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Dominance of Deformation in Nuclear Physics, a Link to Symplectic Symmetry, and Roots in Effective Field Theory

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Abstract: A brief historical review of the important role symmetries have played in our gaining a deeper understanding of nuclear structure is presented. We then focus our attention on the special role that symplectic symmetry plays in exposing a “Dominance of Deformation” that is observed through enhanced B(E2) rates across the Chart of the Nuclides, and in addition, we will show how the No-Core Symplectic Shell Model (NC-SpSM) seems to emerge from a Symplectic Effective Field Theory (Sp-EFT), where the latter prepares a path forward for potentially gaining a truly *ab initio* understanding of the structure of atomic nuclei. As space permits, various spectra, B(E2) transition rates, and nuclear radii of selected light to medium-mass nuclei are shown

Keywords No-Core Shell Model (NCSM), Symplectic (Sp-NCSM) and Symmetry-Adapted (SA-NCSM) versions of the NCSM, Symplectic Effective Field Theory (Sp-EFT) for Atomic Nuclei

INTRODUCTION

The subatomic physics timeline spans the 20th Century starting with the work of Ernest Rutherford [1] (England, Nobel Prize 1908) that led to the nuclear model of the atom that was advanced by his colleague Niels Bohr [2] (Denmark, Noble Prize 1922) who in 1913 proffered a text-book view of the structure of the atom, and ultimately led him into nuclear physics starting with a simple liquid-drop picture of nuclei, supporting vibrational as well as rotational modes and even nuclear fission. This was followed by two game-changing developments of the late 40s and early 50s; specifically, work built upon that of Niels Bohr by his son Aage Bohr and Ben Mottelson (Copenhagen School, Nobel Prize 1975, shared with Rainwater), known as the collective model of nuclear structure [3], and another based upon the pioneering work of Maria Goeppert-Mayer and J. Hans D. Jensen [4] (Noble Prize 1963, shared with Eugene Wigner) for advancing a particle-based shell-model view of nuclei, which in its simplest form places neutrons and protons in a three-dimensional harmonic oscillator (3D-HO) that is augmented with a spin-orbit and orbit-orbit interaction.

The evolution towards modern views of nuclear structure proceeded along two lines of discovery: quantization of a liquid-drop that rotates and vibrates - the Rotation-Vibration Model (RVM) that grew into the Generalized Collective Model [5] (GCM; Frankfurt School led by Walter Greiner in the 60s) along with associated mean-field efforts and attempts to expand the single-particle picture into a many-particle fermion-based shell model theory for atomic nuclei. The former required the quantization of the ‘nuclear fluid’, and the latter a discrete-particle picture that can give rise to the collective modes that were recognized as an integral part of the GCM. So going from the late 50s into the 60s the challenge was clear: Explain collective features in nuclei in terms to a many-body shell model theory, or vice-versa; that is, identify key features of a shell model theory that can expose collectivity in atomic nuclei, which is a call that continues to dominate the nuclear physics landscape.

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This led in 1958 to the development of the SU(3) shell-model [6] (British/Sussex School led by J.P. (Phil) Elliott, which showed that the valence space of a many-particle, three-dimensional harmonic-oscillator (3D-HO) based shell-model theory could be reorganized into irreducible representations (irreps) of SU(3), where its two (Casimir) invariants - one of 2nd and another of 3rd order - could be directly linked to the β (prolate) and γ (triaxial) measures of the collective model. The latter led to a search for algebraic approaches to nuclear structure, that relied on a group-theoretical framework with subgroup chains related to physical phenomena. What follows is an abbreviated recounting of the “rest of the story” for fermion-based shell-model theories.

