On the relation of the shell, collective and cluster models

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Abstract. The intersection of the shell, collective and cluster models is described for multi-major-shell problems.

1. Introduction
The fundamental models of nuclear structure are based on different physical pictures. The shell model indicates that the atomic nucleus is something like a small atom, the cluster model suggests that it is similar to a molecule, while the collective model says that it is a microscopic liquid drop. Therefore, in order to understand the nuclear structure we need to study (among others) the interrelation of these models, find their common intersection, etc.

The basic connections were found in the fifties. Elliott [1] showed how the quadrupole deformation and collective rotation can be derived from the spherical shell model: the states belonging to a collective band are determined by their specific SU(3) symmetry. Wildermuth and Kanellopoulos [2] established the relation between the shell and cluster models. They proved that the Hamiltonians of the two models can be rewritten into each other exactly in the harmonic oscillator approximation. This relation results in a close connection between the corresponding eigenvectors, too: the wavefunction of one model is a linear combination of those of the other, which belong to the same energy. Later on this relation was interpreted by Bayman and Bohr [3] in terms of the SU(3) symmetry. As a consequence, the cluster states are also selected from the shell model space by their specific SU(3) symmetries. (In fact only one kind of cluster states have this feature, and there are other kinds, too, as discussed later.)

We will refer to this interrelation among the three basic structure models as the SU(3) connection. It was established in 1958 for a single major shell problem. Here we consider its extension to multi-major-shells.

The connection of the shell model and the cluster model is especially interesting due to the fact that both models have a complete set of basis states, i.e. any nuclear states can be expanded in both bases. Depending on the simple or complicated nature of these expansions we can distinguish four different cases. i) If it is simple in the shell basis, but complicated in the cluster one, then we can speak about a simple shell state, which is a poor cluster state. ii) If it is simple in the cluster basis, but complicated in the shell basis, one has a good cluster state, which is a poor shell state. (Later on we will refer to these states as rigid molecule-like cluster
states.) iii) The expansion may be simple in both bases. We call this situation as a shell-like cluster state. iv) If it is complicated in both bases, than the state is not a simple one.

Of course it is not the name that matters. The important point is that there are three different kinds of simple states when we investigate them from the viewpoint of the cluster-shell competition. Sometimes only the kind ii), i.e. rigid molecule-like states are considered as cluster states. The reason for our vocabulary, i.e. speaking about two kinds of cluster states: shell-like and molecule-like is inspired by their experimentally observable characteristics. Both of them prefer a certain reaction channel, have a large cluster spectroscopic factor, etc. They represent two different quantum phases of the nucleus, as discussed in [4]. By choosing these names we are in line with the general definition of a simple nuclear state in terms of experimental observation: a state is called simple if its wavefunction has a large overlap, or form a large matrix element with the wavefunction of a reaction channel, in which it can be observed [5].

2. Models of different pictures

2.1. Shell models

Elliott’s U(3) model bridges the spherical shell model and the collective model, and describes rotational states in the p and sd shell nuclei. Here the U(3) symmetry is that of the space part, while the spin-isospin section is characterized by Wigner’s U^{ST}(4) [6]. Thus the group structure of the model is U^{ST}(4) \otimes U(3). In constructing the model space the spin-isospin degrees of freedom are essential, of course. The physical operators, however, often contain simply spin-isospin zero terms, in which case only the generators of the U(3) group contribute. The space part of the basis states is defined by the representation labels of the group chain: U(3) \supset SU(3) \supset SO(3) \supset SO(2).

The quadrupole-quadrupole interaction plays a major role, and it can be written as a linear combination of the quadratic invariant operators (\(C^{(2)}\)) of the group-chain: SU(3) \supset SO(3):

\[ QQ = \frac{1}{2} C^{(2)}_{SU(3)} - \frac{3}{2} C^{(2)}_{SO(3)}. \]

The electromagnetic transition rates are obtained by applying effective charge. The many-nucleon states are classified according to their SU(3) symmetry, and in the simplest case the interactions are expressed in terms of its generators.

