On the intersection of the shell, collective and cluster models of atomic nuclei II: Symmetry-breaking and large deformations

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We discuss the role of the broken symmetries in the connection of the shell, collective and cluster models. The cluster-shell competition is described in terms of cold quantum phases. Stable quasi-dynamical U(3) symmetry is found for specific large deformations for a Nilsson-type Hamiltonian.

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INTRODUCTION

The connection of the shell, collective [1] and cluster models [2, 3], found in terms of the SU(3) symmetry in 1958, was based on a single-shell problem, described in spherical basis, related to simple symmetries. In a previous paper [4] the extension to multi-major shells was addressed, and the U(3) ⊗ U(3) ⊇ U(3) dynamical symmetry was found as the common intersection of the three models. Here we consider the role of more general symmetries and the case of large deformation.

So far two kinds of the SU(3) symmetry were applied in this respect. i) The exact symmetry, in which case both the Hamiltonian is symmetric, i.e. it is an SU(3) scalar, and its eigenvectors are symmetric, i.e. they transform according to irreducible representations (irreps). ii) The dynamical SU(3) symmetry (sometimes called dynamically broken symmetry), when the eigenvectors are still symmetric, but the interactions are not. This kind of special breaking is achieved by incorporating an interaction which is expressed in terms of the invariant operator of the SO(3) subgroup, in addition to the SU(3) scalar part.

The relation between the shell and collective models, established by Elliott [1] was based on the SU(3) ⊇ SO(3) dynamical symmetry. The Wildermuth-connection between the shell and cluster models was originally based on harmonic oscillator Hamiltonians of exact SU(3) symmetry, but it turns out to be valid also for the dynamical symmetry, as discussed e.g. in [2].

Here we consider the more general quasi-dynamical SU(3) symmetry [6] which turns out to be important, too. Therefore, in the next section we discuss very briefly the hierarchy of symmetries (or symmetry-breaking), relevant for the connection of the fundamental structure models. We also describe the cluster-shell competition in terms of quantum phases, being closely related to symmetries. Then we investigate the case of large deformations, with special emphasis on the symmetries of the super- and hyperdeformation, in the presence of realistic (Nilsson-type) interactions. Before the concluding part we devote a short section to the comparison of different kinds of extensions of Elliott’s original SU(3) symmetry, which are relevant from the present viewpoint. The 20Ne nucleus is applied for illustrative purposes, just like in [4].

SYMMETRIES AND SYMMETRY-BREAKING

Hierarchy

The quasi-dynamical (or effective) U(3) symmetry [6] is a generalization of the concept of the U(3) dynamical symmetry in the following sense. The Hamiltonian breaks the symmetry in such a way that the U(3) quantum numbers are not valid for its eigenvectors (contrary to the case of the real U(3) dynamical symmetry). In other words neither the operator is symmetric, nor its eigenvectors [6]. (For comparison with the exact and dynamical symmetries see Table I.) Yet, the symmetry is present in some sense, and it may survive even for strong symmetry-breaking interactions [6]. Then the energy eigenstates are:

$$\psi_{\alpha KJM} = \sum_{\xi \lambda \mu} C_{\alpha \xi \lambda \mu K} \phi_{\xi \lambda \mu KJM}, \quad (1)$$

where $\phi_{\xi \lambda \mu KJM}$ is a basis vector for an SU(3) irreducible representation, $\xi$ and $\alpha$ are additional quantum numbers needed to specify the wavefunction [6]. The $C_{\alpha \xi \lambda \mu K}$ coefficients of the linear combination are independent of $JM$, i.e. within a band the contribution of different SU(3) basis states is the same. (This situation is called adiabatic approximation.) When calculating the matrix elements of the SU(3) generators between these states the result may approximate the matrix elements of an exact representation. In such a case we speak about an approximate embedded representation, and related to it, about an approximate quasi-dynamical or effective SU(3) symmetry.

An asymptotic Nilsson-state serves as an intrinsic state for the quasi-dynamical SU(3) representation. Thus
the effective quantum numbers are determined by the Nilsson-states in the regime of large deformation. When the deformation is not large enough, then we can expand the Nilsson-states in the asymptotic basis, and calculate the effective quantum numbers based on this expansion.

The concept of effective U(3) symmetry is applicable also for the case when the simple leading representation approximation is valid, and then the real and effective U(3) quantum numbers usually coincide. The quasi-dynamical symmetry appears in the investigation of both quantum phases and the large deformation.

