Geometrical interpretation of the semimicroscopic algebraic cluster model

P. O. Hess*
Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de Mexico, Circuito exterior, C.U., Apartado Postal 70-543, Delegación Coyoacán, 04510 México Distrito Federal, Mexico

G. Lévai† and J. Cseh‡
Institute of Nuclear Research of the Hungarian Academy of Sciences, H-4001 Debrecen, Pf. 51, Hungary
(Received 29 February 1996; revised manuscript received 27 June 1996)

A geometrical mapping of the semimicroscopic algebraic cluster model is given. The geometrical variables are the relative radius vector and the quadrupole deformation parameters. The last ones correspond to absolute β and γ values, while the orientation of the deformed nucleus in the laboratory can be changed. We show that the position of the minimum of the nuclear molecular potential is determined by the minimal number of π bosons describing the relative motion. The minimal number of π bosons is determined by the implementation of the Pauli principle. Applications to simple systems ($^{16}O+\alpha$ and $^{12}C+\alpha$) are presented. [S0556-2813(96)00711-X]

PACS number(s): 21.60.Cs, 21.60.Ev, 21.60.Fw, 21.60.Gx

I. INTRODUCTION

In recent years the semimicroscopic algebraic cluster model (SACM) was introduced [1] in order to describe in a unified way the low-lying collective spectrum and the nuclear molecular resonances. In this model the rotational-vibrational relative motion of the clusters is described in terms of the vibron model [2]. This is an algebraic model of the dipole collective motion with $U_R(4)$ group structure. (The subscript R is used to indicate the relative motion.) The group generators are expressed in terms of π and σ bosons, having $l=1$ and $l=0$ angular momenta, respectively. The π bosons are identical with the phonons of the three-dimensional harmonic oscillator. With the help of the σ bosons the model space can be truncated to a finite number of bosons, which denotes a representation of $U_R(4)$.

The internal structure of the clusters is accounted for by the SU(3) shell model [3]. The model space of the SACM is constructed microscopically [4]; therefore, it is free from Pauli-forbidden states and from the spurious excitations of the center-of-mass motion. The physical operators are treated phenomenologically; they are expressed in terms of group generators.

The success of the model lies in the simultaneous description of the low-lying spectra and high-lying molecular states. However, it has the disadvantage of nearly all algebraic models, namely, that it is difficult to visualize the geometric properties of the cluster system. It would also be desirable to look for a connection to a geometrical picture which can be compared to already existing geometrical models for nuclear molecules [5].

The objective of the present contribution is to fill this gap. In Sec. II the algebraic model is introduced very briefly, while in Sec. III we give the mapping to a geometrical picture. For this we will define for the relative motion a coherent state depending on some parameters. The potential is then given by the expectation value of the Hamiltonian with respect to this trial state. The parameters are related to the components of the relative distance vector. We shall see that the minimal number of π bosons, which is necessary to satisfy the Pauli principle, is directly related to the position of the minimum of the nuclear molecular potential. The quadrupole deformation variables are introduced in the same way as given in Ref. [6]. In Sec. IV we apply the mapping to the systems of $^{16}O+\alpha$ and $^{12}C+\alpha$. As will be seen, the results are in agreement with what is expected. Also the dependence of the potential on the relative orientations can be described, which is important for the second system where the ^{12}C nucleus is strongly deformed. Finally, in Sec. V the summary and conclusions are given.

Although in this contribution only asymmetric cluster systems are discussed, we show in Appendix B, for completeness, how to treat symmetric systems.

II. SEMIMICROSCOPIC ALGEBRAIC CLUSTER MODEL

The building blocks of the SACM are π and σ bosons in the section of the relative motion and quanta of the harmonic oscillators in the shell models of the clusters. Their creation and annihilation operators are denoted by $\pi^\dagger_m, \sigma^\dagger, a^\dagger_m$ and $\pi^m, \sigma, a^m (m=-1,0,+1)$, respectively. Note that we use covariant and contravariant indices in order to distinguish between the different transformation properties of the creation operators with respect to the annihilation operators. The contravariant component of the annihilation operator is related to its covariant component via

$$\pi^m=(-1)^{1-m}\pi_{-m}, \quad a^m=(-1)^{1-m}a_{-m}. \tag{1}$$

This deviates from the usual definition. In Ref. [1] the $\tilde{\pi}_m$ corresponds here to π^m. The commutation relations of these operators are

*Electronic address: HESS@ROXANNE.NUCLECU.UNAM.MX
†Electronic address: LEVAIG@TIGRIS.KLTE.HU
‡Electronic address: CSEHJ@TIGRIS.KLTE.HU

$$[\pi^{m'},\pi^{\dagger}_{m}]=\delta^{m'}_{m}, \quad [\sigma,\sigma^{\dagger}]=1, \quad [a^{m'},a^{\dagger}_{m}]=\delta^{m'}_{m}; \quad (2)$$

all the rest gives zero.

The fact that the π bosons of the relative motion correspond to oscillator quanta, just like the a bosons of the internal structure of the clusters, has important consequences. This circumstance enables us to take into account the Pauli-blocking effect. As for the construction of the model space this implementation is one of the main ingredients of the semimicroscopic algebraic model. This leads to the condition that the number of π bosons is bounded from below to a number greater than zero. This can be seen immediately by counting the number of quanta in the shell model oscillator of each cluster. The sum will be less than the total number of quanta of the united system. As an example take $^{12}\mathrm{C}+\alpha$. The number of quanta for α is zero, because all nucleons occupy the shell with zero quanta. The ^{12}C has eight nuclei in the p shell and thus carries eight quanta. The total sum is 8. The united system is ^{16}O and has 12 nuclei in the p shell and, therefore, carries 12 quanta. As can be seen, four nucleons have to be lifted to the p shell of the united system and four quanta have to be added in order to satisfy the Pauli principle. In the literature, this is known as the Wildermuth condition [4].

