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# Localized versus shell-model-like clusters

J. Cseh
*Institute of Nuclear Research of the Hungarian Academy of Sciences,*
*Debrecen, Pf. 51, Hungary-4001,*
*e-mail:cseh@atomki.hu*

J. Darai
*Institute of Experimental Physics, University of Debrecen,*
*Debrecen, Bem tér 18/A, Hungary-4026.*

A. Algora
*Institute of Nuclear Research of the Hungarian Academy of Sciences,*
*Debrecen, Pf. 51, Hungary-4001,*
*IFIC (CSIC-Universidad de Valencia) A.C. 22085, E-46071 Valencia, Spain.*

H. Yépez-Martínez
*Universidad Autónoma de la Ciudad de México,*
*Prolongación San Isidro 151, Col. San Lorenzo Tezonco,*
*Del Izatapalapa, México, D.F. 09790, México.*

P.O. Hess
*Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México,*
*Apartado Postal, 70-543, México, D.F. 04510, México.*

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In light of the relation of the shell model and the cluster model, the concepts of localized and shell-model-like clusters are discussed. They are interpreted as different phases of clusterization, which may be characterized by quasi-dynamical symmetries, and are connected by a phase-transition.

*Keywords:* Cluster models; models based on group theory.

En la búsqueda de la relación entre el modelo de capas y el modelo de cúmulos, los conceptos de cúmulo localizado y cúmulo tipo modelo de capas son discutidos. Estos son interpretados como diferentes fases de clusterización, las cuales pueden ser caracterizadas por simetrías cuasi-dinámicas, y están conectadas por una transición de fase.

*Descriptores:* Modelos de cúmulos; modelos con base en la teoría de grupos.

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## 1. Introduction

The history of cluster studies is as long as that of nuclear structure. It was largely inspired by the analogy with molecular physics. In many articles cluster states and molecule-like states are used as synonyms. Though molecules themselves may have different features, usually one has in mind the physical picture of a rigid molecule. The experimental signature for such a structure can be that of a rotational band with alternating parities and following an exact $L(L+1)$ energy sequence, where $L$ stands for the angular momentum (of an even-even nucleus).

On the other hand the shell model became the most widely used theory of nuclear structure. Finding the cluster states among those of the shell model is also a long-standing task. They may or may not be simply connected to each other. When this relation is simple, we speak about shell-model-like clusters. The experimental signature of this kind of cluster structure is that the bands of positive and negative parities are separated, due to the fact that between the major shells of different parities there is a considerable energy gap.

Some authors apply the name of cluster state only for the structure of the rigid molecule type, while others (including ourselves) speak both about localized and shell-model-like clusters. A major argument in favour of this latter vocabulary is provided by the definition of the cluster state by its experimental observability. This is what we follow here, too. In particular a state is called cluster state if its wave-function largely overlaps with that of a reaction channel [1]. In light of this criterium the existence of localized and shell-model-like clusters turns out to be natural. On the other hand identifying the clusterization only with the rigid molecule like structure, and consider all the others as shell model states, could result in much bigger difference between two shell model states than that between a shell model and a cluster state (*e.g.* in terms of cluster spectroscopic factor).

A question of utmost interest is, of course, whether or not the extreme limits of the shell-like and rigid molecule-like

clusters are observed experimentally. The first case seems to be easier. In light nuclei the SU(3) symmetry is known to be approximately valid, *i.e.* the wave-function of some real nuclear state is dominated by a single SU(3) basis state. Furthermore, for such a basis state the shell model and cluster model state may have a very large overlap. Thus, several nuclear states with approximately good SU(3) symmetry can be considered not only as a good shell-model state, but at the same time as good cluster model state, too.

