Shell and cluster structure in atomic nuclei

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Abstract. The shell and cluster structure of the atomic nucleus, as well as their interrelation (the SU(3) connection) is discussed. Some recent results indicating the importance of the shell-like clusterization are reviewed. Special attention is paid to the aspects of symmetries and phases. The important role of the SU(3) connection in the no-core shell model studies is mentioned.

1. Introduction
The fundamental structure models of the atomic nucleus are based on different physical pictures. The shell model indicates that the nucleus is something like a miniature atom. The cluster model is associated to the molecular picture. The investigation of the cluster–shell competition is a problem in nuclear structure studies with a great tradition.

In this contribution we discuss some aspects of this question, and investigate examples, in which there are very good reasons to talk about shell and cluster structure at the same time. This observation is not a new one, of course. The reason why we think that it is proper to present it here is manyfold. First, sometimes this kind of discussion is carried out in an oversimplified way, and important aspects of the problem remain hidden. Second, new results are available, which are worth investigating from this aspect. Third, this interrelation seems to play an important role in the recent ab initio calculations within the framework of the no-core shell model.

In what follows first we look at the question of the shell or cluster structure from the logical viewpoint. It turns out that there are not only two, rather three different simple states from this aspect: good shell-model states, good cluster-model states and good shell-model-like cluster-states. Then we recall some historical background of the problem, followed by a brief description of two recent works. Both of them are concerning the spectrum of the ground-state band of \( N = Z \) nuclei, and indicate the importance of shell-like clusterization. One of them is a new analysis of old experimental data on the \(^{20}\text{Ne}\) and \(^{24}\text{Mg}\) nuclei, the other one is a new experiment determining the ground and low-spin yrast states of the \(^{92}\text{Pd}\) nucleus, combined with a shell model calculation. Then we discuss the relation between the shell and cluster models from the viewpoints of symmetries and phases. Finally we mention very briefly the important role of the SU(3) connection between the shell and cluster models as well as quadrupole collective states in the new no-core shell model studies.

2. Logical arguments and historical background
Both the shell model and the cluster model provide us with a complete set of basis states in their general form, i.e. without applying simplifying model assumptions or basis truncation. (In fact the basis of the microscopic cluster model is overcomplete.) Therefore, the wavefunction of
any real nuclear state can be expanded in both bases. i) If the expansion is simple in the shell
model basis, but very complicated in the cluster basis, then we speak about a good shell model
state, which is a bad cluster model state. ii) If the expansion is simple in the cluster basis, but
complicated in the shell model, then the state is a good cluster state, and bad shell model state.
The rigid molecule-like states are like this. iii) But it may also happen that the expansion is
simple in both sets of basis states, then we speak about shell-model-like cluster states. One can
apply, of course, different names; what really matters is that the simple states from this aspect
are of three different kinds, not only two. In other words putting the question, like "shell or
cluster structure" may be an oversimplified one. iv) If the expansion is complicated in both
bases, then the state is not a simple state.

These considerations are very closely related, of course, to what we exactly mean by
clusterization, or by a cluster state. Different definitions are possible, and applied. A natural
one is to characterize the cluster state by its experimental observation. Therefore, in the present
discussion the definition we have in mind is that a state is considered to be a cluster state, if its
wavefunction has a large overlap with that of a reaction channel, in which it can be populated,
or decay [1].

The connection between the shell and cluster models was established already in 1958. In
particular Wildermuth and Kanellopoulos showed [2] that the Hamiltonian of the shell model
can be rewritten exactly into that of the cluster model in the harmonic oscillator approximation.
This relation gives, of course, a very close relation between the states of the two models. The
harmonic oscillator approximation indicates SU(3) symmetry, thus very soon after this work
Bayman and Bohr discussed [3] the connection based on the SU(3) group.

It is important to recall here, that the crucial role of the SU(3) symmetry in relating the
nuclear structure models was realised a short time beforehand by Elliott [4], who showed that
states with a well-defined quadrupole deformation and their rotation can be obtained from the
spherical shell model, by selecting according to the SU(3) symmetry. It also turned out that
the ground state in particular, and the low-energy spectrum in general, is dominated by SU(3)
basis states, corresponding to large deformation, i.e. to large eigenvalues of the (second order)
Casimir-operator.

