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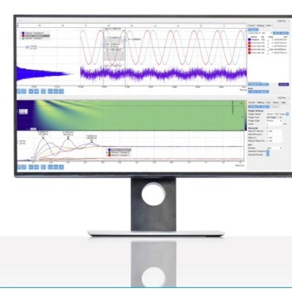

Symmetries and Canonical Transformations in Nuclei

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Abstract. We begin with a brief historical overview of the importance of special symmetries in atomic nuclei, especially the symplectic symmetry. We then show how deforming the symplectic algebra through canonical transformations that are unitary can be used to describe the same physics that in a non-deformed picture requires huge model spaces in far smaller deformed spaces, a simplification that should proportionally reduce the complexity of using the symplectic symmetry in applications. The overarching objective is to exploit this strategy to probe more deeply into the (*ab initio*) structure of nuclei, short cutting a need to await the development of evermore robust computational resources for carrying out advanced microscopic nuclear structure investigations.

INTRODUCTION

Symmetries are essential to understanding emergent phenomena in nuclear physics. They offer insight into important physical properties of nuclei and help us reduce the size of the nuclear problem by identifying the most relevant degrees of freedom that give rise to those symmetries. Perhaps the most important of these symmetries is the SU(3), the symmetry of the harmonic oscillator (HO), which is central to the Elliott Model [1], the first theory to simply reveal rotational collectivity within a microscopic shell model framework. One can find its roots in the Nilsson Model [2] which is a deformed version of the single-particle spherically symmetric HO, where the deformation is achieved by adding a quadrupole-quadrupole interaction ($Q \cdot Q$) to a very simple one-body HO dominated Hamiltonian. The Elliott model is a many-particle theory that replaces Q with Q^a, which is the single-shell preserving algebraic part of the total quadrupole operator. While Q reduces to Q^a within a single shell, it includes couplings to neighboring shells, couplings that are essential for building up collectivity that is required to reproduce observed strongly enhanced B(E2) strengths in nuclei. Including the total quadrupole moment in the algebra elevates the Elliott Model to the far more complex and intriguing symplectic model, Sp(3,$\mathbf{R}$). The primary focus of this paper is on a simplification of the latter via a canonical transformation of its underpinning algebra.

The Interacting Boson Model (IBM) developed by Arima and Iachello [3, 4] is another very insightful algebraic theory that treats nucleons as bosons and offers a very good description of low-lying states in even-even nuclei in terms of representations of a U(6) boson framework. The latter is a relatively simple algebraic theory that can be used to describe rotational and vibrational spectra in nuclei in terms of subgroup limits – U(5) for vibrations, O(6) for triaxial shapes, and SU(3) [not to be confused with SU(3) of the Elliott Model] for rotations – of this U(6) boson structure. The beauty and power of this approach and its various extensions is that it allows one to readily describe a broad spectrum of nuclei and nuclear phenomena in the simplest of terms. In short, the IBM stands in sharp contrast to the far more complex multi-shell symplectic theory, which in its simplest limit is a true many-particle generalization of the Nilsson Model. The advantage of the latter is that it proffers an opportunity for us to study nuclei from an *ab initio* (first principles) perspective. However, significant to both – whether bosonic or fermionic in nature, is the insight that one can gain regarding the structure of atomic nuclei through the use of special symmetries.

Symplectic symmetry plays a dominant role in nuclear dynamics. Numerous studies reveal that a few irreducible representations (irreps) of Sp(3,$\mathbf{R}$) are sufficient to capture typically in excess of 80% of the relevant physics in nuclei [5, 6]. Studies using the No-Core Symplectic Shell Model (NCSpM) [7, 8] show convergence to measured B(E2) values without the use of effective charges, with the corresponding energy spectra in light up to intermediate-mass nuclei also in remarkably good agreement with experiment. The importance of symplectic symmetry has also been

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confirmed through fully *ab initio* symmetry-adapted no-core shell-model (SA-NCSM) studies up through medium-mass nuclei using symmetry-adapted SU(3) coupled basis states [9, 10, 11, 12].

