Phase transitions in algebraic cluster models

H Yépez-Martínez¹, L Parra Rodríguez², P O Hess², J Cseh³ and G Lévai³

¹ Universidad Autónoma de la Ciudad de México, Prolongación San Isidro 151, Col. San Lorenzo Tezonco, Del. Iztapalapa, 09790 México, D.F., Mexico
² Instituto de Ciencias Nucleares, UNAM, A.P. 70-543, 04510 México, D.F., Mexico
³ Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Pf. 51, Hungary-4001

E-mail: hess@nucleares.unam.mx

Abstract. Two algebraic cluster models are studied from the point of view of phase transitions: one in which the Pauli exclusion principle is taken into account and one in which it isn’t. A third-order interaction is introduced to avoid instabilities in the model spectra, which is generally not taken into account. It is shown that both first- and second-order phase transitions occur. The $^{20}\text{Ne} \rightarrow ^{16}\text{O} + ^4\text{He}$ system is considered as an example. Without taking into account the Pauli exclusion principle the transition from the $SU(3)$ to the $SO(4)$ dynamical symmetry is of first or second order, depending on the strength of the quadrupole-quadrupole interaction. It is shown that the inclusion of the Pauli-principle can be simulated by higher-order interactions when the model space is not truncated.

1. Introduction

The study of phase transitions enjoys a substantial interest in algebraic models of nuclear structure. The first examples [1, 2] were related to the Interaction Boson Approximation (IBA) [3] and the vibron model [4, 5]. In these approaches a coherent state is constructed in terms of collective variables and a semi-classical potential is defined as the expectation value of the Hamiltonian with respect to the coherent state. Phase changes are identified with discontinuities in the derivatives of the potential with respect to specific parameters taken at the potential minima. An important conjecture was that phases are determined by quasi-dynamical symmetries. This approximate symmetry is also denoted as an effective symmetry and its mathematically sound definition, called embedded symmetry [6] has been applied to the shell model of the nucleus in [7]. The role of the quasi-dynamical symmetry in relation with the phase-transition was discussed in [8, 9, 10].

Here we discuss phase transitions within algebraic cluster models, in which the relative motion is described by the vibron model. It was found that the corresponding phase transition is of second order [11]. In [12] phase transitions in $U(n)$ algebraic models were discussed using interaction terms up to second order and the existence of a second-order phase transition was confirmed. In [13] a numerical study was performed within a realistic cluster system and it was argued (without proof) that the transition might be of first order.

Here we revisit phase transitions within a particular set of cluster models. One is the Phenomenological Algebraic Cluster Model (PACM), while the other is the Semimicroscopic Algebraic Cluster Model (SACM) [14, 15]. The first set does not obey the Pauli exclusion
principle, while the latter does. We apply the coherent state method to investigate phase transitions and their order. We consider two spherical clusters in order to discuss the following points: i) What changes when we implement the Pauli exclusion principle? ii) Will the order of phase transition change when third-order interactions are introduced to stabilize the spectrum? We will show that there are first- and second-order phase transitions in the PACM. iii) We will show that when the Pauli exclusion principle is taken into account, it corresponds to introducing higher-order interactions (in the PACM language). This changes significantly the structure of phase transitions and may involve a critical point.

In Section 2 we resume the cluster models considered including the Hamiltonian, which will be the same for the two groups of cluster models. This section also deals with the determination of the order of phase transitions using standard methods [16, 17]. In Section 3 the system $^{20}\text{Ne} \rightarrow ^{16}\text{O} + \alpha$ is considered as a particular example, while in Section 4 conclusions are drawn.

