Phases of clusterized nuclei

J Cseh
Institute for Nuclear Research, Hung. Acad. Sci., Debrecen, POB 51, Hungary-4001
E-mail: cseh@atomki.hu

Abstract. After reviewing some basic features of the temperature-governed phase-transitions in macroscopic systems and in atomic nuclei we consider non-thermal phase-transitions of nuclear structure in the example of cluster states. The vibron model, as the algebraic model of the relative motion, is considered from this aspect. The extension by the coupling to the internal degrees of freedom of the clusters is discussed. Phenomenological and semimicroscopical algebraic cluster models with identical interactions are applied to binary cluster systems of closed and non-closed shell clusters. A phase-diagram for the binary cluster systems is proposed, as well as its relation to that of the shell-model. The role of the quasi-dynamical symmetry, as a possible signature of the phase of a finite quantum system, is supported.

1. Introduction
1.1. Phase-transitions in macroscopic systems
One of the best-known phase-transition is that of the water. E.g. at fixed pressure the system changes from the liquid phase to the gas phase by increasing the temperature. At the transition point the temperature \(T\), the pressure \(p\) and the chemical potential \(\mu\) of the two phases are equal. The equilibrium of the system is determined by the second law of thermodynamics, via requiring the minimum of the free enthalpy \(G\), (or its portion for one particle \(\mu = G/N\), where \(N\) stands for the number of particles). Crossing the curve of phase-transition the chemical potential changes continuously, but its derivatives can be discontinuous. The order of phase-transition refers to the order of derivative, which is discontinuous. Below the critical point (at 647.1K, 22.06MPa) the transition is of first order, at the critical point it is of second order, and above that point it is analytical, or cross-over, i.e. each derivative is continuous.

1.2. Thermal phase-transitions in nuclei
In the ground-state region the atomic nucleus is usually considered to be a microscopic liquid drop. It is a long-standing question if there is a phase-transition to the gas phase with increasing temperature. After much experimental and theoretical investigations along this line the answer seems to be affirmative [1]. This is a first order phase-transition of the nucleonic matter.

At even higher temperature the nucleons dissolve and quarks and gluons move freely. As a consequence a drastic phase-transition may take place from the hadronic to the deconfined phase. At the RHIC, LHC and Early Universe energies (and densities) this transition is predicted to be analytical, but lower-order transitions are also expected (at smaller temperatures and larger densities). [2, 3].

These phase-transitions are governed by the temperature, thus we call them thermal transitions. The finite-size effects of the nucleus are very important, of course, they have to
be taken into account and they modify the results in comparison with the infinite limit.

1.3. Non-thermal phase-transitions

In atomic nuclei other kind of phase-transitions can also be observed, which are not governed by the temperature, thus we call them non-thermal phase-transitions. Their appearance is even more closely related to the finite-size effects; in a sense we can say that they show up due to the finite size effects, since they have to do with the nuclear shape, or with the collective motion of the nucleus as a whole. These phenomena are sometimes called quantum phase-transitions, shape-phase transitions, $T = 0$ phase transitions, or ground-state phase-transitions.

In relation with the quadrupole collectivity of nuclei a large amount of work has been carried out along this line, and excellent review papers are available [4]. Here we discuss the basic concepts from the viewpoint of the dipole collectivity, which is the basic degrees of freedom of clusterization. Partly because the dipole collectivity is simpler than the quadrupole one, and also because it is less known, and it might be interesting to look at the problem from a different angle.

2. Algebraic cluster models

The clusterization of atomic nuclei is usually described by cluster models. The basic assumption of all the cluster models is that the relevant degrees of freedom of the nucleus are classified into two categories. Some of them account for the relative motion of the clusters, while others are related to the internal degrees of freedom of the clusters. The phenomenological and the semimicroscopical models apply cluster-cluster interactions, the difference between the two kinds is in the model space. In the semimicroscopical models the Pauli-forbidden states are excluded from the model space, while in the phenomenological model they are not, or not completely. (The fully microscopical models incorporate antisymmetrization, of course, and apply effective nucleon-nucleon forces, instead of cluster-cluster interactions.)