When constructing the model space one has to deal with the spin and isospin degrees of freedom as well [3]. However, in the physical operators they do not necessarily show up explicitly. In case the clusters have spin and isospin zero, the spin- and isospin-dependent interactions are not essential in most of the problems. Then the group structure of the model has relatively simple form

$$\begin{array}{l} \mathrm{U}_{C_1}(3) \otimes \mathrm{U}_{C_2}(3) \otimes \mathrm{U}_R(4) \\ |[n_1^{C_1},n_2^{C_1},n_3^{C_1}],[n_1^{C_2},n_2^{C_2},n_3^{C_2}],[N',0,0,0], \\ \supset U_C(3) \otimes U_R(3) \supset \mathrm{SU}_C(3)\otimes \mathrm{SU}_R(3) \supset \mathrm{SU}(3)\supset \mathrm{O}(3)\supset \mathrm{O}(2) \\ [n_1^C,n_2^C,n_3^C],[n_\pi,0,0,], \ (\lambda_C,\mu_C) \ , \ (n_\pi,0) \ , (\lambda,\mu), \quad K_L,L \ , \ M\rangle. \end{array} \quad (3)$$

Here we also indicated the labels of the irreducible representations (irreps), which define the set of basis states. [Note the different notation of the U(4) irrep: N' with respect to that of Ref. [1].] Further simplification takes place when the clusters have a closed shell structure, and their excitations are omitted. It should be noted here that the total number of relative oscillation number N' is used as a cutoff parameter. In actual calculations, stable results for the states in consideration are reached for already low numbers of excitation quanta (three to six shell excitations). Contrary to other models of molecules, e.g., atomic molecules [2,8], no physical meaning can be associated with the quantum number N'. This is reflected by the structure of the Hamiltonian which only depends on the π bosons.

For a core-plus-alpha-particle system with a core of even proton and neutron numbers the model has a group structure of $\mathrm{U}_C(3)\otimes\mathrm{U}_R(4)$. In general the operators of physical quantities (including the Hamiltonian) are expressed in terms of the generators of this direct product group, and then the eigenvalue problem is solved by numerical diagonalization. As in many other algebraic models, however, there is a very important limiting case, called dynamic symmetry. This holds when the Hamiltonian can be expressed in terms of the invariant operators of the following group chain:

$$\begin{array}{l} \mathrm{U}_C(3) \otimes \mathrm{U}_R(4) \supset \mathrm{U}_C(3)\otimes \mathrm{U}_R(3) \supset \mathrm{SU}_C(3)\otimes \mathrm{SU}_R(3) \\ |[n_1^C,n_2^C,n_3^C],[N',0,0,0], \quad [n_\pi,0,0,], \ (\lambda_C,\mu_C),(n_\pi,0) \\ \supset \mathrm{SU}(3)\supset \mathrm{O}(3)\supset \mathrm{O}(2) \\ (\lambda,\mu),K,L,M\rangle. \end{array} \quad (3')$$

A simple Hamiltonian corresponding to this dynamic symmetry is given by

$$E=\epsilon+\gamma n_\pi+\delta n_\pi^2+\eta C_2(\lambda,\mu)+\theta K^2+\beta L(L+1). \quad (4)$$

If the core has a closed shell structure as well, then one has $(\lambda_C,\mu_C)=(0,0),(\lambda,\mu)=(n_\pi,0)$, and $K=0$.

Since in the limiting case of the dynamic symmetry the energy eigenvalue problem has an analytical solution, it makes the application of the model very easy. So far practical applications have been carried out in this approximation; therefore, in the following discussion we concentrate mainly on this kind of Hamiltonian. It is proper to note, however, that the forthcoming formalism enables us to build a geometrical relation of more general Hamiltonians as well.

III. GEOMETRY OF THE ALGEBRAIC CLUSTER MODEL

The principal idea is to define a coherent state as trial wave function and to define the potential as

$$V(\boldsymbol{\alpha})=\langle\boldsymbol{\alpha}|\hat{H}_{\mathrm{mic}}|\boldsymbol{\alpha}\rangle, \quad (5)$$

where $\hat{H}_{\mathrm{mic}}$ is the semimicroscopic algebraic Hamiltonian, $|\boldsymbol{\alpha}\rangle$ the coherent state, and $\boldsymbol{\alpha}=(\alpha_m)$ a set of parameters yet to be related to the relative vector. For simplicity, we do not include in the trial state explicitly the dependence on the internal structure of the clusters. This is assumed implicitly and will be discussed later. The deformation variables of each cluster will be introduced when necessary. Later we will also relate the parameters α_m to the relative distance vector. Note that Eq. (5) is the expression we get applying the generator coordinate method in the Gaussian overlap approximation [7], except for a constant term.

A. Coherent state of the relative motion

As the coherent state we propose

$$|\boldsymbol{\alpha}\rangle = \mathcal{N}_{N,n_0}(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)^{n_0}[\sigma^\dagger + (\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^N|0\rangle$$
$$= \frac{N!}{(N+n_0)!}\mathcal{N}_{N,n_0}\frac{d^{n_0}}{d\gamma^{n_0}}[\sigma^\dagger + \gamma(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^{N+n_0}|0\rangle|_{\gamma=1}, \tag{6}$$

where n_0 gives the minimal number of π bosons needed in order to satisfy the Pauli principle and the total number of bosons is given by $N+n_0 \equiv N'$. The second line gives an equivalent expression needed to simplify calculations. It is understood that at the end of the differential operation the value of γ has to be set equal to 1. The factor $\mathcal{N}_{N,n_0}$ is the normalization of the state which depends on the minimal number of π bosons and the total number of bosons $(N+n_0)$. In the case of $n_0=0$ the above equation reduces to the equivalent formula obtained in the relation of the Algebraic model for atomic molecules [8,9] to the geometrical model [10]. In this presentation we extend the consideration to a nonzero minimal number of π bosons. Note that the coherent state of Eq. (6) has no definite angular momentum but can be expanded into states of definite angular momentum (and number of π bosons greater or equal to n_0). In defining the potential $V(\boldsymbol{\alpha})$ we follow Ref. [7] and use the coherent state as a trial state. Its advantage is that it contains all physically relevant states in the relative motion.

The scalar product of $\boldsymbol{\alpha}$ with the creation operator is given by

$$(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger) = \sum_m \alpha^m \pi^\dagger_m = \sum_m \alpha_m \pi^{\dagger m}$$
$$= \sum_m (-1)^{1-m}\alpha_{-m}\pi^\dagger_m, \tag{7}$$

and a similar formula holds for all other scalar products.