2. The cluster models and phase transitions

2.1. The model space

We consider two different kinds of cluster model: the Hamiltonian in both is exactly the same and they differ in their model space. In the PACM the model space includes states which are forbidden by the Pauli exclusion principle, while within the SACM the Pauli exclusion principle is taken into account. The basic degrees of freedom are dipole bosons $\pi_{\text{in}}^\dagger$ and scalar bosons $\sigma_{\text{in}}$. The latter are introduced in order to generate a cutoff $N$, such that the total number of bosons, $n_{\pi} + n_{\sigma} = N$ is kept constant. In the SACM the relevant group chain defining the basis is $SU_{C_1}(3) \otimes SU_{C_2}(3) \otimes SU_R(3) \supset SU_C(3) \otimes SU_R(3) \supset SU(3) \supset SO(3) \supset SO(2)$, from the viewpoint of the space degrees of freedom. The individual clusters are described by the irreducible representation (irrep) of $SU_{C_1}(3)$ and are denoted by $(\lambda_C, \mu_C)$. The two cluster irreps are coupled to the irrep $(\lambda, \mu)$ of $SU_C(3)$. The relative motion is described by the $SU_R(3)$ group with its irrep $(n_{\pi}, 0)$, where $n_{\pi}$ is the number of oscillator quanta in the relative motion. $(\lambda, \mu)$ is the total irrep of $SU(3)$. $L$ and $M$ are the angular momentum and its projection of the $SO(3)$ and $SO(2)$ group, respectively, and there is a multiplicity index from $SU(3) \supset SO(3)$ in order to distinguish multiple occurrences of a given $L$ in $(\lambda, \mu)$. The individual clusters are described in terms of Elliott’s $SU(3)$ model [18]. All possible $SU(3)$ irreps $(\lambda, \mu)$ are determined. Within the PACM no restriction is applied and the number of $\pi$ bosons starts from zero. Within the SACM the list of the $SU(3)$ irreps is compared to the list of possible irreps within the $SU(3)$ shell model and only those appearing in the latter list are taken into account. (A similar selection is applied also for the irreps of the $U^{ST}(4)$ spin-isospin group.) As a consequence, there is a minimal number of $\pi$ bosons, denoted by $n_0$. In what follows only the case of two spherical clusters is considered, which implies $(\lambda, \mu) = (0, 0)$, $\alpha = 1, 2$ and $(\lambda, \mu) = (n_{\pi}, 0)$.

2.2. The Hamiltonian

The Hamiltonian, for the case of two spherical clusters is given by

$$H = xH_{SU(3)} + (1-x)\left(H_{O(4)} - \frac{1}{2}\right), \quad (1)$$

where the term $-\frac{1}{2}$ is introduced for convenience. Here

$$H_{SU(3)} = \hbar \omega n_{\pi} + y(a - \hbar \Delta n_{\pi})n_{\pi}(n_{\pi} + 3) + \gamma L^2$$

$$H_{O(4)} = \frac{c}{4}[(\pi^1 \cdot \pi^1) - (\sigma^1)^2][[(\pi \cdot \pi) - (\sigma)^2] + \gamma L^2, \quad (2)$$

with $\Delta n_{\pi} = n_{\pi} - n_0$, $n_0$ being the minimal number of quanta, which, in the PACM is equal to zero, while in the SACM it differs from zero. For the case of two spherical clusters the second-order Casimir operator of $SU(3)$ is just given by $n_{\pi}(n_{\pi} + 3)$. The variable $y$ gives the intensity
of the quadrupole-quadrupole interaction. It is used as parameter which defines the strength of the quadrupole-quadrupole interaction and, therefore, varies only from $y = 1$ (full interaction) to $y = 0$ (no quadrupole-quadrupole interaction). $H_{SU(3)}$ contains a third-order interaction $\Delta n_\pi n_\pi^2$, too. This term is of utmost importance in stabilizing the spectrum. In order to get a stable spectrum (with no high $n_\pi$ states getting below the ground state), the parameter $a$ has to be negative (corresponding to an attractive quadrupole-quadrupole interaction) and the parameter $b$ has to have the same sign as $a$. Without this term states with large enough $n_\pi$ would come below the ground state. The justification of the third-order term is given in [19] within the context of the symplectic model.

The proposed correction to the strength of quadrupole-quadrupole interaction is the simplest possible one. In principle it could be replaced by the third-order Casimir operator of $SU(3)$ too.