EVOLUTION OF FERMION-BASED MODELS OF NUCLEAR STRUCTURE

This story line will be told below in a word only format: The single-particle picture of the late 40s and early 50s of the last century was one of two competing coupling schemes, one a so-called *jj*-coupling scheme and the other an *LS*-coupling scheme. The first is the easiest to describe as one can construct a properly anti-symmetrized set of basis states out of Slater determinants of all available single-particle states, where the angular momentum (\mathbf{l}) and spin (\mathbf{s}) of individual nucleons are coupled to total angular momentum $\mathbf{j} = \mathbf{l} + \mathbf{s}$, with the total angular momentum $\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2 + \dots + \mathbf{j}_n$ of a system (or subsystem) that is made up of n identical nucleons. Except for the proton, the usual case is an A(Z,N) nucleus, made up of Z protons and N neutrons with $A = Z+N$, in which case the total angular momentum is then $\mathbf{J}_A = \mathbf{J}_Z + \mathbf{J}_N$, a *np*-representation of the *jj*-coupling scheme, or one can move into an isospin representation in which case an isotopic spin is assigned to each nucleon ($t_z = +1/2$ for proton and $t_z = -1/2$ for neutrons) so the total isospin, $\mathbf{T}_A = \mathbf{T}_Z + \mathbf{T}_N$ where as for angular momentum $\mathbf{T}_X = \mathbf{t}_1 + \mathbf{t}_2 + \dots + \mathbf{t}_X$, enters as a direct product of the neutron and proton parts, which is the *np*-representation of the *jj*-coupling scheme. Antisymmetrization requirements are met within each sector as the protons and neutrons are distinguishable nucleons and not subject of the Pauli Exclusion Principle. The No-Core Shell Model (NCSM) is a modern (no-core) version of this type of theory [7].

The *LS*-coupling scheme is different as it separates the spatial part of the basis states from the spin and isospin parts that are typically handed in the same way, that is $\mathbf{L} = \mathbf{l}_1 + \mathbf{l}_2 + \dots + \mathbf{l}_A$, which is the total orbital angular momentum of the system, added to $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2 + \dots + \mathbf{s}_A$, which is total spin with $\mathbf{J} = \mathbf{L} + \mathbf{S}$. This alternative provides a direct first-step connection to the collective model picture: \mathbf{L} and \mathbf{S} logically connected to the \mathbf{L} of an ellipsoid in space that carries the spin \mathbf{S} . This is the first step, with two to follow below, for aligning the shell-model with the collective model through the exploitation of symmetries, in this case via SO(3) which is the rotation group in 3 dimensions. Note that this can also be achieved within an *np*-representation, with $\mathbf{L}_A = \mathbf{L}_Z + \mathbf{L}_N$ and $\mathbf{S}_A = \mathbf{S}_Z + \mathbf{S}_N$ just as above and then one can visualize the system as a two-rotor problem, one for the protons and another for neutrons. Such a picture is interesting because it gives rise to scissor plus twist modes of the two ellipsoids depending on their respective geometries, if both are axially symmetric, or only one or both triaxial. As above, this can also be managed within a spin-isospin framework which is called a Wigner Supermultiplet, [8]: $\{U_p(\text{space}) \times U_n(\text{space})\} \times \{SU_{ST}(4) \supset [SU_S(2) \times SU_T(2)]\}$.

While either of the above forms are valid and workable, a major game-changer came in 1958 with the introduction of the Elliott SU(3) model, wherein Elliott's recognition that the symmetry group of the three-dimensional harmonic oscillator (3D-HO) is SU(3), a rank 2 group with 2 invariants that track with irreducible representations (irreps) labels (λ, μ) that are integer variables that can be directly related to the (β, γ) variables of a collective model as shown in Figure 1.

This discovery represents one of two major leaps forward in nuclear structure studies, since for the first time one can now establish within a single-shell of the 3D-HO a mapping of ellipsoidal shapes of the collective model to irreps of SU(3), see Fig. 1. This connection raised the number of

contact points between the microscopic and collective models from just 1, the orbital angular momentum L labeling of the $SO(3)$ shell-model symmetry to 3, the first being L plus 2 new ones, these being shape variables of an ellipsoid of the collective model, where the (β, γ) to link is spelled out in Fig. 1. It is interesting to note that the number of generators of $SU(3)$ is 8, with 3 of the 8 being generators of the $SO(3)$ subgroup of $SU(3)$ and the other 5 associated with the transfer of quanta between the z , the x , and the y axes of the (λ, μ) -defined irrep of $SU(3)$.

