Phenomenological and microscopic cluster models I. The geometric mapping

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The geometrical mapping of algebraic nuclear cluster models is investigated within the coherent state formalism. Two models are considered: the Semimicroscopic Algebraic Cluster Model (SACM) and the Phenomenological Algebraic Cluster Model (PACM), which is a special limit of the SACM. The SACM strictly observes the Pauli exclusion principle while the PACM does not. The discussion of the SACM is adapted to the coherent state formalism by introducing the new SO(3) dynamical symmetry limit and third-order interaction terms in the Hamiltonian. The potential energy surface is constructed in both models and it is found that the effects of the Pauli principle can be simulated by higher-order interaction terms in the PACM. The present study is also meant to serve as a starting point for investigating phase transitions in the two algebraic cluster models.

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I. INTRODUCTION

Phase transitions in algebraic models have been discussed since the 1970’s. The principal method is the use of coherent states. The expectation value of the algebraic Hamiltonian, with respect to a coherent state, is defined as the semi-classical potential. Through the behavior of that potential, as a function in the parameter space, phase transitions and their order can be studied. The basic description, applied to the IBA, was presented in [2]. The method of coherent states also delivers a geometrical mapping of the algebraic model in consideration, providing in this manner an easy interpretation of the dynamical symmetry limits. Other studies on phase transitions in the IBA are published in [4].

In [2], a complete classification of phase transitions in algebraic models is presented, restricted to Hamiltonians with up to two-body interactions. For the vibron models [6, 7] the transitions turned out to be of second order. In [8], a second order phase transition was also encountered. In [9] the U(3) boson model was studied and it was noted that for very large number of bosons, the transition may turn over into one of first order. The transitions were investigated using the overlap of the ground state with that of the O(2) limit and searching for a step like behavior. In other words, no discontinuities of the derivatives of the potential were considered.

Coherent states have not only been applied to the IBA or atomic molecules, but also to other algebraic models, which have a microscopic origin within the shell model. In [10] the geometrical mapping, using the vector coherent state method [11] was applied, mapping the pseudo-symplectic model to the geometric model of the nucleus [12]. The geometrical mapping turned out to be very useful in calculations of nuclear spectra and predicting the spectra of super heavy nuclei. In [17], the coherent state method was used to obtain a geometrical mapping of the Semimicroscopic Algebraic Cluster model (SACM) [18, 19]. The SACM is an algebraic cluster model which takes into account the Pauli exclusion principle. It allows for investigation of the effects of the Pauli exclusion principle on the geometric potentials and on the order of the phase transition. Phase transitions in single nuclear systems were also investigated in [20, 21], related to the symplectic model of the nucleus.

Note that phase transitions in nuclei, though not explicitly stated as such, were already studied in 1972 in the first edition of [13]. A standard curve discussion was applied, while a phase transition was denoted as a shape transition. In the recent treatments, the main difference is the classification in terms of the order of phase transitions.

Since its initial use, interest in the geometrical mapping, using the coherent state method, has not been lost. One of the main reasons is that multiple particle systems in conjunction with phase transitions can be easily treated. These methods can provide important insight into how to treat, in general, complicated many-body systems.

In recent years, phase transitions in atomic and nuclear molecules were investigated in [22, 24], with the help of the coherent state method. The type of phase change discussed there, important for the context of studies presented in this contribution, is related to the SU(3) and SO(4) limit and the transition between them in a molecule, which can consist of two atoms or of two nuclei. Here we will restrict ourselves to nuclear clusters only. Two groups of models will be discussed: the Phenomenological Algebraic Cluster Model (PACM) and the Semimicroscopic Algebraic Cluster Model (SACM). The Vibron Model belongs to the group PACM [22, 26]. In the PACM the minimal number of relative oscillation quanta
is always zero. In contrast, in the SACM there is a minimal number of relative oscillation quanta, $n_0$, due to the Wildermuth condition $[27]$, which is necessary in order to observe the Pauli exclusion principle. Though there is a lot of investigation in the PACM on phase transitions, applications to actual nuclei are very rare. Only in $[28]$, from the beginning of the vibron model, and in $[29]$ have we found applications to real cluster systems.

Some of the important questions we would like to discuss in this and a forthcoming publication are: What is the difference between taking into account or not the Pauli exclusion principle? What are the orders of the phase transitions in the models discussed? How does one define the thermodynamical limit? Normally, only second-order phase transitions appear between the $SU(3)$ and $SO(4)$ dynamical symmetries $[8]$. So, is it also possible to obtain, under certain circumstances, a first order phase transition?

This contribution restricts itself to the geometric mapping of an algebraic Hamiltonian within the PACM and SACM. Already there some important differences arise. One main result will be that in order that the PACM reproduces the same results as the SACM, higher order interaction terms are necessary which simulate the effects of the Pauli exclusion principle. Differences and common features between the PACM and SACM will be discussed. The main reason for the differences is the large overlap of the clusters, making it necessary to antisymmetrize the many nucleon system. The PACM, which ignores the Pauli exclusion principle, will consequently fail in satisfying basic conditions. For atomic molecules this problem does not arise, because the two atomic nuclei are separated in space, and thus no exchange effects play a role. Some caution must be exercised when comparing; because the structures of the individual clusters are described within the SACM by the shell model, we are obliged to compare to a PACM that also uses the $SU(3)$ model. In general, the IBA model has been used in the literature $[26, 29]$. Additionally, the parameter by which the number operator of $\pi$ bosons is multiplied is fixed in the SACM because it describes the mean field. Within the PACM this parameter can be chosen arbitrarily.

This all refers to the first question. The others will be addressed in the second part, dedicated to the study of phase transitions.

The paper is structured as follows: In section II the Semimicroscopic Algebraic Cluster Model is revisited, introducing some novel features, including the definition of the Phenomenological Algebraic Cluster Model (PACM) as a special limit of the SACM not observing the Pauli principle. In section III the coherent state formalism will be implemented in both models. The PACM coherent state can be recovered from the SACM when one sets the minimal number of relative oscillation quanta, $n_0$, to zero. In section IV the geometrically mapped potentials are derived for the two models, and finally, in section V conclusions are drawn and a discussion is presented on the differences of the PACM to the SACM.

II. THE SEMIMICROSCOPIC ALGEBRAIC CLUSTER MODEL RECONSIDERED

In this section we present a brief overview of the Semimicroscopic Algebraic Cluster Model (SACM) $[18, 19]$ and introduce further amendments of it necessary for our study. These new elements appear in all three subsections. Previous applications of the SACM concerned describing the spectroscopic properties of core+$\alpha$-type $[30]$ and other $[31]$ two-cluster systems.

A. The group structure

We start with reviewing the vibron model $[27]$, in which the relevant degrees of freedom are oscillations in the relative motion of two structureless clusters in three dimensions. The operators describing them are boson creation and annihilation operators with angular momentum one:

$$\pi^+_m, \pi^-_m, \ m = 0, \pm 1 \ .$$

(1)

To this system one adds the spinless $\sigma^+_m$ boson creation and $\sigma$ annihilation operators. They define a cut-off, through the condition that the total number of bosons $N = n_{\pi} + n_{\sigma}$ is kept constant. The $\sigma$-bosons have no physical significance, which will play a role later on if one intends to define a thermodynamical limit. The $\pi^m$ operators satisfy the relation

$$\pi^m = (-1)^{1-m} \pi^{-m} \ .$$

(2)