The single major shell model has an algebraic structure defined by a larger group, which contains the symmetry groups of both the space part U(3), and the spin-isospin part U^{ST}(4). It is the unitary group of U(4\(\Omega\)), where \(\Omega\) denotes the orbital degeneracy: \(\Omega=1, 3, 6, ...\) for the the s, p, sd, ... shells, respectively. U(4\(\Omega\)) is a dynamical group of the single major shell model in the sense that the physical operators are obtained in terms of its generators, and the whole spectrum is provided by a single irreducible representation (irrep) of it.

The description of the electromagnetic transitions without an effective charge requires the incorporation of the major shell excitations; i.e. a vertical extension of the SU(3) shell model. For this purpose the symplectic group proved to be very useful [7].

The Sp(3,R) group is generated by the position vectors of the nucleons, and their canonically conjugate momenta. An alternative set of its generators is expressed in terms of harmonic oscillator operators, containing the 9 generators of the U(3) group, which preserve the number of oscillator quanta, and in addition 6 creation \(B_{l}^{+}(m) = [\pi^{+} \times \pi]^{(l)}(m)\), \(l = 0, 2\) and 6 annihilation \(B_{l}^{(m)} = [\pi \times \pi^{(l)}]^{(l)}(m)\) operators, which ladder by 2 or -2 quanta. The creation operators are \([2, 0, 0]\) U(3) tensors, therefore, their products also carry U(3) labels: \([n_{1}^{e}, n_{2}^{e}, n_{3}^{e}]\) (\(e\) stands for excitation).

The algebraic structure of the symplectic shell model is provided by the Sp(3,R) group in the sense that the physical operators are expressed in terms of its generators, and the collective bands are given by its (infinite dimensional) irreducible representations (which are built on U(3) irreps).
2.2. Collective model

Several algebraic collective models have been developed. In what follows we focus on a model with a simple algebraic structure, which is very illuminative from the viewpoint of the interrelation of the fundamental structure models. It is the large \( n \) limit of the \( \text{Sp}(3,\mathbb{R}) \) symplectic model.

The dynamical group in this limit simplifies to \( \text{U}_s(3) \otimes \text{U}_b(6) \), i.e. to a compact group, as opposed to the noncompact \( \text{Sp}(3,\mathbb{R}) \). Technically the simplification is achieved by replacing the creation and annihilation operators of the \( \text{Sp}(3,\mathbb{R}) \) model (in which the description is based on nucleon degrees of freedom) by boson operators. The \( \text{U}_s(3) \) is Elliott’s shell model symmetry of the \( 0\hbar \omega \) shell, and \( \text{U}_b(6) \) is the group of the six dimensional oscillator, generated by the bilinear products of the \( (l = 0 \text{ and } 2) \) boson creation and annihilation operators. It is realised in a similar way as the \( \text{U}(6) \) group of the interacting boson model (IBM) \[8\], nevertheless physically it is different, because in the case of the contracted symplectic model the bosons are associated to intershell excitations, not to intrashell ones.

This model is called \( \text{U}(3) \) boson model \[9\], or contracted symplectic model \[10\]. The contracted boson operators which generate the intershell excitations do introduce here a simplifying approximation. Therefore, the antisymmetry requirement is not fully incorporated in this description. This model is more easily applicable (compared to the \( \text{Sp}(3,\mathbb{R}) \) model), e.g. it has an orthonormal set of basis states.

The algebraic structure of the contracted simplectic collective model is provided by the \( \text{U}_s(3) \otimes \text{U}_b(6) \) group in a sense (similarly to that of the symplectic model) that the physical operators are expressed in terms of its generators, and the collective bands are given by its (finite dimensional) irreducible representations (which are built on \( \text{U}(3) \) irreps).

2.3. Cluster models

There are different kinds of cluster models, which all share the general picture of dividing the relevant degrees of freedom into two categories: those belonging to the relative motion of the clusters (usually in a large variety) and those of the internal structure of them (usually in a rather limited number).

In searching for the symmetry-based relations to the shell and collective models, two aspects of the models are especially important: i) how much they are microscopic, and ii) to what extent they are equipped with an algebraic structure.

