Phase transitions in algebraic cluster models

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We study the phase transitions of two algebraic cluster models, which have similar interactions, but differ from each other in their model spaces. The semimicroscopical model incorporates the Pauli exclusion principle, while the phenomenological one does not. The appearance of the quasidynamical SU(3) symmetry is also investigated in the presence of an explicitly symmetry-breaking interaction. Examples of binary cluster configurations with two, one, or zero closed-shell clusters are studied.

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I. INTRODUCTION

Phase transitions in nuclear systems are of utmost interest. An example is provided by the experimental study of the heat capacity in highly excited nuclei [1], which resulted in an S shape, as a function of the temperature. The reason for this dependence is related to a transition from a pairing-dominated phase to another phase without pairing [2–5].

Another very interesting class of phase transitions can be seen in algebraic models of nuclear structure [6–8]. They are called shape-phase transitions for the following reason. These models have analytically solvable limiting cases, called dynamical symmetries, which are characterized by a chain of nested subgroups. They correspond to a well-defined geometrical shape and behavior, e.g., rotation of an ellipsoid or spherical vibration. The general case of the model, which includes interactions described by more than one group chain, breaks the symmetry; and by changing the relative strengths of these interactions, one can go from one shape to the other. In doing so, a phase transition can be seen. A phase transition is defined as a discontinuity of some quantity as a function of the control parameter, which gives the relative strength of the interactions of different symmetries. Real phase transitions can take place only in infinite systems, as in the classical limits of these algebraic models, when the particle number N is very large: $N \to \infty$. For finite N, the discontinuities are smoothed out; nevertheless, some indications of the phase transitions can still be there.

A controlled way of breaking the dynamical symmetries may reveal another very interesting phenomenon, i.e., the appearance of a quasidynamical (or effective) symmetry [9]. This rather general symmetry concept of quantum mechanics corresponds to a situation in which the symmetry-breaking interactions are so strong that the energy eigenfunctions are not symmetric (i.e., they are not basis states of an irreducible representation of the symmetry group), rather they are linear combinations of these basis states. However, they are very special linear combinations in the sense that their coefficients are (approximately) identical for states with different spin values. When this is the case, then the underlying intrinsic state is the same, and the states are said to form a (soft) band. The quasidynamical symmetry is based on the mathematical concept of embedded representation [10]. (In particular for the quasidynamical SU(3) symmetry, which plays an important role in the following considerations, a method is developed in [11] for the determination of the effective SU(3) quantum numbers in the case of large prolate deformation, and it was extended in [12] for oblate deformation).

The phase transitions as well as the persistence of the quasidynamical symmetries in the algebraic models of quadrupole collectivity have been extensively studied [6,8,13]. The aim of the present paper is to address these questions in relation to another important collectivity of nuclei, i.e., clusterization.

Fully algebraic cluster models, in which the basis states are characterized by the irreducible representations of some groups, and the physical operators are expressed in terms of their generators, have been constructed on both the phenomenological, and the semimicroscopical levels. A description is called semimicroscopical if the phenomenological treatment of the operators (which have some parameters to fit to the experimental data) is combined with a microscopical model space, which is free from the Pauli-forbidden states. When no (proper) distinction is made between the Pauli-allowed and Pauli-forbidden states, the model is called phenomenological.

The basic assumption of the cluster models is that the relevant degrees of freedom of the nucleus can be classified into two categories, which are related to the relative motion of the clusters and to their internal structure. For the algebraic description of relative motion, the vibron model [14] proved to be successful. This model has a scalar (i.e., $l = 0$)σ boson and a set of vector (i.e., $l = 1$)π_i ($i = 0, +1, -1$) bosons as building blocks. It has a U(4) group structure, and there are

two analytically solvable limiting cases of the model, denoted by the SU(3) and SO(4) algebras as

$$\begin{array}{llll} \mathrm{U}_R(4) \supset & \mathrm{SU}_R(3) \supset & \mathrm{SO}_R(3) \supset & \mathrm{SO}_R(2) \\ [N,0,0,0] & (n_\pi,0) & L_R & M_R, \end{array}$$

$$\begin{aligned} n_\pi &= N, N-1, \ldots, 1, 0, \\ L_R &= n_\pi, n_\pi - 2, \ldots, 1 \text{ or } 0, \\ M_R &= L_R, L_R - 1, \ldots, -L_R, \end{aligned} \tag{1}$$

and

$$\begin{array}{llll} \mathrm{U}_R(4) \supset & \mathrm{SO}_R(4) \supset & \mathrm{SO}_R(3) \supset & \mathrm{SO}_R(2) \\ [N,0,0,0] & (\omega,0) & L_R & M_R, \end{array}$$

$$\begin{aligned} \omega &= N, N-2, \ldots, 1 \text{ or } 0, \\ L_R &= \omega, \omega - 1, \ldots, 1, 0, \\ M_R &= L_R, L_R - 1, \ldots, -L_R, \end{aligned} \tag{2}$$

where the subscript R is applied for relative motion, in order to avoid confusion later on. Here we have indicated the labels of the irreducible representations as well as their relations. The SU(3) limit corresponds to the vibration of the system around a spherical equilibrium shape, while the SO(4) describes static dipole deformation. (These questions will be discussed further in Sec. III.)

The internal structure of the clusters can also be described by algebraic models, e.g., by the Elliott model (SU(3) shell model) [15], or by the U(6) interacting boson model (IBM) [6].

In the semimicroscopical algebraic cluster model (SACM) [16,17], the internal structure of the clusters are described by the shell model, having an $\mathrm{U}^{\mathrm{ST}}(4) \otimes \mathrm{U}(3)$ group structure, where $\mathrm{U}^{\mathrm{ST}}(4)$ stands for the spin-isospin sector, while U(3) refers to the space part. Then the model for a binary clusterization has a $\mathrm{U}^{\mathrm{ST}}_{C_1}(4) \otimes \mathrm{U}_{C_1}(3) \otimes \mathrm{U}_R(4) \otimes \mathrm{U}^{\mathrm{ST}}_{C_2}(4) \otimes \mathrm{U}_{C_2}(3)$ algebraic structure, where C_i stands for the ith cluster, and R indicates the relative motion. The model space is constructed to be free from the Pauli-forbidden states, and the physical operators are expressed in terms of the group generators. If we consider spin-isospin zero clusters, which is going to be the case here, then the role of the $\mathrm{U}^{\mathrm{ST}}_{C_i}(4)$ groups are important only in the construction of the model space, but they do not play a role in physical operators. Therefore, from the viewpoint of building up, e.g., the interactions, we can say that the group structure is simplified to $\mathrm{U}_{C_1}(3) \otimes \mathrm{U}_R(4) \otimes \mathrm{U}_{C_2}(3)$. (This model has been applied in realistic studies [18].)

With the exactly same group structure, one can construct a phenomenological algebraic cluster model (PACM), simply forgetting about the exclusion principle. In this sense, we can have a semimicroscopical and a phenomenological model for clusterization with the same group structure and the same interactions.

Since we wish to study the effects of the Pauli principle on the phase transitions and on the persistence of the quasidynamical symmetry in the cluster models, we will study these two models, which are very closely related to each other. As for the relation of the PACM to the better known nuclear vibron model [19], which was historically the first fully algebraic cluster model and has been widely applied [19–21], the following can be said. Their model spaces and groups structures are different, but the interactions are very similar. In particular, the SU(3) dynamically symmetric Hamiltonian, as discussed in the next section, is relevant also for the nuclear vibron model.

The specific aims of the present study and the structure of this paper are as follows. In Sec. II, we present the algebraic cluster models and their Hamiltonians. Section III gives the geometric mapping of the models, which provides us with their large N limits. In this section, the phase transitions are investigated analytically. Then in Sec. IV, examples of binary cluster systems are studied numerically. We chose three examples in such a way that in one of them both clusters have a closed-shell structure, in the other there is one cluster with a closed shell and another with an open-shell structure, and in the third example, both clusters have open shells. In these finite-N systems, we study numerically the signatures of the phase transitions, as well as the question of whether the quasidynamical SU(3) symmetry survives when we move away from the $\mathrm{SU}_R(3)$ limit of the vibron model toward the $\mathrm{SO}_R(4)$ one. Finally some conclusions are drawn in Sec. V.