The sixteen boson number conserving operators

$$\pi^m \pi^{-m}, \ \pi^+_m \sigma^- \ , \ \sigma^+ \pi^- \ , \ \sigma^- \sigma^- \ (3)$$

act as the generators of the $U_R(4)$ group, where $R$ stands for relative motion. There are two subgroup chains that contain the $SO_R(3)$ rotation group. The irreducible representations of the subgroups supply quantum numbers to define bases that are associated with the two dynamical symmetries:

$$U_R(4) \supset SU_R(3) \supset SO_R(3) \supset SO_R(2) \ \ [N,0,0,0] \ \ \ (n_\pi,0) \ \ \ L_R \ \ \ M_R, \ (4)$$

where

$$n_{\pi} = N, N-1,...,1,0, \ \ L_R = n_{\pi}, n_{\pi} - 2,...,1 or 0, \ \ M_R = L_R, L_R - 1, ...,-L_R, \ (5)$$

and

$$U_R(4) \supset SO_R(4) \supset SO_R(3) \supset SO_R(2) \ \ [N,0,0,0] \ \ \ (\omega,0) \ \ \ L_R \ \ \ M_R, \ (6)$$

where

$$\omega = N, N-2,...,1 or 0, \ \ L_R = \omega, \omega - 1, ... , 1, 0, \ \ M_R = L_R, L_R - 1, ...,-L_R. \ (7)$$
The $SU(3)$ dynamical symmetry is generally believed to be the vibrational limit of the system around a spherical equilibrium shape, while the $SO(4)$ dynamical symmetry describes static dipole deformation.

The vibron model formalism reviewed up to this point handles only the relative motion of the clusters and neglects their internal structure. In order to incorporate these degrees of freedom too, the SACM applies Elliott’s $SU(3)$ model \cite{22}. The orbital structure of the clusters is then described by the $SU_C(k)$ group, where $C_k$ refers to the $k$th cluster, $k = 1, 2$. The Elliott model applies LS coupling, but in many cases the $S$ spin degree of freedom does not play a role. This is the case, for example with even-even clusters, and for the sake of simplicity we shall consider clusters of this type in what follows.

It is essential that in the SACM the $SU(3)$ group appears not only in the description of the relative motion and the individual clusters, but also in the description of the unified nucleus. The typical group structure associated with a two-cluster system in the SACM is then

$$SU_C(3) \otimes SU_C(3) \otimes SU_R(3) \supset SU_C(3) \otimes SU_R(3) \supset (\lambda_1, \mu_1) \otimes (\lambda_2, \mu_2) \otimes (n_\pi, 0) \otimes (\lambda_C, \mu_C) \supset SU(3) \supset SO(3) \supset SO(2) \supset (\lambda, \mu) \otimes \kappa L \otimes M,$$

(8)

where $(\lambda_k, \mu_k)$ refers to the $SU_C(k)$ irreducible representations (irreps) of the individual clusters, which are then coupled to intermediate irrep $(\lambda_C, \mu_C)$. These irreps are the ones associated with the ground-state configuration of the $k$th cluster. $n_\pi$ is the number of relative oscillator quanta, while $(\lambda, \mu)$ is the total $SU(3)$ irrep. $L$ and $M$ are the angular momentum and its projection, and $\kappa$ is used to distinguish multiple occurrences of a given $L$ in $(\lambda, \mu)$.

The model space of the SACM is obtained by comparing all possible irreps $(\lambda, \mu)$, as given in (8), contained in the product $(\lambda_{C_1}, \mu_{C_1}) \otimes (\lambda_{C_2}, \mu_{C_2}) \otimes (n_\pi, 0)$, with those of the shell model and retaining only those irreps which appear in the shell model. Computer codes determining the model space are available and can be obtained on request. In most cases, however, it is easy to retrieve the irreps by hand. In this manner the Pauli exclusion principle is observed (for some illustrative examples, see Refs. \cite{18, 19}). The $SU(3)$ basis is also useful in eliminating the spurious center of mass motion.

We note that the above $SU(3)$ matching procedure also reproduces the Wildermuth condition \cite{23} in a natural way. This condition prescribes a minimal number of oscillator quanta (i.e. $n_\pi$) in the relative motion. Apart from the case of closed-shell clusters, however, it is only a necessary condition for the handling of the Pauli exclusion principle.

It is now worthwhile to discuss the possible dynamical symmetries of the SACM based on those of the vibron model. The $SU(3)$ dynamical symmetry is clearly associated with the $SU(3)$ group chain. The equivalent of the $SO(4)$ dynamical symmetry of the vibron model, however, can be considered only an approximate dynamical symmetry in the SACM. The reason is that due to the Pauli principle part of the set of $SO(4)$ basis states has to be excluded from the model space. Although $n_\pi$ is not a good quantum number in the $SO(4)$ limit, the $SO(4)$ basis states can be written as linear combinations of $SU(3)$ states, so excluding these below the minimal allowed $n_\pi$ value distorts the structure of the $SO(4)$ basis. Finally, a third dynamical symmetry can also be derived from the $SU(3)$ dynamical symmetry of the vibron model. The group structure associated with this $SO(3)$ dynamical symmetry is

$$SU_C(3) \otimes U_R(4) \supset SO_C(3) \otimes SO_R(3) \supset SO(3) \supset SO(2) \supset (\lambda_C, \mu_C) |N, 0, 0, 0 \rangle L_C L_R L M.$$

(9)

The difference between the previously mostly ignored $\mathfrak{G}$ chain and the one appearing in (8) is of dynamical nature in the sense that the interaction in the former case does not contain terms typical of the coupled $SU(3)$ degrees of freedom. In fact, the $SU(3)$ groups do not play a role other than supplying labels for classification of the states. In terms of interactions we can call the scenarios associated with the $\mathfrak{G}$ and $\mathfrak{E}$ chains as weak and strong coupling limits, respectively. The two limits are the same when the two clusters are both closed-shell nuclei, but when at least one of them is not (i.e. its internal $(\lambda_k, \mu_k)$ irrep is different from $(0,0)$), a clear difference between the two limits arises.

Before closing this subsection it is worthwhile to comment on the typical selection rules characterizing the dynamical symmetries. This is also related to the band structure determined by the appropriate group structure. In the basis associated with the $SU(3)$ dynamical symmetry of the SACM the bands are defined by the $(\lambda, \mu)$ and $\kappa$ quantum numbers (see Eq. (8)), where $\kappa$ is obsolete when either $\lambda$ or $\mu$ is zero, as is the case in the $SU(3)$ limit of the vibron model too (see Eq. (3)). The states belonging to the same $SU(3)$ irrep are connected by the quadrupole operator, the $SU(3)$ tensorial character of which is $(1,1)$. This operator leaves $n_\pi$ and the parity intact and changes the angular momentum by two units, so it describes electric quadrupole transitions. On the other hand, bands associated with the $SO(4)$ dynamical symmetry are characterized by the $\omega$ quantum number defining the $SO(4)$ irreps (see Eq. (6)) and contain states with both even and odd angular momentum, i.e. with both positive and negative parity. The in-band transitions are described by the $SO(4)$ generators, which play the role of the electric dipole operator. The two dynamical symmetries thus lead to different selection rules, and this has to be taken into account when they are applied to some concrete physical problem.
B. The Hamiltonian

Let us now turn to the Hamiltonian associated with the SACM. While in most typical applications it is sufficient to consider interaction terms constructed as two-body terms, here we argue that a specific third-order interaction term is also necessary to stabilize the spectrum. Furthermore, as another new element we shall separate the Hamiltonian into terms associated with the three dynamical symmetries identified above. The parametrization introduced this way allows interpolation between the dynamical symmetries, changing certain parameters of the Hamiltonian, like $x$ and $y$ (see equation below).

We consider two cases: i) both clusters spherical and ii) one spherical cluster plus a deformed one. Examples for these two scenarios are the $^{16}$O+$^{4}$He and $^{20}$Ne+$^{14}$Ne systems, examined in Paper-II of this series.

