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

Clustering in nuclei has been known since the early days of modern nuclear physics. Its importance manifests itself not only in well-known clustering phenomena like the α-cluster sructure of light nuclei, but also in nuclear molecular states in heavy-ion reactions and the decay of heavy nuclei via the emission of both α particles and heavier clusters [1,2]. More recently, the importance of the cluster structure of nuclei has also been revealed in reactions playing a key role in nuclear astrophysics. In describing this special excitation of the nucleus, cluster models [3] have to take into account the fact that the nucleus is a strongly interacting many-body system consisting of protons and neutrons, i.e. fermions, therefore the Pauli exclusion principle has to be observed by the application of fully antisymmetrized wave functions. Microscopic cluster models take this requirement strictly into account in constructing both the model space and the interactions [4]. Fully microscopic treatment can become prohibitively complicated beyond light nuclei, so cluster models making use of various approximations have also been constructed. In phenomenological cluster models [5] the antisymmetrization requirement is not observed strictly, and the interactions are also approximated by intercluster forces. Semimicroscopic models also apply phenomenologic interactions but combine them with a microscopic model space.

In order to exploit various symmetries of nuclei and nuclear cluster systems, algebraic models have been developed. The first model of this kind was the vibron model [6], which was originally developed for molecular physical applications [7–9], but it was also applied to nuclear molecular states of the $^{12}C + {}^{12}C$ system [10]. It was also developed further to describe internal excitations of the clusters [11,12]. The vibron model and its extensions belong to the family of phenomenological cluster models for reasons described previously.

In another algebraic model, called the *semimicroscopic algebraic cluster model* (SACM) [13,14], the Pauli exclusion principle is taken into account in an elegant manner, such that explicit antisymmetrization is not necessary, which simplifies the calculation considerably. The semimicroscopic nature of the model is represented by combining the microscopic model space with phenomenologic interactions, as will be discussed in Sec. II.

Recently, there has been much interest in the analysis of various phases of nuclear systems and phase transitions between them. The first such studies date back to the 1970s [15]. The principal method here is the use of coherent states [16], which are especially suited to algebraic models. The expectation value of the algebraic Hamiltonian with respect to a coherent state is defined as the semiclassical 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 interacting boson approximation (IBA) [17], was presented in Ref. [16] and more recent reviews can be found in Refs. [18–21]. 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 Ref. [22].

In Ref. [18] a complete classification of phase transitions in algebraic models is presented, restricted to Hamiltonians with up to two-body interactions. For the vibron model [23,24] the transitions turned out to be of second order. In Ref. [25], a second-order phase transition was also encountered. In Ref. [26] 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 steplike behavior. In other words, no discontinuities of the derivatives of the potential were considered.

Coherent states have been applied not only to the IBA or atomic molecules [7,9,18,23,24] but also to other algebraic models, which have a microscopic origin within the shell model. In Ref. [27] the geometrical mapping, using the vector coherent state method [28], was applied mapping the

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pseudosymplectic model [29] to the geometric model of the nucleus [30]. The geometrical mapping turned out to be very useful in calculations of nuclear spectra [31,32] and predicting the spectra of superheavy nuclei [33]. Phase transitions in single nuclear systems were also investigated in Refs. [34,35], 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 Ref. [30]. 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. A more general discussion on quantum phase transitions can be found in Ref. [36].

Recent results concerning the phase transitions in atomic and nuclear molecules [25,37–39] inspired us to extend these studies to the SACM [13,14], too. The coherent state formalism and the geometric mapping already have been developed for this model [40], offering a suitable starting point for the present study. Similarly to other algebraic models, phase changes can be investigated here, too, between limits defined by dynamical symmetries, notably the SU(3) and SO(4) limits describing various types of nuclear two-cluster systems. Two groups of models will be discussed: the *phenomenological algebraic cluster model* (PACM) and the SACM. The *vibron model* belongs to the group PACM [6,11]. 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, required by the antisymmetrization.

Some of the important questions we would like to discuss in this and a forthcoming publication are as follows: 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 [18,25]. 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 some important differences arise. One main result will be that in order for the PACM to reproduce 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 using the comparison; 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 [11,12]. Additionally, the parameter by which the number operator of π bosons is multiplied is fixed in the SACM because it describes the mean field. Within the PACM this parameter can be chosen arbitrarily.

The paper is structured as follows: In Sec. II the SACM is revisited, introducing some novel features, including the definition of the PACM as a special limit of the SACM not observing the Pauli principle. In Sec. III the coherent state formalism will be implemented to 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 Sec. IV the geometrically mapped potentials are derived for the two models, and, finally, in Sec. 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

Previous applications of the SACM concerned describing the spectroscopic properties of core + α-type [41] and other [42] two-cluster systems. In this section we present a brief overview of the SACM [13,14] and introduce further amendments of it necessary for our study. These new elements appear in all three subsections.