Algebraic models are especially suitable for the studies of phase-transitions, thus we apply here algebraic cluster models. The group-theoretical methods guide us in constructing the physical operators and calculating their matrix elements, but they do not decide about the inclusion of the Pauli-principle. Therefore, it is possible to build up phenomenological and semimicroscopical models with the same algebraic structure, including the same interactions, but having different model spaces.

We consider here binary cluster systems and describe them by phenomenological and semimicroscopical algebraic cluster models in such a way that the interactions of the two models are the same. We do so in order to check if the exclusion principle has an influence on the appearance of the phase-transition.

The relative motion is accounted for by the vibron model of $U(4)$ group-structure [5]. The building blocks of this model are the dipole and scalar bosons (as opposed to the interacting boson model of quadrupole collectivity [6], in which quadrupole and scalar bosons are taken). The vibron model has two dynamical symmetries, described by the (I) $U(4) \supset U(3) \supset O(3)$ and (II) $U(4) \supset O(4) \supset O(3)$ group-chains.

The internal structure of the clusters is described by the Elliott-model [7] of $U^{ST}(4) \otimes U(3)$ group structure, where $U^{ST}(4)$ is the spin-isospin group of Wigner [8], while $U(3)$ refers to the orbital part. The product wavefunctions of these models are contaminated by the Pauli-forbidden states, resulting in a phenomenological algebraic cluster model (PACM). When the Pauli-principle is appreciated, and the forbidden states are excluded from the model space we end up with the semimicroscopical algebraic cluster model (SACM)[9].

The interactions of the models are constructed from the group-generators, as usual in the algebraic description. When we are interested only in a single sector of the spin-isospin space, then Wigner’s group is important only in the construction of the model space, but from the
viewpoint of the interaction the group structure simplifies to: $U_{C_1} \otimes U_{C_2} \otimes U_R \supset U(3) \supset O(3)$, where $C_i$ stands for the $i$th cluster, and $R$ indicates relative motion. The Hamiltonian built up from the invariant operators of this chain has a $U(3)$ dynamical symmetry: $H_{U^3}$.

The $U(3)$ limit of the algebraic cluster models corresponds to a soft vibrator in the collective model terms. (More precisely we should call it soft vibrational-rotational motion, but we follow here the simplified terminology.) In order to characterize the rotational-vibrational behaviour one can apply the parameter $R = (2E_{\text{rot}})/(E_{\text{vib}})$, where $E_{\text{rot}}$ stands for the first rotational energy, while $E_{\text{vib}}$ denotes the lowest-lying vibrational one. When $R \approx 1$ then the spectrum is considered to be a soft vibrator, and $R \ll 1$ corresponds to the rigid rotor [10]. From the microscopic viewpoint the $U(3)$ dynamical symmetry describes shell-model-like clusterization, when the cluster model state can be expressed in terms of a few (or a single) shell model basis states [11].

In the vibron model, applied for the description of the relative motion, there is also an $O(4)$ dynamical symmetry. We denote the $O(4)$ dynamically symmetric interaction by $H_{O^4}$. This limit corresponds to a rigid rotor (in the language of the collective model), or to a rigid molecule-like cluster-configuration (from the microscopic viewpoint). This latter name indicates that the cluster wavefunction can be expressed only in a large number of shell-model basis states.

One can apply [12] a general Hamiltonian: $H = xH_{U^3} + (1 - x)H_{O^4} + aH_{O^3}$, thus $x = 0$ corresponds to the $O(4)$ limit, while $x = 1$ gives the $U(3)$ dynamical symmetry.

3. Phase-transitions in the Vibron Model

The vibron model, as an algebraic description of dipole motion, is extensively applied in molecular physics [10, 13], as well as in hadron spectroscopy [14], in addition to the studies of nuclear clusterization [15]. The characteristic features of the applications in different fields are discussed in [16]. The shape-phase-transition in the vibron model has been studied by different methods [17, 18].

First we consider the limiting case of large $N$, when the calculations can be carried out analytically. Here $N$ is the number of particles, i.e. the total number of bosons. Its physical meaning is the largest possible number of dipole phonons (oscillator quanta) in the relative motion of the two clusters.