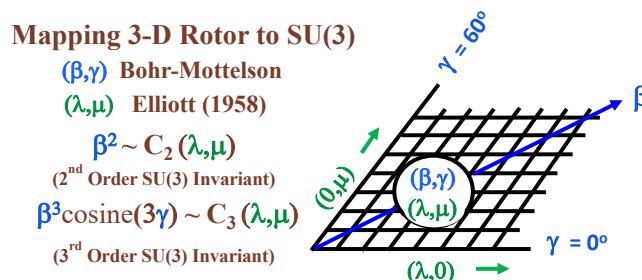


Fig. 1. Mapping continuous shape variables (β, γ) of an ellipsoid of revolution (collective model) onto a lattice of allowed discrete (λ, μ) values that label $SU(3)$ irreps of a microscopic theory.

This breakthrough called out a need for $SU(3)$ coupling and recoupling coefficients if the Elliott $SU(3)$ Model was to ever become a utilitarian theory. This need was met with the publication in 1973 of a $SU(3)$ Package [9] for calculating Wigner coupling and Racah recoupling coefficients for $SU(3)$, a FORTRAN code that stood the test of time for 45 years, but that I can now happily announce as having been overhauled and updated to a new C^{++} version published just this year [10], that represents another important step forward that is now publicly available and that provides a further incentive to continue efforts in support of the next major breakthrough in our story line.

Missing from the above picture is another “obvious” need, that remained “hidden in plain sight” because it seemed like a daunting task to move from the symmetry group of a single-shell of the 3D-HO to a multi-shell picture, since it was clear that this would be accompanied by an explosion in the overall dimensionality of the model space, and with the computer resource available in the 70s-80s there was no way to move to this direction - even if a new analytic theory could be put forward, as there would be no way to test it using *ab initio* interactions. Thankfully, this did not detour George Rosentsteel & David Rowe (R&R in what follows, George was a PhD student of David at that time), who published a breakthrough algebraic framework in 1977 [11] that built forward from the Elliott $SU(3)$ Shell Model. What was missing from the Elliott picture? One could say courage, but a kinder and more straightforward response is wiser: No matter what, it was clear that experimentally measured $B(E2)$ strengths would never be reproduced using a single-shell theory. So while the $SU(3)$ Shell Model results show them to be stronger than expected from simply a flat single-particle picture; it also showed that one could never reach experimentally measured values within such a framework. This was “swept under the rug” simply because introducing the concept of an effective charge that varied smoothly with nucleon numbers seemed to work surprising well, negating the need to address the real problem from a ground up perspective. Missing from this is strong couplings to the so-called giant resonances: an $E0$ mode (“S”, with $L=0$ character), and a $E2$ mode (“D”, with $L=2$ character) where the latter should not be confused with the “s” and “d” modes of very popular Interacting Boson Model (IBM) brought forward in 1975 by Arima and Iachello [12,13].

The solution is “obvious and simple”, so much so that it is also “brilliant”: Extend Elliott’s SU(3) to include Sp(3,**R**), which contains SU(3) as a subgroup, since it is the dynamic group of the 3D-HO, where the latter includes everything that is included in the Elliott SU(3) Model plus vertical excitations through the addition of 12 new $2\hbar\omega$ operators, 6 raising and 6 lowering, that act on any SU(3) irrep to add (or subtract) two harmonic oscillator quanta to the system. The latter is exactly what is needed to expand every single SU(3) irrep (each serving as a “band head” for the addition of zero up to an infinite number of such symplectic excitations) vertically to capture all the missing B(E2) strength. For this reason, Sp(3,**R**) is called a non-compact group. These excitations have, respectively, the SU(3) tensor character (2,0) for raising operators and (0,2) for lowering operators. So, adding the Sp(3,**R**) extension to the Elliott SU(3) Model represent a very significant advance that brings into the foreground the following key structure: $\text{Sp}(3,\mathbf{R}) \supset \text{U}(3) \supset [\text{U}(1) \times \text{SU}(3)] \supset \text{SU}(3) \supset \text{SO}(3)$ which has 21 generators as follows: 3 for SO(3), 8 for SU(3) that includes the 3 for its SO(3) subgroup, 9 for [U(1) X SU(3)] that adds in an operator that counts the total number of oscillator quanta to the 8 of SU(3), a necessary feature because in going up to Sp(3,**R**) from U(3) one adds oscillator quanta to the system. This a beautiful picture, which might at first blush seem scary, but in reality is simply the final missing group structure that clearly and directly flows for the underpinning physics of the 3D-HO and is directly tied to specific physical features of the system it represents.