Now we are able to calculate the normalization factor in Eq. (6). Using the second line of Eq. (6) for the expression of the coherent state and that by definition $\langle 0|0\rangle = 1$, the inverse square of the normalization factor is given by

$$\mathcal{N}^{-2}_{N,n_0} = \left[\frac{N!}{(N+n_0)!}\right]^2 \frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}$$
$$\times\langle 0|[\sigma+\gamma_1(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})]^{N+n_0}[\sigma^\dagger+\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^{N+n_0}|0\rangle$$
$$= \left[\frac{(N!)^2}{(N+n_0)!}\right]\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}[1+\gamma_1\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^{N+n_0}, \tag{8}$$

where again at the end of the calculation γ_1 and γ_2 have to be set equal to 1. In the last step we used that the annihilation operators act like derivatives on the right-hand side. Evaluating the derivatives we finally can identify the inverse square of the normalization factor with

$$\mathcal{N}^{-2}_{N,n_0} = N!\,n_0!\,(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^{n_0}[1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^N$$
$$\times {}_2F_1\left(-n_0,-N;1;\frac{(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}{1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}\right), \tag{9}$$

with ${}_2F_1(\ldots)$ being a hypergeometric function. It can be easily checked that for $n_0=0$ this reduces to the known formula [8] for the normalization of the coherent state.

In the next step we present how to calculate the expectation value of an arbitary generator of $U_R(4)$ with respect to the coherent state. The general expression we have to calculate is of the form

$$\langle\boldsymbol{\alpha}|\mathbf{O}|\boldsymbol{\alpha}\rangle = \mathcal{N}^2_{N,n_0}\left[\frac{N!}{(N+n_0)!}\right]^2\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}$$
$$\times\langle 0|[\sigma+\gamma_1(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})]^{N+n_0}$$
$$\times\mathbf{O}[\sigma^\dagger+\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^{N+n_0}|0\rangle, \tag{10}$$

which is of the same structure as in Eq. (8) except for the appearence of the operator $\mathbf{O}$. We will give an explicit derivation for one particular generator of $U_R(4)$. For the other ones only the final result will be given. The calculation to obtain them is completely equivalent to the example.

Let us take the generator $([\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[S]}_m)$, where we used the notation of the usual angular momentum coupling:

$$[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[S]}_m = \sum_{m_1 m_2}(1m_1 1m_2|Sm)\,\pi^\dagger_{m_1}\pi_{m_2}, \tag{11}$$

with $(1m_1 1m_2|Sm)$ being the Clebsch-Gordan coefficient and S the total spin. The action of π_{m_2} to the right gives $(N+n_0)\gamma_2\alpha_{m_2}$ and the action of $\pi^\dagger_{m_1}$ to the left gives $(N+n_0)\gamma_1\alpha_{m_1}$ and in each case the power of the square brackets is reduced from $(N+n_0)$ to $(N+n_0-1)$. Taking into account the angular momentum coupling, we arrive at

$$\langle 0|[\sigma+\gamma_1(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})]^{N+n_0}[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[S]}_m[\sigma^\dagger+\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^{N+n_0}|0\rangle$$
$$= (N+n_0)^2\gamma_1\gamma_2[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[S]}_m\langle 0|[\sigma+\gamma_1(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})]^{N+n_0-1}[\sigma^\dagger+\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^{N+n_0-1}|0\rangle. \tag{12}$$

Using the same steps as in the calculation of the normalization we obtain finally

$$\langle \boldsymbol{\alpha}|[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[S]}_m|\boldsymbol{\alpha}\rangle=(N+n_0)[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[S]}_m\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!}\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\gamma_1\gamma_2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^{N+n_0-1}. \tag{13}$$

After having applied the derivatives in γ_1 and γ_2 and setting them equal to 1 at the end, we obtain a sum which can be rewritten in terms of the normalization constants $\mathcal{N}_{Nn_0}$ [using Eq. (8) which gives the definition of the normalization constant]. We will not present the final expression here and instead maintain the compact expression.

For the other generators of the $U_R(4)$ group (and their combinations) we obtain

$$\langle \boldsymbol{\alpha}|\sigma^\dagger\pi_m|\boldsymbol{\alpha}\rangle=(N+n_0)\alpha_m\mathcal{N}^2_{Nn_0}\frac{(N!)^2}{(N+n_0)!}\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}\gamma_2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^{N+n_0-1},$$

$$\langle \boldsymbol{\alpha}|\sigma^\dagger\sigma|\boldsymbol{\alpha}\rangle=N^2\frac{\mathcal{N}^2_{Nn_0}}{\mathcal{N}^2_{(N-1)n_0}},$$

$$\langle \boldsymbol{\alpha}|[[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}^\dagger]^{[S_1]}\times[\boldsymbol{\pi}\times\boldsymbol{\pi}]^{[S_2]}]^{[S_3]}_m|\boldsymbol{\alpha}\rangle=(N+n_0)(N+n_0-1)[[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[S_1]}\times[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[S_2]}]^{[S_3]}_m\mathcal{N}^2_{Nn_0}$$
$$\times\frac{(N!)^2}{(N+n_0)!}\frac{d^{n_0}}{d\gamma_1^{n_0}}\frac{d^{n_0}}{d\gamma_2^{n_0}}(\gamma_1\gamma_2)^2[1+\gamma_1\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^{N+n_0-2}. \tag{14}$$

For $\sigma^\dagger\sigma$ we applied the operator directly on the original form of the state, because it is trivial. The fourth-order term in the creation and annihilation operators is also given explicitly because it will appear in the second-order Casimir operator. As can be seen, it has the same structure, except that the above-mentioned procedure of calculating the expectation value has to be applied twice. The situation is similar for the expression of sixth order in the creation and annihilation operators. This one is needed for the third-order Casimir operator. Taking the Hermitian conjugate of expressions in Eq. (14) we obtain the expectation value of the Hermitian conjugate operators. By construction, they are the same.