A. The model space

We start with reviewing the vibron model [6], 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 1:

$$\boldsymbol{\pi}_m^\dagger, \boldsymbol{\pi}_m, \quad m = 0, \pm 1. \tag{1}$$

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

$$\boldsymbol{\pi}^m = (-1)^{1-m}\boldsymbol{\pi}_{-m}. \tag{2}$$

The 16 boson number-conserving operators

$$\boldsymbol{\pi}_m^\dagger \boldsymbol{\pi}^{m'}, \quad \boldsymbol{\pi}_m^\dagger \boldsymbol{\sigma}, \quad \boldsymbol{\sigma}^\dagger \boldsymbol{\pi}^m, \quad \boldsymbol{\sigma}^\dagger \boldsymbol{\sigma} \tag{3}$$

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

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

where

$$\begin{aligned} n_\pi &= N, N-1, \ldots, 1, 0, \\ L_R &= n_\pi, n_\pi - 2, \ldots, 1 \quad \text{or} \quad 0, \\ M_R &= L_R, L_R - 1, \ldots, -L_R, \end{aligned} \tag{5}$$

and

$$\begin{array}{ccccccc} \mathrm{U}_R(4) & \supset & \mathrm{SO}_R(4) & \supset & \mathrm{SO}_R(3) & \supset & \mathrm{SO}_R(2) \\ [N,0,0,0] & & (\omega,0) & & L_R & & M_R, \end{array} \tag{6}$$

where

$$\begin{aligned} \omega &= N, N-2, \ldots, 1 \quad \text{or} \quad 0, \\ L_R &= \omega, \omega-1, \ldots, 1, 0, \\ M_R &= L_R, L_R-1, \ldots, -L_R. \end{aligned} \tag{7}$$

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 [43]. The internal structure of the clusters is then described by the $\mathrm{SU}_{C_k}(3)$ group, where C_k refers to the kth 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

$$\begin{array}{l} \mathrm{SU}_{C_1}(3) \otimes \mathrm{SU}_{C_2}(3) \otimes \mathrm{SU}_R(3) \supset \mathrm{SU}_C(3) \otimes \mathrm{SU}_R(3) \ \supset \\ (\lambda_1, \mu_1) \quad (\lambda_2, \mu_2) \quad (n_\pi, 0) \qquad (\lambda_C, \mu_C) \\ \qquad\qquad \mathrm{SU}(3) \supset \mathrm{SO}(3) \supset \mathrm{SO}(2) \\ \qquad\qquad (\lambda, \mu) \quad \kappa L \quad M, \end{array} \tag{8}$$

where (λ_k, μ_k) refers to the $\mathrm{SU}_{C_k}(3)$ irreducible representations (irreps) of the individual clusters, which are then coupled to intermediate irrep (λ_C, μ_C). These irreps are the ones associated with the ground-state configuration of the kth cluster. 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 occurrences of a given L in (λ, μ).

The model space of the SACM is obtained by determining the direct product

$$(\lambda_1, \mu_1) \otimes (\lambda_2, \mu_2) \otimes (n_\pi, 0) = \sum_{\lambda\mu} m_{\lambda\mu}(\lambda, \mu), \tag{9}$$

where the result is a sum of the irreps of SU(3) with multiplicity $m_{\lambda\mu}$. The sum still contains irreps which are not allowed by the Pauli-exclusion principle. In order to determine which irreps are allowed, one has to match the result with the fully antisymmetrized shell-model space. *The overlap constitutes the model space* of the SACM. 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. [13,14]). 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 [3] in a natural way. This condition prescribes a minimal number of oscillator quanta (i.e., n_π) in the relative motion. For example, consider the cluster system $^{16}\mathrm{O} + \alpha \rightarrow {}^{20}\mathrm{Ne}$. Within the shell model, the number of oscillation quanta in ^{16}O is 12, while for the α particle it is zero. The number of oscillation quanta for ^{20}Ne is 20. Thus, in order to satisfy the Pauli exclusion principle one has to add the difference, i.e., eight oscillation quanta corresponding to lifting the four nucleons of the α particle to the sd shell. States with less oscillation quanta automatically do not fulfill the condition of antisymmetry and are by construction excluded in the above-mentioned procedure. For closed-shell clusters, the Wildermuth condition is sufficient to assure antisymmetrization. However, for open clusters this condition is not sufficient and one has to apply additionally the comparison with the shell-model space.

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 (8) 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_π 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_π 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 SACM. Strictly speaking, this is not a dynamical symmetry according to the standard definition. Our definition [44] is that the following chain corresponds to a Hamiltonian which does not contain any SU(3) coupling but only interactions on the level of the SO(3) groups. In other words, apart from $\hbar\omega \boldsymbol{n}_\pi$ only the interaction terms $\boldsymbol{L}_C^2$, $\boldsymbol{L}_R^2$, and $\boldsymbol{L}^2$ appear. The group structure associated with this SO(3) dynamical symmetry is

$$\begin{array}{llllllll} \mathrm{SU}_C(3) & \otimes & \mathrm{U}_R(4) & \supset & \mathrm{SO}_C(3) & \otimes \mathrm{SO}_R(3) \supset & \mathrm{SO}(3) \supset & \mathrm{SO}(2) \\ (\lambda_C.\mu_C) & & [N,0,0,0] & & L_C & L_R & L & M. \end{array} \tag{10}$$

The difference between the previously mostly ignored chain [Eq. (10)] and the one appearing in Eq. (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, e.g., quadrupole-quadrupole terms. 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 Eqs. (8) and (10) chains as weak and strong coupling limits, respectively. The two limits are the same when the two clusters are both closed-shell nuclei (then $L_C = 0$ and $L_R = L$), but when at least one of them is not [i.e., its internal (λ_k, μ_k) irrep differs 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 (λ, μ) and κ quantum numbers

[see Eq. (8)], where κ is obsolete when either λ or μ is zero, as is also the case in the SU(3) limit of the vibron model [see Eq. (4)]. 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_π 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 $(\omega, 0)$ irrep of SO(4) [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 using control parameters. We consider two cases: (i) both clusters spherical and (ii) one spherical cluster plus a deformed one. Examples for these two scenarios are the $^{16}\mathrm{O} + \alpha \rightarrow {}^{20}\mathrm{Ne}$ and $^{20}\mathrm{Ne} + \alpha \rightarrow {}^{24}\mathrm{Mg}$ systems, examined in second paper of this series.