Furthermore, it has been shown by Moshinsky [13] that Sp(3,**R**) is the group of linear canonical transformations in phase space. We use this fact to define a linear unitary canonical transformation that maps the generators of the sp(3,**R**) algebra into a deformed equivalent set while preserving the symplectic symmetry and argue that a deformed basis tailored to capture the observed deformation and collective properties of real nuclei should enable one to capture the dominant physics of an *ab initio* inspired Hamiltonian in relatively small model spaces, thus saving computational resources while extending the reach of more traditional NCSM [14] applications that skirt the use of special symmetries, relying instead on the Hamiltonian to sort out relevant subspaces of the full model space, an approach that quickly runs up against the exponential grow of model spaces with increasing particle numbers and the number of major shells included in an analysis.

The Symplectic Symmetry Group and the sp(3,R) Algebra

The Sp(3,**R**) symmetry group [15, 16], is an approximate symmetry of the nuclear Hamiltonian. However, as noted above, it extends the simplest Elliott SU(3) picture by including the physical quadrupole operator Q_{ij} rather than the more restricted algebraic Q^a_{ij} one so that the action is not limited to a single-shell picture but incorporates couplings to the neighboring HO shells. In addition to the three angular momentum operators L_{ij} and six mass quadrupole operators Q_{ij}, the Sp(3,**R**) also includes six symmetric vorticity operators S_{ij} which describe the deformation flow in nuclei and six symmetric kinetic energy operators K_{ij}. Altogether these 21 generators form a Lie algebra of the symplectic group Sp(3,**R**), which is the group of all possible real linear transformations of a nucleon's six position and momentum coordinates such that the overarching Heisenberg algebra is preserved:

$$[q_{in}, p_{jn}] = i\delta_{ij}. \tag{1}$$

where i, j=1,2,3 and n denotes the n-th nucleon. The generators of the sp(3,**R**) algebra, within this formulation, are expressed in the following way

$$Q_{ij} = \sum_n^A q_{in}q_{jn}, \tag{2}$$

$$K_{ij} = \sum_n^A p_{in}p_{jn}, \tag{3}$$

$$L_{ij} = \sum_n^A \left(q_{in}p_{jn} - q_{jn}p_{in}\right), \tag{4}$$

$$S_{ij} = \sum_n^A \left(q_{in}p_{jn} + p_{in}q_{jn}\right). \tag{5}$$

where A is the total number of nucleons. It is also possible to express this set of generators in terms of the raising and lowering HO ladder operators b^+_{in} and b_{in} where the former creates the n-th nucleon in the i-th direction and the latter annihilates it. These operators are defined as follows:

$$q_{in} = \frac{1}{\sqrt{2\omega}}(b^+_{in} + b_{in}), \tag{6}$$

$$p_{in} = i\sqrt{\frac{\omega}{2}}(b^+_{in} - b_{in}). \tag{7}$$

where ω is the oscillator length and $\hbar = m = 1$ for simplicity. Then, the symplectic generators are given by

$$Q_{ij} = (2Q^a_{ij} + A_{ij} + B_{ij})/2, \tag{8}$$

$$K_{ij} = (2Q^a_{ij} - A_{ij} - B_{ij})/2, \tag{9}$$

$$L_{ij} = -i(C_{ij} - C_{ji}), \tag{10}$$

$$S_{ij} = i(A_{ij} - B_{ij}). \tag{11}$$

where

$$A_{ij} = \sum_{n}^{A} b^+_{in} b^+_{jn}, \tag{12}$$

$$B_{ij} = \sum_{n}^{A} b_{in} b_{jn}, \tag{13}$$

$$Q^a_{ij} = (C_{ij} + C_{ji})/2, \tag{14}$$

$$C_{ij} = \sum_{n}^{A} (b^+_{in} b_{jn} + b_{jn} b^+_{in})/2. \tag{15}$$

All the operators mentioned above are written in their Cartesian representation. One can also cast them as spherical tensors [17] or express them in terms of fermion creation and annihilation operators [18].

