Progression towards an effective shell-model theory of rotational nuclei

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Abstract. A goal of nuclear physics is to determine the validity of the nuclear shell model and to express the various models of nuclear phenomena as sub-models of this model. It is also profitable to start from a phenomenological model interpretation of nuclear data and use the results to design an effective shell-model description of the data. This paper suggests a method for deriving effective shell-model spaces for rotational nuclei and indicates that new methods are needed for deriving effective interactions for rotational nuclei.

1. Introduction
As a practical matter, it is necessary to restrict nuclear shell-model calculations to finite-dimensional subspaces of the full many-nucleon Hilbert space and to treat the nucleons as elementary particles. Thus, the interactions between the nucleons of the shell model are effective interactions and the properties of calculated shell-model states must be interpreted in terms of appropriate effective operators.

An A-nucleon Hilbert space is an anti-symmetrised, i.e., exterior, product,

\[ \mathcal{H}^{(A)} = \mathcal{H}^{(1)} \wedge \mathcal{H}^{(1)} \wedge \cdots \wedge \mathcal{H}^{(1)}, \ A \text{ copies}, \]

of single-nucleon Hilbert spaces. To facilitate the separation of the centre-of-mass component of \( \mathcal{H}^{(A)} \), and exploit the symmetry properties of the many sub-models of the shell model, it is convenient to define basis wave functions for \( \mathcal{H}^{(A)} \) in terms of anti-symmetric products of single-nucleon harmonic-oscillator wave functions.

Derivations of effective shell model operators on a finite-dimensional subspace of \( \mathcal{H}^{(A)} \) proceed in essentially two steps. The first step restricts the single-nucleon space, \( \mathcal{H}^{(1)} \), to a (very) large but finite-dimensional subspace, \( \mathcal{H}^{(1)} \subset \mathcal{H}^{(1)} \). Because two- and three-nucleon problems can be solved to a high degree of accuracy with bare-nucleon interactions, it is possible to derive an effective Hamiltonian, \( \tilde{H}^{(A)}_{\text{eff}} \), appropriate for the truncated many-nucleon space, \( \tilde{\mathcal{H}}^{(A)} = \tilde{\mathcal{H}}^{(1)} \wedge \tilde{\mathcal{H}}^{(1)} \wedge \cdots \), with the understanding that the effective three- and more-nucleon interactions generated from bare two-nucleon interactions are negligible provided the truncated subspace \( \tilde{\mathcal{H}}^{(1)} \) is sufficiently large (cf. [1] for a review of methods). The second step is to derive the effective interactions and operators appropriate for the chosen effective A-nucleon shell-model space, \( \tilde{\mathcal{H}}^{(A)}_{\text{eff}} \), for which calculations are to be carried out.

This talk addresses the question of how the effective space \( \tilde{\mathcal{H}}^{(A)}_{\text{eff}} \) should be chosen. Calculations to date have generally adopted the strategy of ordering the many-particle configurations by
increasing energy with respect to the conventional spherical harmonic-oscillator independent-particle shell model Hamiltonian with a spin-orbit interaction. The effective shell-model space is then chosen to be that spanned by as many of the lowest-energy configurations as can be handled. This makes sense for many states of light nuclei and medium-light singly-closed-shell nuclei which appear to be spherical in their lowest-energy states. However, there is much evidence to show that even the so-called spherical nuclei exhibit highly-deformed rotational states at low excitation energies [2, 3]. These states are commonly described as intruder states and are associated with higher-energy harmonic-oscillator configurations that are not included in the standard effective shell-model space. In fact, it appears that such higher-energy harmonic oscillator configurations become the lowest-energy states in doubly-open shell nuclei. Thus, ordering shell-model subspaces by increasing energies with respect to a spherical harmonic-oscillator Hamiltonian with spin-orbit interactions appears to be inappropriate for the majority of doubly-open shell nuclei, which are deformed and exhibit rotational structure.

Much of what I have to say in addressing these questions has been known for 30 years. However, only recently has its relevance to effective interaction theory [4] and the widely observed phenomenon of shape coexistence [2, 3] become apparent.