The Hamiltonian is given by

$$\boldsymbol{H} = xy\boldsymbol{H}_{\mathrm{SU}(3)} + y(1-x)\boldsymbol{H}_{\mathrm{SO}(4)} + (1-y)\boldsymbol{H}_{\mathrm{SO}(3)} \quad (11)$$

with

$$\begin{aligned}
\boldsymbol{H}_{\mathrm{SU}(3)} &= \hbar\omega\boldsymbol{n}_\pi + a_{\mathrm{Clus}}C_2(\lambda_C, \mu_C) + (a - b\Delta\boldsymbol{n}_\pi)C_2(\lambda, \mu) \\
&\quad + (\bar{a} - \bar{b}\Delta\boldsymbol{n}_\pi)C_2(\boldsymbol{n}_\pi, 0) + \gamma\boldsymbol{L}^2 + t\boldsymbol{K}^2 \\
\boldsymbol{H}_{\mathrm{SO}(4)} &= a_C\boldsymbol{L_C}^2 + a_R^{(1)}\boldsymbol{L_R}^2 + \gamma\boldsymbol{L}^2 + \frac{c}{4}[(\boldsymbol{\pi}^\dagger \cdot \boldsymbol{\pi}^\dagger) - (\sigma^\dagger)^2] \\
&\quad \times [(\boldsymbol{\pi} \cdot \boldsymbol{\pi}) - (\sigma)^2] \qquad (12) \\
\boldsymbol{H}_{\mathrm{SO}(3)} &= \hbar\omega\boldsymbol{n}_\pi + a_{\mathrm{Clus}}C_2(\lambda_C, \mu_C) + a_C\boldsymbol{L_C}^2 \\
&\quad + a_R^{(1)}\boldsymbol{L}_R^2 + \gamma\boldsymbol{L}^2,
\end{aligned}$$

with $\Delta\boldsymbol{n}_\pi = \boldsymbol{n}_\pi - n_0$, n_0 being the minimal number of quanta. The a_{Clus} 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* parts, respectively. Further interaction terms are the total angular-momentum operator, $\boldsymbol{L}^2$, and the $\boldsymbol{K}^2$ operator, defined in Refs. [13,14] 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 $\boldsymbol{n}_\pi(\boldsymbol{n}_\pi + 3)$. 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 Eq. (12) 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 $\boldsymbol{L}^2$ operator can be written as $(\boldsymbol{L_C} + \boldsymbol{L}_R)^2 = [\boldsymbol{L}_C^2 + \boldsymbol{L}_R^2 + 2(\boldsymbol{L}_C \cdot \boldsymbol{L}_R)]$. The first and second terms 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 $\boldsymbol{L}_C = (\boldsymbol{L}_{C_1} + \boldsymbol{L}_{C_2})$.

The division according to dynamical symmetries in Eq. (12) 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 $\mathrm{SU}_C(3)$ and SU(3) have to appear. The SO(3) limit couples only at the SO(3) level, i.e., only the angular-momentum operators appear [no second- and higher-order SU(3) Casimir operators, except $\boldsymbol{n}_\pi$]. These were introduced in the previous subsection as the *strong*- and *weak*-coupling limits, respectively. This is a deviation from the literature, where these two limits are both referred to as the SU(3) limit. 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 $(\boldsymbol{L}_k^2, k = 1, 2)$. We exclude this interaction for the moment.

The new higher-order interaction appearing in the third term of $\boldsymbol{H}_{\mathrm{SU}(3)}$ needs some explanation. The whole term is related to the quadrupole-quadrupole interaction, *which is present in any nuclear system*. However, without the $-b\Delta\boldsymbol{n}_\pi$ (with $-b > 0$) correction, states which contain a sufficiently large n_π will be lower in energy than states with the minimal number of $\boldsymbol{\pi}$ bosons, n_0. This is due to the dependence on $\boldsymbol{n}_\pi^2$ in the second-order Casimir operator, which will finally dominate over the $\hbar\omega\boldsymbol{n}_\pi$ term for a sufficiently large number of $\boldsymbol{\pi}$ bosons. In the standard treatment, when n_π is conserved, a simple restriction to small Δn_π suffices to circumvent the problem, i.e., states with large Δn_π are simply not taken into account in the model space.

This effect was studied in Ref. [45] within the context of the symplectic model of the nucleus [29,46,47]. In addition, the quadrupole-quadrupole interaction dominates over the kinetic energy and, finally, will promote high-n_π 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 [45], 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 Ref. [14], where correction terms of the type Δn_π, mentioned here, were included. Without these corrections the problem increases significantly when interactions mixing states with different n_π are considered. Then, avoiding states with large n_π is not an option, as is in the case of conserved n_π, when the model space can be limited in n_π using physical arguments.