It should be clear from this discussion that unlike the Elliott Model which is a 'compact' algebraic theory with basis states that are confined to a single HO shell, the Symplectic Model, which is simply a reorganization of the Shell Model (SM), is a 'non-compact' algebraic theory, with basis states that are infinite in number because its defining algebra structure includes raising operators (A_{ij}) that add (create) a pair of HO quanta to the system as well as lowering (B_{ij}) operators that subtract (annihilate) a pair of HO quanta from the system, in addition to the subset of generators L_{ij} and Q^a_{ij} of the Elliott su(3) algebra that only act within a single HO shell. This hierarchical symplectic structure, which maps the SM onto the symplectic model – a non-trivial but faithful reorganization of basis states of the former, is a key feature of the theory, one that can be used to parse the entire (infinite) HO shell-model space into a collection of symplectic subspaces each of which is itself infinite in size.

Unitary Canonical Transformations of the sp(3,R) Algebra

Classically, canonical transformations are transformations that preserve the Poisson brackets between the coordinates and momenta

$$\left\{q_i, p_j\right\} = \left\{\widetilde{q}_i, \widetilde{p}_j\right\} = \delta_{ij}. \tag{16}$$

This definition can be generalized for the quantum mechanical case as a transformation that preserves the commutation relation between the coordinate and momentum operators

$$[q_i, p_j] = [\widetilde{q}_i, \widetilde{p}_j] = i\delta_{ij}. \tag{17}$$

Further, in classical mechanics, a canonical transformation is a unitary transformation. However, this is not necessarily the case for the quantum case [19]. In quantum mechanics, a canonical transformation can be unitary or non-unitary [20, 21]. Here, for constructing a deformed basis, we will limit ourselves to unitary transformations.

Now we define the following unitary canonical transformations

$$\widetilde{q}_i = \frac{1}{\sqrt{\epsilon_i}} q_i, \tag{18}$$

$$\widetilde{p}_i = \sqrt{\epsilon_i} p_i. \tag{19}$$

where '$\sim$' denotes the quantities in the canonically deformed space, and the ϵ_i's are the deformation parameters (real positive quantities) that define the specifics of the transformation. The physical implication of ϵ_i depends on the system being studied. If we choose $\epsilon_i = \omega/\omega_i$ where ω_i is the HO frequency in the $i - th$ direction then ϵ_i could be interpreted as a deformation parameter that transforms the non-deformed canonical set (q_i, p_i) into the deformed canonical set $(\widetilde{q_i}, \widetilde{p_i})$. It is important to note that these canonical transformations not only preserve the Heisenberg algebra, but also preserve the symplectic algebra [22]. This means that the commutation relations between all of the symplectic generators in the deformed space is the same as in the non-deformed space, and so, for example, the deformed symplectic algebra closes under commutation just as the non-deformed algebra does.

Since the symplectic generators could be expressed in terms of raising and lowering operators, see Eqs.(8-11), one needs to define the deformed equivalent of those operators in such a way that the symplectic algebra and its underlying Heisenberg algebra are preserved. To do this we define the deformed operators in the following way

$$\widetilde{b}^+_{in} = \frac{1}{2}\left(\frac{1}{\sqrt{\epsilon_i}}\left(b^+_{in} + b_{in}\right) + \sqrt{\epsilon_i}\left(b^+_{in} - b_{in}\right)\right), \tag{20}$$

$$\widetilde{b}_{in} = \frac{1}{2}\left(\frac{1}{\sqrt{\epsilon_i}}\left(b^+_{in} + b_{in}\right) - \sqrt{\epsilon_i}\left(b^+_{in} - b_{in}\right)\right). \tag{21}$$

It is easy to see that the canonical tranformations in Eqs.(20,21) are equivalent to Eqs.(18,19), and therefore

$$[b_{in}, b^+_{jn}] = [\widetilde{b}_{in}, \widetilde{b}^+_{jn}] = \delta_{ij}. \tag{22}$$

which are equivalent to Eq.(17).