The Hamiltonian is given by

$$H = xyH_{SU(3)} + y(1-x)H_{SO(4)} + (1-y)H_{O(3)}$$

with

$$H_{SU(3)} = \hbar \omega n_{\pi} + a_{C}\{\lambda \lambda (\lambda, \mu) + (\lambda - \frac{b}{a}\Delta n_{\pi})C_{2}(n_{\pi}, 0) + \gamma L^{2} + \frac{i}{2}K^{2}$$

$$H_{SO(4)} = a_{C}L^{2} + a_{R}^{(1)}L^{2} + \gamma L^{2} + \frac{\sigma^{2}}{4}[(\pi \cdot \pi) - (\sigma^{2})]$$

$$H_{O(3)} = \hbar \omega n_{\pi} + a_{C}L^{2} + a_{R}^{(1)}L^{2} + \gamma L^{2}$$

with $\Delta n_{pi} = n_{\pi} - n_{0}$, $n_{0}$ being the minimal number of quanta. The $a_{C}$ is the strength of the quadrupole-quadrupole interaction, restricted to the cluster part, while $R$ and $C$ denote the contributions related to the relative and cluster part respectively. Further interaction terms are the total angular momentum operator, $L^{2}$, and the $K^{2}$ operator, defined in [13, 16] which classifies the rotational bands, giving the projection of the angular momentum onto the intrinsic $z$ axis. For the case of two spherical clusters, the second-order Casimir operator of $SU(3)$ is just given by $n_{\pi}(n_{\pi} + 3)$. Note that in the case of deformed clusters the information about the deformation only enters in the $SU(3)$ dynamical limit.

Note that the division in (11) is done according to dynamical symmetry limits and not according to two terms, referring to each cluster, one to the relative motion and one to the interactions between them. If one wishes to do that, all what has to be done is to decouple the different contributions. For example, the $L^{2}$ operator can be written as $[L_{C} + L_{R}]^{2} = [L_{C}^{2} + L_{R}^{2} + 2(L_{C} \cdot L_{R})]$. The first and second term refer to the cluster and relative angular momentum, respectively, while the last term refers to the coupling between the channels. This can be further divided by writing the cluster angular momentum as $L_{Cm} = (L_{C1m} + L_{C2m})$.

The division according to dynamical symmetries in (11) was done as follows: In the $SU(3)$ limit the coupling of interaction operators is on the level of $SU(3)$, i.e., Casimir operators of $SU(3)$ and $SU(3)$ have to appear. This is called the strong coupling limit. The $SO(3)$ limit couples only at the $SU(3)$ level, i.e. only the angular momentum operators appear (no second- and higher-order $SU(3)$ Casimir operators, except $n_{\pi}$ and functions in it). This is called the weak coupling limit. This is reflected by the appearance of interaction terms related only to angular momentum ($L_{R}^{2}$, $L_{C}^{2}$ and $L^{2}$). In the literature one usually refers to this latter limit as the $SU(3)$ limit, where the Hamiltonian contains only the $\hbar \omega n_{\pi}$ term plus at most some weak anharmonic terms. Here we feel it necessary to change the notation because we understand the $SU(3)$ limit to include also terms such as a strong quadrupole-quadrupole interaction. In order to compare with results in the literature, this has to be kept in mind when we report on phase transitions between different dynamical symmetries. The $SO(4)$ limit is defined through the appearance of the second-order Casimir operator of $SO(4)$. This limit is called the deformed limit because the interaction will always produce a potential with a deformed minimum.

In principle, one can add the angular momentum operator of the deformed clusters ($L_{k}^{2}$, $k = 1, 2$). We exclude this interaction for the moment.

The new higher-order interaction appearing in the third term of $H_{SU(3)}$ needs some explanation. The whole term is related to the quadrupole-quadrupole interaction, which is present in any nuclear system. However, without the $-b\Delta n_{\pi}$ (with $b > 0$) correction, states which contain a sufficiently large $n_{\pi}$ will be lower in energy than states with the minimal number of $\pi$ bosons, $n_{0}$. This is due to the dependence on $n_{\pi}^{2}$ in the second-order Casimir operator, which will finally dominate over the $\hbar \omega n_{\pi}$ term for a sufficiently large number of $\pi$-bosons. In the standard treatment, when $n_{\pi}$ is conserved, a simple restriction to small $\Delta n_{\pi}$ suffices to circumvent the problem, i.e., states with large $\Delta n_{\pi}$ are simply not taken into account in the model space.

This effect was studied in [33] within the context of the symplectic model of the nuclei [12, 34, 35]. Also there, the quadrupole-quadrupole interaction dominates over the kinetic energy and finally will promote high $n_{\pi}$ states to low energies, even below the physical ground state. This problem was solved by subtracting from the quadrupole-quadrupole interaction the so called Trace Equivalent part [33], which insures that the average mean field is still represented by a harmonic potential. When no correction is applied, the mean field shell structure is destroyed and a mean oscillator structure, one of the main assumptions of the shell model, cannot be assumed anymore. This was also noted within the SACM in [13], where correction terms of the type $\Delta n_{\pi}$, mentioned here, were included. Without these corrections the problem increases significantly when interactions mixing states with different $n_{\pi}$ are considered. Then, avoiding states with
large $n_\pi$ is not an option, as is in the case of conserved $n_\pi$, when the model space can be limited in $n_\pi$ using physical arguments.

C. PACM: the phenomenological limit of the SACM

The minimal number of $\pi$ bosons is an essential requirement in the SACM to incorporate the Pauli principle. However, the formalism allows setting this minimal number to zero. This limit of the SACM can be defined as the Phenomenological Algebraic Cluster Model (PACM). It has to be stressed that the difference between the SACM and the PACM manifests itself only in the model space, while the two models share the same Hamiltonian and other operators. Obviously, the different model space will lead to different matrix elements in the two models. Note that the minimal number of relative model space will lead to different matrix elements in Hamiltonian and other operators. We define the SACM to incorporate the Pauli principle, while the two models share the same formalism arising due to it.

The coherent state is presented, which is used to obtain a geometrical mapping of the SACM and PACM in the next section.

One of the main objectives of the present work is to investigate the similarities and differences between the two approaches. This is especially interesting within the context of the coherents state formalism, because in other models restrictions similar to those in the SACM (i.e. restricting the boson number) are unknown. In this sense the formalism of the PACM is closer to that of other models. Due to the minimal number of $\pi$ bosons the formalism of the SACM will obviously become more involved. It is our aim to explore this conflict between the physical importance of a fundamental principle (i.e. the Pauli principle) and the technically more complicated formalism arising due to it.

III. COHERENT STATES AND THE GEOMETRICAL MAPPING

In this section the coherent state is presented, which is used to obtain a geometrical mapping of the SACM and PACM in the next section.

The use of coherent states is the most common method of applying a geometrical mapping. One advantage is that the coherent state can be expanded in terms of the complete set of states for a given total number of bosons, $N_\pi$, in the SACM, this refers to all allowed basis states for a given total number of quanta). The ground-state energy is usually reproduced very well. The coherent state also provides a transparent relation to collective variables. Its use is justified by noting that it corresponds to the Gaussian Overlap Approximation within the Generator Coordinate Method, skipping the term of the zero-point energy. As shown in [36], this method allows the definition of a potential with usually good results. However, the mass parameters of the kinetic energy are usually not reproduced very well. In order to obtain a kinetic energy too, the coherent state variables have to be defined as complex variables [6, 7]. We do not consider the kinetic energy due to the reason mentioned above, and focus on the potential.

The coherent state within the SACM was introduced in [17]

$$|\alpha\rangle = \mathcal{N}_{N_\pi n_\pi}(\alpha \cdot \pi)^{n_\pi} \left[\sigma^+ + (\alpha \cdot \pi)^t\right]^N |0\rangle$$

$$= \mathcal{N}_{N_\pi n_\pi} \frac{N!}{(N + n_\pi)!} \frac{d^{n_\pi}}{d\gamma_1^{n_\pi}} \left[\sigma^+ + \gamma_1 (\alpha \cdot \pi)^t\right]^{N+n_\pi} |0\rangle,$$

(12)

where, for convenience, we redefined the total number of relative oscillation quanta as $(N + n_\pi)$, while the $\gamma_1$ parameter has to be set equal to 1 after the differentiation.