The observation of pure rigid molecule-like state is a more delicate question. A band in the $^{18}$O was reported to follow this sequence [2], which is associated to the $^{14}$O+$^{4}$He rigid binary structure. Later studies [3], however, showed that other band assignments are also possible (and can classify more cluster-bands). Some well-known states of the $^{12}$C has been associated to a triangle structure [4], but this interpretation is not unicvocal either; several authors claim that some of the states have different nature [5]. More recently new candidates showed up for the rigid structure from among the non-alpha-like nuclei. There the extra neutrons are thought to stabilize the molecular structure, via the "covalent binding" (by occupying molecular orbitals). The $^{10}$Be [6], and $^{14}$C [7] nuclei are considered as example for this phenomenon.

The best-known example of $^{20}$Ne, showing several well-developed $^{16}$O+$^{4}$He cluster bands [8] does not show a complete degeneracy of bands with positive and negative parities, but there is a tendency of approaching each other (for the bands of inversion doublets). Thus the overall qualitative picture suggests a transitional character between the rigid molecule and the shell-like nature (although the specific bands are not uniformly mixed).

In what follows first we review very briefly some aspects of the interrelation between the shell model and the cluster model, and discuss a few important consequences. Then we present the results of a recent schematic study in the framework of algebraic (phenomenologic and semimicroscopic) cluster models, aiming at the investigation of phases and phase transitions. A short comparison with the recent microscopic calculations along a similar line is also made. Finally some conclusions are drawn.

## 2. Shell model versus cluster model

### 2.1. Historical background

#### *2.1.1. Basic relations*

The relation of the cluster model to the shell model was established by Wildermuth and Kanellopoulos [9], who have shown that in the harmonic oscillator approximation the Hamiltonians of the two models can be rewritten into each other exactly:

$$H_{SM} = H_{C_1} + H_{C_2} + H_R \tag{1}$$

where $H_{C_i}$ is the internal shell-model Hamiltonian of the $i$th cluster, while $H_R$ is the Hamiltonian of their relative motion. Here we have written the relation for a binary cluster-configuration, for the sake of simplicity, and supposed that the center of mass motion is already separated. As a consequence, the wave function of one of them can be expressed as a linear combination of those wave functions of the other, which belong to the same energy.

The connection between the shell model and the quadrupole collective model was revealed by Elliott [10], who derived the rotational bands from the set of the shell-model states by picking up a definite SU(3) symmetry. Based on these results the SU(3) symmetry was used for interrelating the cluster states and quadrupole deformation, too [11].

This symmetry played an important role in many other works illuminating the connection between the two models (see *e.g.* Ref. 12). The transformations of the SU(3) group and that of the permutation group commute with each other, therefore, all the states belonging to a definite SU(3) irreducible representation (irrep) behave in the same way under the action of the antisymmetrizer operator [13]. The combination of this fact with the relation of the Hamiltonians results in an U(3) selection rule:

$$[n_1 n_2 n_3] = [n_1^{(c_1)} n_2^{(c_1)} n_3^{(c_1)}] \otimes [n_1^{(c_2)} n_2^{(c_2)} n_3^{(c_2)}] \otimes [n_1^{(r)} 00] \tag{2}$$

which says that a binary cluster-configuration characterized by the internal cluster-structure of $[n_1^{(c_1)} n_2^{(c_1)} n_3^{(c_1)}]$ and $[n_1^{(c_2)} n_2^{(c_2)} n_3^{(c_2)}]$, and by the relative motion of $[n_1^{(r)} 00]$, is allowed in the parent state of $[n_1 n_2 n_3]$ if and only if among the triple products on the right hand side the $[n_1 n_2 n_3]$ values are present. The $\otimes$ symbol indicates direct product.

The U(3) basis turned out to be very useful also in the calculation of the cluster spectroscopic factors both on the microscopic [14] and on the semimicroscopic level [15].