2.3. Coherent state and the mapping to a semi-classical potential

In order to map to a semi-classical potential, a coherent state is introduced as [20],

$$ | \alpha > = \mathcal{N}_{N,n_0} \frac{N!}{(N+n_0)!} d^{n_0} \left[ \sigma^+ + \gamma (\alpha \cdot \pi) \right]^{N+n_0} | 0 > $$

where the $\gamma$ parameter has to be set to 1 after the differentiation and the normalization factor $\mathcal{N}_{N,n_0}$ is given in [20]. For convenience here we redefined the total number of relative oscillation quanta by $(N + n_0)$. The coherent state for the PACM is obtained with $n_0 = 0$. The only variable which will play a role is the absolute value of $\alpha_m$, denoted by $\alpha$, with $\alpha^2 = \sum_m \alpha_m \alpha_m^*$. The geometrical potential is obtained by calculating the expectation value of $H$ with respect to the coherent state using $| \alpha \rangle \langle \alpha |$.

$$ \langle \alpha | H | \alpha \rangle = V(\beta) = N\beta^2 \left[ x (h\omega + 4y (a - b)) - (1 - x) c (N - 1) \right] + N (N - 1) \beta^4 [xy (a - 6b) + (1 - x) c] - N (N - 1) (N - 2) \beta^6 xyb . $$

This potential can be reparametrized as

$$ V = N(N - 1)(N - 2)(-bx) \left\{ A\beta^2 - B\beta^4 + \beta^6 \right\} . $$

Finally, it suffices to investigate the effective potential $\tilde{V} = \{ A\beta^2 - B\beta^4 + \beta^6 \}$, which depends on the variable $\beta \in [0, 1]$.

In the SACM the expression gets more involved. For example, the expectation value of $n_\pi$ in the PACM is given by $N\alpha^2/(1 + \alpha^2)$, while within the SACM we obtain

$$ \langle n_\pi \rangle = (N+n_0)\alpha^2 F_{11}(\alpha^2) F_{00}(\alpha^2) . $$

The $F_{pq}$ function is a polynomial in $\alpha^2$ of the order $N + n_0 - \max(p, q)$. Similar formulas are obtained for the other interaction terms. This expression makes it extremely difficult to determine analytically the first and second derivatives of the potential with respect to the parameters of the model, taken at generally more than one minimum of the potential. As we shall see below, there is still a possibility to determine them.

There is one important observation: Inspecting Eq. (6) and noting that within the PACM $\langle n_\pi \rangle = N\frac{\alpha^2}{1 + \alpha^2}$ holds, one can realize that the inclusion of the Pauli exclusion principle corresponds to the introduction of higher-order interactions of the type $n_\pi^k$.

Another observation is related to the $N$-dependence of the potential. In principle, one can renormalize the expression such that no $N$-dependence appears at the end (for example, see [21]). Due to lack of space, we do not apply this renormalization and refer to a later publication.
By inspecting the expressions for the SACM we immediately note some important differences to PACM: the expectation value of the \( \pi \) number operator is proportional to \( \alpha^2/(1 + \alpha^2) \), while within the SACM we get a complicated function in \( \alpha \). This function can also be obtained within the PACM when higher-order interaction terms are included. Thus the ratios \( F_{pq}/F_{00} \) simulate higher-order interactions within the PACM. This already indicates that the phase transitions can be of order higher than two.

2.4. Phase transitions

Phase transitions are investigated using the following steps recommended by [16, 17, 22, 23].

a) First the minima of the Potential Energy Surface (PES) in the space of the collective variables \( \alpha_{im} \) is determined. Now there is only one relevant variable \( \alpha \), because the distance vector between the two clusters can always be aligned along the intrinsic z-axis. Studying the extrema via \( \frac{dV}{d\alpha} = 0 \) determines the potential at the minima \( V(\bar{\alpha}_i) \) and their location \( \alpha = \bar{\alpha}_i \). Now, this index \( i \) now does not refer to a component of \( \alpha \) but to the value of \( \alpha \) at a specific minimum. The \( \bar{\alpha}_i = \bar{\alpha}_i(x) \) are functions of the interaction parameters \( \vec{p} = (p_k) \), with \( k = 1, 2, ..., n_k \) and \( n_k \) being considered as control parameters. In our case there are two, namely \( x \) and \( y \). The \( y \) parameter serves only in fixing the strength of the quadrupole-quadrupole interaction (parameters \( a \) and \( b \)).