The canonical transformations defined in Eqs.(18,19) are symmetric with respect to inverse transformations. The inverse transformations are achieved if one removes '$\sim$' from the deformed quantities and adds it to the non-deformed quantities and then flips the deformation coefficients. To demonstrate this we apply this procedure of inverse transformation on Eqs.(18,19). In Eqs.(18,19) we can make the substitution ($\widetilde{q_i} \rightarrow q_i, \widetilde{p_i} \rightarrow p_i$.), then flip the coefficients $\frac{1}{\sqrt{\epsilon_i}} \rightarrow \sqrt{\epsilon_i}$, $\sqrt{\epsilon_i} \rightarrow \frac{1}{\sqrt{\epsilon_i}}$ and we will get

$$q_i = \sqrt{\epsilon_i}\widetilde{q_i}, \tag{23}$$

$$p_i = \frac{1}{\sqrt{\epsilon_i}}\widetilde{p_i}. \tag{24}$$

which are the inverse transformations. The fact that the canonical transformations defined in Eqs.(18,19) are symmetric with respect to an inverse transformation suggests that the canonical sets (q_i, p_i) and $(\widetilde{q_i}, \widetilde{p_i})$ are mathematically equivalent. The fact that we chose to call the former set non-deformed and the latter deformed is purely formal and is done for clarity. This is also evident from the fact that the canonical transformations defined above are unitary. However, the physical significance of those transformations come from the fact that one can represent the canonical set (q_i, p_i), defined in an infinite phase space through mapping it onto a canonical set $(\widetilde{q_i}, \widetilde{p_i})$ that is defined in a relevant finite phase space achieved by a careful selection of the deformation parameters ϵ_i.

In order to demonstrate this let us first define the deformed equivalent of the symplectic operators given in Eqs.(12-15) as

$$\widetilde{A}_{ij} = \sum_n^A \widetilde{b}^+_{in}\widetilde{b}^+_{jn}, \tag{25}$$

$$\widetilde{B}_{ij} = \sum_n^A \widetilde{b}_{in}\widetilde{b}_{jn}, \tag{26}$$

$$\widetilde{C}_{ij} = \sum_n^A (\widetilde{b}^+_{in}\widetilde{b}_{jn} + \widetilde{b}_{jn}\widetilde{b}^+_{in})/2. \tag{27}$$

By plugging Eqs.(20,21) into Eqs.(25-27), using the fact that $B_{ij} = A^+_{ij}$, $C_{ij} = C^+_{ji}$ and that the same holds for their deformed equivalents, we obtain a relationship between the deformed and non-deformed symplectic operators

$$\widetilde{A}_{ij} = \frac{1}{4}\left(\frac{1}{\sqrt{\epsilon_i\epsilon_j}}(A_{ij}+B_{ij}+C_{ij}+C_{ji})+ \sqrt{\frac{\epsilon_j}{\epsilon_i}}(A_{ij}-B_{ij}-C_{ij}+C_{ji})+ \sqrt{\frac{\epsilon_i}{\epsilon_j}}(A_{ij}-B_{ij}+C_{ij}-C_{ji})+ \sqrt{\epsilon_i\epsilon_j}(A_{ij}+B_{ij}-C_{ij}-C_{ji})\right), \tag{28}$$

$$\widetilde{B}_{ij} = \frac{1}{4}\left(\frac{1}{\sqrt{\epsilon_i\epsilon_j}}(A_{ij}+B_{ij}+C_{ij}+C_{ji})+ \sqrt{\frac{\epsilon_j}{\epsilon_i}}(-A_{ij}+B_{ij}+C_{ij}-C_{ji})+ \sqrt{\frac{\epsilon_i}{\epsilon_j}}(-A_{ij}+B_{ij}-C_{ij}+C_{ji})+ \sqrt{\epsilon_i\epsilon_j}(A_{ij}+B_{ij}-C_{ij}-C_{ji})\right), \tag{29}$$

$$\widetilde{C}_{ij} = \frac{1}{4}\left(\frac{1}{\sqrt{\epsilon_i\epsilon_j}}(A_{ij}+B_{ij}+C_{ij}+C_{ji})+ \sqrt{\frac{\epsilon_j}{\epsilon_i}}(-A_{ij}+B_{ij}+C_{ij}-C_{ji})+ \sqrt{\frac{\epsilon_i}{\epsilon_j}}(A_{ij}-B_{ij}+C_{ij}-C_{ji})+ \sqrt{\epsilon_i\epsilon_j}(-A_{ij}-B_{ij}+C_{ij}+C_{ji})\right), \tag{30}$$

$$\widetilde{C}_{ji} = \frac{1}{4}\left(\frac{1}{\sqrt{\epsilon_i\epsilon_j}}(A_{ij}+B_{ij}+C_{ij}+C_{ji})+ \sqrt{\frac{\epsilon_j}{\epsilon_i}}(A_{ij}-B_{ij}-C_{ij}+C_{ji})+ \sqrt{\frac{\epsilon_i}{\epsilon_j}}(-A_{ij}+B_{ij}-C_{ij}+C_{ji})+ \sqrt{\epsilon_i\epsilon_j}(-A_{ij}-B_{ij}+C_{ij}+C_{ji})\right). \tag{31}$$