B. Coherent state with internal cluster structure

The group $U_R(4)$ is not the only one appearing in the Hamiltonian of the semimicroscopic algebraic model. There are also the $SU_{C_k}(3)$ groups ($k=1,2$), as introduced by Elliott [3], for each cluster and the total $SU_C(3)$ which is contained in the direct product $SU_{C_1}(3)\otimes SU_{C_2}(3)$ as a subgroup. [Here the same notation is used as in Eq. (3), with the difference that the groups appearing there are U(3) groups instead of SU(3) groups appearing here.] In order to take into account their contribution we have to add to the coherent state the dependence on the $SU_C(3)$-irreducible representation (irrep). For that the vacuum state in Eq. (6) is substituted by

$$|0\rangle\rightarrow|n_{C_1}(\lambda_{C_1},\mu_{C_1}),n_{C_2}(\lambda_{C_2},\mu_{C_2})\rho_C(\lambda_C,\mu_C)\kappa_C L_C,M_C=L_C\rangle, \tag{15}$$

where the notation refers to the SU(3) coupling of the representations of the two clusters to a total $SU_C(3)$-irreducible representation (irrep), which is still a vacuum for the bosons of the relative motion. The $U_{C_k}(3)$ quantum numbers in Eq. (3) are related to the $SU_{C_k}(3)$ labels as $\lambda_{C_k}=n_1^{C_k}-n_2^{C_k}$ and $\mu_{C_k}=n_2^{C_k}-n_3^{C_k}$. The n_{C_k} are the total number of oscillation quanta of cluster number k. The numbers ρ_C and κ_C are multiplicity labels. For the operators of the $SU_{C_k}(3)$ groups we then follow the rule as given in Refs. [11,12]. Calculating the expectation value we substitute the algebraic quadrupole operator $Q^a_m(k)$ ($k=1,2$) by

$$\langle Q^a_m(k)\rangle=\sqrt{\frac{5}{\pi}}[n_{C_k}+\tfrac{3}{2}(A_k-1)]\alpha_{2m}(k)$$
$$=\sqrt{\frac{5}{\pi}}N_{0,k}\alpha_{2m}(k). \tag{16}$$

Note that $Q^a_m(k)$ is the algebraic quadrupole operator of cluster number k and acts only on it.

The $\alpha_{2m}(k)$ is the quadrupole deformation variable as introduced in the geometrical model of the nucleus [10]. For the ρ_C, (λ_C,μ_C), κ_C, L_C, and M_C values we take a particular coupling, i.e., the $\kappa_C=1$ ($K_C=0$), $L_C=0$ state of the

most symmetric Pauli-allowed $SU_C(3)$ irrep. [κ_C merely is a multiplicity label with $\kappa_C=1,2,3,\ldots$, where $\kappa_C=1$ corresponds to $K_C=0$ as introduced by Elliott [3]. Also ρ_C is a multipicity label of how many times (λ_C,μ_C) appears in the product $(\lambda_{C_1},\mu_{C_1})$ with $(\lambda_{C_2},\mu_{C_2})$.] Restricting to the lowest $SU_C(3)$ irrep in energy corresponds to probing the lower boundary of the potential. We also can take higher irreps which correspond to an excited cluster system. Note that $Q^a_m(k)$ is sensitive only to the structure of the individual cluster. It does not act on the relative part of the coherent state. So restricting to $L_C=0$ refers to the coupling of the two clusters and *not* on a total L of the coherent state (the coherent state does not have a definite angular momentum). With the dependence on $\alpha_{2m}(k)$ we will be able to describe the dependence of the potential as a function on the relative orientation of the two clusters when we define the nuclear molecular axis as the laboratory systems for the clusters [12].

The definition in Eq. (15) of the vacuum state of the relative motion can be relaxed, if necessary, by not coupling to a total definite SU(3) irrep of the cluster. The main point here is that the annihilation operators σ and π^m applied to this vaccum state have to give zero.

Next we will give the operators, which appear in the Hamiltonian of the semimicroscopic algebraic cluster model, in terms of the generators of all groups appearing in the model. Using the above formulas for the generators of $U_R(4)$, we can obtain their geometrical equivalent in terms of the α_m and $\alpha_{2m}(k)$.

Following the notation of Ref. [1] the relevant generators, which depend on the π bosons, are given by

$$\mathbf{n}_\pi=\sqrt{3}[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[0]}_0,$$

$$\mathbf{L}_{R,m}=\sqrt{2}[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[1]}_m,$$

$$\mathbf{Q}_{R,m}=\frac{\sqrt{3}}{2}[\boldsymbol{\pi}^\dagger\times\boldsymbol{\pi}]^{[2]}_m=\frac{1}{2\sqrt{2}}\mathbf{Q}^a_{R,m}, \tag{17}$$

where $\mathbf{Q}^a_{R,m}$ is the quadrupole operator which corresponds to the usual definition as it is used in the microscopic SU(3) schemes; i.e., it is given by $[2(z^2+p_z^2)-(x^2+p_x^2)-(y^2+p_z^2)]$ with p_x, p_y, and p_z the momenta in x, y, and z. The index a refers to ''algebraic'' and denotes that the operator only acts within a shell. There are also equivalent operators referring to the cluster structure:

$$\mathbf{n}_C,\mathbf{L}_C,\mathbf{Q}^a_C, \tag{18}$$

where the first refers to the total number of oscillation quanta of the two clusters, the second to the coupled angular momentum, and the last to the sum of the quadrupole operators of the two clusters. For each individual cluster the definitions are the same except that the operators carry an index k with $k=1,2$.

With these definitions the second-order Casimir operator of the total SU(3) group is related to the second-order Casimir operator of $SU_C(3)$ by

$$\begin{aligned}\mathbf{C}_2((\lambda,\mu))&=\mathbf{C}_2((\lambda_C,\mu_C))+\mathbf{n}_\pi(\mathbf{n}_\pi+3)\\&\quad-\tfrac{3}{2}(\mathbf{L}_C\cdot\mathbf{L}_R)+4(\mathbf{Q}_C\cdot\mathbf{Q}_R)\\&=\mathbf{C}_2((\lambda_C,\mu_C))+\mathbf{n}_\pi(\mathbf{n}_\pi+3)-\tfrac{3}{2}(\mathbf{L}_C\cdot\mathbf{L}_R)\\&\quad+\tfrac{1}{2}(\mathbf{Q}^a_C\cdot\mathbf{Q}^a_R),\end{aligned} \tag{19}$$

where we used that $\mathbf{C}_2((n_\pi,0))=\mathbf{n}_\pi(\mathbf{n}_\pi+3)$ with the normalization of the Casimir operators such that the eigenvalue, for example, of the $\mathbf{C}_2((\lambda,\mu))$, is given by $\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu$ [similar for the others as, e.g., $\mathbf{C}_2((\lambda_C,\mu_C))$].