2. The Bohr model and its microscopic extension
Collective vibrational and rotational states have been successfully interpreted in terms of collective models based on the Bohr model [5]. The latter is an incompressible liquid drop with a sharply-defined surface defined by a set of deformation parameters, \( \alpha_{\lambda\nu} \), in an expansion

\[
R(\theta, \varphi) = R_0[1 + \sum_{\lambda\nu} \alpha_{\lambda\nu}^* Y_{\lambda\nu}(\theta, \varphi) + \ldots],
\]

of its radius as a function of orientation angles, where \( Y_{\lambda\nu}(\theta, \varphi) \) are standard spherical harmonics. Thus, it has only shape-vibrational and rotational degrees of freedom. For present purposes we restrict to quadrupole shape degrees of freedom for which \( \lambda = 2 \) and for which we define \( \alpha_{\nu} \equiv \alpha_{2\nu} \). The dynamics of the Bohr model is described by a Hamiltonian

\[
\hat{H} = \frac{1}{2B} \sum_{\nu} \hat{\pi}_\nu^* \hat{\pi}_\nu + V(\alpha),
\]

where \( \pi_\nu = B \dot{\alpha}_{\nu} \) is the momentum associated with the coordinate \( \alpha_{\nu} \) and \( \hat{\pi}_\nu = -i\hbar \frac{\partial}{\partial \alpha_{\nu}} \) is its quantisation; \( \hat{\pi}_\nu = -i\hbar \frac{\partial}{\partial \alpha_{\nu}} \). The Hilbert space for the Bohr model is then that of a five-dimensional harmonic oscillator. The spectra and properties of such a Hamiltonian can be calculated quickly and easily using the algebraic methods of ref. [6].

Our strategy is now to extend the Bohr model to a microscopic collective model that has representations carried by subspaces of shell-model states. These subspaces are then identified as the appropriate shell-model spaces needed for a microscopic description of collective-model states. A first step towards construction of such a model is achieved by replacing the quadrupole shape coordinates, \( \{ \alpha_\nu \} \), by the quadrupole and monopole moments of a system of \( N \) point nucleons with position coordinates \( \{ x_{ni} \} \):

\[
Q_{ij} = \sum_{n=1}^{N} x_{ni} x_{nj}, \quad i, j = 1, 2, 3.
\]

These moments have time derivatives \( \dot{Q}_{ij} = \sum_{n=1}^{N} (x_{ni} \dot{x}_{nj} + x_{ni} \dot{x}_{nj}) \). Hence, the canonical momenta are

\[
P_{ij} = \sum_{n=1}^{N} (x_{ni} p_{nj} + p_{ni} x_{nj}), \quad i, j = 1, 2, 3,
\]
where \( \{p_{ni}\} \) are the single-nucleon momenta. The quantisation of a collective model with these coordinates is now given by \( \hat{Q}_{ij} \rightarrow \hat{Q}_{ij} \) and \( \hat{P}_{ij} \rightarrow \hat{P}_{ij} \), where \( \hat{Q}_{ij} \) and \( \hat{P}_{ij} \) act on many-nucleon wave functions according to standard quantum mechanics according to the equations

\[
\hat{Q}_{ij} \psi(x) = \sum_n x_{ni} x_{nj} \psi(x), \quad \hat{P}_{ij} \psi(x) = \sum_n (x_{ni} \hat{p}_{nj} + \hat{p}_{ni} x_{nj}) \psi(x),
\]

with \( \hat{p}_{nj} = -i\hbar \frac{\partial}{\partial x_{nj}} \). Thus, whereas the Bohr model observables satisfy the Heisenberg commutation relations

\[
[\hat{Q}_{ij}, \hat{P}_{kl}] = i\hbar \delta_{ik} \delta_{jl}, \quad [\hat{Q}_{ij}, \hat{Q}_{kl}] = i\hbar \delta_{il} \delta_{jk}, \quad [\hat{P}_{ij}, \hat{P}_{kl}] = i\hbar \delta_{ik} \delta_{jl},
\]

those of the microscopic collective model, satisfy the relations

\[
[\hat{Q}_{ij}, \hat{P}_{kl}] = i\hbar \delta_{ik} \hat{Q}_{jl} + \delta_{il} \hat{Q}_{jk} + \delta_{jl} \hat{Q}_{ik} + \delta_{jk} \hat{Q}_{il},
\]

The collective model group, generated by the operators \( \{\hat{Q}_{ij}, \hat{P}_{ij}\} \), is known by the acronym GCM(3), where G (for general) signifies the inclusion of monopole degrees of freedom.