C. PACM: The phenomenological limit of the SACM

The minimal number of π 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 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 oscillation quanta is either 0 or n_0. It is not allowed to choose a number in between, because each of such a number violates the Pauli exclusion principle. When both clusters are closed-shell nuclei, the PACM essentially recovers the vibron model [6].

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 coherent 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 π 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 that arises 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 [9,15,16,18,21,23,24,27,40]. 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 (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* [48], skipping the term of the zero-point motion. As shown in Ref. [48], 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 [23,24]. 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 Ref. [40]

$$\begin{aligned}|\alpha\rangle &= \mathcal{N}_{N,n_0}(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)^{n_0}[\sigma^\dagger + (\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^N|0\rangle \\ &= \mathcal{N}_{N,n_0}\frac{N!}{(N+n_0)!}\frac{d^{n_0}}{d\gamma_1^{n_0}}[\sigma^\dagger + \gamma_1(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^{N+n_0}|0\rangle, \quad (13)\end{aligned}$$

where, for convenience, we redefined the total number of relative oscillation quanta as $(N + n_0)$, while the γ_1 parameter has to be set equal to 1 after the differentiation. The normalization factor is given by Eq. (A5) in the Appendix. The PACM coherent state is obtained from Eqs. (13) and (A5) by setting $n_0 = 0$.

The $\boldsymbol{\alpha}$ is a short-hand notation for the, in general, complex variables α_m ($m = 1, 0, -1$). The coherent state with complex $\boldsymbol{\alpha}$ coefficients is the most general linear combination of the boson creation operators. For static problems the requirement [23,24]

$$\alpha_m^* = (-1)^{1-m}\alpha_{-m} \quad (14)$$

reduces the number of real parameters to three, namely to α_0, and the real plus the imaginary part of α_{+1}.

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

$$(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}) = \sum_m (-1)^{1-m}\alpha_m\alpha_{-m} = \alpha^2, \quad (15)$$

where α represents a measure of the intercluster distance [40] and α^2 a short-hand notation for $(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})$. Because the only relevant variable is the intercluster distance, we can express the potential in terms of this sole variable α.

The importance of the coherent states resides in the fact that they provide us with the possibility to define a *potential energy surface*

$$V(\boldsymbol{\alpha}) = \langle\boldsymbol{\alpha}|\boldsymbol{H}|\boldsymbol{\alpha}\rangle, \quad (16)$$

in terms of the collective variables α_m.

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

Applying the coherent state for the SACM to the Hamiltonian (11), one obtains the geometrically mapped potential

$$\begin{aligned}\langle\boldsymbol{H}\rangle = \mathcal{C}(x,y) - (b+\bar{b})xy\Bigg[&A(x,y)\alpha^2\frac{F_{11}(\alpha^2)}{F_{00}(\alpha^2)} \\ &- B(x,y)\alpha^4\frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)} + \alpha^6\frac{F_{33}(\alpha^2)}{F_{00}(\alpha^2)} \\ &- C(x,y)\alpha^2\frac{F_{20}^{N-2}(\alpha^2)}{F_{00}(\alpha^2)}\Bigg], \quad (17)\end{aligned}$$

where

$$\begin{aligned}\mathcal{C}(x,y) = &\langle(a_{\mathrm{Clus}} + a + bn_0)C_2(\lambda_C,\mu_C) + \gamma\boldsymbol{L_C}^2 \\ &+ (1-xy)a_C\boldsymbol{L_C}^2\rangle + xyt\langle\boldsymbol{K}^2\rangle \\ &+ \frac{c}{4}(N+n_0)(N+n_0-1)y(1-x) \quad (18)\end{aligned}$$

and the $F_{ij}(\alpha^2)$ functions are defined by Eq. (A15) in the Appendix. Further, the coefficients appearing in Eq. (17) are

defined as

$$
\begin{aligned}
A(x,y) = &-\frac{1}{(b+\bar{b})xy}\Big\{\hbar\omega[yx+1-y] \\
&+2\big[\gamma+(1-yx)a_R^{(1)}\big]+xy[a-b][4+\Gamma_1+\Gamma_2] \\
&+4xy[\bar{a}-\bar{b}]+xybn_0[4+\Gamma_1+\Gamma_2]+4xyn_0\bar{b} \\
&-bxyC_2(\lambda_C,\mu_C)-\frac{c}{2}y(1-x)(N+n_0-1)\Big\} \\
B(x,y) = &\frac{1}{(b+\bar{b})xy}\Big\{xy[a+\bar{a}-6b-6\bar{b} \\
&-b\{\Gamma_1+\Gamma_2\}+n_0(b+\bar{b})]+\frac{c}{2}y(1-x)\Big\} \\
C(x,y) = &-\frac{\frac{c}{2}y(1-x)}{(b+\bar{b})xy},
\end{aligned}
\tag{19}
$$

where Γ_k, according to Ref. [40], is given by

$$
\begin{aligned}
\Gamma_k &= \langle(\lambda_k,\mu_k)|\,\boldsymbol{Q}_m^{\text{Cluster(k)}}|(\lambda_k,\mu_k)\rangle \\
&= \sqrt{\frac{5}{\pi}}\left[n_k+\frac{3}{2}(A_k-1)\right]\alpha_{2m}(k) \\
&= \sqrt{\frac{5}{\pi}}N_{0,k}\beta_k.
\end{aligned}
\tag{20}
$$