II. THE MODELS

The two models we investigate here differ from each other in their model spaces, while their interactions are the same, as mentioned in the previous section.

In the semimicroscopical algebraic cluster model (SACM), the internal structure of the clusters are described by the Wigner-Elliott shell model of $\mathrm{U}^{\mathrm{ST}}_{C_i}(4) \otimes \mathrm{U}_{C_i}(3)$ group structure. Their internal wave functions are completely antisymmetric. When, however, the product wave function of the two clusters and of the relative motion is constructed, it is contaminated by the Pauli-forbidden states, because the antisymmetrization with respect to the interchange of nucleons sitting in the two different clusters has not been taken into account so far. It has to be incorporated as an extra requirement. There are different ways to do this. For light binary cluster configurations, which will be considered here, a simple procedure is provided by taking the intersection of the nonantisymmetric cluster model basis and the fully antisymmetric shell model basis of the united nucleus. We take this approach here, the details of which are discussed in Ref. [17]. When this procedure is applied to a system of two closed shell clusters, then it reduces to the Wildermuth condition, which simply gives a lower limit for the number of quanta of the relative motion [22]. (This number depends, of course, on the clusters.) When one or more clusters are open shell, then in addition to this condition, a more refined selection of the allowed and forbidden single-nucleon states within a major shell is involved. As is obvious from this brief description, in constructing the microscopic model space, the spin-isospin degrees of freedom [the $\mathrm{U}^{\mathrm{ST}}(4)$ group] play an essential role; without them the consequences of the antisymmetrization cannot be taken into account.

If one does not pay attention to the exclusion principle, i.e., the approach is phenomenological (PACM), then the basis provided by the triple product wave functions (cluster-1, cluster-2, relative motion) gives the basis of the cluster model

itself, without any further restrictions. In such a case, the lowest number of quanta in the relative motion is always zero.

In constructing the model Hamiltonians, the difference between the semimicroscopical and the phenomenonological approaches is less significant. In particular, when our interest is restricted to a single sector of the spin-isospin degrees of freedom, which is going to be the case in what follows, exactly the same interactions can be applied. Thus, the formalisms of the two models coincide from the viewpoint of the Hamiltonians. In this respect, both models can be characterized by the

$$\begin{array}{rcl} \mathrm{SU}_{C_1}(3)\otimes\mathrm{SU}_{C_2}(3) & \otimes\mathrm{SU}_R(3)\supset & \mathrm{SU}_C(3)\otimes\mathrm{SU}_R(3)\supset \\ (\lambda_1,\mu_1)(\lambda_2,\mu_2) & (n_\pi,0) & (\lambda_C,\mu_C) \\ \mathrm{SU}(3)\supset & \mathrm{SO}(3)\supset & \mathrm{SO}(2) \\ (\lambda,\mu) & \kappa L & M, \end{array} \tag{3}$$

group structure, where (λ_k,μ_k) refers to the $\mathrm{SU}_{C_k}(3)$ irreducible representations (irreps) of the individual clusters, which are coupled to the intermediate irrep (λ_C,μ_C). n_π is the number of relative oscillator quanta, while (λ,μ) is the total SU(3) irrep. L and M are the angular momentum and its projection, and κ is used to distinguish multiple. Accurrances of a given L in (λ,μ). It is worth mentioning here that the same dynamical symmetry is relevant for the interactions of the nuclear vibron model.

We apply the Hamiltonian

$$\boldsymbol{H} = x(\hbar\omega\boldsymbol{n}_\pi - a_1\boldsymbol{C}_2(\mathrm{SU}(3))) + (1-x)a_2\boldsymbol{P}_4 + a\boldsymbol{L}^2. \tag{4}$$

The first and the third terms correspond to the SU(3) dynamical symmetry of the model, as described by group chain (3). The second and third terms represent the SO(4) dynamical symmetry of the vibron model, describing the relative motion. x is a control parameter that we vary between 0 and 1, thus $x=0$ indicates the SO(4) limit, while $x=1$ corresponds to the SU(3) dynamical symmetry. In particular, the first member of the interactions $\hbar\omega\boldsymbol{n}_\pi$ contains the linear invariant operator of the $\mathrm{U}_R(3)$ subgroup of the vibron model, and the $\hbar\omega$ is usually chosen as $(45A^{-1/3}-25A^{-2/3})$ for light [23] and $41A^{-1/3}$ for heavy nuclei [24]. $\boldsymbol{C}_2(\mathrm{SU}(3))$ is the second-order Casimir-invariant of the united SU(3) group of (3), having contributions from both the internal cluster part and the relative motion:

$$\begin{aligned} \boldsymbol{C}_2(\mathrm{SU}(3)) &= \tfrac{1}{4}\boldsymbol{Q}^2 + \tfrac{3}{4}\boldsymbol{L}^2, \\ &\rightarrow (\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu), \\ \boldsymbol{Q} &= \boldsymbol{Q}_C + \boldsymbol{Q}_R, \\ \boldsymbol{L} &= \boldsymbol{L}_C + \boldsymbol{L}_R, \end{aligned} \tag{5}$$

where $\boldsymbol{Q}$ and $\boldsymbol{L}$ stand for the quadrupole momentum and angular momentum, respectively. The relations of the momentum operators to the $C^{(1,1)}_{2m}$ generators of the SU(3) group, expressed in terms of SU(3)-coupled π-boson creation and annihilation operators [25], are

$$\begin{aligned} \boldsymbol{Q}_{2m} &= \tfrac{1}{\sqrt{3}}C^{(1,1)}_{2m}, \\ \boldsymbol{L}_{1m} &= C^{(1,1)}_{1m}, \end{aligned} \tag{6}$$

$$\boldsymbol{C}^{(1,1)}_{lm} = \sqrt{2}[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}]^{(1,1)}_{lm}. \tag{7}$$

Here the superscripts denote SU(3), while the subscripts denote SO(3) and SO(2) quantum numbers. The parameters a_1 and a_2 are introduced in order to allow a similar scale in energy for the $x=0$ and $x=1$ cases

The SO(4) part consists of the pairing operator [26]

$$\begin{aligned} \boldsymbol{P}_4 &= \tfrac{1}{4}((\boldsymbol{\pi}^\dagger\cdot\boldsymbol{\pi}^\dagger)-(\boldsymbol{\sigma}^\dagger)^2)((\boldsymbol{\pi}\cdot\boldsymbol{\pi})-(\boldsymbol{\sigma})^2) \\ &= \tfrac{1}{4}\boldsymbol{N}(\boldsymbol{N}+2) - \tfrac{1}{4}\boldsymbol{C}_2(\mathrm{SO}(4)) \\ &\rightarrow \tfrac{1}{4}N(N+2) - \tfrac{1}{4}\omega(\omega+2) \end{aligned} \tag{8}$$

[where the second-order Casimir operator of $C_2(\mathrm{SO}(4))$ deviates from the definition given in [26] by a factor of $\frac{1}{2}$]. The eigenvalue, shown in the last line in (8), is correct only in the full SO(4) basis, i.e., when it is not truncated by the Pauli principle. When a truncation is applied due to the exclusion principle, one has to diagonalize $\boldsymbol{P}_4$ in the SU(3) basis of (3) with a minimal number of relative oscillation quanta larger than zero. Then the eigenvalues will differ from those given in (8). The angular momentum term $\boldsymbol{L}^2$ is common in both of the dynamical symmetries.

The matrix elements of the interaction terms can be calculated by standard SU(3) coupling and recoupling techniques [25]; the relevant formulas are collected in the Appendix.