The expression for the third-order Casimir operator is rather lengthy. One has to recouple the terms such that the factors depending only on the π-boson operators are coupled together. The normalization of the third-order Casimir operator is chosen in a way that the eigenvalue is given by $(\lambda-\mu)(2\lambda+\mu+3)(2\mu+\lambda+3)$. After tedious calculation we arrive at

$$\begin{aligned}\mathbf{C}_3((\lambda,\mu))&=[\mathbf{C}_3((\lambda_C,\mu_C))+\mathbf{C}_3((n_\pi,0))]-9(1-\tfrac{2}{3}\mathbf{n}_C)\mathbf{C}_2((\lambda_C,\mu_C))+\mathbf{n}_C^3-9(1-\tfrac{2}{3}\mathbf{n}_\pi)\mathbf{C}_2((n_\pi,0))\\&\quad+\mathbf{n}_\pi^3+9[1-\tfrac{2}{3}(\mathbf{n}_C+\mathbf{n}_\pi)]\mathbf{C}_2((\lambda,\mu))+(\mathbf{n}_C+\mathbf{n}_\pi)^3+3\mathbf{n}_C\mathbf{n}_\pi(\mathbf{n}_c+\mathbf{n}_\pi)+\frac{9}{2}\{\mathbf{n}_\pi[(\mathbf{L}_C\cdot\mathbf{L}_C)+2(\mathbf{L}_C\cdot\mathbf{L}_R)]\\&\quad+\mathbf{n}_C[(\mathbf{L}_R\cdot\mathbf{L}_R)+2(\mathbf{L}_C\cdot\mathbf{L}_R)]\}+\frac{27}{4}\sqrt{\frac{3}{2}}([[\mathbf{L}_C\times\mathbf{L}_C]^{[1]}\times\mathbf{L}_R]^{[0]}_0+[[\mathbf{L}_R\times\mathbf{L}_R]^{[1]}\times\mathbf{L}_R]^{[0]}_0)\\&\quad+\frac{3}{2}\sqrt{5}\{\mathbf{n}_\pi([\mathbf{Q}^a_C\times\mathbf{Q}^a_C]^{[0]}_0+2[\mathbf{Q}^a_C\times\mathbf{Q}^a_R]^{[0]}_0)+\mathbf{n}_C([\mathbf{Q}^a_R\times\mathbf{Q}^a_R]^{[0]}_0+2[\mathbf{Q}^a_R\times\mathbf{Q}^a_C]^{[0]}_0)\}\\&\quad+\frac{3}{4}\sqrt{\frac{35}{2}}\{[[\mathbf{Q}^a_C\times\mathbf{Q}^a_C]^{[2]}\times\mathbf{Q}^a_R]^{[0]}_0+[[\mathbf{Q}^a_R\times\mathbf{Q}^a_R]^{[2]}\times\mathbf{Q}^a_C]^{[0]}_0\},\end{aligned} \tag{20}$$

where $(\mathbf{n}_C+\mathbf{n}_\pi)$ is the sum of the number of quanta in the cluster system and the π quanta. Having deduced relations (17)–(20), the expectation values are obtained by using the steps presented from Eqs. (8) – (16).

C. Relation of α_m to the radius parameter

Up to now we expressed every operator, which are functions in the π bosons, in terms of the parameter values α_m of the coherent state of Eq. (6). In what follows they will be related to the radial distance of the clusters r_m. For that we require the relation

$$\langle 0|\mathbf{r}_m|0\rangle = r_m, \tag{21}$$

where the operator on the left is the distance operator. However, the distance operator cannot have the usual form $(\sqrt{\hbar/2m\omega})(\pi_m^\dagger+\pi_m)$ because a cutoff was introduced using the $U_R(4)$ group. ($\sqrt{\hbar/m\omega}$ is the oscillation length with m being the nucleon mass and $\hbar\omega$ the distance in energy of the shells in the nucleus composed by the two clusters. This value sets the length scale in a nucleus.) Because of that, we work in a space where the total number of σ plus π bosons is conserved. The usual distance operator does not conserve the total number of bosons and, thus, does not give an expectation value different from zero. In order to account for the conservation of the total number of bosons we have to modify the expression of the distance operator. This is done by *proposing* (i) to substitute $\pi_m^\dagger$ and π_m by $\pi_m^\dagger\sigma$ and $\sigma^\dagger\pi_m$, respectively, and (ii) to divide by the square root of the expectation value of $\sigma^\dagger\sigma$, i.e., by the number of σ bosons. We use the convention that for zero σ bosons this part of $\mathbf{r}_m$ is zero, which can be understood as a limiting process of the numerator versus the denominator. With this we *define* the modified distance operator as

$$\mathbf{r}_m = \sqrt{\frac{\hbar}{2m\omega}}\frac{(\pi_m^\dagger\sigma+\sigma^\dagger\pi_m)}{\sqrt{\langle 0|\sigma^\dagger\sigma|0\rangle}}+r_{0,m}, \tag{22}$$

where $r_{0,m}$ does not depend on the boson operators and, thus, does not change the total number of bosons either. $r_{0,m}$ is determined by requiring, in order to be consistent, that the expectation value of the normal-ordered square of the original distance operator $(\sqrt{\hbar/2m\omega})(\pi_m^\dagger+\pi_m)$ with respect to the state with $N=0$ has to be equal to $\langle(\mathbf{r}_0\cdot\mathbf{r}_0)\rangle$. (The normal ordering is used because $r_{0,m}$ should vanish when the minimal number of π bosons is zero. Then one has to obtain the modified form of the relative distance operator for this case. If the normal ordering is not used, there would always remain a constant term.) In such a way we take into acount that there is a minimal number of π bosons. We obtain

$$r_{0,m}=r_0\hat{r}_m,$$

$$r_0^2=\frac{\hbar}{2m\omega}\mathcal{N}_{0,n_0}^2\sum_m(-1)^m\langle 0|:(\boldsymbol{\alpha}\cdot\boldsymbol{\pi})^{n_0}(\pi_m^\dagger+\pi_m)$$
$$\times(\pi_{-m}^\dagger+\pi_{-m})(\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)^{n_0}:|0\rangle, \tag{23}$$

where : . . . : stands for normal ordering, $\hat{r}_m$ is the unit vector of r_m, and r_0^2 nothing else than the expectation value of the square of the real distance operator with respect to the state where no σ bosons appear but only the minimal number of π bosons. This corresponds in Eq. (6) to the case with $N=0$.