Later on the connection between the shell model and cluster model states has been
investigated from different aspects. Some important works are cited in [5], but the list is
necessarily incomplete.

3. New evidences for shell-like clusterization
The $N = Z$ nuclei have long been known as good examples for showing clusterization. Recently
the ground-state bands of the $^{20}$Ne and $^{24}$Mg was analysed from a new aspect [6]. In particular a
generator coordinate method calculation have been completed, by applying an antisymmetrized
quasicluster basis. The special feature of this calculation is that it starts from the cluster
picture, i.e. an $^{16}$O core and alpha-particle(s), but with a change of a continuous parameter
of the wavefunction it can go to the shell model limit of $^{16}$O core plus 4 (or 8) nucleons. The
parameter is related to the strength of the spin-orbit interaction. By applying this method one
can check quantitatively how much the wave function cluster or shell-model like is. It turned
out that the best description of the ground-state band is provided by a wavefunction, which is
close to the shell-model like cluster configuration.

This recent study from the cluster side seems to complete very nicely some previous results
from the shell model side. In particular, shell-model calculations revealed the fact that the
SU(3) symmetry is approximately valid in the states of the ground-bands of these nuclei [7].
And good SU(3) symmetry indicates simple shell and cluster structure at the same time (if the
clusterization is allowed).

The heavier $N = Z$ nuclei are not stable, therefore, their experimental study is rather
complicated. The ground-state band of $^{92}$Pd was detected only recently [8], from an EXOGAM-DIAMANT-Neutron-Wall experiment, in which different particles were detected in coincidence. The energy sequence of the states with $0^+$, $2^+$, $4^+$, and $6^+$ spin-parities were found to be nearly equidistant. According to a state-of-the-art shell-model calculation this feature can be understood as a consequence of the isospin-zero, spin-aligned proton-neutron pairing of the valence nucleon(-hole)s [8, 9]. This nucleus is just 4 protons and 4 neutrons away from the $^{100}$Sn closed shell nucleus, i.e. its low-lying yrast states found in the experiment can be considered as two-quartet-hole states. Quarteting corresponds to shell-model-like clusterization, too.

### 4. Symmetries

Symmetry-based models can be useful also in describing different kinds of clusterization on an equal footing, as well as accounting for extended spectra in detail. In particular the semimicroscopic algebraic cluster model (SACM) [10] contains both rigid molecule-like, and shell model like clusterization, and it is easy to apply for the description of the gross features of experimental spectra. In this approach the relative motion of the clusters is accounted for by the vibron model [11], while the internal structure of the clusters is described by the SU(3) shell model [4]. The Pauli exclusion principle is taken into account in the construction of the model space.

The SACM proved to be successful in describing the detailed spectra of some cluster systems in terms of an approximate SU(3) dynamical symmetry [12]. It is also worth mentioning that the unified description of different cluster systems can be carried out in this framework by the extensions of this symmetry. Different cluster-configurations of the same nucleus can be treated in a unified framework by applying the multichannel dynamical symmetry [13], while similar clusterizations (e.g. core-plus-alpha-particle) of different nuclei can be described by the supersymmetric model [14]. By applying large multiplet-structures of the microscopic model space, and unified physical operators, these schemes handle the problem with serious constraints, and consequently they have strong predictive power.

### 5. Phases

The studies of phases and phase transitions of algebraic models are usually carried out as follows [15]. A group-theoretical model is considered with a well-defined model space and with interactions which are varied continuously. The model has limiting cases, called dynamical symmetries. When a dynamical symmetry holds, the eigenvalue-problem has an analytical solution, due to the fact that the Hamiltonian can be expressed in terms of the invariant operators of a chain of nested subgroups. In such a case the eigenstates of the Hamiltonian have a complete set of good quantum numbers. 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 [16] 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 [16, 17], 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 SACM of a binary cluster system has three dynamical symmetries. Two of them come from the vibron model of the relative motion: SU(3) corresponds to shell-like clusterization, or in the language of the collective motion to a soft vibrator, while SO(4) represents a rigid molecule-like rotator. The third symmetry, SO(3) corresponds to a situation, when the coupling between the relative motion and internal degrees of freedom of the clusters is weak. Therefore, the phase diagram of a binary system is two-dimensional, and can be illustrated by a triangle [18].

