pre-thesis) Examples
(Now onto Beta Decay)



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



^{48}Ca



^{48}Ti

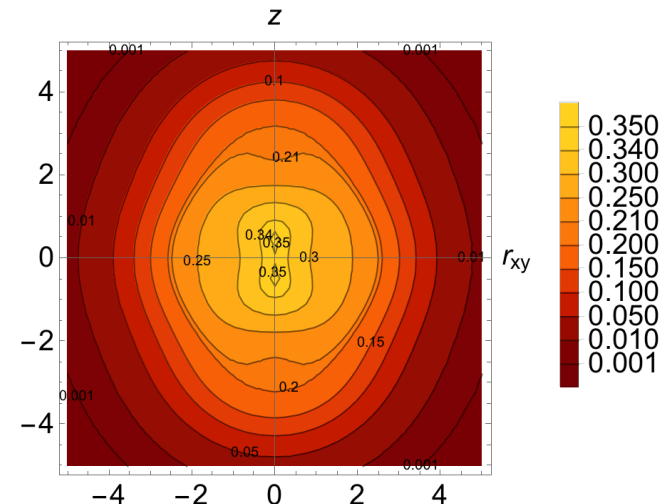
8 shells, N2LOopt
 0^+

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)	



Symplectic Effective Field Theory for Nuclear Structure Studies

(David Kekejian, Thesis Research @ LSU 10/21 & Currently Post Doc, UNC)

Generic (Scalar) Field Theory

Quantum (Scalar) Field Theory

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \varphi)(\partial^\mu \varphi) + \frac{1}{2} m^2 \varphi^2 \xrightarrow{\text{canonical quantization}} H = \sum_k E_k (b_k^+ b_k^- + \frac{1}{2})$$

$$\varphi(r, t) = \frac{1}{\sqrt{V}} \sum_k b_k^- \frac{1}{\sqrt{|2k^0|}} e^{-ik^\mu x_\mu} + \frac{1}{\sqrt{V}} \sum_k b_k^+ \frac{1}{\sqrt{|2k^0|}} e^{ik^\mu x_\mu}$$

$$\mathcal{L}^{(n)} = \frac{\alpha^n}{2(n+1)!} (\partial_\mu \varphi \partial^\mu \varphi^* + m^2 \varphi \varphi^*)^{n+1}$$

$$\mathcal{H}^{(n)} = \frac{\alpha^n}{2(n+1)!} (\dot{\varphi} \dot{\varphi}^* - \varphi' \cdot \varphi'^* + m^2 \varphi \varphi^*)^n ((2n+1) \dot{\varphi} \dot{\varphi}^* + \varphi' \cdot \varphi'^* - m^2 \varphi \varphi^*)$$

$$H^{(n)} \sim \left(\frac{\alpha}{V} \hbar \Omega\right)^n \times (g^2 Q \cdot Q)^n, (K \cdot K)^n, (gQ \cdot K)^n, (gK \cdot Q)^n \quad \text{Where: } \frac{\alpha}{V} \hbar \Omega = \frac{\beta^2}{8N_\sigma} \quad g = \frac{m^2}{\hbar^2 \omega^2}$$

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(DOI: 10.1103/PhysRevC.106.014304)

Kekejian (Thesis), Draayer & Mokeev, Roberts

Conclusion: Symplectic Symmetry emerges naturally from a quantum effective Field Theory!



Back to the Future: ~~Recent Examples and~~ Bridge Building

Nuclear (LE-QED) Discoveries!

Particle (HE-QCD) Challenges?

20th Century Subatomic Physics

Great Minds and Creative Models
Numerous Prestigious Awards Won
Major New Facilities Commissioned
Simplicity within Complexity Good
Analytic Solutions Well Regarded

- 100 -
Years

- 100 -
Years

Physics Changed Technology
1990s – HPC/ERA – 2010s
Technology Changed Physics

21st Century Subatomic Physics

Bigger Computers! -> Better Results?

Symmetries Important

Partial Symmetries Expose Coherent Features

Lunch (~5 years back) at JLab: 'Is the nucleon deformed (round)?'



Nucleons Communicate with one another via Scalar Fields!

Our job is to learn the grammar of that new language, perhaps in a `nucleon speakeasy' such as this meeting?

In any case, thanks to the organizers for their efforts in pulling this meeting together and letting me `speakeasy' (of perhaps `speakhard' for some ... sorry about details!

A special thank you to Craig Roberts and Volker Mokeev who kindly took our earliest ramblings on this seriously and have continued to proffer guidance ... sharing in a vision that there is value in seeking and finding simplicity within complexity!

Thanks to One & All!
From the extended (non-compact)
LSU Team



- Exploit the KISS (Keep It Simple Stupid) Principle! -

$$H = T(\text{kinetic Energy}) + V(\text{potential Energy})$$

$$V(\text{potential Energy}) = V(\text{rotor: } \sim Q \cdot Q) \ \& \ V(\text{pairs: } \sim N_s + \sim N_d + \dots) + V(\text{cross-couplings})$$

[Recall: Terms in "V" terms must be Rotational Scalars due to Isotropy of Space]