(This was obtained by a geometric mapping of the symplectic model [27,31,32].) The (λ_k,μ_k) denotes the SU(3) irrep of the deformed cluster number k. In the case that it is spherical, $\Gamma_k=0$. The N_{0k} 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 kth 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 Eq. (20) we used only the $m=0$ component of $\alpha_{2m}(k)$ and defined it β_k, the deformation of cluster k. This implies that the deformed cluster is assumed to be axially symmetric and it is in line with the intercluster 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 θ, the deformation value β_k is multiplied by a matrix element of the rotation matrix, which only changes the numerical value of β_k, i.e., $\beta_k'=d_{00}^2(\theta)\beta_k$. 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 model. This structure will be used in the second paper investigating the possible phase transitions and the phase diagram.

For $x=0$ in Eq. (11), 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 Eq. (19). In this case the potential maps to

$$
\begin{aligned}
V &= \langle\boldsymbol{H}\rangle \\
&\to \left[\overline{A}\alpha^2\frac{F_{11}(\alpha^2)}{F_{00}(\alpha^2)}-\overline{B}\alpha^4\frac{F_{22}(\alpha^2)}{F_{00}(\alpha^2)}-\overline{C}\alpha^4\frac{F_{20}^{N-2}(\alpha^2)}{F_{00}(\alpha^2)}\right]+\mathcal{C}
\end{aligned}
\tag{21}
$$

with

$$
\overline{A} = \left\{\hbar\omega[1-y]+2\big[\gamma+a_R^{(1)}\big]-\frac{c}{2}y(N+n_0-1)\right\} \tag{22}
$$

$$
\overline{B} = -\left(\frac{c}{2}y\right) \tag{23}
$$

$$
\overline{C} = \frac{c}{2}y = -\overline{B}. \tag{24}
$$

In this case only two independent parameters $\overline{A}$ and $\overline{B}$ 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 Eq. (17) 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.

A very useful consideration is the investigation of the potential in the $\alpha\to\infty$ and $\alpha\to 0$ 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 α the coherent state contains only π bosons and cannot increase the energy any further. The second limit ($\alpha\to 0$) is necessary to adjust $V(\alpha=0)=0$.

(i) Limit $\alpha\to\infty$:

The relevant formulas are

$$
\begin{aligned}
\alpha^2\frac{F_{11}}{F_{00}} &\to (N+n_0) \\
\alpha^4\frac{F_{22}}{F_{00}} &\to (N+n_0)(N+n_0-1) \\
\alpha^6\frac{F_{33}}{F_{00}} &\to (N+n_0)(N+n_0-1)(N+n_0-2) \\
\alpha^2\frac{F_{20}^{N-2}}{F_{00}} &\to N(N-1)\frac{1}{\alpha^2}\to 0.
\end{aligned}
\tag{25}
$$

With this, the limit of the complete geometric potential (18) is given by

$$
\begin{aligned}
V \to \mathcal{C} &- bxy\{A(N+n_0)-B(N+n_0)(N+n_0-1) \\
&+(N+n_0)(N+n_0-1)(N+n_0-2)\}.
\end{aligned}
\tag{26}
$$

Depending on the signs and values of A and B, this limit is either positive or negative. For the positive value the limit for $(N+n_0)\to\infty$ 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 $\alpha\to 0$:

The relevant formulas are

$$
\begin{aligned}
\alpha^2\frac{F_{11}}{F_{00}} &\to n_0 \\
\alpha^4\frac{F_{22}}{F_{00}} &\to n_0(n_0-1) \\
\alpha^6\frac{F_{33}}{F_{00}} &\to n_0(n_0-1)(n_0-2) \\
\alpha^2\frac{F_{20}^{N-2}}{F_{00}} &\to N(N-1)(n_0+1)(n_0+2)\frac{\alpha^2}{2}\to 0.
\end{aligned}
\tag{27}
$$

With this, the limit of the complete geometric potential (18) is given by

$$V(\alpha = 0) \to \mathcal{C} - bxy\{An_0 - Bn_0(n_0 - 1) + n_0(n_0 - 1)(n_0 - 2)\}, \quad (28)$$

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

B. The PACM

In this subsection it is more convenient to use the parameter

$$\beta^2 = \frac{\alpha^2}{1 + \alpha^2}. \quad (29)$$

While the range of α is from zero to ∞, the range of β is from zero to 1.

Using the Hamiltonian as introduced in Sec. II and the coherent state of Sec. III, 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

$$\begin{aligned}\langle \boldsymbol{H} \rangle &= V(\beta) \\ &= (a_{\rm Clus} + a)\mathcal{C}_2(\lambda_C, \mu_C) + \frac{c}{4}N(N-1)y(1-x) \\ &\quad + N\beta^2\big\{[\hbar\omega(xy + 1 - y) + (a - b)(4 + \Gamma_1 + \Gamma_2) \\ &\quad + 4(\bar{a} - \bar{b}) - b\,\mathcal{C}_2(\lambda_C, \mu_C)] - (1 - x)yc(N - 1) \\ &\quad + 2\big[\gamma + (1 - xy)a_R^{(1)}\big]\big\} + N(N-1) \\ &\quad \times \beta^4\{xy[a + \bar{a} - 6b - 6\bar{b} - b(\Gamma_1 + \Gamma_2)] \\ &\quad + (1 - x)yc\} - N(N-1)(N-2)\beta^6 xy(b + \bar{b}) \\ &\quad + \mathcal{C}_2(\lambda_C, \mu_C)axy + \frac{1}{4}(1 - x)ycN(N-1). \end{aligned} \quad (30)$$