The normalization factor is given by [17]

$$\mathcal{N}_{N_\pi n_\pi}^{-2} = \frac{N!^2}{(N + n_\pi)!} \frac{d^{n_\pi}}{d\gamma_1^{n_\pi}} \frac{d^n}{d\gamma_2^n} \left[1 + \gamma_1 \gamma_2 (\alpha^* \cdot \alpha)\right]^{N+n_\pi},$$

(13)

Again, the $\gamma_k$ to have be set equal to 1 after the application of the derivatives.

The $\alpha$ is a short-hand notation for the, in general, complex variables $\alpha_m$ ($m = 1, 0, -1$). The coherent state with complex $\alpha$ coefficients is the most general linear combination of the boson creation operators. For static problems the requirement $\alpha^* = -1$ reduces the number of real parameters to three, namely to $\alpha_0$ and the real plus the imaginary part of $\alpha_{\pm 1}$.

In the Appendix we present the results for the geometrical mapping for the important interaction terms appearing in the Hamiltonians. We define

$$\alpha^*_m = (-1)^{1-m} \alpha_{-m},$$

(14)

where $\alpha$ represents a measure of the inter-cluster distance and $\alpha^2$ a short-hand notation for $(\alpha \cdot \alpha)$. Because the only relevant variable is the inter-cluster distance, we can express the potential in terms of this sole variable $\alpha$.

The importance of the coherent states resides in the fact that they provide us with the possibility to define a Potential Energy Surface (PES)

$$V(\alpha) = \langle \alpha | H | \alpha \rangle,$$

(16)

in terms of the collective variables $\alpha_m$.

A. Renormalization of the variable $\alpha$

It is often convenient to transform $\alpha$ to other related variables. In the literature there are different conventions, which often contradict each other...
Here we present some arguments to justify our choice, restricting for simplicity to the PACM, where \( n_0 = 0 \).

In [6, 7] the renormalization of the interaction parameters is proposed using the following reasoning: the expectation value of a one-body interaction with respect to the coherent state is proportional to the total number of quanta. As an example, the expectation value of \( a_1 n_\pi \) is given by

\[
\langle a_1 n_\pi \rangle = a_1 N \frac{\alpha^2}{(1 + \alpha^2)} .
\]  

(17)

Assuming that \( \alpha \) is of the order of one, this expectation value increases with \( N \), which is unnatural because \( \langle n_\pi \rangle \) is of the order of one (note that this argument assumes that \( \alpha \) is of the order of one, too). In order to avoid this, it is recommended in [6, 7] to redefine the interaction as

\[
\frac{a'_1}{N} n_\pi
\]  

(18)

In this manner, it is expected that the parameter \( a'_1 \) does not change significantly with increasing \( N \). A similar argument holds for the two-body interaction, recommending to divide the corresponding interaction parameter by \( N(N - 1) \), and so on.

This argument is supported by considerations given in [40]. There it is shown that one- and two-body interactions scale like \( N \) and \( N(N - 1) \), respectively. This dependence has to be canceled in order to define a thermodynamic limit \( N \to \infty \). However, the \( N \) used in [40] can always be related to the number of particles. For example, in the IBA \( N \) is given by half the number of valence nucleons and in Lipkin-type models (two-level systems) the \( N \) is given by the number of states in the lower level which are completely filled in its lowest states.

In the algebraic cluster models, however, the \( N \) is not related to a number of particles but rather to a boson cut-off. The \( \sigma \)-boson is introduced merely to define a cut-off for the number of \( \pi \)-bosons \( (n_\pi \leq N) \). Physics requires that the final results do not depend on this cut-off.

In what follows we present a proposal on how to treat the cut-off in algebraic cluster models. Note that in [13] a conceptual problem arises already, which has not been considered before in the literature. Here we try to convince the reader that the former renormalization (simply dividing the interaction parameters by a power in \( N \)) is too simple and a more sophisticated renormalization has to be applied. Here we illustrate the situation in three different ways.

a) Consider first the \( \hbar \omega n_\pi \) term, which represents the mean field of the harmonic oscillator in the SACM. Dividing it by \( N \) implies that \( \hbar \omega' = \frac{\hbar \omega}{N} \) tends to zero as \( N \to \infty \). The contradiction becomes apparent because \( \hbar \omega \) is a physical value, which has to be kept independent of \( N \), while \( a_1 \) in Eq. (17) is used as an abstract parameter.

b) Looking at it from a different angle, let us consider the operator \( n_\pi \) alone. When applying \( n_\pi \) in an harmonic oscillator basis, in the lowest states the eigenvalues of \( n_\pi \) are small numbers. The geometrical mapping gives \( N \frac{\alpha^2}{(1 + \alpha^2)} \), which suggests an increase proportional to \( N \). The only way to maintain numbers of the order of one is to redefine \( \alpha \) by

\[
\alpha^2 \sim \frac{\delta^2}{N} ,
\]  

(19)

such that the \( \alpha \) tends to zero for \( N \to \infty \). In this way, with \( \delta \) of the order of one, the geometrical mapping also gives results of the order of one. Thus, restricting for example to the PACM \( (n_0 = 0) \), the coherent state in [12] is redefined as

\[
|\delta\rangle = \frac{1}{\sqrt{N!(1 + \frac{1}{N}[\delta \cdot \delta])^N}} \left[ \sigma^1 + \frac{1}{\sqrt{N}} (\delta \cdot \sigma^1) \right]^N |0\rangle.
\]  

(20)

The expectation value of \( n_\pi \) then leads to

\[
\langle n_\pi \rangle = \frac{\delta^2}{(1 + \frac{1}{N}\delta^2)} .
\]  

(21)

The global dependence on \( N \) vanishes, while for \( N \to \infty \), the \( N \)-dependence disappears.

The same happens for most of the two-body interactions, as we will discuss further below, with some differences when the \( \sigma \)-operators are involved.

c) The above choice of the new variable \( \delta \) can be justified in a third way. To prove this, let us consider the coordinate operator defined without \( \sigma \)-bosons, i.e. without cut-off \( (N) \), namely

\[
r_m = \sqrt{\frac{\hbar}{2m\omega}} (\pi^\dagger_m + \pi_m) .
\]  

(22)

When the \( \sigma \)-bosons are introduced, this operator has to be changed. The new operator, called the algebraic coordinate operator, should satisfy the following minimal conditions: i) The total number of bosons has to be kept constant, i.e., each \( \pi^\dagger_m \) has to be multiplied by \( \sigma \) and each \( \pi_m \) has to be multiplied by a \( \sigma^\dagger \); ii) the definition of the distance operator should be independent of the basis and Hamiltonian used; and iii) for \( N \to \infty \) it should converge to the standard form given in [22]. The proposed algebraic coordinate operator is given by

\[
r^a_m = \sqrt{\frac{\hbar}{2N\omega}} (\pi^\dagger_m \sigma + \sigma^\dagger \pi_m) .
\]  

(23)

The “\( a \)” refers to an algebraic operator. The operator itself does not change the total number of bosons, as required by the above condition i). The \( N \) in the denominator of the square root is introduced because in the harmonic oscillator basis the matrix elements of the \( \sigma \)-operators behave like \( \sqrt{N - n_\pi} \), which for large \( N \) and small number of \( \pi \) bosons is approximated by \( \sqrt{N} \). This
approximate value of the $\sigma$ operators is satisfied in any basis, with the condition that the average number of $\pi$ bosons is much smaller than $N$ (though, the structure is particularly simple in the harmonic oscillator basis). Thus the $1/\sqrt{N}$ factor cancels approximately the contributions due to the addition of the $\sigma^1$ and $\sigma$ operators. In this form, the algebraic coordinate operator does not depend on the basis used (the $r_{\alpha}^a$ can be applied to any kind of basis) and nor on the Hamiltonian, thus, satisfying condition ii). For very large $N$ the expressions of the physical and the algebraic coordinate operators tend to each other, satisfying condition iii).