III. GEOMETRICAL MAPPING

The algebraic models usually have the advantage of being simple in structure and easy to solve numerically. On the other hand, their disadvantage is that they are fairly abstract and have no connection to the familiar geometrical concepts, such as shape. To overcome this difficulty, the study of the geometrical mapping of the group theoretical models can be very helpful. The geometrical connection can be developed via the concept of the mean field. In boson models, like the models studied here, the mean field emerges as a result of the interaction of the bosons. The shape can be determined via the energetically most favored state.

Several algebraic models have been studied in this respect (see, e.g., Refs. [26–31], and their relation to the geometrical models [24] have been revealed.

In this section, we discuss the geometrical mapping of the two algebraic cluster models that we introduced in the previous section (PACM and SACM) from the viewpoint of the phase transitions. First, we do so for the phenomenological model, which is the simpler one, and then for the semimicroscopical model.

As is usual in studies of the phase transitions of algebraic models in the large N limit [6,8], we investigate the behavior of the energy minimum as a function of the control parameter x.

A. Phenomenological approach

We concentrate on the relative motion part of the model. The lowest energy state will be a boson condensate, which can be written as [32]

$$|\alpha\rangle = \frac{1}{\sqrt{N!(1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}))^N}}(\boldsymbol{\sigma}^\dagger + (\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger))^N|0\rangle. \quad (9)$$

Here, α is a short-hand notation for α_m ($m = 1, 0, -1$). Please note that the operator with complex α coefficients is the most general linear combination of the boson creation operators of the vibron model. For static problems, the requirement of time reversibility,

$$\alpha_m^\star = (-1)^m\alpha_{-m}, \quad (10)$$

reduces the number of real parameters to three. In relation to the interacting boson models, the (9) type of state is called a projective coherent state [6]. It can also be considered as a trial state of the generator coordinate method [33] in the Gaussian overlap approximation without the zero point energy. The geometrical mapping of the relevant operators are given in Table I.

The potential $V(\alpha) = \langle\alpha|\boldsymbol{H}|\alpha\rangle$, sometimes also called the energy functional, is given (for $L = 0$) by

$$V(\alpha) = xN\left(\hbar\omega\frac{(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}{(1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}))} - a_1\left[C_2(\lambda_C,\mu_C) + 3\frac{N}{(1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}))}(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}) + \frac{N(N-1)}{(1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}))^2}(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^2\right]\right) + (1-x)a_2\frac{N(N-1)}{4(1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}))^2}[(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})-1]^2 + \cdots, \quad (11)$$

TABLE I. Geometrical mapping of some relevant operators in terms of the coherent state variable $\alpha : \alpha_m (m = 1, 0, -1)$ in the limit of $N \to \infty$ [when $(\alpha\cdot\alpha) \ll 1$] for $L = 0$. The $\hat{\boldsymbol{\alpha}}_2 : \hat{\alpha}_{2m}(k) (m = 2, 1, 0, -1, -2, k = 1, 2)$ are the quadrupole variables of the cluster number k. $N_{0,k}$ is the total number of oscillation quanta plus $\frac{3}{2}(A_k - 1)$ for the cluster k, where A_k is the number of nucleons in that cluster. $\boldsymbol{C}_2(\lambda,\mu)$ is the second-order Casimir operator of the SU(3) group, while $C_2(\lambda_C,\mu_C) = (\lambda_C^2 + \lambda_C\mu_C + \mu_C^2 + 3\lambda_C + 3\mu_C)$ is the eigenvalue of the second-order Casimir operator of $SU_C(3)$. The mapping in terms of the relative distance vector r_m is obtained via $\alpha_m = \sqrt{\frac{\mu\omega_r}{2N\hbar}}\tilde{r}_m$, where $\tilde{r}_m$ is r_m for the PACM while it is $(r_m - r_{0,m})$ for the SACM. Here, the absolute value r_0 of the vector r_0 is given by Eq. (18). The number operator of the π bosons is given by $[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}]_0^{[0]}$.

Operator	α map
$[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}]_M^{[L]}$	$N[\boldsymbol{\alpha}\otimes\boldsymbol{\alpha}]_M^{[L]}$
$\boldsymbol{Q}_m^a(k)$	$\sqrt{\frac{5}{\pi}}N_{0,k}\hat{\alpha}_{2m}(k)$
$(\boldsymbol{\pi}^\dagger\cdot\boldsymbol{\pi}^\dagger)(\boldsymbol{\pi}\cdot\boldsymbol{\pi})$	$N^2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^2$
$(\boldsymbol{\pi}^\dagger\cdot\boldsymbol{\pi}^\dagger)(\boldsymbol{\sigma})^2$	$N^2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})$
$(\boldsymbol{\sigma}^\dagger)^2(\boldsymbol{\pi}\cdot\boldsymbol{\pi})$	$N^2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})$
$(\boldsymbol{\sigma}^\dagger)^2(\boldsymbol{\sigma})^2$	N^2
$\boldsymbol{C}_2(\lambda,\mu)$	$C_2(\lambda_C,\mu_C) + 3N(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}) + N^2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^2 + ([N_{0,1}\hat{\boldsymbol{\alpha}}_2(1) + N_{0,2}\hat{\boldsymbol{\alpha}}_2(2)]\cdot[\boldsymbol{\alpha}\otimes\alpha]^{[2]})$

where terms, indicated by "+...", which depend on the deformation of the individual clusters, have been skipped. They introduce a dependence on the relative orientation [21], but they do not change our main conclusions. Using the relation of the relative distance to the variables α_m [34]

$$r_m \approx \langle\alpha|\boldsymbol{r}_m|\alpha\rangle \approx \sqrt{\frac{2N\hbar}{\mu\omega_r}}\alpha_m, \quad (12)$$

where r_m is the approximate distance between the clusters, μ is the reduced mass, and $\omega_r = \sqrt{\frac{A_1+A_2}{A_1A_2}}\omega$ such that $\mu\omega_r^2 = m\omega^2$ (in [34]$m\omega$ was used but later it was corrected in [35]), and with the procedure explained in Ref. [34] the potential acquires the form

$$W(r) \approx x\left(\frac{\mu\omega_r^2}{2}r^2 - a_1\left[C_2(\lambda_C,\mu_C) + 3\left(\frac{\mu\omega_r}{2\hbar}\right)r^2 + \left(\frac{\mu\omega_r}{2\hbar}\right)^2 r^4\right]\right) + (1-x)a_2\left(\frac{\mu\omega_r}{2\hbar}\right)^2 \times\left(r^2 - \frac{2N\hbar}{\mu\omega_r}\right)^2 + \cdots. \quad (13)$$

In this expression, there is a minimum corresponding to the SU(3) limit at $r = 0$, and another one corresponding to the SO(4) limit (for positive sign in front of $\boldsymbol{P}_4$) at $r = (2N\hbar/\mu\omega_r)^{\frac{1}{2}}$. (This latter minimum increases with N, indicating a dissociation of the two clusters for $N \to \infty$; it could be kept at finite distance only with some renormalization. This observation is in line with the procedure of [36], where the parameter R^2 in front of $(\boldsymbol{\sigma}^\dagger)^2$ and $(\boldsymbol{\sigma})^2$ was introduced, which may cancel the N dependence; if R^2 is proportional to $1/N$, however, it moves the system away from the SO(4) limit.)

The competition of the SU(3) and SO(4) minima (by changing the control parameter x) determines the global energy minimum. A simplified analysis can be carried out easily for the $a_1 = 0$ case (this parameter is normally small). The minimum values of the SU(3) and SO(4) parts at the relevant r values (as mentioned above) are $W_{SU(3)}(0) = (1-x)a_2N^2$ and $W_{SO(4)}(\sqrt{2N\hbar/\mu\omega_r}) = xN\hbar\omega_r$. They are equal at

$$x_0 = \frac{1}{1+\frac{\hbar\omega_r}{a_2N}}, \quad (14)$$

and this value gives an *estimation* of where the transition sets in.