### Phases

Symmetry-adapted models are especially suitable for the studies of the phases and phase-transitions in finite quantum systems. The usual scenario is to consider an algebraic model with a well-defined model space and with interactions which are varied continuously. The model has limiting cases, i.e. dynamical symmetries. When a dynamical symmetry holds, the eigenvalue-problem has an analytical solution. The general Hamiltonian, however, which has contributions from interactions with different dynamical symmetries, has to be diagonalized numerically. The relative weight of the dynamically symmetric interactions serves as a control parameter, and it defines the phase-diagram of the system. When there are more than two dynamical symmetries, more than one control parameters appear.

In the limit of large particle number phase-transitions are seen in the sense that the derivative of the energy-minimum, as a function of the control-parameter, is discontinuous. The order of the derivative, showing the discontinuity, gives the order of the phase-transition. Thus the phase-transition is investigated quantitatively, like in the thermodynamics. A phase is defined as a region of the phase diagram between the endpoint of the dynamical symmetry and the transition point. It is also conjectured that such a quantum phase is characterised by a quasi-dynamical symmetry. Therefore, although the real dynamical symmetry is valid only at a single point of the phase-diagram, the more general quasi-dynamical symmetry may survive, and in several cases does survive, in a finite volume of the phase diagram. If this conjecture really turns out to be true, then the situation is similar to Landau’s theory: different phases are determined by different (quasi-dynamical) symmetries, and phase transitions correspond to a change of the symmetry.

In the case of the finite particle number the discontinuities are smoothed out, as the consequence of the finite size effect, but still remarkable changes can be detected in the behaviour of the corresponding functions.

The semimicroscopic algebraic cluster model (SACM) of a binary cluster system has three dynamical symmetries, see (2). Two of them come from the vibron model of the relative motion: $U_R(3)$ corresponds to shell-like clusterization, or in the language of the collective motion to a soft vibrator, while $O_R(4)$ represents a rigid molecule-like rotator. The third symmetry, $SU(3)$ corresponds to a rigid molecule-like (O

A triangle-like phase diagram has been proposed for the shell model, too, which in addition to the SU(3) and SU(2) symmetries has the independent-particle model as the third corner. The limiting cases correspond to the situations, in which the quadrupole-quadrupole, pairing (both of them are two-body) interactions, and the single-particle energies dominate, respectively. (When a single shell calculation is performed then

\[
\begin{align*}
U_C(3) & \otimes U_C(3) \otimes U_R(4) \supset U_C(3) \otimes U_R(3) \supset U(3) \supset SU(3) \supset SO(3) \supset SO(2) \\
U_C(3) & \otimes U_C(3) \otimes U_R(4) \supset U_C(3) \otimes O_R(4) \supset SO_C(3) \supset SO(3) \supset SO(2) \\
U_C(3) & \otimes U_C(3) \otimes U_R(4) \supset U_C(3) \otimes U_R(3) \supset SO_C(3) \supset SO_R(3) \supset SO(3) \supset SO(2)
\end{align*}
\]
the spin-orbit interaction may be the most relevant part of the single-particle contribution.) The two phase diagrams match each other at the SU(3) corner, as shown in Figure 1. The real nuclear systems can be allocated to this diagram. The control parameters measure the distance from the dynamical symmetries, as mentioned before.

Here we refer to the results of three different calculations on the ground-band of the $^{20}$Ne nucleus. Vargas et al. [17] performed a full shell calculation for the 4 nucleons outside the core (accounting for many other states in addition to the ground band, of course). They applied SU(3) basis, and the Hamiltonian included, in addition to the harmonic oscillator potential, quadrupole-quadrupole, pairing interactions of the alike nucleons, and spin-orbit force (as well as some rotor-like terms to fine tune the moment of inertia and the position of different $K$-bands). For the purpose of illustration the parameters of their Hamiltonian can be rewritten into the form

$$H = yzH_{SU3} + (1 - z)H_{LS} + (1 - y)zH_{SU2}$$

(3)

where the control parameters $y, z$ take values between 0 and 1, in such a way that $z = 1, y = 1$ corresponds to the SU(3) dynamical symmetry, $z = 1, y = 0$ corresponds to the SU(2) dynamical symmetry, and $z = 0$ refers to the limit of the large LS interaction. (More specifically we took the parametrization, as follows: $H = \Sigma_i a_i H_{SU3} + bH_{LS} + cH_{SU2}, |a| = \Sigma_i |a_i|, y = |a|/(|a| + |c|), z = (|a| + |c|)/(|b| + |a| + |c|)$, where $|w|$ indicates the absolute value of $w$.) The location of the system on the shell model diagram is $y = 0.99, z = 0.77$.