Defining

$$\begin{aligned} A &= -[(b + \bar{b})xy(N-1)(N-2)]^{-1} \\ &\quad \times \big\{\hbar\omega(yx + 1 - y) + 2\big[\gamma + (1 - yx)a_R^{(1)}\big]. \\ &\quad + 4xy(\bar{a} - \bar{b}) + xy(a - b)(4 + \Gamma_1 + \Gamma_2) \\ &\quad - bxyC_2(\lambda_C, \mu_C) - y(1 - x)c(N - 1)\big\} \\ B &= \frac{xy[a + \bar{a} - 6(b + \bar{b}) - b(\Gamma_1 + \Gamma_2)] + cy(1 - x)}{(N - 2)(b + \bar{b})xy} \\ \mathcal{C} &= \langle (a_{\rm Clus} + a)C_2(\lambda_C, \mu_C) + \gamma \boldsymbol{L_C}^2 + (1 - xy)\boldsymbol{L_C}^2 \rangle \\ &\quad + xyt\langle \boldsymbol{K}^2 \rangle + \frac{c}{4}N(N-1)y(1-x), \end{aligned} \quad (31)$$

the potential acquires the form [49,50]

$$V = N(N-1)(N-2)[-(b + \bar{b})xy]\{A\beta^2 - B\beta^4 + \beta^6\} + \mathcal{C}. \quad (32)$$

This allows us to define a new, normalized potential,

$$\widetilde{V} = \{A\beta^2 - B\beta^4 + \beta^6\}. \quad (33)$$

In the definition of $\widetilde{V}$ we extracted the factor $(b + \bar{b})xy$, such that there appears no factor in front of the β^6 term. However, for the SO(4) to SO(3) transition, the x value is always zero. For this case we include the x value within the parenthesis, yielding a vanishing factor of the six-order 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 differs rather markedly from its PACM counterpart; however, a similar potential can also be generated within the latter framework. This can be achieved by including higher-order interactions of the type $F_1(\boldsymbol{n}_\pi)/F_2(\boldsymbol{n}_\pi)$, with appropriate functions $F_k(\boldsymbol{n}_\pi)$. 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 higher-order 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 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 Ref. [44] 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 interactions 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_π quantum number.

The PACM was introduced as a special limit of the SACM with the minimal number of the π 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 as well 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.

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APPENDIX : THE COHERENT STATE FOR THE SACM

We choose the most general structure for the coherent state, allowing arbitrary parameters, a_m, which only coincide with α_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 Refs. [51,52]. Nevertheless, as long as we are only interested in the potential energy surface for systems without rotation, the parameters α_m will form a simple tensor.

We use the definition

$$(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)=\sum_m \alpha_m \boldsymbol{\pi}^\dagger_m. \tag{A1}$$

The α_m are in general complex and arbitrary. The complex conjugate is denoted by α^*_m. We also use

$$\tilde{\alpha}_m=(-1)^{1-m}\alpha_{-m}. \tag{A2}$$

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

The conjugate coherent state is given by

$$\langle\boldsymbol{\alpha}|=\mathcal{N}_{Nn_0}\langle 0|[\boldsymbol{\sigma}+(\boldsymbol{\alpha}^*\cdot\boldsymbol{\pi})]^N(\boldsymbol{\alpha}^*\cdot\boldsymbol{\pi})^{n_0}, \tag{A3}$$

with

$$(\boldsymbol{\alpha}^*\cdot\boldsymbol{\pi})=\sum_m \alpha^*_m\boldsymbol{\pi}^m. \tag{A4}$$

Thus, the $\boldsymbol{\pi}^\dagger_m$ acts on the left as an annihilation operator. Note that here we do not assume a tensorial behavior of the α_m, contrary to what we used in the body of the paper. In order to relate this α_m to the one used in the paper, we 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.

$\mathcal{N}_{Nn_0}$ is the normalization factor, given by

$$\mathcal{N}^{-2}_{Nn_0}=\frac{N!^2}{(N+n_0)!}\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0}, \tag{A5}$$

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

Acting with $\boldsymbol{\pi}^\dagger_m$ to the left, commutators of the type $[\boldsymbol{\pi}^{m_1},\boldsymbol{\pi}^\dagger_{m_2}]$ appear and will give expressions proportional to α^*_m. However, acting with $\boldsymbol{\pi}_m$, as it appears in a coupled expression, to the right, it will give expressions proportional to $\tilde{\alpha}_m=(-1)^{1-m}\alpha_{-m}$, because we, first, have to lift the index of the annihilation operator, obtaining $(-1)^{1-m}\boldsymbol{\pi}^{-m}$. Note that

$$(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})=\sum_m \alpha^*_m\alpha_m=\sum_m|\alpha_m|^2 \tag{A6}$$

is a real number.