The derivative shows a jump at the point of transition, as can be seen using Eq. (13): taken at the minimum position of the SU(3) part ($r = 0$) and putting $a_1 = 0$, we obtain $\frac{dW(r)}{dr}|_{r=0,a_1=0} = 0$; while taken at the minimum position of the SO(4) part [$r = r_0 = \sqrt{2N\hbar/\mu\omega_r}$)], we obtain $\frac{dW(r)}{dr}|_{r=r_0,a_1=0} = x\omega_r\sqrt{2N\hbar\omega_r\mu}$. Since the first derivative of the energy-minimum is discontinuous at the transition, it is called a first-order phase transition.

An alternative derivation gives a similar result in the following way. Starting from Eq. (11) and setting $a_1 = 0$, the extrema of the potential are (given by the absolute value of

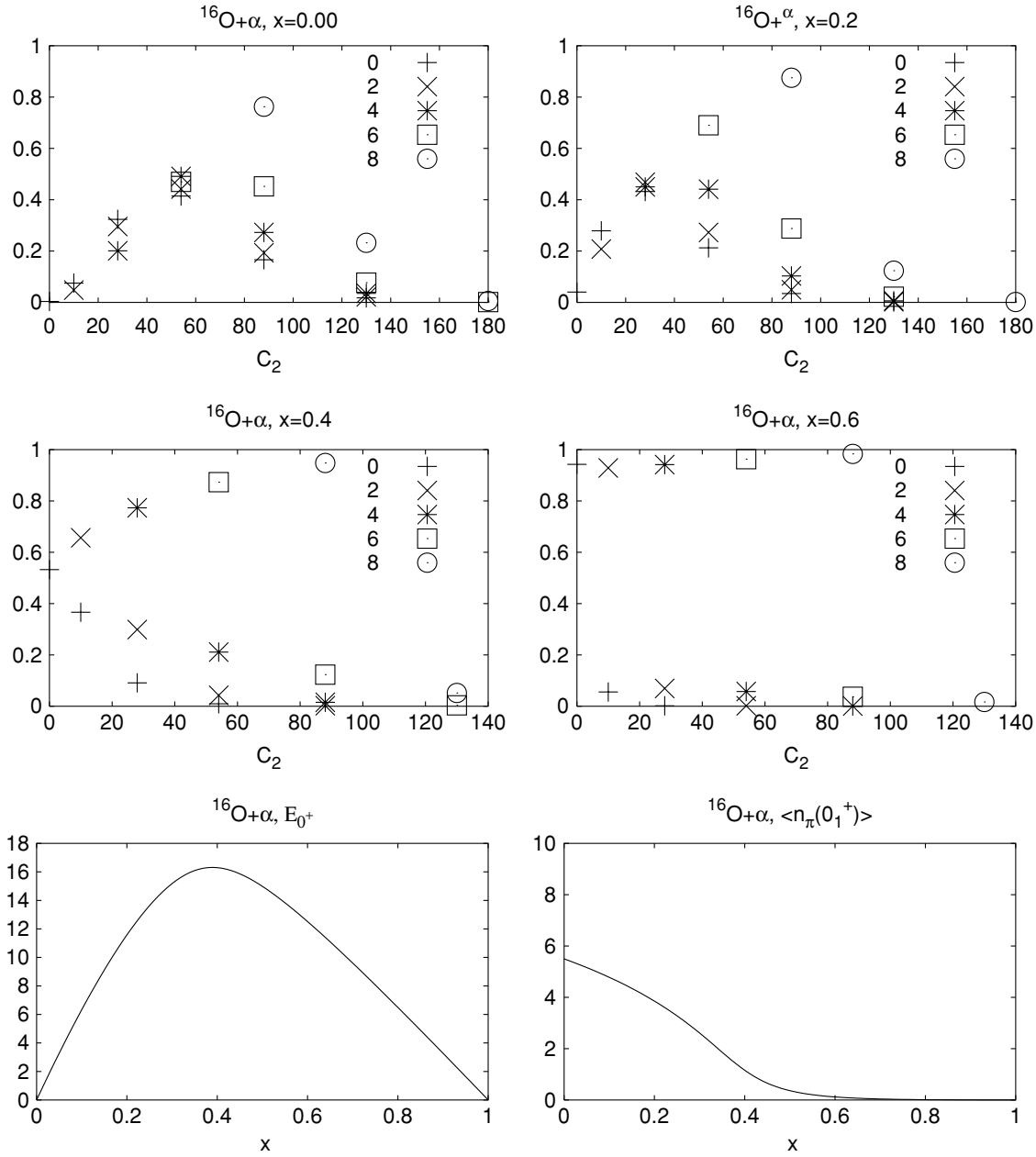

FIG. 1. Phenomenological model calculations for the ^{16}O+α system. Parameters of the Hamiltonian are $\hbar\omega = 13.2$, $a_1 = 0.1$, $a_2 = 1.0$, $a = 0.1$ (all in MeV), while $x_0 = 0.46$.

$\alpha_m)\,\alpha = 0$, and

$$\alpha^2 = \frac{(1-x)a_2(N-1) - x\hbar\omega}{(1-x)a_2(N-1) + x\hbar\omega}. \tag{15}$$

α^2 is positive (as it has to be) in the range of x

$$0 \leqslant x \leqslant \frac{1}{1 + \frac{\hbar\omega}{a_2(N-1)}} = x_l. \tag{16}$$

It turns out that $\alpha = 0$ is an absolute minimum when $x > x_l$, and it is a maximum when $x < x_l$. In the latter case, the root value of Eq. (15) gives the position of the minimum. For large N values, the estimation of Eqs. (14) and (16) coincide.

B. Semimicroscopical approach

When the Pauli principle is taken into account, there is a minimal number (n_0) of n_π bosons; therefore, the coherent state for the relative motion has a different form [34]:

$$|\alpha\rangle = \mathcal{N}_{N'n_0}(\alpha\cdot\pi)^{n_0}[\sigma^\dagger + (\alpha\cdot\pi^\dagger)]^{N'}|0\rangle, \tag{17}$$

where the total number of quanta is $N = N' + n_0$. In the limit $N \to \infty$, the corresponding potential has the same form as in (13), except that the distance variable r has to be substituted