b) Once the extrema are obtained, one determines at each minimum the derivatives \( \frac{\partial V(\bar{\alpha}_i(\vec{p}))}{\partial p_k} \) of the potential with respect to the control parameters: in most cases the first and second derivatives are sufficient. In this contribution the free parameters are \( x \) and \( y \), although the interaction parameters can, in principle, be varied, too. Nevertheless, here we shall fix the interaction constants to the spectrum of realistic systems at the points of exact dynamical symmetries and then vary the \( x \) and \( y \) variables only.

c) The places of phase transitions are determined identifying the borders in the parameter space where at least two minima are at equal energy, i.e., \( V(\bar{\alpha}_{i_1}) = V(\bar{\alpha}_{i_2}) \) for some index values \( i_1 \) and \( i_2 \) of the minima. This provides us with a relation \( f(p_1, ..., p_{n_p}) = 0 \) between the parameters, which allows, in principle, to express one parameter in terms of the others.

d) The phase transition is of order \( m \), when the \( m \)'th derivative of the potential is discontinuous at the point of the phase transition, i.e.,

\[
\frac{\partial^m V(\bar{\alpha}_{i_1})}{\partial p_k^n} = \frac{\partial^m V(\bar{\alpha}_{i_2})}{\partial p_k^n}, \quad \text{for } n < m, \quad \frac{\partial^m V(\bar{\alpha}_{i_1})}{\partial p_k^n} \neq \frac{\partial^m V(\bar{\alpha}_{i_2})}{\partial p_k^n}. \quad (7)
\]

The derivative of \( \bar{V}(\bar{\alpha}_i) \) with respect to a parameter has to be understood as a derivative of \( \bar{V}(\alpha) \) with respect to this parameter and after that \( \alpha \) is set to \( \bar{\alpha}_i \). Note that this procedure of determining the order of a phase transition is quite general and does not depend on identifying the phase by a dynamical symmetry.

The derivatives of the potential are easily determined within the PACM, however, within the SACM this is not so any more. We consider the particular potential structure, valid only for the particular case discussed in this contribution,

\[
\bar{V}(\alpha) = x\bar{V}_1(\alpha) + (1 - x)\bar{V}_2(\alpha),
\]

implying the division into a \( SU(3) \) and \( SO(4) \) part given in Eq. (1). The difference to Eq. (5) consists in the division of a simple factor, or just the expectation value calculated within the curly bracket. The minima of \( \bar{V} \) are obtained using algebraic and numerical routines. Taking the values of the potential \( \bar{V}(\alpha) \) at the minima, the derivative with respect to \( x \) is given by

\[
\frac{d\bar{V}(\bar{\alpha}_i)}{dx} = \frac{\partial \bar{V}(\bar{\alpha}_i)}{\partial x} + \frac{\partial \bar{V}(\bar{\alpha}_i)}{\partial \bar{\alpha}_i} \frac{\partial \bar{\alpha}_i}{\partial x} = \frac{\partial \bar{V}(\bar{\alpha}_i)}{\partial x} = \bar{V}_1(\bar{\alpha}_i) - \bar{V}_2(\bar{\alpha}_i). \quad (9)
\]
with \( i = 1 \) or 2. We exploited the fact that the first derivatives of the potential at a minimum are equal to zero. These expressions have to be calculated at the point of phase transition.

In case \( \tilde{V}(\bar{\alpha}_i) \) turns out to be identically zero or constant for a given \( i \) (as will be the case in our example for \( \bar{\alpha}_1 \), which will be related to the spherical minimum where \( V = 0 \)), then by construction all higher derivatives also give zero. Therefore, in what follows, higher derivatives are only computed when \( \tilde{V}(\bar{\alpha}_i) \) is not a constant.