This procedure is in analogy with the one used by Roosmalen [13] in the description of atomic molecules, except for the additional contribution $r_{0,m}$ which has its origin in the requirement of a minimal number of π bosons.

In order to evaluate the expectation value of $\sigma^\dagger\sigma$ we can use the second equation of Eq. (14). This gives a rather complicated expression. We can simplify it by considering that N of Eq. (6) goes to ∞. The same is done for the evaluation of r_0. We get

$$\mathbf{r}_m\approx\sqrt{\frac{\hbar}{2Nm\omega}}\sqrt{1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}(\pi_m^\dagger\sigma+\sigma^\dagger\pi_m)+r_{0,m}, \tag{24}$$

where r_0 is computed by Eq. (23) with the result

$$r_0\approx\sqrt{\frac{\hbar}{m\omega}n_0}. \tag{25}$$

This gives, for the expectation value,

$$r_m\approx\sqrt{\frac{2N\hbar}{m\omega}}\sqrt{1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}\alpha_m+r_{0,m}. \tag{26}$$

Note that the first term of r_m is proportional to $\sqrt{N}\alpha_m$, and so for the limit of $N\to\infty$, and assuming that r_m has always values of the order of several fm, the α_m will be a very small number. For this reason we can identify, approximately for α_m [with $\sqrt{1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}\approx 1$],

$$\alpha_m\approx\sqrt{\frac{m\omega}{2N\hbar}}(r_m-r_{0,m}). \tag{27}$$

Note that α_m gives the *difference* of the radius variable to the value of $r_{0,m}$. The last is only different from zero when the minimal number of π bosons (n_0) is *different from zero*. This will produce in the potential a minimum value at r_0 and, therefore, n_0 plays a very important role in determining the structure of the nuclear molecular potential.

As was seen from the previous discussion, we can consider the limit of $N\to\infty$ in order to get approximate values for the expectation values. In fact, this should be the limit to be considered when the cutoff is raised. In this limit the expressions for the expectation values acquire a particularly simple form, namely, the one as if n_0 is set to zero. One can then ask if all the effort done in the first sections is of practical value. This is indeed the case because, first, calculations are done with $N=$ finite and one has to discuss to which potential these calculations correspond. Second, the fact that n_0 is different from zero survives in the appearence of $r_{0,m}$ in Eq. (27). In what follows, we will for simplicity only consider the limit $N\to\infty$ in order to deduce the potential in the case of two-cluster systems.

As a next step we have to express the expectation values of the operators, which appear in the Hamiltonian, in terms

of r_m and $r_{0,m}$. We will see that in the limit $N\to\infty$ all dependence on N will vanish. This should be so because the cutoff, given by N, is an arbitray value introduced by hand.

The rule is simple: We have to calculate the expectation value of any operator with respect to the trial state. In the limit of $N\to\infty$ it is sufficient to calculate the expectation value with respect to the coherent state with $n_0=0$. As we saw above, it will give the correct value for the real case in this limit. Next, the parameter value α_m has to be substituted by Eq. (27). As an example, consider the operators $\mathbf{n}_\pi$ and $\mathbf{n}_\pi^2$. Following the steps, we obtain

$$\langle \mathbf{n}_\pi\rangle \approx N(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}) \approx \frac{m\omega}{2\hbar}(r-r_0)^2,$$

$$\langle \mathbf{n}_\pi^2\rangle \approx N(N-1)(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^2 \approx \left(\frac{m\omega}{2\hbar}\right)^2 (r-r_0)^4. \tag{28}$$

A particular application is the expectation value of the operator $[L_R\times L_R]_0^{[0]}$. Using Eq. (13) and Eq. (17) we arrive at

$$\langle\boldsymbol{\alpha}|[L_R\times L_R]_0^{[0]}|\boldsymbol{\alpha}\rangle = \frac{2}{\sqrt{3}}\langle\boldsymbol{\alpha}|\mathbf{n}_\pi|\boldsymbol{\alpha}\rangle.$$

The expectation value of the total L^2 operator is obtained by using that the operator L_m is a sum of $L_{R,m}$ and of the cluster part $L_{C,m}$ and that the two clusters are coupled to zero L_C.

A little more involved is the calculation of the expectation value of the second-order Casimir operator $\mathbf{C}_2((\lambda,\mu))$. The expectation value of the expression of Eq. (19) has to be calculated. Using also Eq. (17) we obtain

$$\begin{aligned}\langle \mathbf{C}_2((\lambda,\mu))\rangle \approx{}& C_2(\lambda_C,\mu_C)+3\left(\frac{m\omega}{2\hbar}\right)(r-r_0)^2\\ &+\left(\frac{m\omega}{2\hbar}\right)^2(r-r_0)^4+\frac{1}{2}\sqrt{\frac{30}{\pi}}N[N_{0,1}\boldsymbol{\alpha}_2(1)\\ &+N_{0,2}\boldsymbol{\alpha}_2(2)]\cdot[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[2]},\end{aligned} \tag{29}$$

where $N_{0,k}$ gives the total number of oscillation quanta of cluster number k [plus $\frac{3}{2}(A_k-1)$; see Eq. (16)] and $\boldsymbol{\alpha}_2(k)$ is the deformation of the kth cluster which is defined via its $SU_k(3)$ irrep as given in Refs. [6,12] and its relation to the quadrupole operator is also given in Eq. (16). The ''$\cdot$'' defines the scalar product between the $\mathbf{Q}_{C,m}$ and the function in $\boldsymbol{\alpha}$. Substituting α_m by Eq. (27) we obtain finally

$$\begin{aligned}\langle \mathbf{C}_2((\lambda,\mu))\rangle ={}& C_2(\lambda_C,\mu_C)+3\left(\frac{m\omega}{2\hbar}\right)(r-r_0)^2\\ &+\left(\frac{m\omega}{2\hbar}\right)^2(r-r_0)^4+\frac{1}{2}\sqrt{\frac{30}{\pi}}\left(\frac{m\omega}{2\hbar}\right)\\ &\times[N_{0,1}\boldsymbol{\alpha}_2(1)+N_{0,2}\boldsymbol{\alpha}_2(2)]\cdot[\tilde{\mathbf{r}}\times\tilde{\mathbf{r}}]^{[2]},\end{aligned} \tag{30}$$

with

$$\tilde{r}_m = r_m - r_{0,m},$$

$$C_2((\lambda_C,\mu_C)) = \lambda_C^2+\lambda_C\mu_C+\mu_C^2+3\lambda_C+3\mu_C. \tag{31}$$

In Appendix A we show how, for the case of one deformed, axially symmetric cluster and another spherical one, the deformation-dependent term in Eq. (30) can be expressed in the deformation variable $\beta(1)$ of the deformed cluster and its orientation with respect to the molecular z axis. This we will need in the applications. Similarly, the expectation value of other operators can be determined. In the next section we apply the procedure to two simple systems.