#### *2.1.2. More general interactions*

It is important to note that the U(3) connection of the cluster model states to those of the shell model (and via this path also to those of the collective model) is valid for more general interactions, too. Therefore, the same relation may hold for realistic cases as well, not only for the simple example of the harmonic oscillator. *E.g.* the (algebraic) quadrupole operator, which plays a crucial role in the description of the structure of light nuclei [10], can be split up into internal cluster and relative contributions in the same way, like the oscillator Hamiltonian. This problem was discussed more in detail in Ref. 16. The key point of the relation is that the energy eigenvectors can be symmetric (*i.e.* transform according to a definite irrep) even in cases when the Hamiltonian is not symmetric (scalar). This special dynamical breaking of the symmetry describes a more general situation, than the exact symmetry (*e.g.* that of the harmonic oscillator) [17].

### 2.1.3. *Deformed oscillators*

The deformed harmonic oscillator is known to explain the stability of the superdeformed (ratio of axes 2:1:1), and hyperdeformed (3:1:1), etc. shapes. As it was noticed by Rae [18], based on the decomposition of the deformed magic numbers, it also indicates the appearance of clusterization in these states. This observation, which was extended to more realistic models, too establishes the interrelation of the shape isomers and cluster configurations via their shell-model-correspondence.

From the viewpoint of the symmetry-based relation of the different model states (or from the viewpoint of the corresponding mathematical background) the work of Rosensteel and Draayer [19] illuminates the situation: they have shown that the symmetry algebra of any (three dimensional) harmonic oscillator Hamiltonian with commensurate frequencies is that of U(3). (See also [20].)

### 2.1.4. *Quasi-dynamical symmetries*

The validity of the U(3) symmetry, as discussed so far is limited in mass number, energy, etc. to the regions, where the relative importance of the symmetry-breaking interactions, like spin-orbit and pairing is small. It turned out, however, that in some sense the U(3) symmetry may survive even in cases when the symmetry-breaking interactions are so strong, that the leading-representation-approximation is not valid, *i.e.* the nuclear states are not dominated by a single U(3) basis states, rather they are superpositions of many basis states belonging to different U(3) irreps [21]:

$$\psi_{\alpha KJM} = \Sigma_{\xi\lambda\mu} C_{\alpha\xi\lambda\mu K} \phi_{\xi\lambda\mu KJM}, \qquad (3)$$

where $\phi_{\xi\lambda\mu KJM}$ is a basis vector for an SU(3) irrep, and $\xi$ stands for all the quantum numbers not belonging to the SU(3) group [22]. Please, note that 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 are the same. (This is called adiabatic coupling between the single-particle and collective degrees of freedom.) In particular the matrix elements of the SU(3) generators between these states 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 quasidynamical or effective SU(3) symmetry. The states of Eq. (3) with different $J$-s are said to form a soft SU(3) band.

The quasi-dynamical symmetry describes a situation, when neither the (Hamiltonian) operator, nor its eigenvectors are symmetric, yet the symmetry acts [17]. Obviously this very general concept enlarges the territory of the applicability of symmetry considerations very much.

## 2.2. Recent applications

In this subsection we consider some aspects of the shape-stability, based on the simple (cylindrically symmetric) Nilsson-model, and the relation of these shapes to cluster configurations, based on the U(3) selection rule.

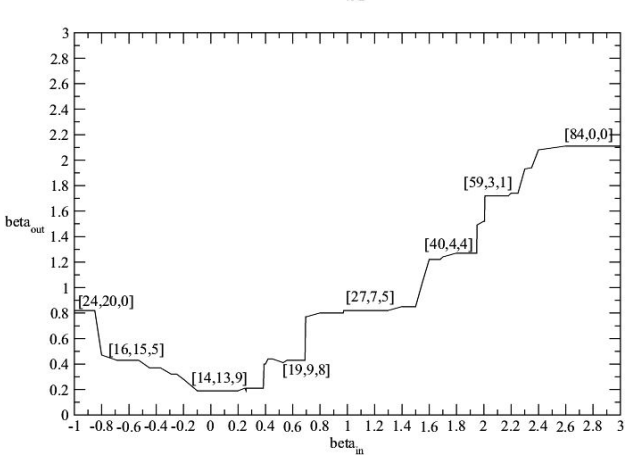


FIGURE 1. Absolute value of the deformation of the $^{28}$Si nucleus from the simple Nilsson-model.