There are now two possibilities. i) The two minima are separated, i.e., at the point of phase transition the deformed minimum is at a value \( \bar{\alpha}_2 \) different from zero, while the spherical minimum is at \( \bar{\alpha}_1 = 0 \). ii) The two minima coincide at the point of phase transition, i.e., \( \bar{\alpha}_1 = \bar{\alpha}_2 \) at \( x = x_0 \), with \( x_0 \) denoting the value \( x \) at which the phase transition takes place.

For case i) the expression in (9) is in general different for the two minima, except for a rare coincidence when \( \tilde{V}_1(\bar{\alpha}_1) - \tilde{V}_2(\bar{\alpha}_1) = \tilde{V}_1(\bar{\alpha}_2) - \tilde{V}_2(\bar{\alpha}_2) \) for \( \bar{\alpha}_1 \neq \bar{\alpha}_2 \). Thus we can conclude that in this case the first derivatives at the point of phase transition are different, taken at \( \alpha_1 \) in one case and at \( \alpha_2 \) in the other case. Therefore, the phase transition is of order one.

In the second case the second derivative also has to be calculated:

\[
\frac{d^2\tilde{V}(\bar{\alpha}_i)}{dx^2} = \left[ \frac{\partial \tilde{V}_1(\bar{\alpha}_i)}{\partial \bar{\alpha}_i} - \frac{\partial \tilde{V}_2(\bar{\alpha}_i)}{\partial \bar{\alpha}_i} \right] \frac{\partial \bar{\alpha}_i}{\partial x}.
\]

For the case when the positions of the two minima coincide, the expression in the squared parenthesis for \( \alpha = \bar{\alpha}_1 \) and \( \alpha = \bar{\alpha}_2 \) are equal. However, the derivatives of \( \bar{\alpha}_i \) with respect to \( x \) are, in general, different except for the coincidence, when the factor of the derivative of \( \bar{\alpha}_i \) is the same for \( \bar{\alpha}_1 \) and \( \bar{\alpha}_2 \). Thus we can conclude that the phase transition is of second order here. Of course, the numerical values have to be checked in order to exclude the rare coincidence. In order to do that higher derivatives have to be determined, which is cumbersome in the SACM.

This new consideration makes it manageable to determine the order of a phase transition within the SACM. All we have to do is to determine if the two minima are separated at the point of phase transition (first-order) or merge at the point of phase transition (second-order).

The general phase diagram has the following structure (see left panel Fig. 1): For \( A > 0 \) and \( B \leq 0 \) only a spherical minimum exists, while for \( A < 0 \) only a deformed minimum exits. For \( B > 0 \) and \( 0 \leq A \leq \frac{B^2}{3} \) a spherical and a deformed minimum co-exist. For \( A > \frac{B^2}{3} \) the global minimum is the spherical one, while for \( A < \frac{B^2}{3} \) it is the deformed one. At \( A = \frac{B^2}{3} \) a phase transition takes place which is of first order. Thus the phase diagram shows a much richer structure, including first- and second-order phase transitions.

3. A particular application: \( ^{20}\text{Ne} \rightarrow ^{16}\text{O} + \alpha \)

In this section we consider a system that has the same model space as \( ^{20}\text{Ne} \rightarrow ^{16}\text{O} + \alpha \). In reality we do not consider the physical \( ^{20}\text{Ne} \), because this is given by a fixed value of \( x \) and \( y \) adjusted to the physical spectrum. Rather, we describe a hypothetical cluster system with the same \( SU(3) \) representation as \( ^{20}\text{Ne} \), changing its structure going from \( x = 1 \), the \( SU(3) \) dynamical symmetry limit, to \( x = 0 \), the \( SO(4) \) dynamical symmetry limit. In the first step we considered the PACM only. We adjusted the interaction parameters of the model such that the energy levels, both within the \( SU(3) \) and \( SO(4) \) dynamical symmetry limit exhibit the same scale and resemble the physical spectrum in the \( SU(3) \) dynamical symmetry limit. As a result we obtained for the parameters of (4) the values \( a = -2.311 \text{ MeV}, \ b = -0.17 \text{ MeV}, \ c = 0.335 \text{ MeV} \) and we used \( n_0 = 8, \ N = 20 \) and \( (\lambda, \mu) = (8, 0) \). In Fig. 1 the corresponding phase diagram is plotted in the left panel.