IV. APPLICATION TO $^{16}O+\alpha$ AND $^{12}C+\alpha$

The first system is particularly simple, because both clusters are characterized by the scalar (0,0) SU(3) irrep. The second one represents the next more complicated situation with one cluster deformed. In both cases the Hamiltonian has a particularly simple structure and, therefore, can illustrate in a transparent way the geometrical mapping.

In the following we use model parameters obtained from the new, standardized Hamiltonian of the semimicroscopic algebraic cluster model [14]. The new ingredient of this is selecting a harmonic oscillator parameter appropriate for the mass number of the given unified nucleus, which then results in a consistent set of parameters. Previously the harmonic oscillator constant was fitted together with the other parameters, as a result of which a direct comparison of different cluster systems was difficult.

A. $^{16}O+\alpha$

The Hamiltonian of this system is given by [14]

$$\mathbf{H} = \epsilon+\gamma\mathbf{n}_\pi+\eta\mathbf{C}_2((n_\pi,0))+\beta\mathbf{L}^2, \tag{32}$$

with $\mathbf{L}^2$ as the total angular momentum operator and ϵ the zero-point energy, adjusted to experimental data. The values used are $\epsilon=-63.998$ MeV, $\gamma=\hbar\omega=13.185$ MeV, $\eta=-0.4641$ MeV, and $\beta=0.1562$ MeV. γ has been determined from the formula $\hbar\omega=45A^{-1/3}-25A^{-2/3}$ [15] as a harmonic oscillator parameter characteristic for nuclei with $A=20$ nucleons. Taking the same $\hbar\omega$ value and 8 as the minimal number of π bosons (n_0) Eq. (25) yields $r_0=5.01$ fm as the minimum of the nuclear molecular potential. This value is consistent with the estimation based on the picture of two touching clusters with a distance of 1.2 fm $\times(A_1^{1/3}+A_2^{1/3})=4.93$ fm; i.e., the two clusters slightly overlap. For the potential we finally get (in MeV)

$$V(r) = -63.998+1.9078(r-r_0)^2-0.0118(r-r_0)^4. \tag{33}$$

This corresponds to a shifted oscillator with the minimum at r_0 containing also a slight anharmonic contribution of the fourth order. The negative sign of the fourth-order term, implying an unstable behavior for large r, should not worry us very much. First, this term becomes important only for very large values of r. The maximum of the potential in Eq. (33) is at $r=14$ fm and the potential has there a value of $\approx$ 77 MeV above the minimum. Second, the wave functions of

physical interest are not sensitive to this unphysical range and, therefore, the potential deduced is sensitive only to not too large values of r. The negative factor is a consequence of how the model Hamiltonian of Eq. (32) is adjusted to experimental data at low energies. As a result the Hamiltonian contains a quadratic term in $\mathbf{n}_\pi$ (in the second-order Casimir operator) with negative coefficient. This term lowers higher shells (large n_π values) too much. One has, however, to keep in mind that the above consideration is for $N\rightarrow\infty$ and finite distance; i.e., according to Eq. (27) the variable α_m is always very small. In actual calculations the number of excited quanta, i.e., N, is of the order of 3–6. In this case deviations appear for large values of α_m. These deviations appear at unphysically large distances, i.e., to which the states fitted are not sensitive. We will consider now the limit of $\alpha\rightarrow\infty$ but finite N. [The general discussion is very complicated and not intuitive. This is due to the complex expressions of, e.g., the normalization given in Eq. (9).] In this case the inverse square of the normalization [Eq. (9)] can be approximated by

$$\mathcal{N}^{-2}_{Nn_0}\rightarrow(N+n_0)!(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^{N+n_0}. \tag{34}$$

Also the factor $[1+\gamma_1\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^{N+n_0-k}$ in Eqs. (13) and (14) can be approximated by

$$[1+\gamma_1\gamma_2(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^{N+n_0-k}\rightarrow(\gamma_1\gamma_2)^{N+n_0-k}(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})^{N+n_0-k}. \tag{35}$$

These are the terms which become important for the expectation value of $\mathbf{n}_\pi$ and $\mathbf{n}^2_\pi$ which is proportional to the total spin 0 in Eq. (13) and also the intermediate spins equal to 0 in Eq. (14). With these approximations, the expectation value of $\mathbf{n}_\pi$ is given by $(N+n_0)$ and for $(\mathbf{n}_\pi)^2$ by $(N+n_0)(N+n_0-1)$. So they approach a constant value. The expectation value of the sum $[\gamma\mathbf{n}_\pi+\eta\mathbf{C}_2((n_\pi,0))+\beta\mathbf{L}^2]$ is given in this limit by

$$\langle\boldsymbol{\alpha}|[\gamma\mathbf{n}_\pi+\eta\mathbf{C}_2((n_\pi,0))+\beta\mathbf{L}^2]|\boldsymbol{\alpha}\rangle \rightarrow(N+n_0)\left[\left(\gamma+3\eta+\frac{2}{\sqrt{3}}\beta\right)+\eta(N+n_0-1)\right]. \tag{36}$$

With the parameter values given in Eq. (32) the potential approaches for $N=8$ the value $+80.2$; i.e., now the bending over of the potential has been avoided. One can also see when the bending over approximately starts by determining at which value this assymptotic constant is zero. This is the case for $N\approx18$. The explanation, given here, is the same for the next case studied in this contribution.