### 2.2.1. *Shape-stability*

The determination of the effective (or average) $\lambda$ and $\mu$ values can be carried out by applying the asymptotic Nilsson states due to the fact that these states serve as intrinsic states for the soft SU(3) bands of Eq. (3) [22]. This procedure which was invented originally for large prolate deformation can be generalized for oblate shape and for small deformation, too, by expanding the Nilsson-orbitals in terms of asymptotic states [23]. The $\lambda$ and $\mu$ quantum numbers are uniquely related to the $\beta$ and $\gamma$ quadrupole shape-parameters [24]:

$$\beta^2 = \frac{16\pi}{5N_0^2}(\lambda^2+\mu^2+\lambda\mu), \quad \gamma = \arctan\left(\frac{\sqrt{3}\mu}{2\lambda+\mu}\right) \qquad (4)$$

where $N_0$ is the number of oscillator quanta, including the zero-point contribution.

We have investigated, how the effective SU(3) symmetry content, and related to that the deformation of the nucleus, changes as a function of the input-parameter of $\beta$. A typical result is shown in Fig. 1. The stair-like functional form can be understood as the influence of the crossings of the single-partical Nilsson-orbitals on the shape of the many-body system. It is interesting to note that the location of the symmetry, or shape-stability regions resemble to that of the local energy-minima of the Nilsson-Strutinsky calculations [25]. An interesting question is: what kind of clusterizations are allowed in these states.

### 2.2.2. *Deformation and clusterization*

In order to study the deformation-dependence we have investigated the appearance of cluster-configurations in the ground, superdeformed and hyperdeformed states of some

nuclei. The first two (at least in some cases) are known experimentally, the hyperdeformed states were predicted theoretically.

The main motivation of these studies was that in addition to taking into account the energetic preferences of different cluster-configurations we tried to incorporate the consequences of the exclusion principle as well. This latter one is done by the application of the real or quasi-dynamical $SU(3)$ symmetry for light and heavy nuclei, respectively, as mentioned above. In this way the effect of the Pauli-principle is handled only approximately, of course, but in a microscopic and well-controlled way, and its results can be tested by comparing with those of the fully microscopic calculations, where they are available. The forbiddenness of the cluster-configurations are characterized quantitatively. The deformation of the clusters (and parent nuclei) are taken into account, and no constraint is applied for their relative orientation.

The energetic preference of the clusterization is measured by the binding-energy difference (combined with the no-dipole constraint) of [26], on the one side, and in some cases with the more detailed double-folding potential energy of the dinuclear system model [27] on the other side. This latter quantity is determined both for the usual pole-to-pole configuration, and for the one, which is preferred by the selection rule.

We have considered the possible binary configurations for the $^{36}$Ar, $^{40}$Ca and $^{252}$Cf nuclei, [28,29], and some ternary configurations [30] for the $^{36}$Ar and $^{252}$Cf.

The main conclusion of these calculations can be summarized as follows. The preference of the exclusion principle and the energy-calculation do not necessarily coincide. Therefore, we think that when searching for the most probable cluster-configuration(s), one has to take into account not only the energetic circumstances, but the exclusion principle, too. It also turned out that sometimes the same clusterization can be present both in the ground and in the superdeformed, as well as in the hyperdeformed state. The difference between them is the spatial arrangement of the deformed clusters.

## 3. Phases and phase transitions

### 3.1. The algebraic method

Phases and phase-transitions are usually investigated in systems with very large numbers of degrees of freedom. More recently, however, much interest has been concentrated on the phase-transitions in finite quantum systems *e.g.* atomic nuclei [31,32]. Algebraic models seem to be especially useful for this kind of studies. In these models one usually considers finite number ($N$) of particles, but it is possible to go to the large $N$ limit, where real phase-transitions can take place. For finite $N$ it can be investigated, whether or not some less robust changes survive. As a control parameter one has the relative weight of the Hamiltonians belonging to the different dynamical symmetries (analytically solvable limits). The energy-minimum is investigated as a function of the control parameter, and the degree of its derivative showing discontinuity (in the large $N$ limit) defines the order of the phase-transition.