This definition agrees with [37, 38] where an algebraic model for atomic molecules is discussed. Often (see for example [39]) one defines the radial distance as a function of the dynamical symmetry, relating it indirectly to the matrix element of the dipole operator, without any further considerations. This violates condition ii) above. We insist that the definition of the radial coordinate operator can always be chosen along the z-axis. The square of $\sigma$ suggests we redefine

$\alpha = \sqrt{m^2 h^2 r^a_m}$. 

We define this as the algebraic distance $r^a_m$, which is, by definition, of the order of one. Inverting this relation gives

$$\frac{\alpha_m}{(1 + \alpha^2)} = \sqrt{\frac{m\omega}{2Nh^a_m}},$$

which again provides the dependence of $\alpha_m$ on $N$. It suggests we redefine $\alpha_m$ in terms of $\delta_m$ and $N$ as given above, i.e.,

$$\alpha_m = \frac{\delta_m}{\sqrt{N}}.$$ 

with $\delta_m$ given by

$$\frac{\delta_m}{(1 + \frac{\alpha^2}{N})} = \sqrt{\frac{m\omega}{2h^a_m}},$$

a dimensionless measure of the distance between the two nuclear clusters. We claim that this is a consistent way to define the distance between clusters trough the variable $\delta_m$.

The validity of [24], the definition of $r^a_m$, depends on the fluctuations of the related expectation value. This will be discussed shortly. The inter-cluster distance vector can always be chosen along the z-axis. The square of the variation $(\langle r^a_0 \rangle^2 - \langle r^a_0 \rangle^2)$ can then also be calculated, giving

$$\langle (r^a_0)^2 - \langle r^a_0 \rangle^2 \rangle = - \left( \frac{4h}{m\omega} \right) \left( \frac{\delta^2}{N} \right) + \left( \frac{h}{2m\omega} \right) \left( \frac{1 + \delta^2}{1 + \frac{\alpha^2}{N}} \right),$$

$$\rightarrow \left( \frac{h}{2m\omega} \right),$$

where the arrow gives the limit for large $N$. As long as the expectation value of the algebraic distance operator is greater than the square root of this expression, it is safe to identify the $r^a_0$ as the distance between the two clusters. The square root of [25] gives numbers of the order of 1 fm.

When applying the PACM the usage of another variable

$$\beta^2 = \frac{\alpha^2}{(1 + \alpha^2)}.$$ 

will be found more favorable. The range of $\beta^2$ is $0 \leq \beta^2 \leq 1$, because the range of $\alpha$ is $0 \leq \alpha^2 < \infty$. The $\beta^2$ variable can be related to $\delta^2$ as it was to $\alpha^2$. The main reason to use $\beta$ is that within the PACM it simplifies most expressions, as can be seen further below. For the SACM we will return, for convenience, to the variable $\alpha$.

Before closing this subsection we note that in the SACM the relation between $\alpha$ and the relative distance of the two clusters is given by $\alpha \sim (r - r_0)$, [17], with $r_0 \sim \sqrt{n_0}$. This means that there is a minimal difference in the inter-cluster distance due to the presence of a minimal number of $\pi$-bosons, i.e., clusters can not overlap completely. In the PACM, $n_0 = 0$ and thus $r_0 = 0$. Defining the minimum at $\alpha = 0$ as the “spherical” minimum then loses its meaning, because in the SACM it already corresponds to a minimal distance. Nevertheless, we will continue to call a minimum at $\alpha = 0$ a “spherical” minimum and $\alpha \neq 0$ as a “deformed” minimum.

IV. THE GEOMETRICALLY MAPPED POTENTIAL

As discussed previously, the difference between the SACM and PACM model spaces manifests itself in the difference of the matrix elements of physical operators, even if the operators themselves are the same in the two approaches. In this section we determine the potential energy surfaces in both models and explore the relation between them.

A. The SACM case: Pauli principle taken into account

Applying the coherent state for the SACM to the Hamiltonian [10], one obtains the geometrically mapped
potential

\[
\langle H \rangle = C(x, y) - (b + \bar{b})xy \frac{A(x, y)\alpha^2 F_{11}(\alpha^2)}{F_{00}(\alpha^2)}
- B(x, y)\alpha^4 \frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)} + \alpha^6 \frac{F_{33}(\alpha^2)}{F_{00}(\alpha^2)}
- C(x, y)\alpha^2 \frac{F_{20}^{-2}(\alpha^2)}{F_{00}(\alpha^2)}
\]

(30)

where

\[
C(x, y) = \langle (a_{C_{1us}} + a + b n_0) xy C_2(\lambda_C, \mu_C) + \gamma L_C^2 + (1 - xy) L C_2^2 \rangle
+ xyt(K^2) + \frac{c}{4} (N + n_0) (N + n_0 - 1) y (1 - x)
\]

(31)

and the \(F_{ij}(\alpha^2)\) functions are defined as

\[
F_{00}(\alpha^2) = \frac{(N!)^2}{(N + n_0)!} \\
\times \sum_{k=n_0}^{N+n_0} \left( \frac{k!}{(k-n_0)!} \right)^2 \alpha^{2k}
\]

\[
F_{11}(\alpha^2) = \frac{(N!)^2}{(N + n_0 - 1)!} \\
\times \sum_{k=\max(n_0-1,0)}^{N+n_0-1} \left( \frac{k!}{(k-n_0)!} \right)^2 \alpha^{2k}
\]

\[
F_{22}(\alpha^2) = \frac{(N!)^2}{(N + n_0 - 2)!} \\
\times \sum_{k=\max(n_0-2,0)}^{N+n_0-2} \left( \frac{k!}{(k-n_0)!} \right)^2 \alpha^{2k}
\]

\[
F_{20}^{-2}(\alpha^2) = \frac{(N!)^2}{(N + n_0 - 2)!} \\
\times \sum_{k=n_0}^{N+n_0-2} \left( \frac{k!}{(k-n_0)!} \right)^2 \alpha^{2k}
\]

\[
F_{33}(\alpha^2) = \frac{(N!)^2}{(N + n_0 - 3)!} \\
\times \sum_{k=\max(n_0-3,0)}^{N+n_0-3} \left( \frac{k!}{(k-n_0)!} \right)^2 \alpha^{2k}
\]

(32)

Further, the constants appearing in (30) are defined as

\[
A(x, y) = - \frac{1}{(b + \bar{b}) xy} \left( \hbar \omega [yx + 1 - y] \\
+ 2 \left[ \gamma + (1 - xy) \alpha_2^0 \right] \\
+ x y [a - b] [4 + \Gamma_1 + \Gamma_2] \\
+ 4 x y [\pi - \bar{b}] + x y n_0 [4 + \Gamma_1 + \Gamma_2] + 4 x y n_0 \bar{b} \\
- b x y C_2(\lambda_C, \mu_C) - \frac{c}{2} y (1 - x) (N + n_0 - 1) \right)
\]

\[
B(x, y) = \frac{1}{(b + \bar{b}) xy} \left( x y [a + \pi - 6 b - 6 \bar{b}] \\
- b \{ \Gamma_1 + \Gamma_2 \} + n_0 (b + \bar{b}) + \frac{c}{2} y (1 - x) \right)
\]

\[
C(x, y) = - \frac{c}{2} y (1 - x) \frac{\gamma x}{(b + \bar{b}) xy} ,
\]