The formulas are now similar to those of Ref. [40], but without the use of a possible tensor character of the α_m and with the appearance of complex conjugate α^*_m and $\tilde{\alpha}_m$. One of the interesting matrix element is given by Ref. [40]

$$\left\langle[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}]^{[S]}_m\right\rangle=(N+n_0)[\boldsymbol{\alpha}^*\times\tilde{\boldsymbol{\alpha}}]^{[S]}_m\mathcal{N}^2_{Nn_0}\frac{N!^2}{(N+n_0)!}\times\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\gamma_1\gamma_2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0-1}.$$

We have

$$[\boldsymbol{\alpha}^*\times\tilde{\boldsymbol{\alpha}}]^{[S]}_m=\sum_{m_1m_2}(1m_1,1m_2|S\mu)\alpha^*_{m_1}\tilde{\alpha}_{m_2}, \tag{A7}$$

where the coupling sign "$\times$" instead of "$\otimes$" was used in order to indicate that we do not couple tensors. This is just a shorthand notation.

In the geometrical mapping one has to take into account that

$$(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)=\alpha_0\boldsymbol{\pi}^\dagger_0+\alpha_1\boldsymbol{\pi}^\dagger_{+1}+\alpha_{-1}\boldsymbol{\pi}^\dagger_{-1} \tag{A8}$$

and, thus,

$$\begin{aligned}&[\boldsymbol{\pi}_m,(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]=(-1)^{1-m}\alpha_{-m}=\tilde{\alpha}_m,\\&[(\boldsymbol{\alpha}^*\cdot\boldsymbol{\pi}),\boldsymbol{\pi}^\dagger_m]=\alpha^*_m.\end{aligned} \tag{A9}$$

Note the difference in the phase.

In this sense, the mapping of different operators is completely parallel to the one given in Ref. [40], with the exception of the definition in the coupling of α_m. The geometrical mapping of more relevant operators is given by

$$\begin{aligned}&\langle\boldsymbol{\alpha}|\boldsymbol{\sigma}^\dagger\boldsymbol{\pi}_m|\boldsymbol{\alpha}\rangle\\&\quad=(-1)^{1-m}(N+n_0)\tilde{\alpha}_m\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!}\\&\qquad\times\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}[\gamma_2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0-1}]\\&\langle\boldsymbol{\alpha}|\boldsymbol{\pi}^\dagger_m\boldsymbol{\sigma}|\boldsymbol{\alpha}\rangle\\&\quad=(-1)^{1-m}(N+n_0)\alpha^*_m\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!}\\&\qquad\times\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}[\gamma_2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0-1}]\end{aligned}$$

$$
\begin{aligned}
&\langle\boldsymbol{\alpha}|\boldsymbol{\sigma}^\dagger\boldsymbol{\sigma}|\boldsymbol{\alpha}\rangle \\
&\quad = N^2\frac{\mathcal{N}^2_{Nn_0}}{\mathcal{N}^2_{(N-1)n_0}} \\
&\langle\boldsymbol{\alpha}|[[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{[S_1]}\otimes[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{[S_2]}]^{[S_3]}_m|\boldsymbol{\alpha}\rangle \\
&\quad = (N+n_0)(N+n_0-1)\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!} \\
&\qquad\times[[\boldsymbol{\alpha}^*\times\boldsymbol{\alpha}^*]^{[S_1]}\times[\tilde{\boldsymbol{\alpha}}\times\tilde{\boldsymbol{\alpha}}]^{[S_2]}]^{[S_3]}_m \\
&\qquad\times\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}(\gamma_1\gamma_2)^2[1+\gamma_1\gamma_2(\alpha^*\cdot\alpha)]^{N+n_0-2} \\
&\langle\boldsymbol{\alpha}|[\boldsymbol{\pi}^\dagger\otimes\boldsymbol{\pi}^\dagger]^{[S]}_\mu(\boldsymbol{\sigma})^2|\boldsymbol{\alpha}\rangle \\
&\quad = (N+n_0)(N+n_0-1)\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!}[\boldsymbol{\alpha}^*\times\boldsymbol{\alpha}^*]^{[S]}_\mu \\
&\qquad\times\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\left\{\gamma_2^2[1+\gamma_1\gamma_2(\alpha^*\cdot\alpha)]^{N+n_0-2}\right\} \\
&\langle\boldsymbol{\alpha}|(\boldsymbol{\sigma}^\dagger)^2[\boldsymbol{\pi}\otimes\boldsymbol{\pi}]^{[S]}_\mu|\boldsymbol{\alpha}\rangle \\
&\quad = (N+n_0)(N+n_0-1)\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!}[\tilde{\boldsymbol{\alpha}}\times\tilde{\boldsymbol{\alpha}}]^{[S]}_\mu \\
&\qquad\times\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\left\{\gamma_1^2[1+\gamma_1\gamma_2(\alpha^*\cdot\alpha)]^{N+n_0-2}\right\} \\
&\langle\boldsymbol{\alpha}|(\boldsymbol{\sigma}^\dagger)^2(\boldsymbol{\sigma})^2|\boldsymbol{\alpha}\rangle \\
&\quad = N(N-1)\frac{\mathcal{N}^2_{Nn_0}}{\mathcal{N}^2_{(N-2)n_0}}.
\end{aligned}
\tag{A10}
$$