A model is called fully microscopic if the antisymmetrization is completely involved, and the interactions are (effective) nucleon-nucleon forces. It is semimicroscopic, if the exclusion principle is appreciated, but the interactions are (phenomenological) cluster-cluster interactions. It is fully phenomenological, if cluster-cluster interactions are applied in a model space, which is constructed phenomenologically, i.e. without taking into account the Pauli-principle.

The algebraic structure on the other hand reveals the symmetries of the model, and this can provide us with a connection to the shell and collective picture.

For the sake of simplicity we consider here binary cluster configurations. When the \( \text{SU}(3) \) shell model \[1\] is applied for the description of the internal structure of the clusters then the spin-isospin degrees of freedom of the clusters are coupled together, while the space-part is characterized by the group-chain:

\[
U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_{R}(3) \supset U_{C}(3) \otimes U_{R}(3) \supset U(3) \supset SU(3) \supset SO(3) \supset SO(2),
\]

here \( U_{C}(3) \) stands for the coupled space symmetry of the two clusters.

This basis is especially useful for treating the exclusion principle, since the \( U(3) \) generators commute with those of the permutation group, therefore, all the basis states of an irrep are either Pauli-allowed, or forbidden \[11\].
On the fully microscopic level much work has been done in developing an algebraic description. Especially great progress was made in the works [11, 12], in calculating the necessary matrix elements in an U(3) basis.

In the fully microscopic description usually effective nucleon-nucleon forces are applied without specific symmetry character. Therefore, this is not a fully algebraic description (the physical operators are not expressed in terms of the generators of a dynamical group), contrary to the single major shell model of U(4Ω), the symplectic model of Sp(3,R), and the contracted symplectic model of \( U_s(3) \otimes U_b(6) \).

The semimicroscopic algebraic cluster model (SACM) [13] is a fully algebraic approach with transparent symmetry-properties. The internal structure of the clusters is described here by the Elliott model [1] too, therefore, this part of the wavefunction has a \( U^{ST}_C(4) \otimes U_C(3) \) symmetry. The relative motion of the clusters is accounted for by the modified vibron model [14].

The coupling between the relative motion and internal cluster degrees of freedom for a binary cluster system results in a group structure: 
\[
G_{2C} \equiv U_{C1}^{ST}(4) \otimes U_C(3) \otimes U_{C2}^{ST}(4) \otimes U_C(3) \otimes U_R(4).
\]
The spin and isospin degrees of freedom are essential in this case, too, from the viewpoint of the construction of the model space. However, if one is interested only in a single supermultiplet \( [U^{ST}_C(4)] \) symmetry, which is typical in cluster problems, then the relevant group structure simplifies to that of the space part. In particular the U(3) (strong) coupled basis is defined by the group chain:
\[
U_C(3) \otimes U_R(4) \supset U_C(3) \otimes U_R(3) \supset U(3) \supset SU(3) \supset SO(3) \supset SO(2).
\] (2)

The exclusion of the Pauli-forbidden states amounts up to a truncation of the coupled U(3) basis from the side of the small number of oscillator quanta. Some major shells are completely missing, and from some other ones parts of the single-nucleon states are excluded. This is the modification [13] with respect to the original vibron model, as it is applied e.g. in molecular physics [15].

The relation of the SACM and fully microscopic description from the viewpoint of the model space is that they contain the same U(3) [and \( U^{ST}_C(4) \)] irreps, but the complete antisymmetrization is carried out only in the fully microscopic descriptions. Therefore, the calculation of the cluster spectroscopic amplitude in the semimicroscopic model is being done by the introduction of phenomenologic parameters [16].

The connection between the fully microscopic and the semimicroscopic cluster models is somewhat similar to the relation between the symplectic shell model and the contracted symplectic model. The previous ones are fermionic models, accounting for the antisymmetrization to full details, while the latter ones are their simplifying (bosonic) approximations. Therefore, their wavefunctions are not the same, though the U(3) content is identical in both cases.