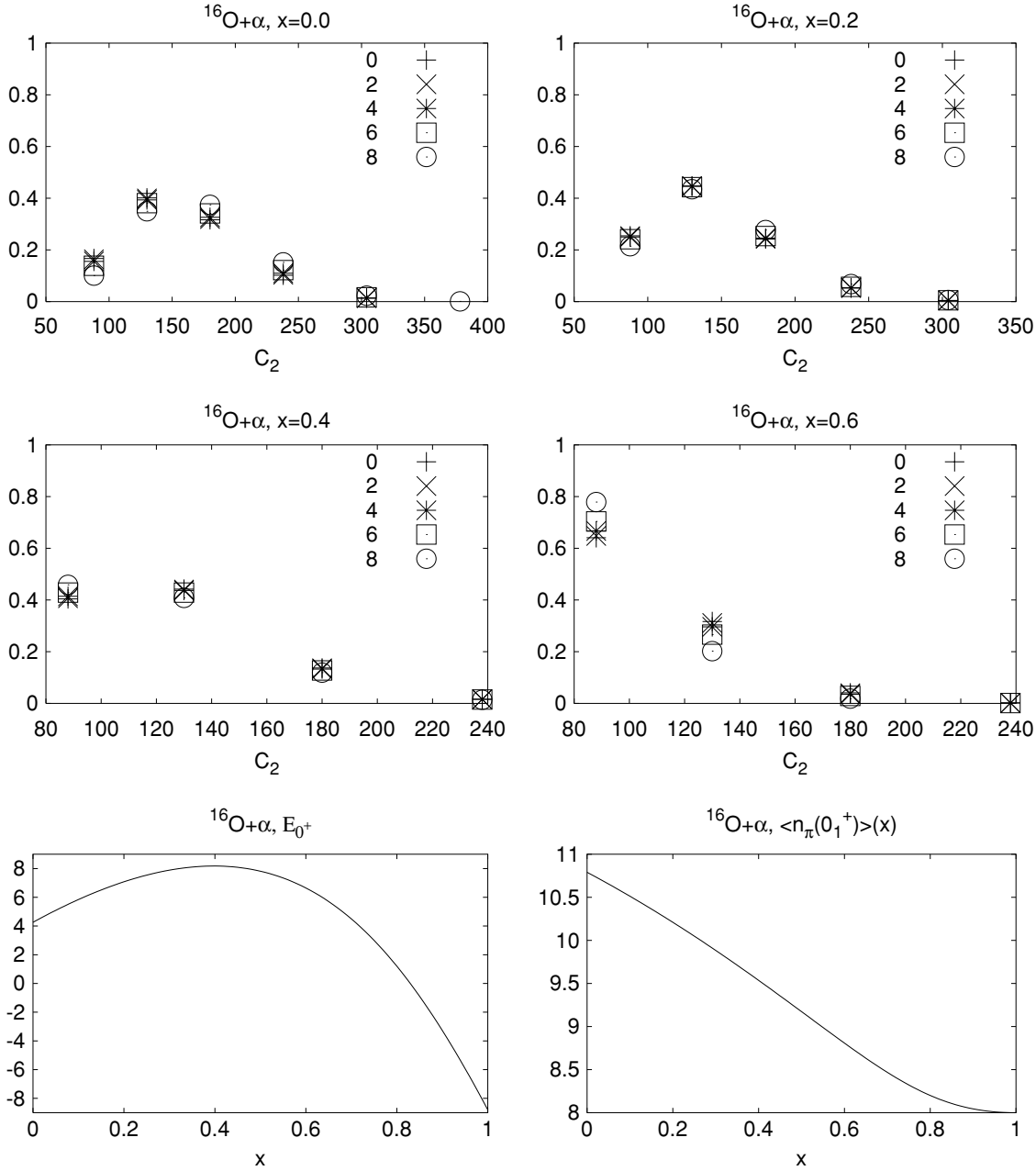

FIG. 2. Semimicroscopical model calculations for the ^{16}O+α system.

by $\tilde{r}$, with $\tilde{r} = (r - r_0)$, and r_0 is given by [34]

$$r_0 \approx \sqrt{\frac{\hbar}{\mu\omega_r} n_0}, \tag{18}$$

$$W(r) \approx x\left(\frac{\mu\omega_r^2}{2}(r-r_0)^2 - a_1\left[C_2(\lambda_C,\mu_C) + 3\left(\frac{\mu\omega_r}{2\hbar}\right)\right.\right.$$
$$\left.\left.\times\ (r-r_0)^2 + \left(\frac{\mu\omega_r}{2\hbar}\right)^2 (r-r_0)^4\right]\right) + (1-x)a_2$$
$$\times \left(\frac{\mu\omega_r}{2\hbar}\right)^2 \left((r-r_0)^2 - \frac{2N\hbar}{\mu\omega_r}\right)^2 + \cdots. \tag{19}$$

This potential has a minimum in both its SU(3) and its SO(4) parts at finite distance ($r > 0$). (Please note that the exclusion principle moves the minimum of the potential from zero to a finite value even for the Hamiltonian of SU(3) dynamical symmetry.) The two minima are at $r_1 = r_0$, and $r_2 = r_0 + \sqrt{2N\hbar/\mu\omega_r}$, respectively. [The SO(4) part also has an extremum at $r_1 = r_0$; however, it is a maximum; furthermore, it has another local minimum at $r = 0$, but it turns out that this can never become a global minimum.] Their competition determines the global minimum, similar to the case of the phenomenological model. The transition takes place again at the x_0 value of Eq. (14), and the first derivative of the potential is again discontinuous at this point; thus, the phase transition is of first order in this case, too.

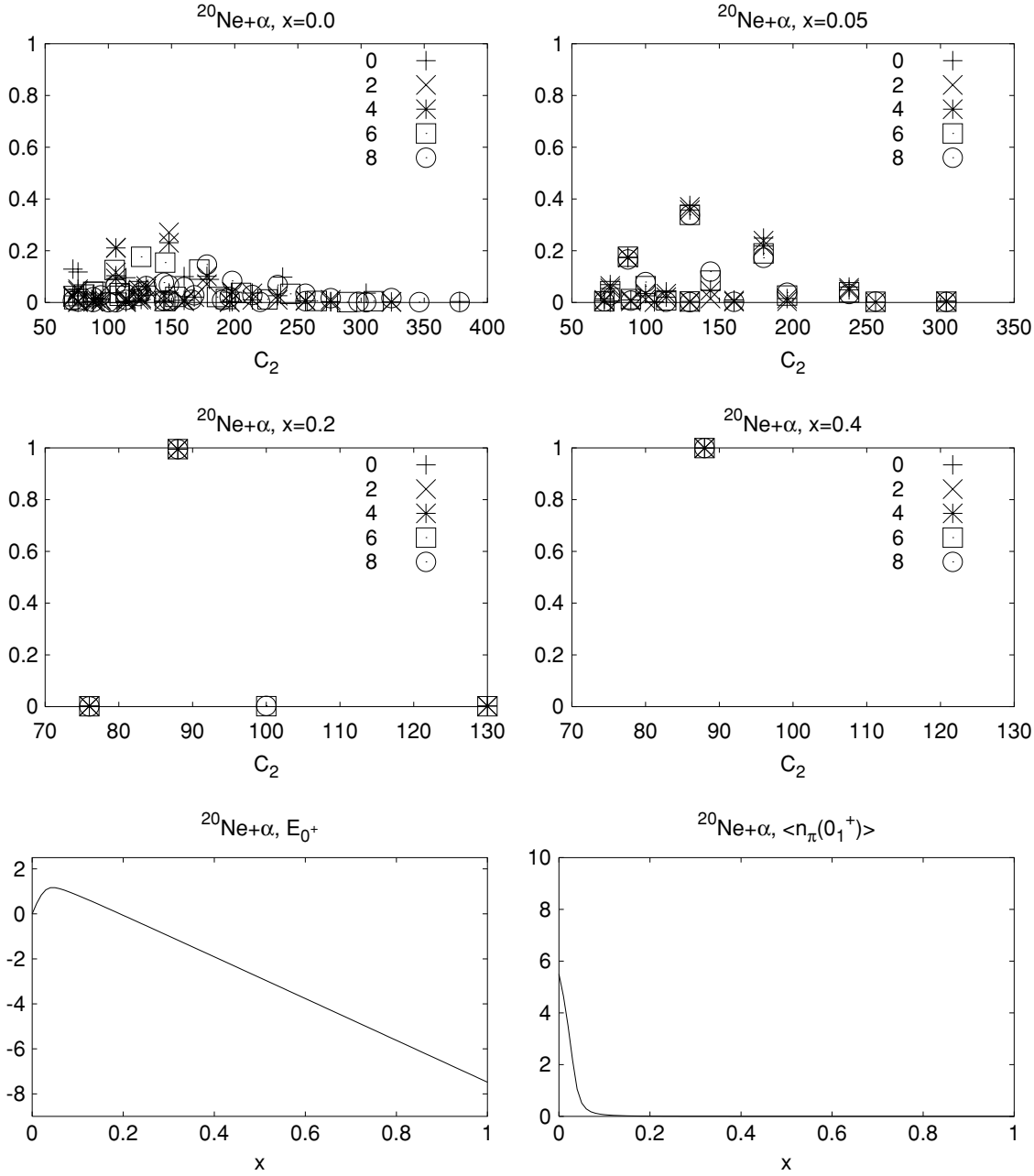

FIG. 3. Phenomenological model for the ^{20}Ne+α system. Parameters of the Hamiltonian are $\hbar\omega = 12.6$, $a_1 = 0.085$, $a_2 = 0.055$, $a = 0.1$ (all in MeV), while $x_0 = 0.08$.

IV. NUMERICAL STUDIES

In this section, we present the results of the numerical solution of the energy-eigenvalue problem for the Hamiltonian (4), for various x. In this way we can see how the phase transition shows up in finite N systems, as well as the persistence of the quasidynamical SU(3) symmetry. The three examples we have chosen represent binary cluster systems with zero (^{16}O+^{4}He), one (^{20}Ne+^{4}He), and two (^{12}C+^{8}Be) open-shell clusters.