Whereas the Bohr model has only one unitary representation, the GCM(3) model has many [7], each of which is characterised by an intrinsic vorticity quantum number which can take any non-negative integer value. Thus, the microscopic collective model corrects one of the deficiencies of the Bohr model which is its restriction to irrotational quantum-fluid flows.

3. Embedding the microscopic collective model in the shell model

We now consider the microscopic collective model as a submodel of the shell model and relate the basis states for its irreps to those of a shell-model coupling scheme. This is achieved by extending the GCM(3) model to a larger symplectic model with an \( \text{Sp}(3, \mathbb{R}) \supset \text{GCM}(3) \supset \text{SO}(3) \) dynamical group [8]. This extension is useful because the Lie algebra of \( \text{Sp}(3, \mathbb{R}) \) contains the moments of momenta,

\[
\hat{K}_{ij} = \sum_n \hat{p}_{ni} \hat{p}_{nj},
\]

as well as the elements of the GCM(3) Lie algebra. In particular, it contains the many nucleon kinetic energy operator \( \hat{T} = \frac{1}{2\hbar} \sum_{ni} \hat{p}_{ni}^2 \). Moreover, \( \text{Sp}(3, \mathbb{R}) \) is a dynamical group for the spherical harmonic oscillator Hamiltonian and its representations are easy to construct within the harmonic-oscillator shell-model space. The construction is greatly facilitated by the classification of shell-model states by means of the subgroup chain

\[
\text{Sp}(3, \mathbb{R}) \times U(4) \supset \text{U}(3) \times \text{U}(2)_S \times \text{U}(2)_T \supset \text{SO}(3) \times \text{SU}(2)_S \times \text{SU}(2)_T,
\]

where \( U(4) \supset SU(2)_S \times SU(2)_T \) is Wigner’s supermultiplet group; it contains the spin and isospin groups as subgroups. The group \( U(3) \supset U(1) \times SU(3) \) is the symmetry group of the spherical harmonic oscillator Hamiltonian and contains \( SU(3) \), the dynamical group of Elliott’s model [9], as a subgroup. An important observation is that the whole (multi-shell) Hilbert space of the shell model is spanned by irreducible representations of this chain of subgroups. In fact, this subgroup chain defines an LST coupling scheme.

\( \text{Sp}(3, \mathbb{R}) \) irreps can be labelled by \( U(1) \times SU(3) \) quantum numbers \( N(\lambda\mu) \) where \( N\hbar\omega \) is the harmonic oscillator energy of the lowest-weight state; e.g., \( N = 36 \) for the closed-shell state of \( ^{16}\text{O} \) before removal of the centre-of-mass energy. They are simply constructed from the observation that the nuclear (mass) quadrupole tensor \( \hat{Q} \) can be separated into three components:

\[
\hat{Q}_{ij} = \hat{Q}_{ij}^{(0)} + \hat{Q}_{ij}^{(+2)} + \hat{Q}_{ij}^{(-2)}.
\]
When acting on a shell-model state, $\hat{Q}_{ij}^{(0)}$ conserves the quantum number $N$ and $\hat{Q}_{ij}^{(\pm 2)}$ change $N$ to $N \pm 2$, respectively. Observe also that $\hat{Q}$ is a sum of irreducible $L = 0$ and $L = 2$ spherical tensors, $\hat{Q}_0$ and \{\hat{Q}_{2\nu}\}. Thus, $\hat{Q}^{(0)}$ is a $\Delta N = 0$, U(3) tensor of the Elliott type, whereas the components of $\hat{Q}^{(\pm 2)}$ are, respectively, $\Delta N = \pm 2$ raising and lowering operators for giant monopole and quadrupole excitations. We refer to the U(3) irreps that are annihilated by the $\hat{Q}^{(-2)}$ lowering operators as lowest-grade representations. Sp(3, $\mathbb{R}$) has three kinds of irreps:

(i) **Spherical representations**

These representations are based on a closed-shell state, which spans a trivial one-dimensional representation of U(3). The $\hat{Q}^{(-2)}$ operators annihilate this state and the $\hat{Q}^{(+2)}$ operators act on it to create giant monopole and giant quadrupole vibrational excitations. Acting twice, they create two phonon giant resonance excitations, etc., as illustrated in figure 1.