(33)

where \(\Gamma_k\), according to [17], is given by

\[
\Gamma_k = \langle (\lambda_k, \mu_k) \rangle \langle Q^m_{\text{Cluster}}(k) \rangle (\lambda_k, \mu_k)
= \sqrt{\frac{5}{\pi}} \left[ s_k + \frac{3}{2} (\Lambda_k - 1) \right] \alpha_{2m}(k)
= \sqrt{\frac{5}{\pi}} N_{0,k,b} \beta_k .
\]

(34)

This was obtained by a geometric mapping of the symplectic model [10, 14, 15]. The \((\lambda_k, \mu_k)\) denotes the \(SU(3)\) irrep of the deformed cluster number \(k\). In the case that it is spherical, \(\Gamma_k = 0\). The \(N_{0,k}\) is the sum of the total number of quanta \(n_k\) of the deformed cluster plus \(\frac{3}{2}(A_k - 1)\), where \(A_k\) is the number of nucleons in the \(k^{th}\) cluster. This last term is the zero-point energy with the contribution of the center of mass already extracted. The \(\alpha_{2m}(k)\) is the deformation variable of cluster number \(k\). In [24] we used only the \(m = 0\) component of \(\alpha_{2m}(k)\) and defined it \(\beta_k\), the deformation of cluster \(k\) (not to be confused with the \(\beta\) variable appearing in Eq. (29)). This implies that the deformed cluster is assumed to be axially symmetric and it is in line with the inter-cluster \(z\)-axis, which connects both clusters. When the \(z\)-axis of the deformed cluster is inclined with respect to the molecular \(z\)-axis by an angle \(\theta\), the deformation value \(\beta_k\) is multiplied by a matrix element of the rotation matrix, which only changes the numerical value of \(\beta_k\), i.e., \(\beta_k' = d_{00}(\theta) \beta_k\). For simplicity we do not include these orientations in the discussion. Furthermore, it will not change the basic results.

In discussing the phase transitions it is possible to choose as the independent parameters of the theory \(A\), \(B\) and \(C\), which themselves are the functions of all interaction parameters of the theory. This structure will be used in the second paper, investigating the possible phase transitions and the phase diagram.

For \(x = 0\), i.e. in the case of the \(SO(4)\) to \(SO(3)\) phase transition, the discussion has to be modified due to the \(xy\) factor appearing in the denominators in (33).
In this case the potential maps to
\[
V = \langle H \rangle \\
\rightarrow \left( A\alpha^2 \frac{F_{11}(\alpha^2)}{F_{00}(\alpha^2)} - \frac{1}{2} \alpha^4 \frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)} - C\alpha^4 \frac{F_{00}^{N-2}(\alpha^2)}{F_{00}(\alpha^2)} \right) + C \\
\tag{35}
\]
with
\[
\xi = \left( \frac{\hbar}{2} (1 - y) + 2 \left[ \frac{\gamma + \alpha R}{2} \right] - \frac{c}{2} (N + n_0 - 1) \right) \\
\frac{\gamma}{2} = - \frac{c}{2} y \\
\frac{\gamma}{2} = - \frac{c}{2} y . \\
\tag{36, 37, 38}
\]

In this case only two independent parameters \( \xi \) and \( \frac{\gamma}{2} \) appear.

Note that for \( c > 0 \), the \( C \) is positive (remember that \( -b > 0 \)). When \( C < 0 \), the situation corresponds in the \( SO(4) \) limit to a ground state where all bosons are decoupled and the highest state is the one where all bosons are coupled in pairs.

In [31], we have to add a constant term, such that the geometrically mapped potential is zero at \( \alpha = 0 \). This is a permitted renormalization of the zero-point energy. This constant will be determined further below.

It also has to be noted that the \( SO(4) \) dynamical symmetry needs special care due to the truncation of the \( SU(3) \) basis required by the Pauli principle. Eliminating these components leads to the destruction of the \( SO(4) \) dynamical symmetry. However, we will still denote it a \( SO(4) \) dynamical symmetry, because the operators in the Hamiltonian will be the same. Instead of the \( SO(4) \) basis we will stay within the \( SU(3) \) basis, because only there can the Pauli principle be implemented easily, canceling all states with \( n_\pi < n_0 \). Note also that the total number of bosons is now \( (N + n_0) \) and not just \( N \).

A very useful consideration is the investigation of the potential in the \( \alpha \rightarrow \infty \) and \( \alpha \rightarrow 0 \) limits. In the first limit we will see that the potential approaches a constant value depending on \( (N + n_0) \), which is due to the finite size of the boson space. For large values of \( \alpha \) the coherent state contains only \( \pi \)-bosons and cannot increase the energy any further. The second limit \( \alpha \rightarrow 0 \) is necessary to adjust \( V(\alpha = 0) = 0 \). These consideration will be important in the second paper, when the general structure of the SACM phase diagram will be discussed.

i) Limit \( \alpha \rightarrow \infty \):

The relevant formulas are
\[
\alpha^2 \frac{F_{11}}{F_{00}} \rightarrow (N + n_0) \\
\alpha^4 \frac{F_{22}}{F_{00}} \rightarrow (N + n_0) (N + n_0 - 1) \\
\alpha^6 \frac{F_{33}}{F_{00}} \rightarrow (N + n_0) (N + n_0 - 1) (N + n_0 - 2) \\
\alpha^6 \frac{F_{00}^{N-2}}{F_{00}} \rightarrow N (N - 1) \left( \frac{1}{\alpha^2} \right) \rightarrow 0 . \\
\tag{39}
\]

With this, the limit of the complete geometric potential [31] is given by
\[
V \rightarrow C - (b + \bar{b}) \{ A(N + n_0) - B(N + n_0)(N + n_0 - 1) + (N + n_0)(N + n_0 - 1)(N + n_0 - 2) \} . \\
\tag{40}
\]

Depending on the signs and values of \( A \) and \( B \), this limit is either positive or negative. For the positive value the limit for \( (N + n_0) \rightarrow \infty \) is then \( +\infty \), leading to a stable potential, while if it is negative the limit leads to \( -\infty \), leading to an unstable potential.

ii) Limit \( \alpha \rightarrow 0 \):

The relevant formulas are
\[
\alpha^2 \frac{F_{11}}{F_{00}} \rightarrow n_0 \\
\alpha^4 \frac{F_{22}}{F_{00}} \rightarrow n_0 (n_0 - 1) \\
\alpha^6 \frac{F_{33}}{F_{00}} \rightarrow n_0 (n_0 - 1) (n_0 - 2) \\
\alpha^6 \frac{F_{00}^{N-2}}{F_{00}} \rightarrow N (N - 1) (n_0 + 1)(n_0 + 2) \left( \frac{\alpha^2}{2} \right) \rightarrow 0 . \\
\tag{41}
\]

With this, the limit of the complete geometric potential [31] is given by
\[
V(\alpha = 0) \rightarrow C - (b + \bar{b}) \{ A n_0 - B n_0 (n_0 - 1) + n_0 (n_0 - 1)(n_0 - 2) \} . \\
\tag{42}
\]

which is independent of \( N \). This result can be used to adjust the potential to zero at \( \alpha = 0 \).