The model spaces, characterized by n_π, are as follows. ^{16}O+^{4}He phenomenological: $0 \leqslant n_\pi \leqslant 12$, semimicroscopical: $8 \leqslant n_\pi \leqslant 20$; ^{20}Ne+^{4}He phenomenological: $0 \leqslant n_\pi \leqslant 12$, semimicroscopical: $8 \leqslant n_\pi \leqslant 20$; i.e. the size of the model space is the same for these cases. For the third system, ^{12}C+^{8}Be, we took a bit smaller space because of the large dimensions caused by the coupling to two open-shell clusters; phenomenological: $0 \leqslant n_\pi \leqslant 10$, semimicroscopical: $8 \leqslant n_\pi \leqslant 18$.

Figures 1–6 show the results for the phenomenological and semimicroscopical description of the three systems. The parameters of the Hamiltonian, shown in the figure captions, were identical in the phenomenological and semimicroscopical calculations. In each figure, the upper four parts give the decomposition of the wave function of the lowest-lying states

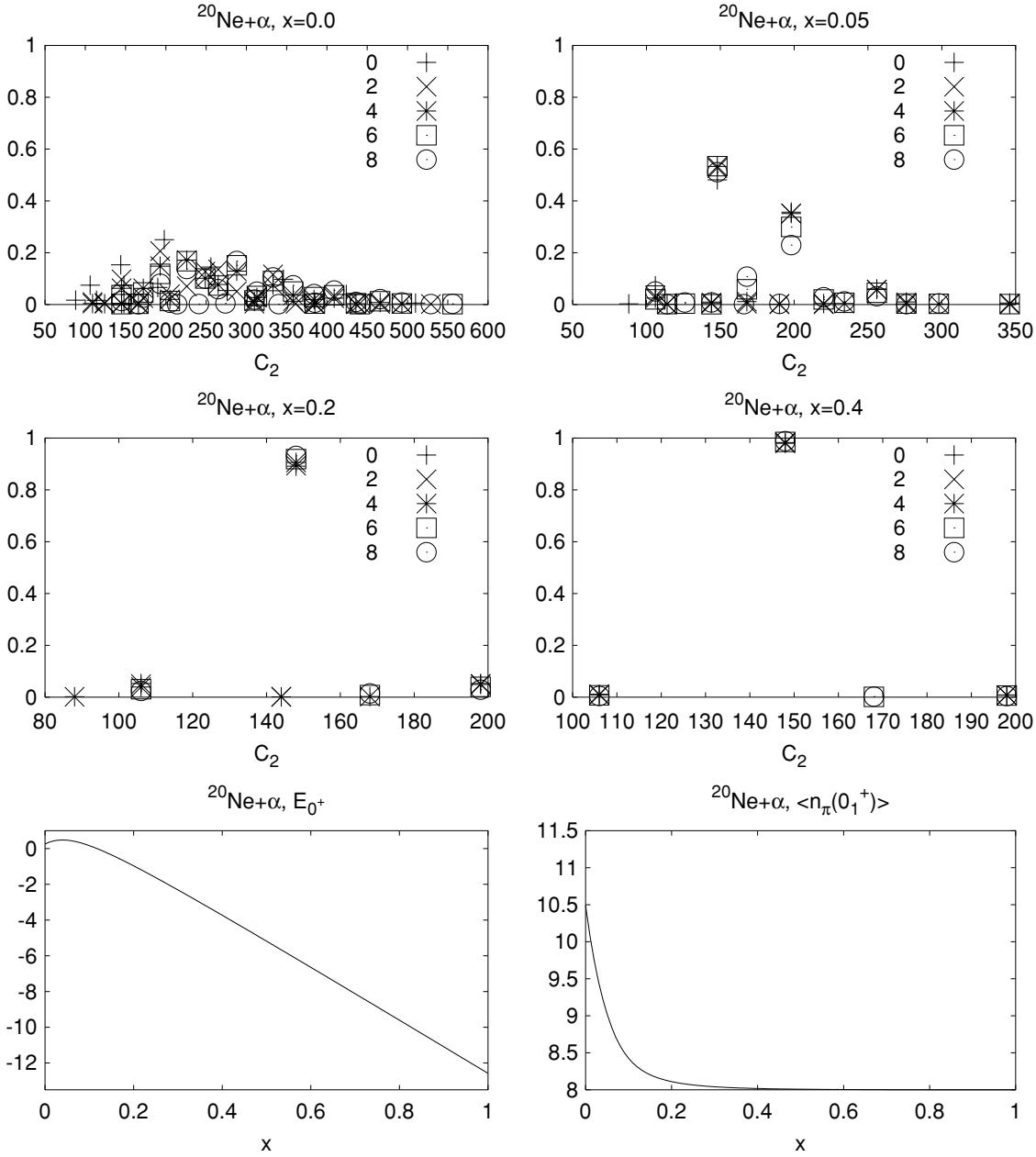

FIG. 4. Semimicroscopical model calculations for the ^{20}Ne+α system.

with angular momentum 0, 2, 4, 6, and 8 in terms of SU(3) basis states for different x values. The weights of the basis states are plotted vs the expectation value of the second-order Casimir operator. The x values are chosen such that the region of expected phase transition is displayed as well as some points beforehand and afterward. The critical x_0 values, based on the estimation of the previous section, are also given in the figure captions. These parts indicate whether the quasidynamical symmetry is present in the system (at a given x) in the following way. When the contribution of an SU(3) basis state is similar to the energy eigenstates with different angular momentum, i.e., their symbols are close to each other, then the quasidynamical symmetry is (approximately) valid. (This is relevant, of course, for the nonzero contributions. Some missing coincidence of the symbols for different L values on the horizontal axis are unimportant in this respect, reflecting merely the uncertainty of the plotting procedure for the practically zero contributions.)

The two lower parts of each figure show the behavior of the ground-state energy and the expectation value of the number of π bosons $\langle n_\pi \rangle$ as a function of x. The expectation value $\langle n_\pi \rangle$ is given by

$$\langle n_\pi \rangle = N \frac{\alpha^2}{1+\alpha^2}. \tag{20}$$

Due to Eq. (15), $\langle n_\pi \rangle$ is different from zero for $x < x_l$, and it is zero for $x > x_l$. The abrupt change in these quantities indicate the phase transition; however, for finite systems, it may be smoothed out or even disappear. (That is why we investigate