Yepez-Martinez et al. have carried out a similar calculation on the cluster-side of the phase diagram [18]. They applied the semimicroscopic algebraic cluster model [13] with a Hamiltonian:

$$H = xvH_{SU3} + (1 - x)vH_{SO4} + (1 - v)H_{SO3},$$

(4)

therefore, $v = 1, x = 1$ corresponds to the SU(3) dynamical symmetry, $v = 1, x = 0$ shows the SO(4) dynamical symmetry, and $v = 0$ refers to the SO(3) limit. They have found $v = 1.00, x = 0.78$. (In this calculation several other cluster bands were obtained, too.)

Itagaki et al. applied the antisymmetrized quasi-cluster model [19] for the description of the ground band. This model can take a direct route from the rigid molecule-like (SO(4)) clusterization via the shell-like cluster limit (SU(3)) to the $jj$-coupled shell model dominated by a strong $LS$ interaction. Thus, it is especially illuminative from the viewpoint of the cluster-shell competition. It does not have, however, a well-defined algebraic structure, therefore, the control parameters can not be introduced in terms of the relative weights of interactions with different dynamical symmetries. It has two parameters to characterize the situation, but they are parameters of the wavefunction. One of them ($R$) refers to the distance of the (quasi) clusters, the other ($\Lambda$) is related to the strength of the spin-orbit force. A qualitative correspondence can be found between these parameters and the ones mentioned before in relation with the algebraic shell and cluster models. In short: the small $R$ and small $\Lambda$ is located near the matching point of the two diagrams (SU(3) dynamical symmetry), increasing $R$ takes towards the rigid molecule-like (SO(4)) corner, while increasing $\Lambda$ moves to the large $LS$ limit. The result of this study showed that the experimental situation corresponds to the shell like clusterization, i.e. close to the crossing point between the shell and cluster model.

It is remarkable that three different model calculations have similar conclusion on the closeness of the ground-band of $^{20}$Ne to the matching point between the shell and cluster models.

### LARGE DEFORMATIONS

The SU(3) connection from 1958 is based on the symmetry of the spherical shell model. In light of the fact that today very largely deformed states are known experimentally, it is an important question, what happens to this symmetry with increasing deformation. The superdeformed states e.g. represent a situation which is close to the axially symmetric spheroid with ratios of main axes of 2:1:1, the hyperdeformed state corresponds to 3:1:1.
Deformed harmonic oscillator

In \[20\] it was shown that the symmetry algebra of the anisotropic harmonic oscillator is SU(3), whenever its frequencies are commensurate, i.e. expressed as ratios of integer numbers. As a special case it includes the spherical oscillator, as well as the superdeformed or hyperdeformed shapes. More details, concerning the axially symmetric case with 2:1, 3:1, and 3:2 ratios are discussed in \[21\], and the triaxially deformed oscillator in \[22\]. (For previous works on this problem we refer to the citations in these papers.)

The connection between the anisotropic harmonic oscillator and clusterization have been discussed in \[23–26\].

Realistic interactions

In considering realistic interactions the Nilsson model plays an important role: it gives the single particle orbits of a Hamiltonian with spin-orbit, as well as \(l^2\) terms \[27\]:

\[
H = \hbar \omega N + \hbar \omega r^2 \beta Y_{20}(\theta, \phi) + Cls + DL^2.
\]  

Soon after the experimental discovery of the superdeformed states, Sugawara-Tanabe et al have realised that the \(L - S\) coupling recovers for the superdeformed shape, first in a simple \[28\], then in more realistic Nilsson model calculations \[29\]. In particular they found that the \(L - S\) coupled spherical wavefunction components became more than 85% of the total wavefunction. The reason for this is the dominant role of the quadrupole interaction due to the large deformation. This phenomenon provides an explanation for the appearance of the parity doublet levels.