While the length constraints on this document does not allow us to elaborate on this theme in greater detail, hopefully it is clear that the genius of Elliott complemented by that of R&R - taking all Elliott SU(3) band heads into account, spans the full (infinite space) to the 3D-HO. Fortunately, as I hope is exposed here - albeit in condensed form, this is the reason for proclaiming the “Dominance of Deformation” in the title of this paper as this feature is clearly dominant and it allows one to winnow down the infinite space to manageable subspaces tuned to where real nuclei choose to go land, exposing their structure in ways heretofore by-and-large overlooked.

Sp(3,**R**) & SA-NCSM RESULTS FOR VARIOUS EXEMPLAR APPLICATIONS

Space limitations require that this section is limited to two figures: Fig. 2 is included as an illustration and advertisement to students regarding what can be done once one keys in on the dominant features in play in nuclear physics. This figure was created early on to help build team spirit in what we had been working on for nearly two decades. It served as a learning exercise for the members of our team, including myself, regarding what was, and what now is, as well as what can be if we stay the course and methodically work each problem as it arises, underpinned with an assurance that the outcomes will represent what we believe to be a major step forward in our effort to advance an ab initio microscopic theory with potentially significant implications for our gaining a simple but comprehensive understanding of major features that define the low-energy structure of nuclei.

Fig. 3 tells another story [15]. It is a collage as well, but in this case, it represents a very serious dive into the structure of three representative nuclei shown in separate panels in the figure. In this case it is from the thesis work of Grigor Sargsyan (student recruited from Armenia, LSU PhD 2021). Grigor’s thesis supervisor is Kristina Launey (originally a Bulgarian student, and soon to be an Associate Professor at LSU). Grigor, with strong interest for high-performance computing, worked very closely with our team’s “Code Master” Tomas Dytrych (former Czech student, who is now back in the Czech Republic building his own group, and the “go-to” person on any and all questions regarding the development and use of what is now called SA-NCSM [16] - the Symmetry Adapted NCSM - which is publicly available - but if interested you should reach out to Tomas directly as he is - as suggested above - our “Code Master”, bringing advanced technologies forward as we continue to push our program forward, taking advantage of any and all options for speed-ups as well as exploring

for example possibilities for integrating AI (Artificial Intelligence) and QIS (quantum information science) concepts into future nuclear physics studies.

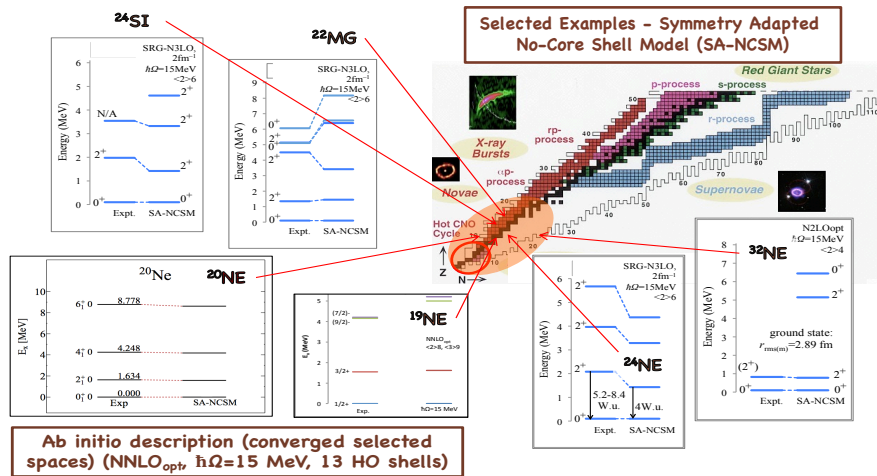


Fig. 2. A collage of examples [14], see also [15]; https://abinitio.triumf.ca/2016/Baker_TRIUMF_pres_final.pdf