B. The PACM case: Pauli principle not taken into account

Using the Hamiltonian as introduced in the section [1] and the coherent state of section [11] for the case when the Pauli exclusion principle is not taken into account, the potential is obtained by calculating the expectation.
value of the Hamiltonian as
\[ \langle H \rangle = V(\beta) \]
\[ = (a_{clus} + a) \, xyC_2(\lambda_C, \mu_C) + \frac{c}{4}N(N-1)y(1-x) \]
\[ + N\beta^2 \left[ \left( \hbar \omega (xy + 1 - y) + (a - b)(4 + \Gamma_1 + \Gamma_2) \right) \right. \]
\[ + 4 \left( \bar{a} - \bar{b} \right) - bC_2(\lambda_C, \mu_C) \left. - (1 - x) yc(N - 1) \right] \]
\[ + 2 \left( \gamma + (1 - xy)a_R^{(1)} \right) \]
\[ + N(N - 1) \beta^4 \left[ xy(a + \bar{a} - 6\bar{b} - 6\bar{b} - b(\Gamma_1 + \Gamma_2)) \right. \]
\[ + (1 - x) yc \left. - N(N - 1)(N - 2) \beta^6xy(b + \bar{b}) + C_2(\lambda_C, \mu_C)axy \right] \]
\[ + \frac{1}{4}((1 - x) ycN(N - 1)) . \] (43)

Defining
\[ A = \left[ \left( b + \bar{b} \right) xy(N - 1)(N - 2) \right]^{-1} \]
\[ \times \left[ \hbar \omega (xy + 1 - y) + 2 \left( \gamma + (1 - xy)a_R^{(1)} \right) \right. \]
\[ + 4xy(\pi - \bar{b}) + xy(a - b)(4 + \Gamma_1 + \Gamma_2) \]
\[ - bxyC_2(\lambda_C, \mu_C) - y(1 - x)c(N - 1) \left. \right] \]
\[ B = \frac{xy(a + \pi - 6(b + \bar{b}) - b(\Gamma_1 + \Gamma_2)) + cy(1 - x)}{(N - 2)(b + \bar{b})xy} \]
\[ C = \langle a_{clus} + a \rangle \, xyC_2(\lambda_C, \mu_C) + \gamma LC^2 + (1 - xy) LC^2 \]
\[ + xyt(K^2) + \frac{c}{4}N(N - 1)y(1 - x) \] , (44)

the potential acquires the form \[ \text{[41, 42]} \]
\[ V = N(N - 1)(N - 2)(-b(b + \bar{b})xy) \left\{ A\beta^2 - B\beta^4 + \beta^6 \right\} \]
\[ + C \] , (45)

which allows us to define a new, normalized potential
\[ \tilde{V} = \left\{ A\beta^2 - B\beta^4 + \beta^6 \right\} \] . (46)

In the definition of \( \tilde{V} \) we extracted the factor \( (b + \bar{b})xy \), such that there appears no factor in front of the \( \beta^6 \) term. This poses no problem as long as \( x \) is varied from 0 to 1. In the limit of \( x \to 0 \) the \( A \) and \( B \) values also approach \( \pm \infty \), depending on the sign. However, for the \( SO(4) \) to \( SO(3) \) transition, the \( x \) value is always zero. For this case we include \( x \)\'s value within the parenthesis, yielding a vanishing factor of the sextic term.

Comparing the potentials obtained from the same Hamiltonian in the SACM and PACM approaches leads to a remarkable finding. The potential in the SACM framework is rather different from its PACM counterpart, however, a similar potential can also be generated within the latter framework too. This can be achieved by including higher-order interactions of the type \( F_1(n_\pi)/F_2(n_\pi) \), with appropriate functions \( F_k(n_\pi) \). This demonstrates that observing the Pauli exclusion principle acts as if one used high-order interactions in a model which does not observe the Pauli exclusion principle. In fact, the nonlinear terms simulate the presence of the Pauli exclusion principle.

V. CONCLUSIONS

In order to investigate possible phase transitions between different limits corresponding to various dynamical symmetries, we reparametrized the Hamiltonian of the Semimicroscopic Algebraic Cluster Model (SACM) such that it allowed interpolation between the three possible limits. These were the strong coupling limit \( (SU(3)) \), the deformed limit \( (SO(4)) \) and the weak coupling limit \( (SO(3)) \). The latter limit was proposed in the present work and it differs from the strong coupling limit in the level on which the interaction terms of the relative motion and those of the internal cluster structure are coupled: in the weak coupling limit this is done on the \( SO(3) \) (i.e. angular momentum) level, while in the strong coupling limit the \( SU(3) \) algebra plays a role, introducing, e.g. quadrupole–quadrupole interaction between the two sectors. In the case of a system with two spherical clusters the weak coupling Hamiltonian is a simplified version of the strong coupling one, so it does not stand as a separate limit in itself. The \( SO(4) \) limit also has its limitations due to the truncation of the model space in the \( n_\pi \) quantum number.

The Phenomenological Algebraic Cluster Model (PACM) was introduced as a special limit of the SACM with the minimal number of the \( \pi \) bosons set to zero. This choice corresponds to neglecting the effects of the Pauli exclusion principle. Although this means giving up a fundamental physical requirement, this decision was inspired by the fact that the formalism of the PACM is closer to other similar models using the coherent state method. It appears instructive to study the differences and similarities between the SACM and PACM within this latter approach.

The present work is meant to be the basis for a further study in which phase transitions are investigated by interpolating between two dynamical symmetry limits. This method requires the application of large boson numbers, so as another new ingredient, the Hamiltonian was implemented with a third-order term in order to stabilize the energy spectrum in this situation. The potential energy surface was constructed in terms of a variable controlling the relative distance of the clusters. This was done both in the SACM and PACM framework. It was found that the potential obtained from the SACM can be reproduced within the PACM approach too by including higher-order terms in the Hamiltonian. This indicates that studying only the Hamiltonian, the effects of the Pauli principle can be simulated by higher-order interactions.

The present results will be used in a forthcoming publication that focuses on phase transitions between phases determined by different dynamical symmetries of the
SACM and the PACM.

**APPENDIX A: The Coherent State for the SACM**

We choose the most general structure for the coherent state, allowing arbitrary parameters, \( \alpha_m \), which only coincide with \( \alpha_m \) when the static problem is considered. This will be important in future work, when we intend to treat the cranking formalism within the PACM and SACM, similar to the formalism presented in \([43, 44]\). Nevertheless, as long as we are only interested in the potential energy surface for systems without rotation, the parameters \( \alpha_m \) will form a simple tensor.

We use the definition

\[
(\alpha \cdot \pi^\dagger) = \sum_m \alpha_m \pi_m^\dagger .
\]

The \( \alpha_m \) are in general complex and arbitrary. The complex conjugate is denoted by \( \alpha_m^* \). We also use

\[
\tilde{\alpha}_m = (-1)^{1-m} \alpha_{-m} .
\]

This will be important when we apply \( \pi^m = (-1)^{1-m} \pi_{-m} \) to the coherent state on the right.

The conjugate coherent state is given by

\[
\langle \alpha^* \rangle = \mathcal{N}_{Nn0} \langle 0 | [\sigma + (\alpha^* \cdot \pi)]^N (\alpha^* \cdot \pi)^{n_0} ,
\]

with

\[
(\alpha^* \cdot \pi) = \sum_m \alpha_m^* \pi^m .
\]

Thus, the \( \pi_m^\dagger \) acts on the left as an annihilation operator. Note that here we do not assume a tensorial behavior of the \( \alpha_m \), contrary to what we used in the body of the paper. In order to relate this \( \alpha_m \) to the one used in the paper, or to make \( \alpha_m \) to the coherent state on the right, we will have to assume \( \alpha_m^* = (-1)^m \alpha_{-m} \). This is justified for a static problem, as discussed in the paper. The situation changes, when for example the cranking formalism is applied or not only the potential is intended to derive but also the kinetic energy.

\( \mathcal{N}_{Nn0} \) is the normalization factor, given by

\[
\mathcal{N}_{Nn0}^{-2} = \frac{N!^2}{(N+n_0)!} \frac{d^n_0}{d\gamma_1^n} \frac{d^{n_0}}{d\gamma_2^n} [1 + \gamma_1 \gamma_2 (\alpha^* \cdot \alpha)]^{N+n_0} ,
\]

taken at \( \gamma_1 = \gamma_2 = 1 \), after performing the derivation.