In what follows we investigate the survival (or appearance) of the SU(3) symmetry systematically as a function of the quadrupole deformation (including triaxiality). We do so in terms of the Nilsson-model combined with the concept of the quasi-dynamical symmetry, discussed in the previous section. We obtain the shape isomers from a selfconsistent calculation concerning the quadrupole deformation. In particular: one varies systematically the parameters \((\beta_{in}, \gamma_{in})\), as an input for the Nilsson-model. The calculations provide us with the effective U(3) quantum numbers, which can be translated into the \((\beta_{out}, \gamma_{out})\) quadrupole deformation, since they are uniquely related to each other \[30\]. Then one can check if the selfconsistency is satisfied, as well as the question whether or not the result is stable with respect to the (small) changes of the input values. This method for the determination of the shape isomers is an alternative to the standard energy-minimum calculation and has been shown to be effective for a range of light nuclei \[31–33\].

The result of the Nilsson model + quasi-dynamical SU(3) calculation for \(^{20}\)Ne is shown in Figure 2 for \(\gamma_{in} = 60^\circ\) and \(\gamma_{in} = 0^\circ\). In this figure, the horizontal plateaus rather than the minima correspond to stable shapes. (The calculations with \(\gamma\) in between 0\(^\circ\) and 60\(^\circ\) do not show other shape isomers. In fact those of 10\(^\circ\), 20\(^\circ\) and 30\(^\circ\) are very similar to the right side of Figure 2 while the 40\(^\circ\) and 50\(^\circ\) resemble to its left side.)

Table II compares the results of the present calculations with those of the earlier determination of shape isomers using Nilsson model potential energy surfaces \[34\], and the Bloch-Brink alpha-cluster model \[35–37\]. Leander and Larsson list three shape isomers \[34\], each of

| State | Q.no. | \(h\omega\) | U(3) | \(\beta\) | \(\gamma\) | a:b:c | BB | LL |
|-------|-------|-------|------|-------|-------|-------|-----|-----|
| GS    | e     | 0     | [11,5,4] | 0.43  | 7.6   | 1.5:1.1:1 | 0   |
|       | h     | 0     | [12,4,4] | 0.52  | 0.0   | 1.6:1.0:1 | +   |
| SD    | e     | 4     | [14,10,0] | 0.75  | 43.9  | 2.4:2.0:1 | 50  |
|       | h     | 4     | [16,8,0] | 0.84  | 30.0  | 2.6:1.8:1 | +   |
| HD    | e     | 8     | [24,3,1] | 1.24  | 4.5   | 3.1:1.2:1 |     |
|       | h     | 8     | [24,4,0] | 1.25  | 8.9   | 3.4:1.4:1 | +   |
| AC    | e     | 20    | [40,0,0] | 1.85  | 0.0   | 5.0:1.0:1 | 0   |
|       | h     | 20    | [40,0,0] | 1.85  | 0.0   | 5.0:1.0:1 | +   |
which is very close to our present ones. The alpha-cluster studies found all the four shape isomers, we see here. Their U(3) symmetries are in coincidence with those of the simple harmonic oscillator configurations approximating the effective quantum numbers. It is remarkable that the instability of the shape in the ground state region, shown by the curvature in Fig. 2, is observed also in the Bloch-Brink calculations [37]. they mention two close-lying states with very similar configurations.

Connection to clusterization

The U(3) connection [1,3] between the collective, shell and cluster models works well in case i) the U(3) symmetry is approximately valid, and ii) the relation between the cluster and shell model wavefunctions is simple. This latter condition means that the expansion of the cluster U(3) state in terms of shell basis reduces to a few terms. As discussed in the previous subsection the U(3) symmetry recovers for the superdeformed, hyperdeformed, et shapes, in spite of the important role of the symmetry-breaking spin-orbit interaction. The second condition (on the simple shell model expansion) turns out to be valid also for several shape isomers. E.g. in case of the 20Ne nucleus each of the 4 shape isomers (of the U(3) symmetry: [12,4,4], [16,8,0], [24,4,0], [40,0,0]) has single multiplicity in the shell model basis. Therefore, if a cluster state with the same U(3) symmetry is allowed it is identical with the shell state. This is a consequence of the fact that the cluster state can be expanded in terms of shell basis, and basis states of different U(3) irreps are orthogonal to each other. (Both the shell and cluster states are normalized.)