A triangle-like phase diagram has been proposed for the shell model, too, [19], which, in addition to the SU(3) and SU(2) symmetries has the independent-particle model as the third corner. The two phase diagram match each other at the SU(3) corner, as shown in Figure 1.

The real nuclear systems or states are supposed to be allocated to this diagram. The calculations of [6] indicates qualitatively, that the ground-state bands of the 20Ne and 24Mg nuclei are close to the SU(3) intersection. However, quantitative statement is not easily obtainable, because the control parameter of [6] is included in the wavefunction, while that of the algebraic models is related to the relative weights of the interactions with different dynamical symmetries.

6. Ab initio method

No-core shell model (NCSM) calculations [20] apply realistic nucleon-nucleon interactions and are built on fundamental principles. Therefore, they have great predictive power, and represent the forefront research in nuclear structure. Their applicability is, however, largely limited by the combinatorial growth of the dimension of the the model space, with increasing number of nucleons and major shells. The novel approach of the symmetry-adapted no-core shell model (SA-NCSM) [21] seems to solve this problem by winnowing the physically relevant states determined from symmetry considerations.

In this model a proton-neutron \( L - S \) coupled basis is used. The analysis of the full NCSM wavefunction showed a typical overlap of 90 percent or more with basis states of low spin \( S \), and large deformation. In other words: a small fraction of the full model space determines the low-energy dynamics to a large extent. This observation offers the possibility for organizing the model space in a more economic way, and the gain is several orders of magnitude in the dimension. The combination of the symmetry-adapted construction of the model space and advanced computational methods enlarges the capacity of the NCSM calculations very much.

Low-lying states of light and medium mass nuclei can be analysed in this way. E.g. the lowest-lying ten \( 0^+ \) states of the \( 12C \) nucleus have been calculated in [22], and investigated in order to see if they have any cluster structure (which would be revealed by some characteristic SU(3) configurations). It turns out that apart from the ground state only the sixth \( 0^+ \) state shows such a feature. This finding raises interesting question in relation with the experimental observations and/or the bare nucleon-nucleon forces.

7. Conclusions

The fundamental models of nuclear structure are closely related to each other on the microscopic level. In particular, the SU(3) dynamical symmetry sits in the intersection of the shell, cluster and collective models. Symmetry considerations are helpful also in revealing the different possible varieties within a basic model. E.g. they make clear distinction between rigid molecule like and shell model like clusterization, which correspond to different phases of the finite quantum
Figure 1. Relation of the phase diagram of the shell and cluster models. (Ind. part. stands for independent particle.)

Figure 2. Extension of Elliott’s SU(3) symmetry along the dimensions of the mass number and excitation energy. (The scale along the vertical axes is measured in $\hbar \omega$).

system of the many-nucleon system. In this contribution some recent studies were mentioned, which indicate the importance of the shell-like clusterization.

Algebraic models have proven to be useful in many respects in structure studies. They can describe different structures on an equal footing, and offer a possibility for quantitative allocation of nuclear states on the phase diagrams, an interesting task which still remains to be done as far as cluster or shell structure is concerned.

The SU(3) connection of the shell, collective and cluster states seems to play an important role in the new ab initio calculations, too. In particular, the symmetry-adapted no-core shell model calculations revealed the dominance of low-spin and high deformation basis states in the low-energy dynamics, and based on this observation the powerful concepts of the ab initio calculations could be extended to larger mass number and higher lying major shells. This very efficient treatment of the many-nucleon problem seems to enable the nuclear structure studies to formulate direct questions concerning the bare nucleon-nucleon interactions.

Elliott’s SU(3) symmetry was applied in its original form for the description of the low-lying states in light nuclei. Several interesting extensions of it has been proposed in the last decades, and in Figure 2 we tried to summarize them schematically.

Acknowledgments
This work was supported by the OTKA (Grant No. K72357) and by the MTA-JSPS collaboration (project No 119).
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