In this sense, the mapping of different operators is completely parallel to the one given in \([17]\), with the exception of the definition in the coupling of \( \alpha_m \). The geometrical

\[
\frac{d^n_0}{d\gamma_1^n} \frac{d^{n_0}}{d\gamma_2^n} \gamma_1 \gamma_2 [1 + \gamma_1 \gamma_2 (\alpha^* \cdot \alpha)]^{N+n_0-1} .
\]

We have

\[
[\alpha^* \times \tilde{\alpha}]_m^S = \sum_{m_1 m_2} (1m_1, 1m_2|S)m \alpha_{m_1}^* \tilde{\alpha}_{m_2} ,
\]

where the coupling sign “×” instead of “⊗” was used in order to indicate that we do not couple tensors. This is just a short-hand notation.

In the geometrical mapping one has to take into account that

\[
(\alpha \cdot \pi^\dagger) = \alpha_0 \pi_0^\dagger + \alpha_1 \pi_{+1}^\dagger + \alpha_{-1} \pi_{-1}^\dagger
\]

and thus

\[
[\pi_m, (\alpha \cdot \pi^\dagger)] = (-1)^{1-m} \alpha_{-m} = \tilde{\alpha}_m
\]

and

\[
[ (\alpha^* \cdot \pi), \pi_m^\dagger ] = \alpha_m^* .
\]

Note the difference in the phase.

The formulas are now similar to those of Ref. \([17]\), but without the use of a possible tensor character of the \( \alpha_m \) and with the appearance of complex conjugate \( \alpha_m^* \) and \( \tilde{\alpha}_m \). One of the interesting matrix element is given by

\[
\mathcal{N}_{Nn0}^{-2} = \frac{N!^2}{(N+n_0)!} \frac{d^n_0}{d\gamma_1^n} \frac{d^{n_0}}{d\gamma_2^n} [1 + \gamma_1 \gamma_2 (\alpha^* \cdot \alpha)]^{N+n_0-1} .
\]
The mapping of more relevant operators is given by
\[
\langle \alpha |\pi_{m}|\alpha \rangle = (N+n_0)\alpha_{m}N_{N+n_0}^2 \frac{(N!)^2}{(N+n_0)!} \\
\times \frac{d_{n_0}}{d_{\gamma_1}^{n_0}} \frac{d_{n_0}}{d_{\gamma_2}^{n_0}} \left[ \gamma_2 \left[ 1 + \gamma_1 \gamma_2 (\alpha^{*} \cdot \alpha) \right]^{N+n_0-1} \right]
\]
Note that the mapping is more complicated than when no Pauli exclusion principle is taken into account \((n_0 = 0)\), due to the distinct property of \(\alpha_{m}\). (It is not a tensor anymore.) Also note that
\[
[\hat{\alpha} \times \hat{\alpha}]_0 = \frac{1}{\sqrt{3}} \sum_{m} (-1)^{1-m} \alpha_{m} \alpha_{-m} \\
[\alpha^{*} \times \alpha^{*}]_0 = \frac{1}{\sqrt{3}} \sum_{m} (-1)^{1-m} \alpha^{*}_{m} \alpha^{*}_{-m} . \tag{58}
\]
Thus, the sum of both is real. Because they always appear in a sum in the expectation value of the Hamiltonian with respect to the coherent state, the expectation value is always real. This is a remarkable sign of consistency.

The mapping, concerning the individual clusters, is the same as given in [17]. There, one has to take into account that the coherent state acquires the form of a direct product of the state describing the relative motion and the one giving the cluster coupling
\[
\hat{\alpha}^{2} |\alpha \rangle = |C_1 \times C_2|^C , \tag{59}
\]
where the last factor refers to the coupling of the two cluster states, which is fixed [17].

Next we have to expand the above expressions in powers of \((\alpha \cdot \alpha)\). In [17] the \(n_0\) was neglected compared to \(N\). Here, we will take into account the contributions of \(n_0\). The list of expansions is
\[
\frac{d_{n_0}}{d_{\gamma_1}^{n_0}} \frac{d_{n_0}}{d_{\gamma_2}^{n_0}} \left[ \gamma_2 \left[ 1 + \gamma_1 \gamma_2 (\alpha^{*} \cdot \alpha) \right]^{N+n_0-1} \right] \bigg|_{\gamma_1=\gamma_2=1} = \sum_{k=0}^{N+n_0-1} \left( \frac{N+n_0}{k} \right) \left( \frac{k!}{(k-n_0)!} \right)^2 \left( \alpha^{*} \cdot \alpha \right)^k
\]
\[
\frac{d_{n_0}}{d_{\gamma_1}^{n_0}} \frac{d_{n_0}}{d_{\gamma_2}^{n_0}} \left[ \gamma_1 \gamma_2 \left[ 1 + \gamma_1 \gamma_2 (\alpha^{*} \cdot \alpha) \right]^{N+n_0-1} \right] \bigg|_{\gamma_1=\gamma_2=1} = \sum_{k=0}^{N+n_0-1} \left( \frac{N+n_0-1}{k} \right) \left( \frac{(k+1)!}{(k+1-n_0)!} \right)^2 \left( \alpha^{*} \cdot \alpha \right)^k
\]
\[
\frac{d_{n_0}}{d_{\gamma_1}^{n_0}} \frac{d_{n_0}}{d_{\gamma_2}^{n_0}} \left[ \gamma_2 \left[ 1 + \gamma_1 \gamma_2 (\alpha^{*} \cdot \alpha) \right]^{N+n_0-1} \right] \bigg|_{\gamma_1=\gamma_2=1} = \sum_{k=0}^{N+n_0-1} \left( \frac{N+n_0-1}{k} \right) \left( \frac{k!}{(k-n_0)!} \right)^2 \left( \alpha^{*} \cdot \alpha \right)^k
\]\n
\[
\frac{d^{n_0}}{d\gamma_1 d^{n_2}} (\gamma_1 \gamma_2)^2 \left[ 1 + \gamma_1 \gamma_2 (\alpha^* \cdot \alpha) \right]^{N+n_0-2} |_{\gamma_1=\gamma_2=1} = \\
N^{n_0} \sum_{k=\max(n_0,0)}^{N+n_0-2} \left( \frac{(k+2)!}{(k+2-n_0)!} \right) \times (\alpha^* \cdot \alpha)^k
\]

\[
\frac{d^{n_0}}{d\gamma_1 d^{n_2}} (\gamma_2)^2 \left[ 1 + \gamma_1 \gamma_2 (\alpha^* \cdot \alpha) \right]^{N+n_0-2} |_{\gamma_1=\gamma_2=1} = \\
N^{n_0} \sum_{k=\max(n_0,0)}^{N+n_0-2} \left( \frac{(k+2)!}{(k+2-n_0)!} \right) \times (\alpha^* \cdot \alpha)^k
\]

which leads then to Eq. (60).

For example, the leading term in the first expression is \( \frac{N^{n_0}}{N!} (\alpha^* \cdot \alpha)^{n_0} \) which leads in lowest order in \( (\alpha^* \cdot \alpha) \) to the normalization, as defined in Eq. (8) of Ref. [17]. We will, however assume that \( N \gg n_0 \gg 1 \), otherwise the resulting expressions are too involved.

The equations in (60) can be simplified, using the abbreviation

\[
F_{pq}(\alpha^2) = \frac{N!^2}{(N+n_0)!} \\
\times \sum_{k=\max(n_0,0)}^{N+n_0-\max(p,q)} \left( \frac{N+n_0-\max(p,q)}{k} \right) \\
\times \left[ \frac{(k+p)!}{(k+p-n_0)!} \right] \left[ \frac{(k+q)!}{(k+q-n_0)!} \right] \alpha^{2k}
\]

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