Equations (28-31) show that any operator that belongs to the deformed set of operators $\left(\widetilde{A}_{ij}, \widetilde{B}_{ij}, \widetilde{C}_{ij}\right)$ are a superposition of all the other operators that belong to the non-deformed set $\left(A_{ij}, B_{ij}, C_{ij}\right)$ and because of the symmetrical property of the inverse transformation, the opposite is also true. It should be clear from these results that one can map any symplectic-symmetry-preserving Hamiltonian onto another so long as the two can be linked to one another through a unitary canonical transformation, for example – for cases under consideration – from a non-deformed picture to its deformed equivalent, or vice-versa. More generally, this should allow one to capture the dominant features of any quadratic-deformation driving Hamiltonian in a smaller model space through an appropriate choice of the deformation parameters. Our expectation – yet to be manifestly demonstrated – is that the long-range features of the quadratic (E2) electromagnetic interaction that drives the need for higher $N_{\max}$ values, where $N_{\max}$ is the maximum number of HO excitations (quanta) allowed in a given model space, in a non-deformed representation can in this way be captured within lower deformed model spaces.

Many-Body Harmonic Oscillator Hamiltonian in terms of Deformed Symplectic Operators

Consider the many-body HO Hamiltonian and express it in terms of the deformed symplectic operators in $\hbar\omega$ units

$$H = \sum_i C_{ii} = \frac{1}{4}\left(\epsilon_i(\widetilde{A}_{ii} + \widetilde{B}_{ii} + 2\widetilde{C}_{ii}) + \frac{1}{\epsilon_i}(-\widetilde{A}_{ii} - \widetilde{B}_{ii} + 2\widetilde{C}_{ii})\right). \tag{32}$$

where for simplicity, ϵ_x=ϵ_y with the constraint $\epsilon_x\epsilon_y\epsilon_z = 1$ which implies volume conservation of the system. Then Eq.(32) reduces to

$$H = \frac{1}{4}\left((\epsilon_z - \frac{1}{\epsilon_z})(\widetilde{A}_{zz} + \widetilde{B}_{zz}) + +2(\sqrt{\epsilon_z} + \frac{1}{\sqrt{\epsilon_z}})(\widetilde{C}_{xx} + \widetilde{C}_{yy}) + 2(\epsilon_z + \frac{1}{\epsilon_z})\widetilde{C}_{zz}\right). \tag{33}$$

Diagonalizing the Hamiltonian in Eq.(33) for a single particle within a model space of $N_{\max} = 2$ and $N_{\max} = 4$ we get results shown in Figure 1. While one would expect all the eigenvalues to be independent of ϵ_z, Fig.1 shows a slight dependence of the eigenvalues on ϵ_z. This is because we are attempting to map from an infinite Hilbert space onto a finite Hilbert space, which one can only do approximately by going to higher and higher $N_{\max}$ values; that is, the transformation from the non-deformed to deformed set of operators is not truly a unitary one. To get a unitary transformation, that will be independent of ϵ_z, one has to map it onto infinite deformed basis states which is not possible, but as the figures show, with increasing $N_{\max}$ the results seem to converge very nicely to the low-lying eigenvalues by the time $N_{\max} = 4$.