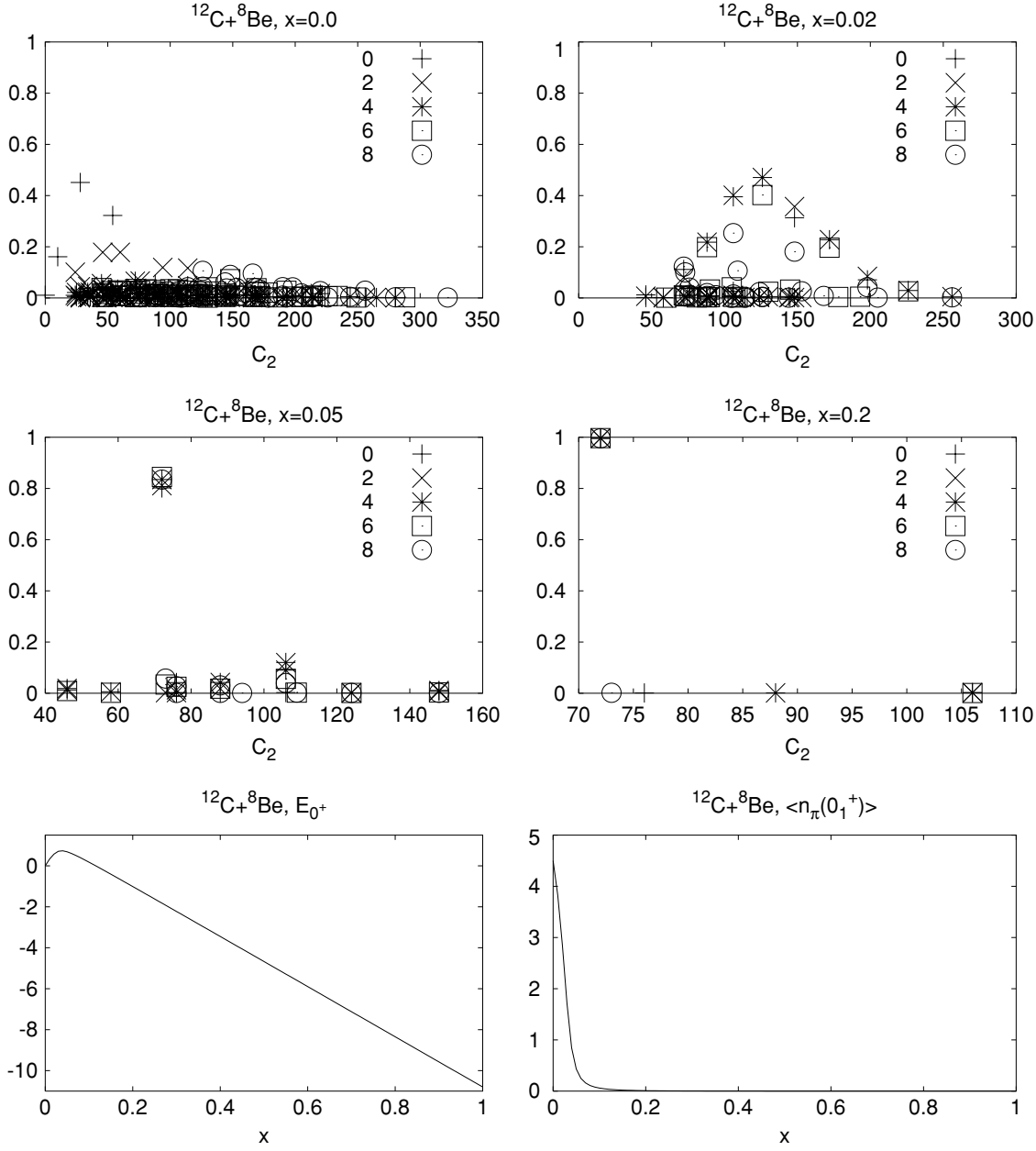

FIG. 5. Phenomenological model calculations for the ^{12}C+^{8}Be system. Parameters of the Hamiltonian are $\hbar\omega = 13.2$, $a_1 = 0.15$, $a_2 = 0.025$, $a = 0.1$ (all in MeV), while $x_0 = 0.04$.

two quantities, instead of the single energy, as we did in the case of the infinite system of the previous section.)

The figures show some changes in both the phenomenological and the semimicroscopical description around the critical values of the control parameter in each system, though the discontinuity of the infinite system is smoothed out to a large extent in each case.

As for the persistence of the quasidynamical symmetry, the following can be said. Those systems that contain some nonclosed-shell clusters (^{20}Ne+α, ^{12}C+^{8}Be) show similar behavior. The SU(3) quasidynamical symmetry survives until the critical point, in both the phenomenological and semimicroscopical descriptions. It seems that the large model space, obtained as a result of the coupling of the relative motion degrees of freedom to some internal structure, helps to develop some similar mixture of basis states in both descriptions.

The system of two closed-shell structures (^{16}O+α) shows some different characteristics. The phenomenological model does not associate a single SU(3) irrep to the ground state (and other) band even in the limit of the SU(3) dynamical symmetry. Therefore, in this case, no quasidynamical symmetry appears. In the semimicroscopic description, however, when the real SU(3) dynamical symmetry associates well-defined SU(3) quantum numbers to the bands, it survives as a quasidynamical symmetry not only up to the critical point of the control parameter, but even farther, up to the real SO(4) limit.

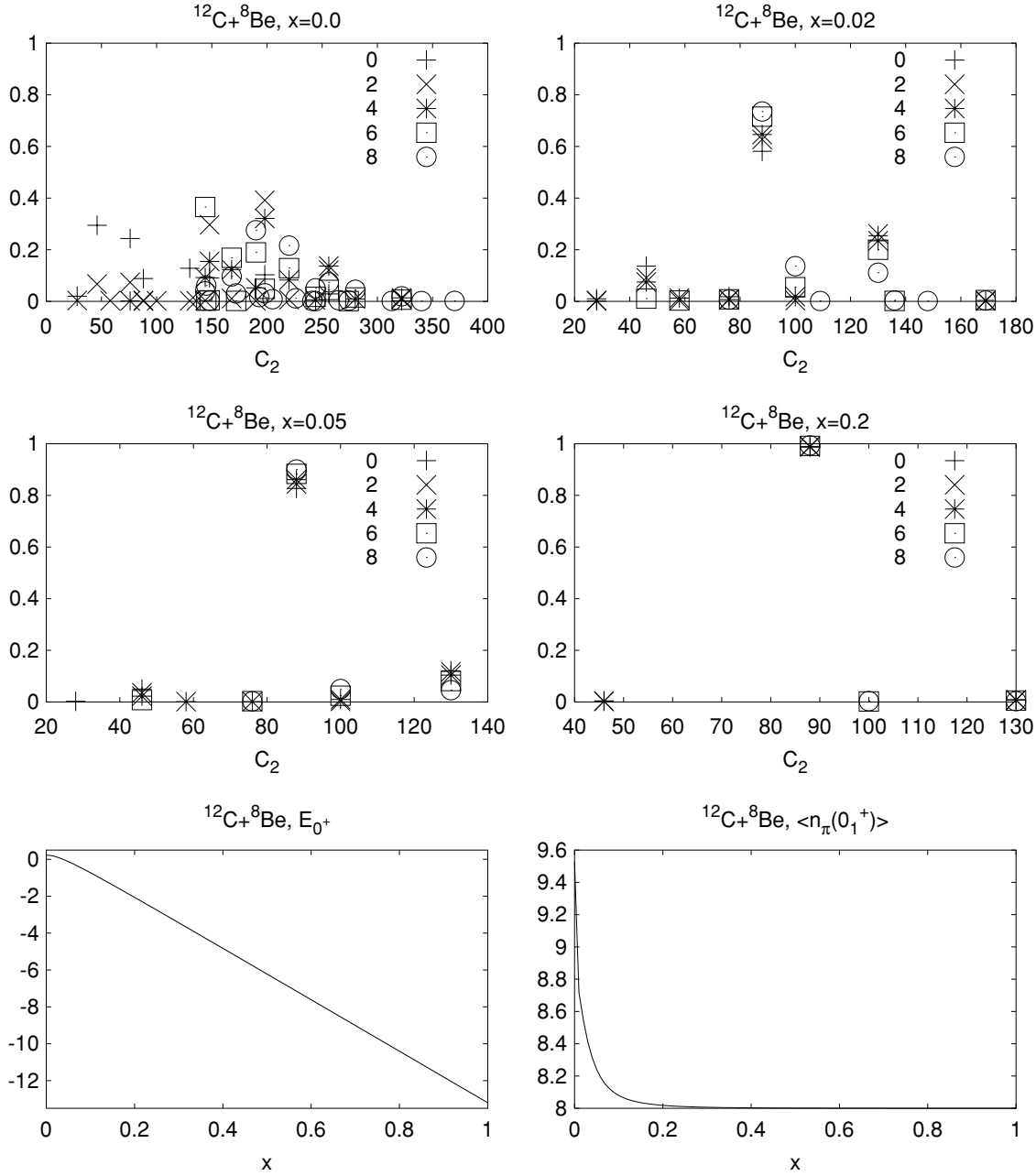

FIG. 6. Semimicroscopical model calculations for the ^{12}C+^{8}Be system.

This might be understood as being the consequence of the close similarity between the rotational spectrum, appearing also in the SO(4) limit, and an SU(3) irrep. (In case there is a coupling to the internal degrees of freedom, this rigid structure in the SU(3) basis content of the relative motion seems to be dissolved.)