3. Intersection
When major shell excitations are incorporated, then both the (symplectic) shell model, and the (contracted symplectic) collective model, as well as the (microscopic or semimicroscopic algebraic) cluster model has a set of basis states characterised by the irreps of the group chain:
\[
U_x(3) \otimes U_y(3) \supset U(3) \supset SU(3) \supset SO(3) \supset SO(2).
\] (3)
group chain, as seen above. For the shell and collective models \( x \) stands for the band-head (valence shell), for the cluster model it refers to the internal cluster structure. \( y \) indicates in each case the major shell excitations; in the shell and collective model cases it takes place in steps of \( 2\hbar\omega \), connecting oscillator shells of the same parity, while in the cluster case it is in steps of \( 1\hbar\omega \), incorporating all the major shells. For the cluster model it has only completely
symmetric (single-row Young-tableaux) irreps: \([n, 0, 0]\), while in the case of the shell and collective models it can be more general. As a consequence the model space of the three models have a considerable overlap, but they are not identical.

As for the relation of the model spaces (wavefunctions) of the three basic structure models (shell, collective and cluster models) is considered the following can be said. When multi major shells are involved then the (quadrupole) collective or (dipole) cluster bands can be picked up from the microscopic shell model basis according to their \(U_x(3) \otimes U_y(3) \supset U(3)\) symmetry. Some irreducible representations are present in each of the three models. Having the same SU(3) basis, however, does not necessarily mean 100\% overlap of the wavefunction, it can be less, too. This situation is similar to what was found for the single major shell problem in terms of the historical SU(3) connection.

Another interesting question of the intersection of the different structure models is how their spectra compare to each other, when similar interactions applied. In this respect first we should note that the Wildermuth-connection between the shell and cluster model states, which was found originally for harmonic oscillator Hamiltonians, turned out to be valid for more general interactions, too [17], just like the Elliott-connection. If the Hamiltonian is expressed in terms of the invariant operators of the group chain (3) then the energy-eigenvalue has an analytical solution i.e. a (broken) dynamical symmetry is present. This \(U_x(3) \otimes U_y(3) \supset U(3)\) dynamical symmetry is the common intersection of the shell, collective and cluster models of multi major shells.

Figure 1. shows a comparison between the experimental and the U(3) dynamically symmetric (3) spectrum of the \(^{20}\text{Ne}\) nucleus. The energy (in MeV) was obtained with the formula

\[
E = 13.19\lambda - 0.4579\lambda(\lambda + 3) + 0.8389\frac{1}{22}L(L + 1).
\]

The oscillator energy is determined according to the systematics [18], while \(\theta\) is the moment of inertia calculated classically for the rigid shape determined by the U(3) quantum numbers. The parameters of the quadratic and the rotational terms were fitted to the experimental data. (The ground state energy is taken to be zero.) The experimental data are from [19]. (For more details, including \(E_2\) transitions, see [20].)

The purpose of this calculation is not to give a detailed description of the experimental data, rather to show how the common intersection of the three basic structure models compares to the experiment. The right panel in Fig. 1. can be considered as a (part of a) shell, collective or cluster spectrum, when the basis states and the operators can be characterized by the SU(3) (and subgroup) symmetries, i.e. for the case of the dynamical symmetry. These circumstances are similar again to those of the single-shell problem.
4. Summary and conclusion
In this paper we have discussed the interrelation of the fundamental nuclear structure models, the shell, collective and cluster models from the viewpoint of symmetries. These models are based on different physical pictures, and their connection was established first in terms of the SU(3) symmetry for a single shell problem [1, 2, 3]. We have considered here the generalization of this relation along the major shell excitations.

Algebraic models have been constructed for the description of this vertical extension in each of the three approaches. The most relevant ones from the viewpoint of the symmetry-based interrelations are the symplectic shell model of Sp(3,R) algebraic structure [7], the contracted symplectic model of U(6)⊗U(3), which is the large n limit of the multi major-shell symplectic model [9, 10], and the fully microscopic [11, 12] as well as the semimicroscopic algebraic cluster models [13], with U_C(3)⊗U_R(3) basis. The common intersection of these models is provided by the U_x(3)⊗U_y(3)⊃U(3) dynamical symmetry, i.e. for the many major-shell problem this symmetry substitutes the simple SU(3). Figure 1 shows how the schematic spectrum of this dynamical symmetry, which can be considered as a shell, collective or cluster description, compares with the experimental one.

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