The horizontal axis gives \( x \) and shows the transition from the \( SO(4) \) dynamical symmetry for \( x = 0 \) towards the \( SU(3) \) dynamical symmetry at \( x = 1 \). The vertical axis shows the value \( y \),
Region I
Region II
Region III
Region IV
\[ B = \frac{2}{3} \]
\[ B = \frac{2}{4} \]
\[ A = 0 \]

Figure 1. The left panel shows the phase space diagram as a function of the two parameters \( A \) and \( B \). See the text for explanations. The right panel shows the phase diagram for the system \( ^{20}\text{Ne} \rightarrow ^{16}\text{O} + \alpha \). Note that there is a first-order phase transition line starting from the upper right side of the curve until reaching the dot. To the left of the dot the phase transition is of second order.

which is a measure of the strength of the quadrupole-quadrupole interaction. One has to read for a fixed \( y \) the horizontal axis \( x \).

Our first observation is that removing the three-body interaction the results of Ref. [12] are recovered, i.e. a second-order phase transition occurs.

The line of phase transition is also plotted for the case when the three-body interaction is included in general. The line is divided into two sections, the division indicated by a dot. The upper right part of the curve indicates a first-order phase transition, while the lower left section indicates a second-order phase transition. For \( y = 1 \) we find a first-order phase transition. When \( y \) is lowered, from one point on, when the quadrupole-quadrupole interaction is sufficiently small, the phase transition turns over to second-order. Thus, we found an example when there exists not only a second-order phase transition, but also a first-order one. A small strength of the quadrupole-quadrupole interaction corresponds to unharmonic corrections in the interaction and reproduces the known results. The new result is that when the interaction is stongly unharmonic (including a cubic term) the transition turns over to a first-order one.

We repeated the investigation for the SACM, when the Pauli exclusion principle is taken into account. Further above we noted that this introduces more involved expressions, corresponding to higher-order interactions within the PACM. The same interaction parameters are used and only \( x \) and \( y \) are varied. We used the method explained in the last section. For the case of \( ^{20}\text{Ne} \), we found that the phase transition changes dramatically: For \( y = 1 \) the phase transition between the \( SU(3) \) and \( SO(4) \) dynamical symmetries vanishes! This is because the potential at \( y = 1 \) has a deformed minimum for all values of \( x \), so no spherical minimum appears! As a consequence, no structural change happens and, thus no phase transition. At \( y = 0 \) the situation changes. Now at \( x = 1 \) there is a spherical minimum. In between \( x = 0 \) and \( x = 1 \) this spherical minimum turns over into a deformed one. Since the two minima merge at the point of phase transition, it is of order two.

We have not done yet he analysis for \( y \) values between 0 and 1. However, one can safely make
the following conjecture: somewhere between $y = 0$ and 1 the phase transition ceases to exist, implying a critical point. All this indicates that the structure of phase transitions exhibits a more dramatic structure than in the previous considerations, including the existence of a critical point.

4. Conclusions
We investigated the phase transition properties within algebraic cluster models, which are divided into two classes called PACM and SACM. In the first class the Pauli exclusion principle is not taken into account, while in the second it is. In order to avoid instabilities we had to include a third-order interaction in the Hamiltonian. The results are the following:
i) The same results are obtained when only up to two-body interactions are considered [12] and the Pauli exclusion principle is neglected. The differences appear with the inclusion of higher-order interactions and/or when the Pauli exclusion principle is taken into account.
ii) When a three-body interaction is included within the PACM, the structure of the phase diagram changes. It now also includes first-order phase transitions.
iii) When the Pauli exclusion principle is taken into account (SACM), from the point of view of the PACM it looks equivalent to introducing complicated higher-order interactions. The structure of phase transitions changes significantly, allowing also the appearance of critical points.

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