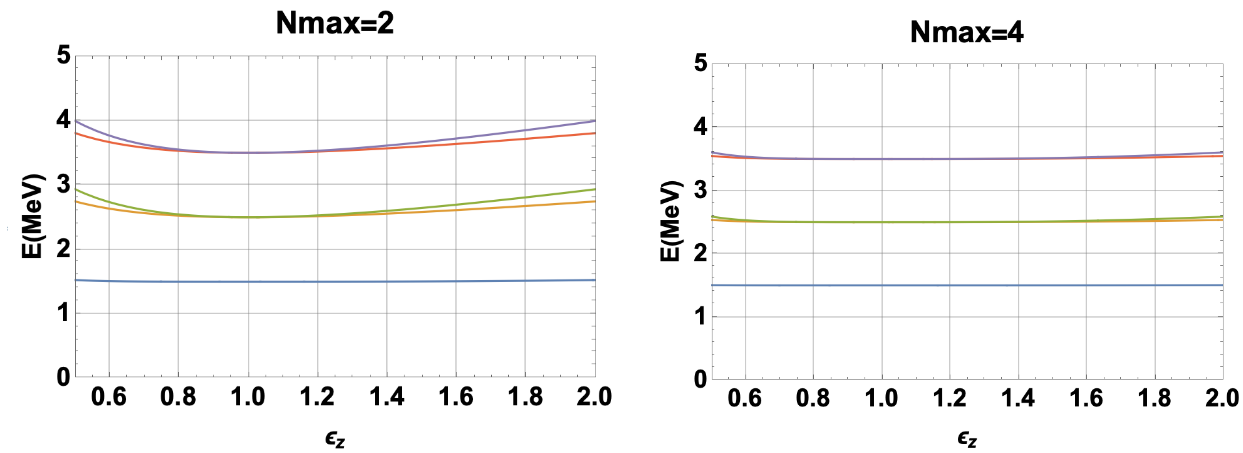

FIGURE 1: The eigenvalues (in $\hbar\omega$ units) of a 3D spherical HO as a function of ϵ_z in the deformed model spaces of N_{max}=2 (a) and N_{max}=4 (b).

Note that when we applied the canonical transformations to the harmonic oscillator Hamiltonian in Eq.(32) the operator C_{ii} includes the zero point energy or the so-called vacuum energy in its definition (Eq. 15). It is usually common practice in quantum mechanics and quantum field theories to renormalize the energy by discarding the vacuum contribution to the energy since it has no physical meaning. However, the vacuum term should be included when applying canonical transformations because it is part of the symplectic algebra sp(3,**R**). In order to unitarily map the symplectic operators to their deformed counterparts one also needs to map the vacuum to its deformed counterpart. After the mapping one could renormalize the energy by throwing away the deformed vacuum. The vacuum term in C_{ii} for a single particle is $\frac{3}{2}$ which, after applying the canonical transformation becomes $6(\sqrt{\epsilon_z} + \frac{1}{\sqrt{\epsilon_z}}) + 3(\epsilon_z + \frac{1}{\epsilon_z})$ for ϵ_x=ϵ_y and $\epsilon_x\epsilon_y\epsilon_z = 1$.

CONCLUSIONS

In this paper we briefly revisited the importance of special symmetries in nuclear physics, whether within a bosonic or fermionic framework, and then focused in on the symplectic extension of the Elliott Model as a model of choice for gaining reasonable *ab initio* results within relatively small model spaces. We then examined the quantum equivalent of a canonical transformation for mapping the non-deformed symplectic algebra onto its deformed counterpart, and vice-versa; and within that framework advanced a unitary canonical transformation that preserves the symplectic symmetry and in so doing established the theoretical underpinning of a deformed symplectic model that is the logical extension of a many-particle generalization of the Nilsson Model. We also noted the obvious, but illusive fact that throughout these consideration it is very important to take proper account of zero-point energy of the HO and its deformed counterpart.

We went on to show that, within this framework, one can recover the eigenvalues of the non-deformed HO in the deformed basis, with good convergence across a broad spectrum of the deformation parameters. The new development presented here portends well for extensions of the non-deformed NCSpM and the SA-NCSM with their respective codes to their deformed counterparts. Within this framework one expects to realize the effects of higher N_{max} configurations of non-deformed calculations at lower N_{max} values, which could serve to further reduce model space requirements and therefore also further reduce the computational challenges of the theory which should simultaneously allow for an extension of the use of these models and the associated codes for even heavier nuclei, all of which should be doable within the context of existing computational resources.

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