3.1. Large $N$ case

The expectation value of the energy, which corresponds to the general Hamiltonian above can be calculated analytically with the coherent state technique [19]. The energy-functional depends on two parameters: $r$ is the distance between the two clusters, and $x$ is the control parameter, i.e. the relative weight of the interactions of different dynamical symmetries. The minimum with respect to the geometrical parameter determines the shape of the nucleus. We investigate the behaviour of this energy-minimum as a function of the control parameter. It varies continuously, as well as its first order derivative, but at a certain $x_0$ value the second-order derivative is discontinuous. Thus we speak about a second order phase-transition.

Let us summarize here the analogy between the macroscopic phase-transitions, and those of the cold finite quantum system, e.g. atomic nucleus. In both cases there is an energy-like physical quantity (e.g. the free enthalpy versus the ground-state energy), which determines the equilibrium of the system via its minimum (as a consequence of the second law of thermodynamics). There is a control-parameter, which governs the system (e.g. temperature versus relative weights of the interactions with different dynamical symmetries). The physical quantities changes continuously as a function of the control parameter, but some derivatives may show discontinuity at a critical point. Then we speak about a phase-transition of the order given by the discontinuous derivative. This similarity is the reason, why the language of phase-transitions is applied in relation with the cold nuclear structure problem.
3.2. Critical behaviour

The potential energies corresponding to the $U(3)$ and $O(4)$ dynamical symmetries have minima at different values of the geometrical parameter $r$. The competition of these two minima, as a function of the control parameter results in the phase-transition, as described in the previous subsection. For the parametrization, applied here, for large $x$ values ($x \approx 1$) the minimum of the $U(3)$ dynamically symmetric parts dominates, and the minimum is at $r = 0$. With decreasing value of $x$ the minimum gets less deep, and at the critical value of $x_0$ it is rather flat. One can try to approximate this flat potential by a square infinite well, in which case the description of the critical-point behaviour can be given analytically, in terms of the Bessel-equation. Then one speaks about the $E(3)$ critical-point symmetry [18], where the number 3 refers to the dimension of the problem, while $E$ stands for the Euclidean group, related to the flat potential. (This symmetry is the 3-dimensional sister of the much studied $E(5)$ critical-point symmetry of the quadrupole model [20].)

3.3. Finite $N$ case

The real physical systems represent the situation of finite boson number $N$. Then the eigenvalue-problem has to be solved by numerical diagonalization for different values of the control parameter. No analytic calculations can be carried out, which could show the appearance of the phase-transition, but numerical studies can show if a precursor of it can be observed as an abrupt but smooth change, due to the finite-size effects.

It turns out that both the energy-spectrum, and other physical quantities show this kind of behaviour, with sharper changes for larger $N$. In [18] the low-lying energy-spectrum, the overlap of the ground-state wave-function with that of the $U(3)$ limit, the expectation value of the dipole bosons over $N$ (as the quantal order parameter), and some characteristic energy-ratios ($E_{21}/E_{02}$, $E_{31}/E_{02}$), as well as electromagnetic transition ratios ($\frac{B(E1;21\rightarrow11)}{B(E1;11\rightarrow01)}$, $\frac{B(E1;02\rightarrow11)}{B(E1;11\rightarrow01)}$) are found as signatures of the phase-transition.

4. Phase-transitions in the algebraic cluster models

4.1. Relative motion

The first straightforward question to investigate in the algebraic cluster model is if the phase-transition of the vibron model survives if we couple the internal cluster degrees of freedom. This problem was investigated in [12]. It turned out that the phase-transition between the $U(3)$ and $O(4)$ dynamical symmetries can be observed independent of the fact if the clusters have closed- or open-shell structure. Furthermore, both the phenomenological and the semimicroscopical description shows its appearance, i.e. the incorporation of the Pauli-principle does not change the situation qualitatively.
4.2. Binary clusterization