I decided against adding a section on symplectic effective field theory (Sp-EFT), even though this was promised in the title, as that topic is based on the thesis work of David Kekejian, who is Armenian as well - a classmate of Grigor Sargsyan - since his thesis defense, which occurred early in December 2021 was not finalized at the time of my presentation so it would have been inappropriate for me to include his results prior to his defense and the acceptance of his thesis. (David Kekejian has as of the final review of this manuscript successfully defended and completed all requirements for a Ph.D. degree in Physics from LSU. A publication based on David's thesis work - with David as the first author - entitled "A Symplectic Effective Field Theory for Atomic Nuclei" should appear in the archives 1st Quarter of 2022.)

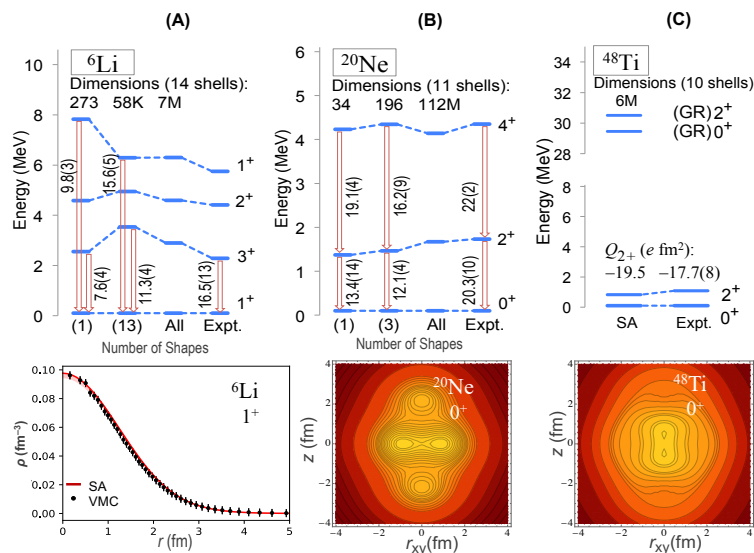


Fig. 3. $Sp(3,R)$ & SA-NCSM results for light (${}^6\text{Li}$ & ${}^{20}\text{Ne}$) medium (${}^{48}\text{Ti}$) mass nuclei. Shapes & dimensions indicated; radial density ${}^6\text{Li}$ & plane densities for ${}^{20}\text{Ne}$ & ${}^{48}\text{Ti}$.

CONCLUSION

I took you down the path I walked, sharing some of the lessons I've learned, stressed the importance of paying close attention to details - not overlooking what might appear to be a daunting task and encouraging each reader to be constantly looking for “gems” along the way that may be “hiding in plain sight” as this - small or big can make or break us as each forges forward down his/her personal scientific journey. In conclusion, I leave you with the following - a one-line equation - that tells a tale of developments in gaining a Fermion-based model of modern nuclear structure studies:

$$\text{Sp}(3, \mathbf{R}) \supset \text{U}(3) \supset [\text{U}(1) \times \text{SU}(3)] \supset \text{SU}(3) \supset \text{SO}(3)$$

Based on my experience as a student, postdoc - multiple times, and ultimately a professor, if a reader gets to this point and can explain in his/her own words the reason for each colored group [hint, work from right to left: blue to red (Elliott's Model), and then red and black to green (R&R Model)] in the above display, and address the “why and what” of each; that is, how each folds into a nuclear physics timeline, and the specific role each plays individually and with respect to the whole of nuclear theory. I believe it is safe to say a reader who can do this in his/her own voice should have a reasonably good understanding of modern 21st Century nuclear theory and therefore a person of interest that I as well as many of my colleagues would be interested in working with either as a student, postdoc, or visiting scholar, support permitting!

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