In general: the U(3) selection rule for determining the allowed clusterization is:

\[ [n_1, n_2, n_3] = \hat{n}^{C_1}_{n_1} \otimes \hat{n}^{C_2}_{n_2} \otimes \hat{n}^{C_3}_{n_3} \otimes \hat{n}^{R}_{0,0} \]

where \( [n_1, n_2, n_3] \) is the U(3) symmetry of the shell model state, \( \hat{n}^{C_i}_{n_i} \) is that of the i-th cluster, and \( \hat{n}^{R}_{0,0} \) stands for the relative motion. When the shell model irrep matches with one of the results of the triple product of the right hand side, the cluster configuration is allowed. In addition to the U(3) selection, there is another simple prescription by Harvey [38] for the determination of the allowed clusterizations. It also applies harmonic oscillator basis, so the two requirements are somewhat similar. Nevertheless, their physical content is not the same; in some sense they are complementary to each other. Therefore, the best way is to apply them in a combined way [39,41]. (Their relation is discussed more in detail in [42].) When a cluster configuration is forbidden, one can characterize its forbiddenness quantitatively [43].

The energetic preference represents a complementary viewpoint for the selection of clusterization. We usually incorporate it in two different ways: i) by applying simple binding-energy arguments [44], and ii) by performing double-folding calculations, according to the dinuclear system model [45,46].

The alpha-like (N=Z=even) cluster configurations are energetically preferred, in general. When considering binary clusterizations with both clusters in their intrinsic ground state, then the GS state of 20Ne allows both 16O+4He, and 12C+8Be clusterizations. The latter configuration is present also in the SD and HD states, while the linear alpha-chain can not be built up from two ground-state clusters. Due to the single shell model multiplicity of these shape isomers, one can say that to the extent the U(3) symmetry is valid, these states can be considered, as the cluster configurations mentioned before.

**EXTENSION OF ELLIOTT’S SU(3) SYMMETRY**

In Fig. 3 we illustrate some generalizations of Elliott’s SU(3) symmetry into different directions. In its original form it proved to be effective for light nuclei of the p and sd shell, for a single major shell problem. The vertical extension along the shell-excitation has been discussed in detail in [3].

Several approaches have been invented in order to export the elegant and powerful technique of the group theory to the medium and heavy nuclei. The interacting boson model [17] uses a method (by introducing bosons of coupled valence nucleons) which is applicable for a single (or a few) major shell. This model has a U(6) group structure, and one of its dynamical symmetries: U(6)⊃SU(3)⊃SO(3) describes the rotational spectra of deformed nuclei. The IBM model has been applied to
heavy nuclei in a very wide range.

The pseudo-SU(3) symmetry associates the SU(3) irrep of the \((n - 1)\)-th major shell to a subset of the states in the \(n\)-th major shell. It appears due to a special ratio of the \(ls\) and \(l^2\) interactions \([48]\). Thus the nucleon states are divided into two categories, and one of them carries the SU(3) symmetry. This approach can treat several major shells in a similar manner.

The quasi-dynamical SU(3) symmetry, as discussed beforehand, builds up from the contribution of many nucleons in a "democratic" way, i.e. no distinction is made between the single particle levels. It turns out that this symmetry may survive in the presence of different symmetry-breaking interactions, like e.g. spin-orbit and pairing \([49]\).

The extension towards the very light nuclei is related to the quasi-SU(3) symmetry (not to be mixed up with the quasi-dynamical symmetry, mentioned before) \([50]\) and no-core shell model (NCSM). The quasi-SU(3) is a symmetry of the shell model, and in the \(LS\) coupled proton-neutron formalism it results in an efficient truncation scheme: only the low spin components and SU(3) basis states of large deformation give important contribution \([17, 51]\). It is interesting that it turned out to be effective also with realistic nucleon-nucleon interactions in \(ab\) into calculations \([52]\).

The generalization to deformed basis and large deformation has been discussed in the previous section.

**SUMMARY**

In the present and the previous paper we have discussed the extension of the SU(3) connection between the shell, collective and cluster models. This relation was established in 1958 \([1, 2]\) for a single major shell, by applying spherical basis of the exact or dynamically broken symmetry. In \([3]\) we considered the vertical extension, i.e. the incorporation of major shell excitations. Here we discussed further generalization along the symmetry-breaking and large deformation.

The cluster-shell competition or coexistence has been interpreted in terms of the joint phase diagram of the shell and cluster models. Three different (shell, cluster and quasi-cluster) calculations indicate the position of the ground-band of \(^{20}\)Ne very close to the SU(3) matching point of the two models.

Concerning the large deformations the quasi-dynamical SU(3) symmetry is found to be stable for Nilsson-type interactions for several shapes with commensurable ratios of the main axes.

All these considerations, as well as many others, are based on the extension of Elliott’s SU(3) symmetry. In Figure 3 we summarized some of its generalization along different directions: excitation energy, mass number and deformation.

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