More recently a conjecture was made [33] that the phases (bounded by the real dynamical symmetries and the phase-transitions in the phase-diagram) can be characterized by a quasi-dynamical symmetry. If it is so then the situation resembles to that of the phase-transitions in Landau's theory, where the different phases are characterized by different symmetries [34]. These questions were investigated thoroughly concerning the quadrupole collective motion.

### 3.2. Cluster models

In Ref. 35 we have investigated the problem of phases and phase-transitions from the viewpoint of clusterization (*i.e.* dipole collectivity). We have concentrated on the relative motion of binary cluster systems. There are two relevant algebra-chains of the relative motion [36, 37], one containing U(3), and the other containing O(4). Their physical content are the following. From the collective motion viewpoint U(3) corresponds to a soft vibrator, while O(4) describes a rigid rotor. From the microscopic viewpoint U(3) corresponds to shell-model-like clusters, while O(4) describes localized clusters.

We have investigated binary cluster systems (with zero, one and two open-shell clusters) both in a phenomenologic and in a semimicroscopic model (in order to study the influence of the Pauli-principle on the question of phase-transition).

Concerning the geometrical picture associated to the two dynamical symmetries we should note the difference between the phenomenologic and the semimicroscopic model. In the former case the U(3) limit has a spherical equilibrium shape, but in the latter one does not. This is because there is a finite (non-zero) distance between the two clusters due to the Pauli-principle. Therefore, the difference between the localized and the shell-like clusterization is not so much the finite equilibrium distance (this is the case in both limits), rather their tendency for melting in the liquid of the shell-model states.

It turned out that phase transition takes place at a critical point both in the phenomenologic and in the semimicroscopic model in the large $N$ limit. For finite systems the transition is smoothed out somewhat, but still observable. (The larger the model space the more abrupt the transition is.)

Another interesting finding was that in both models the quasi-dynamical U(3) symmetry proved to be valid between the endpoint of the real dynamical symmetry and the critical point; *i.e.* throughout the whole phase.

### 3.3. Microscopic studies of phases

The localized (rigid rotor, O(4)) and the shell-like (soft vibrator, U(3)) cluster phases show very remarkable similarities to

the "solid" and "liquid" phases discussed in some recent microscopic cluster studies [6,32]. In these investigations the crystal-like structure, is considered as a solid phase, while the shell-like structure has the liquid properties. The driving force taking the system from one phase to the other is the spin-orbit. It is absent in the cluster-picture, but it becomes important when a cluster breaks up.

Microscopic calculations also indicate the appearance of some loosely bound alpha-condensate, in which alpha-particles occupy the same $0s$ state (apart from some correction due to the antisymmetrization effect). The oscillator parameter of this state is very different from that of the single-nucleon states. This kind of state is associated to the gas phase. The best experimental candidate for this phase is the $0_2^+$ state of $^{12}$C. Four-alpha state is also considered in $^{16}$O, around the break-up threshold [5]. Furthermore, it seems that alpha-condensate can develop in heavier nuclei, too, around a core [32].

## 4. Summary and outlook

In this contribution we have discussed some aspects of the localized and shell-model-like clusterization. Their relation raises several interesting open questions. One of the most exciting ones is how much they can be interpreted as two different phases of the finite nuclear matter. There are remarkable signs pointing at this direction, both from schematic algebraic model calculations, and from microscopic studies. If it turns out to be correct, then the different phases of the clusterized nuclear matter appear in energy closer to each other than the phases of the nucleonic matter. It seems to be very challenging, to try to explore this problem from both sides: by putting the algebraic calculations on a more realistic ground on the one hand, and by transferring the quantitative methods of phase-transitions to the microscopic level on the other hand.

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