These equations also give us the mapping of $\boldsymbol{n}_\pi$ and $\boldsymbol{n}^2_\pi$ as special cases. For completeness we also give the mapping of $\boldsymbol{n}^3_\pi$, which is

$$
\begin{aligned}
&\langle\boldsymbol{\alpha}|\boldsymbol{n}^2_\pi+2\sum_{i,j}\boldsymbol{\pi}^\dagger_i\boldsymbol{\pi}^\dagger_j\boldsymbol{\pi}^i\boldsymbol{\pi}^j+\sum_{i,j,k}\boldsymbol{\pi}^\dagger_i\boldsymbol{\pi}^\dagger_j\boldsymbol{\pi}^\dagger_k\boldsymbol{\pi}^i\boldsymbol{\pi}^j\boldsymbol{\pi}^k|\boldsymbol{\alpha}\rangle \\
&\quad=\langle\boldsymbol{\alpha}|3\{[\,\boldsymbol{\pi}^\dagger\otimes\,\boldsymbol{\pi}^\dagger]^0_0[\,\boldsymbol{\pi}\otimes\,\boldsymbol{\pi}]^0_0 \\
&\qquad+\sqrt{5}[[\,\boldsymbol{\pi}^\dagger\otimes\,\boldsymbol{\pi}^\dagger]^2\otimes[\,\boldsymbol{\pi}\otimes\,\boldsymbol{\pi}]^2]^0_0\}|\boldsymbol{\alpha}\rangle \\
&\qquad+\langle\boldsymbol{\alpha}|\sum_{i,j,k}\boldsymbol{\pi}^\dagger_i\boldsymbol{\pi}^\dagger_j\boldsymbol{\pi}^\dagger_k\boldsymbol{\pi}^i\boldsymbol{\pi}^j\boldsymbol{\pi}^k+\boldsymbol{n}_\pi|\boldsymbol{\alpha}\rangle.
\end{aligned}
\tag{A11}
$$

Note that the mapping is now more complicated than when no Pauli exclusion principle is taken into account due to the distinct property of α_m. (It is not a tensor any more.) Also note that

$$
\begin{aligned}
[\tilde{\boldsymbol{\alpha}}\times\tilde{\boldsymbol{\alpha}}]^{[0]}_0&=\frac{1}{\sqrt{3}}\sum_m(-1)^{1-m}\alpha_m\alpha_{-m}, \\
[\boldsymbol{\alpha}^*\times\boldsymbol{\alpha}^*]^{[0]}_0&=\frac{1}{\sqrt{3}}\sum_m(-1)^{1-m}\alpha^*_m\alpha^*_{-m}.
\end{aligned}
\tag{A12}
$$

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 Ref. [40]. 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

$$
|\boldsymbol{\alpha}\rangle|[C_1\times C_2]^C\rangle, \tag{A13}
$$

where the last factor refers to the coupling of the two cluster states, *which is fixed* [40].

Next we have to expand the above expressions in powers of $(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})$. In Ref. [40] the n_0 was neglected compared to N. Here, we will take into account the contributions of n_0. The list of expansions is

$$
\begin{aligned}
&\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0}|_{\gamma_1=\gamma_2=1} \\
&\quad=\sum_{k=n_0}^{N+n_0}\binom{N+n_0}{k}\left[\frac{k!}{(k-n_0)!}\right]^2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})^k \\
&\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\gamma_1\gamma_2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0-1}|_{\gamma_1=\gamma_2=1} \\
&\quad=\sum_{k=\max(n_0-1,0)}^{N+n_0-1}\binom{N+n_0-1}{k}\left[\frac{(k+1)!}{(k+1-n_0)!}\right]^2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})^k \\
&\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\gamma_2[1+\gamma_1\gamma_2(\alpha^*\cdot\alpha)]^{N+n_0-1}|_{\gamma_1=\gamma_2=1} \\
&\quad=\sum_{k=n_0}^{N+n_0-1}\binom{N+n_0-1}{k}\left[\frac{k!}{(k-n_0)!}\right] \\
&\qquad\times\frac{(k+1)}{(k+1-n_0)}(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})^k \\
&\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}(\gamma_1\gamma_2)^2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0-2}|_{\gamma_1=\gamma_2=1} \\
&\quad=\sum_{k=\max(n_0-2,0)}^{N+n_0-2}\binom{N+n_0-2}{k}\left[\frac{(k+2)!}{(k+2-n_0)!}\right]^2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})^k \\
&\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}(\gamma_2)^2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})]^{N+n_0-2}|_{\gamma_1=\gamma_2=1} \\
&\quad=\sum_{k=\max(n_0,0)}^{N+n_0-2}\binom{N+n_0-2}{k}\left[\frac{(k+2)!}{(k+2-n_0)!}\right] \\
&\qquad\times\left[\frac{k!}{(k-n_0)!}\right](\boldsymbol{\alpha}^*\cdot\boldsymbol{\alpha})^k.
\end{aligned}
\tag{A14}
$$

The equations in (A14) can be simplified using the abbreviation

$$
\begin{aligned}
F_{pq}(\alpha^2)=&\frac{N!^2}{(N+n_0)!}\frac{(N+n_0)!}{[N+n_0-\max(p,q)]!} \\
&\times\sum_{k=\max(n_0-p,n_0-q,0)}^{N+n_0-\max(p,q)}\left[N+n_0-\max(p,q)\atop k\right] \\
&\times\left[\frac{(k+p)!}{(k+p-n_0)!}\right]\left[\frac{(k+q)!}{(k+q-n_0)!}\right]\alpha^{2k}.
\end{aligned}
\tag{A15}
$$

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