(ii) **Axially symmetric representations**

These representations are based on a non-trivial U(3) representation $N(\lambda, \mu = 0)$ or $N(\lambda = 0, \mu)$. (iii) **Triaxial representations**

These representations are based on a generic U(3) representation $N(\lambda \mu)$. For a Hamiltonian of the Elliott type

$$\hat{H} = \hat{H}_{\text{HO}} - \chi \hat{Q}_2^{(0)} \cdot \hat{Q}_2^{(0)},$$

with no mixing between harmonic-oscillator shells, one obtains a low-lying triaxial SU(3)-rotational bands with higher-lying giant monopole and giant quadrupole vibrational bands built upon it, as illustrated in figure 2.

**Figure 1.** Basis states for an Sp(3, $\mathbb{R}$) irrep $N(0, 0)$. The lowest-weight state is a closed-shell $L = 0$ state. The one-phonon giant monopole and giant quadrupole states span a $(2, 0)$ SU(3) irrep. The two-phonon excitations span a reducible $(2, 0) \times (2, 0)$ SU(3) representation.

**Figure 2.** Basis states for an Sp(3, $\mathbb{R}$) irrep $N(\lambda, \mu)$. The lowest-grade states spans a $(\lambda, \mu)$ SU(3) irrep. The one-phonon giant monopole and giant quadrupole states now span a reducible $(\lambda, \mu) \times (2, 0)$ SU(3) representation.

### 4. Selecting an effective shell model space in an SU(3) basis

In adapting the strategy outlined in the introduction to an $A$-nucleon nucleus in which monopole and quadrupole shape fluctuations dominate over other correlations, one should start with basis states for the Hilbert space $\hat{H}^{(A)}$ classified by means of the subgroup chain (10). If the Sp(3, $\mathbb{R}$) irreps were ordered such that the low-energy states of the $A$-nucleon nucleus were expected to have decreasing overlaps with the correspondingly ordered representation spaces, it would then be natural to choose the space spanned by the direct sum of lowest-grade U(3) sub-states for a finite number of the leading Sp(3, $\mathbb{R}$) irreps in this ordered sequence as the Hilbert space for an effective shell-model of the $A$-nucleon nucleus. It would then remain to derive the effective interactions and effective operators appropriate for such a choice of shell-model space.
As shown by Jarrio et al. [10], the dominant $\text{Sp}(3,\mathbb{R})$ irreps needed to describe observed rotational states are determined by experimental observations of quadrupole moments and E2 transition rates. For example, they show that the irrep needed to describe the ground-state band of $^{168}\text{Er}$ has $N \sim N_0 + 16$, $\lambda \sim 88$, and $\mu \sim 11$, where $N_0$ is the minimum possible value of $N$ for an $\text{Sp}(3,\mathbb{R})$ irrep of $^{168}\text{Er}$ states. The results of ref. [10] prove to be consistent with the following self-consistent method based on a generalisation [11] of the Nilsson model.