V. SUMMARY

In this paper, we have studied the phase transitions of algebraic cluster models. Two models were considered, a phenomenological one, containing no Pauli principle, and a semimicroscopical one, which is based on a microscopically determined model space, being free from the Pauli-forbidden states. The interactions were treated in a phenomenological and algebraic way in both cases. In this respect, the two models have similar group structures. We have studied the SU(3)-SO(4) phase transition, related to the description of the relative motion in terms of the vibron model (in its simplest form in the phenomenological model and in a properly truncated form in the semimicroscopical description).

The analytical study of the large-N limit of both models shows a first-order phase transition. We also carried out numerical calculations. Three binary cluster systems were chosen, in which the number of open-shell clusters were zero,

one, and two, respectively. The numerical studies show that the phase transition is smoothed out for finite N systems, but some fingerprints of it still can be seen.

The appearance of the quasidynamical SU(3) symmetry has also been studied, when moving away from the limit of the real SU(3) dynamical symmetry. It turned out that in each case, when there is a real dynamical symmetry in the limiting case (in the sense that a well-defined SU(3) quantum number can be associated to a band), this symmetry survives as quasidynamical at least up to the critical value of the control parameter. This finding is very similar to those of the investigations of the models of quadrupole collectivity [8]. In the case of the semimicroscopical description of the two closed-shell clusters, it turned out to be valid in the whole range of the control parameter.

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APPENDIX

Here we present the formulas needed for the calculation of the matrix elements of the Hamiltonian (4). The only nondiagonal interactions are those related to the SO(4) pairing interaction.

We use the formulas of Ref. [25], as listed in its Appendix. In that work, Eq. (A.7) gives the triple reduced matrix elements of the bilinear products of creation and annihilation operators of the relative quanta. In our notation, they read

$$\begin{aligned}\langle (n'_\pi,0)|||[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{(2,0)}|||(n_\pi,0)\rangle &= \sqrt{n'_\pi(n'_\pi-1)}\,\delta_{n'_\pi,n_\pi+2},\\ \langle (n'_\pi,0)|||[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{(0,2)}|||(n_\pi,0)\rangle &= \sqrt{(n'_\pi+3)(n'_\pi+4)}\\ &\quad\times\delta_{n'_\pi,n_\pi-2}.\end{aligned}\tag{A1}$$

Using Eq. (C.29) of Ref. [25], the triple reduced matrix elements of a pair of boson creation operators is given by

$$\begin{aligned}&\langle \rho'_C(\lambda'_C,\mu'_C),(n's_\pi,0),(\lambda',\mu')|||[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{(2,0)}\\ &\quad\times|||\rho_C(\lambda_C,\mu_C),(n_\pi,0),(\lambda,\mu)\rangle_1\\ &=\begin{Bmatrix}(\lambda_C,\mu_C) & (0,0) & (\lambda'_C,\mu'_C) & 1\\ (n_\pi,0) & (2,0) & (n'_\pi,0) & 1\\ (\lambda,\mu) & (2,0) & (\lambda',\mu') & 1\\ 1 & 1 & 1 & \end{Bmatrix}\langle (n'_\pi,0)|||[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{(2,0)}\\ &\quad\times|||(n_\pi,0)\rangle_1\delta_{(\lambda'_C,\mu'_C),(\lambda_C,\mu_C)}\delta_{\rho'_C,\rho_C}\end{aligned}\tag{A2}$$

and a similar relation holds for the two annihilation operators. Here { } stands for the 9-(λ,μ) symbol. Please note that the total number of bosons N is conserved, thus the number of σ bosons is determined by n_π; so our short-hand notation for the basis states is complete.

The next type of interaction is the product of two creation and two annihilation operators, where Eq. (C.28) of Ref. [25] is used, i.e.,

$$\begin{aligned}&\langle \rho'_C(\lambda'_C,\mu'_C),(n'_\pi,0),(\lambda',\mu')\\ &\quad\times|||\big[[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{(2,0)}\otimes[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{(0,2)}\big]^{(\lambda,\lambda)}\\ &\quad\times|||\rho_C(\lambda_C,\mu_C),(n_\pi,0),(\lambda,\mu)\rangle_1\\ &=\begin{Bmatrix}(\lambda_C,\mu_C) & (0,0) & (\lambda'_C,\mu'_C) & 1\\ (n_\pi,0) & (\lambda,\lambda) & (n'_\pi,0) & 1\\ (\lambda,\mu) & (\lambda,\lambda) & (\lambda',\mu') & 1\\ 1 & 1 & 1 & \end{Bmatrix}\delta_{(\lambda'_C,\mu'_C),(\lambda_C,\mu_C)}\delta_{\rho'_C,\rho_C}\\ &\quad\times\langle (n'_\pi,0)|||\big[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger\big]^{(2,0)}|||(n_\pi-2,0)\rangle_1\\ &\quad\times\langle (n_\pi-2,0)|||[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{(0,2)}|||(n_\pi,0)\rangle_1\\ &\quad\times\mathrm{U}[(n_\pi,0)(0,2)(n'_\pi,0)(20);(n_\pi-2,0)11(\lambda,\lambda)11],\end{aligned}\tag{A3}$$

with $\lambda=0,2$ and U[$\cdots$] is the SU(3) Racah coefficient [25].

In the Hamiltonian, only those products of two creation and two annihilation operators appear, which are coupled to zero angular momentum. Their relation to the SU(3) tensor products are

$$\begin{aligned}(\boldsymbol{\pi}^\dagger\cdot\boldsymbol{\pi}^\dagger) &= \sqrt{3}\langle (1,0)11,(1,0)11||(2,0)10\rangle_1[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{(2,0)}_{100},\\ (\boldsymbol{\pi}\cdot\boldsymbol{\pi}) &= \sqrt{3}\langle (0,1)11,(0,1)11||(0,2)10\rangle_1[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{(0,2)}_{100},\end{aligned}\tag{A4}$$

and

$$\begin{aligned}(\boldsymbol{\pi}^\dagger\cdot\boldsymbol{\pi}^\dagger)(\boldsymbol{\pi}\cdot\boldsymbol{\pi}) = 3\sum_\lambda&\langle (1,0)11,(1,0)11\\ &\times||(2,0)10\rangle_1\langle (0,1)11,(0,1)11||\\ &\times(0,2)10\rangle_1\langle (2,0)10,(0,2)10||(\lambda,\lambda)10\rangle_1\\ &\times\big[[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{(2,0)}\otimes[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{(0,2)}\big]^{(\lambda,\lambda)}_{100},\end{aligned}\tag{A5}$$

where the subindex in the last line refers to the multiplicity κ, angular momentum L, and its projection, respectively.

The matrix elements of the $\sigma^\dagger$ and σ operators are

$$\begin{aligned}\langle n'_\sigma|\boldsymbol{\sigma}^\dagger|n_\sigma\rangle &= \delta_{n'_\sigma n_\sigma+1}\sqrt{n_\sigma+1},\\ \langle n'_\sigma|\boldsymbol{\sigma}|n_\sigma\rangle &= \delta_{n'_\sigma n_\sigma-1}\sqrt{n_\sigma},\\ \langle n'_\sigma|\boldsymbol{\sigma}^\dagger\boldsymbol{\sigma}|n_\sigma\rangle &= \delta_{n'_\sigma n_\sigma}n_\sigma,\\ \langle n'_\sigma|(\boldsymbol{\sigma}^\dagger)^2|n_\sigma\rangle &= \delta_{n'_\sigma n_\sigma+2}\sqrt{(n_\sigma+1)(n_\sigma+2)},\\ \langle n'_\sigma|(\boldsymbol{\sigma})^2|n_\sigma\rangle &= \delta_{n'_\sigma n_\sigma-2}\sqrt{n_\sigma(n_\sigma-1)},\end{aligned}\tag{A6}$$

where we denoted the basis states by the $n_\sigma=N-n_\pi$ quantum number.

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