In fact the algebraic model of a binary cluster system has three dynamical symmetries, not only two, like the vibron model. This is a consequence of the coupling to the internal cluster degrees of freedom, of course. In particular they are, as follows:

\[
\begin{align*}
U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_R(4) &\supset U_{C}(3) \otimes U_R(3) \supset U(3) \supset SU(3) \supset SO(3) \\
U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_R(4) &\supset U_{C}(3) \otimes O_R(4) \supset SO_C(3) \otimes SO_R(3) \supset SO(3) \\
U_{C_1}(3) \otimes U_{C_2}(3) \otimes U_R(4) &\supset U_{C}(3) \otimes U_R(3) \supset SO_C(3) \otimes SO_R(3) \supset SO(3).
\end{align*}
\] (1)

The first two are sort of trivial extensions of the $U(3)$ and $O(4)$ symmetries of the vibron model, the third one is the so-called weak-coupling limit, which contains the $U(3)$ group, but allows only angular momentum interactions (and not quadrupole interactions).

As a consequence of the three dynamical symmetries, the phase-diagram of the binary cluster model is two-dimensional, and can be represented as a triangle, shown in Figure 2.

4.3. Connection to the shell model

The interrelation between the shell-model and cluster model is a longstanding problem, which has been investigated from different aspects. From the viewpoint of the phase diagram the connection of these two approaches is also an interesting question.

The phase-diagram of the shell model is also a triangle [21], as shown in Figure 3. Here the $SU(2)$ limit corresponds to the jj-coupling, while the $SU(3)$ corresponds to the ls-coupling. This latter one is the common intersection with the cluster model. Therefore, the relation between
the phase diagrams of the shell model and cluster model can be illustrated, as shown in Figure 4.

Where the specific nuclei are located on this map is an important open problem, which remains to be investigated.

5. Signature of the phases
In the thermodynamics a phase is homogeneous and shows a common physical behaviour, e.g. it is described by a single (set of) equation of state. In case of the finite quantum systems, e.g. atomic nuclei it is not so trivial what the signature of the phase is (for a finite volume of the phase-space).

For reasons of simplicity let us come back to the one-dimensional phase-diagram of the vibron model (Figure 1) in studying this problem. The diagram is defined by the dynamical symmetries of the model, as ending points. Somewhere in between there is a phase-transition-like phenomenon. Thus the phase is determined by the end-point of the phase-diagram and the critical point of the transition. But the question of the common physical behaviour of a phase is not so simple. The unique and final answer to this question is not known yet, but there is an interesting suggestion put forward by D. Rowe [22], which is based on his numerical studies of the quadrupole collective model. In particular a quasi-dynamical symmetry seems to be present (practically) in the whole phase of the quantum system.

Our numerical studies [12] show that for the cluster-problems the quasi-dynamical $U(3)$ symmetry is the common physical content for the whole phase between the end-point of the real $U(3)$ symmetry at $x = 1$ and (very close to) the transitional point $x_0$.

The quasi-dynamical $U(3)$ symmetry is more general than the dynamical $U(3)$ symmetry[23]. In the latter case the energy-eigenvectors are $U(3)$ basis states in spite of the fact the interaction is not $U(3)$-invariant. In case of the quasi-dynamical symmetry, however, the eigenstates are linear combinations of basis states belonging to different irreducible representations of $U(3)$, but in such a special way that the matrix-elements of the generators between these states approximate those of the real symmetry. In a sense the quasi-dynamical symmetry is the most general symmetry-concept of the quantum mechanics, describing a situation when neither the operator, nor its eigenvectors are symmetric, yet the eigenvalue-equation is symmetric[24].

If this guess is correct, and the signature of the phase of a finite quantum system really proves to be the quasi-dynamical symmetry, then the situation resembles to that of Landau’s theory of phase-transitions[25]. In particular, different phases are characterized by different symmetries, and the phase-transition involves the change of the symmetry.
6. Summary and conclusion

Today we know how the transition of the nucleonic matter takes place from the liquid phase to the gas phase. It is studied very intensively, how the phase transition from the hadronic matter to the deconfined matter happens. It is also an interesting question, what kind of phases the clusterized nuclear matter has, and what kind of transitions show up between them. Work along this line has also started, but it is at the very early stage. In this paper we tried to review the phenomenological aspects of the problem, from the angle of the algebraic models, which offer a convenient possibility for studying these problems quantitatively. Investigations from the side of the microscopic theories have also started [26].