Recall that an $\text{Sp}(3,\mathbb{R})$ irrep is labelled by the quantum numbers $N(\lambda, \mu)$ of its lowest-grade $U(3)$ irrep, defined as follows. A spherical harmonic-oscillator Hamiltonian is a sum of three simple harmonic-oscillator Hamiltonians, $\sum_i h_i$, with common frequencies, $\omega_1 = \omega_2 = \omega_3$. A $U(3)$ highest-weight state is an eigenstate of each $h_i$ with eigenvalue $N_i/\hbar\omega_i$, and the standard labels of an $\text{Sp}(3,\mathbb{R})$ irrep are defined by $N = N_1 + N_2 + N_3$, $\lambda = N_1 - N_2$, and $\mu = N_2 - N_3$. Now, because the group $\text{Sp}(3,\mathbb{R})$ contains quadrupole shape transformations, it can transform the highest-weight state of its lowest-grade $U(3)$ irrep into an eigenstate of a triaxial harmonic oscillator Hamiltonian with arbitrary values of $\omega_1$, $\omega_2$, and $\omega_3$, without changing the values of $N_1$, $N_2$, and $N_3$. Any such state is then a deformed lowest-weight state for the $\text{Sp}(3,\mathbb{R})$ irrep $N(\lambda, \mu)$. Thus, Hartree-Fock methods could be used to determine the minimum energy, $E_{N(\lambda, \mu)}$, for the Hamiltonian $\hat{H}^{(A)}$, among the set of such deformed lowest-weight states. More simply, self-consistency arguments can be used to determine the triaxial harmonic oscillator energy $\sum_i N_i/\hbar\omega_i$ for which the deformed lowest-weight state has the same quadrupole shape as the triaxial harmonic oscillator potential of which it is an eigenstate [11]. These energies can be used to order the $\text{Sp}(3,\mathbb{R})$ irreps.

5. Concluding comments

The above analysis gives an outline of what is required for a realistic effective shell-model description of deformed nuclei. In particular, it gives criteria for identifying a meaningful effective shell-model space in an LST coupling scheme. The proposed scheme is based on an understanding of the character of nuclear rotational correlations gained from experimentally-based model calculations. However, proceeding on to actually deriving effective shell-model interactions and other operators for doubly-open shell nuclei poses numerous challenges and will undoubtedly require major approximations and further guidance from model investigations.

For example, for light nuclei one might initially set aside the shape coexisting states for which higher shells in the model space are required and define the active shell-model space to be the lowest open spherical harmonic-oscillator shell. Standard methods could then be used to renormalise the interactions restricted to this space by taking account of the coupling of each $U(3)$ subspace in this shell to the many-phonon giant monopole/quadrupole states of the $\text{Sp}(3,\mathbb{R})$ irrep built upon it. This approach is being pursued by Draayer and his group [4].

A simple example illustrates how a single effective $U(3)$ model can reproduce the result of a complicated $\text{Sp}(3,\mathbb{R})$ calculation. Figure 3 shows the $U(3)$ amplitudes for the lowest-energy states of $^{168}\text{Er}$ of angular momentum $L = 0$ to 10 for a Hamiltonian $\hat{H} = \frac{1}{2m} \sum n p_n^2 + V(Q)$ on an $\text{Sp}(3,\mathbb{R})$ irrep $826_{10}^{10}(78, 0)$ (with centre-of-mass degrees of freedom removed) obtained by Bahri [12]. The potential $V(Q)$ is a rotationally-invariant collective model potential, expressed in terms of the many-nucleon quadrupole moments, chosen to have a minimum at the experimentally observed mean deformation of the $^{168}\text{Er}$ ground-state rotational band. Note that the lowest-grade $U(3)$ irrep contributes an almost negligible amount to the states calculated, and suggests that a perturbative renormalisation of the lowest-grade $U(3)$ states by coupling to the giant resonance excitations would be unlikely to converge. Nevertheless, as figure 4 shows, an $U(3)$ model calculation with this irrep and just a two-body $Q \cdot Q$ interaction and an effective charge of $e_{\text{eff}} \sim 2$ fits the energy levels and E2 transition rates extraordinarily well.

A few observations give hope that shell-model calculations of rotational states in heavy nuclei with realistic effective interactions might be possible in representative examples. If $\text{Sp}(3,\mathbb{R})$
symmetry were conserved for heavy deformed nuclei, it is feasible (cf. LSU workshop [13]) that
such calculations could be done in the not too distant future. From numerous model studies
of systems with competing dynamical symmetries, it invariably transpires (except in phase
transition regions) that one symmetry is dominant [14]. Thus, for example, one could start
with phenomenological calculations with single Sp(3,R) irreps to describe the rotational bands
of $^{168}$Er. If successful, corresponding shell-model calculations could then be attempted with a
realistic interaction and finally perturbative corrections might be added perturbatively.

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