The atomic nucleus is known to be a good prototype of mesoscopic systems, and several methods worked out in nuclear studies could be exported to other fields of research too. The better understanding of the phase-transitions of finite quantum systems might be fruitful for very exotic applications as well, like e.g. that of the protein-folding[27, 28].

Acknowledgments

This work was supported by the OTKA (Grant No. K72357) and by the exchange program of the Bulgarian and Hungarian Academies of Sciences. The author acknowledges collaboration on some parts of this work with H. Yepez-Martinez, P.O. Hess and J. Darai. Fruitful discussions with D. Rowe, N. Itagaki, M. Ploszajczak and A. Georgieva are also highly appreciated.

References

[1] Elliott J B et al. 2002 Phys. Rev. Lett. 88 042701
[2] Aoki Y et al. 2006 Nature 443/12 675
[3] www.gsi.de/fair/experiments/CBM
[4] Cejnar P, Jolie J 2009 Prog. Part. Nucl. Phys. 62 210; Iachello F 2009 AIP Conf. Proc. 1165 193
[5] Iachello F 1981 Phys. Rev. C 23 2778
[6] Iachello F, Arima A 1987 The Interacting Boson Model, Cambridge University Press, Cambridge
[7] Elliott J P 1958 Proc. Roy. Soc. A 245 128
[8] Wigner E P 1937 Phys. Rev. 51 106
[9] Cseh J 1992 Phys. Lett. B 281 173; Cseh J, Lévai G 1994 Ann. Phys. (NY) 230 165
[10] Iachello F, Levine R D 1995 Algebraic Theory of Molecules, Oxford University Press, Oxford
[11] Cseh J, Darai J, Algora A, Yepez-Martinez H, Hess P O 2008 Rev. Mex. Fis. 54 S3 30
[12] Yepez-Martinez H, Cseh J, Hess P O 2006 Phys. Rev. C 74 024319
[13] Frank A, Van Isacker P 1994 Algebraic Methods in molecular and Nuclear Structure Physics, Wiley, NY
[14] Iachello F Mukhopadhyay N C, Zhang L 1991 Phys. Rev. D 44 898
[15] Lévai G, Cseh J, Scheid W 1992 Phys. Rev. C 46 548; Cseh J, Lévai G, Scheid W 1993 Phys. Rev. C 48 1724; Lévai G, Cseh J 1996 Phys. Lett. B 381 1; Fulop Zs et al. 1996 Nucl. Phys. A 604 286; Cseh J, Léva G, Ventura A, Zuffi L 1998 Phys. Rev. C 58 2144; Lepine-Szily A et al. 1999 Phys. Rev. Lett. 82 3972; L. Hernández de la Peña et al. 2001 J. Phys. G 37, 2019
[16] Iachello F, Cseh J, Lévai G 1995 APH NS Heavy Ion Physics 1 91
[17] Van Roosmalen O S, Dieperink A E L 1982 Ann. Phys. NY 139 198; Leviatan A, Kirson M 1988 Ann. Phys. NY 188 142; Cejnar P, Iachello F 2007 J. Phys. A 40 581
[18] Zhang Y et al. 2008 Phys. Rev. C 78 024314
[19] Hess P O, Lévai G, Cseh J 1996 Phys. Rev. C 45 2345; and references therein.
[20] Iachello F 2000 Phys. Rev. Lett. 85 3580
[21] Frank A, Jolie J, Van Isacker P 2009 Symmetries in Atomic Nuclei, Springer, NY
[22] Rowe D J 2004 Nucl. Phys. A 745 47
[23] Jarrio M, Wood J L, Rowe D J 1991 Nucl. Phys. A 528 409
[24] Cseh J 2006 Proc. IV Int. Symp. on Quantum Theory and Symmetries (Varna) (Sofia: Heron Press) p 918
[25] Landau L D, Lifshiz E M 1976 Teoreticheskaya Fizika V, Nauka, Moskva
[26] Itagaki N, Masui H, Ito M, Aoyama S 2005 Phys. Rev. C 71 064307
[27] Broglia N A, Tiana G, Provasi D 2004 J. Phys: Cond. Matt. 16 R111
[28] Yakubovich A V, Solov’yov I A, Solov’yov A V, Greiner W 2006 Eur. Phys. J. D 40 363