The anharmonic contribution in Eq. (33) being small allows us to *estimate* the position of the first excited 1^- state, representing a relative excitation. Assuming that the radial kinetic energy is quadratic and the mass is nothing but the effective mass $\mu=m_O m_\alpha/(m_O+m_\alpha)=(16\times4/20)m=(16/5)m$ we arrive at

$$\hbar\omega_r=\hbar\sqrt{\frac{C_r}{\mu}}\approx7.024\ \text{MeV}, \tag{37}$$

where $C_r=2\times1.9078$ is the stiffness of the radial potential and we used $\hbar c\approx197$ MeV fm, $mc^2\approx938$ MeV. This has to be compared with the experimental observation of 5.785 MeV [16] which is fairly close, considering the simplicity of our approach.

B. ^{12}C+α

This system represents the next level of complexity with one of the clusters deformed. The Hamiltonian with parameters fitted to the experimental data [14] takes the form

$$\mathbf{H}=-29.416+13.921\mathbf{n}_\pi-0.5738\mathbf{n}_\pi(\mathbf{n}_\pi+3) -0.0896\mathbf{C}_2((\lambda,\mu))+0.5422\mathbf{K}^2+0.2038\mathbf{L}^2. \tag{38}$$

Here $\mathbf{K}^2$ is the K-band splitting operator as introduced in Ref. [6]. This operator splits the degeneracy of the 2^+ states belonging to the γ-vibrational band and to the ground-state one. Since we defined the potential as the expectation value with respect to the 0^+ state with $K=0$, this term does not contribute.

In deriving the potential we use Eq. (30) for the expectation value of the second-order Casimir operator and Ref. [10] for the relation of the quadrupole variables α_{2m} of ^{12}C [see Eq. (16)] to the deformation and orientation variables (β,θ_2) (see Appendix A). An index C will indicate that we deal with ^{12}C. Using Eqs. (28)–(30) and Appendix A the potential can be expressed as

$$V(r)=-41.925+[2.0467+0.2329\beta_C(3\cos^2\theta_{2C}-1)] \times(r-r_0)^2-0.018\,68(r-r_0)^4. \tag{39}$$

Note that for ^{12}C the value of β_C is -0.66 (oblate deformation) and thus the lowest positon in energy is for $\theta_{2C}=0°$. This means that the symmetry axis of the ^{12}C nucleus coincides with the molecular z axis; i.e., the α particle is approaching along the symmetry axis of the ^{12}C nucleus. This is the orientation we will discuss; i.e., we assume that the molecular system is within that minimum and investigate how the potential behaves as a function in the intermolecular distance. Of course, the potential depends also on the angle θ_{2C} and the deformation variable β_C. What we do is to construct a cut through the multidimensional potential energy surface. The stiffness parameters in θ_C as an example can be obtained by expanding in Eq. (39) around the minimum. As in the ^{16}O+α system the potential in r is a shifted harmonic oscillator with a slight anharmonic contribution. As a possible average value of β_C we took the one from Ref. [17]. In what follows we will discuss the orientation where $\theta_{2C}=0°$. The position of the minimum of the nuclear molecular potential is, according to Eq. (25) at $r_0=3.45$ fm. One would expect a deformation-dependent r_0, however, Eq. (25) was derived without reference to the deformation of the clusters, and therefore r_0 is best considered an average value.

When the radius of ^{12}C along the symmetry axis is calculated we obtain, using the formulas given in Ref. [10], a value of 3.595 fm. For the α particle we obtain a spherical radius of 2.064 fm. Therefore, the touching distance of the clusters is 5.659 fm with $\beta_C=-0.66$. This has to be compared to the above value of r_0. Of course, we assumed the formula for a box distribution of the mass for the nuclei. We know that this is not the case for light nuclei, especially for the α particle. The above values suggest that the minimum of the potential is well inside of the touching configuration. Now we discuss the potential.

Using Eq. (39) we obtain

$$V_1(r)=-41.925+1.8138(r-r_0)^2-0.018\,68(r-r_0)^4, \tag{40}$$

from where we can deduce, in analogy to the case $^{12}\mathrm{O}+\alpha$, the position of the first excited 1^- state 6.926 MeV. This has to be compared with the experimental first excited $J^\pi=1^-$ state: 7.117 MeV. We therefore conclude that a good qualitative agreement exists between experiment and the simple procedure. We note that the orientation where the Coulomb energy is highest is lowest in energy, although one would have expected naively the other way around (because of the higher Coulomb repulsion). The difference must come from the nuclear interaction. Following *ab initio* studies in similar systems [18], where the potential energy surface was calculated, we are in agreement with these results.

We mention that the remarkable agreement between the predicted and observed energy of the $J^\pi=1^-$ states can be attributed to the application of the standardized Hamiltonian [14]. The results are definitely poorer using the parameters of the nonstandardized Hamiltonians.

We would like to clarify one paradox. The united system in the last example is ^{16}O, which is a spherical nucleus. Nevertheless, the two clusters are at a finite distance, which seems to present a contradiction. This contradiction is virtual as can be seen in what follows: The spherical structure of the ground state is reflected in the harmonic oscillator [or SU(3)] picture by the fact that the oscillator quanta belonging to the nucleons are distributed isotropically in space; i.e., all the directions are equally important. The same is valid in the cluster approach, together with the extra point that some of the oscillator quanta of the united nucleus are assigned to the *deformed* core nucleus and some to the *relative* motion (the last contains more than zero quanta and thus represents a finite distance between the clusters). Together with the relative oscillation quanta the ground state of ^{16}O has in each direction four quanta.

V. SUMMARY AND CONCLUSIONS

This contribution was motivated by finding a geometrical connection of the semimicroscopic algebraic cluster model. In order to obtain this connection we followed the basic ideas of Ref. [8] with the essential difference that a minimal number of π bosons has to be introduced. This condition stems from the Pauli principle and the fact that the sum of oscillator quanta of the two clusters is less than the number of oscillator quanta of the united system. As a consequence of introducing a minimal number of π bosons the resulting potential by construction will have a *minimum at a relative distance different from zero*. Its distance from the origin is proportional to the square root of this minimal number. In calculating the expectation values we implemented at the end the limit of $N\rightarrow\infty$. In the parameter value α_m the formulas are the same as using $n_0=0$. Nevertheless, the explicit formulas can be used in order to deduce which approximated potential is to be employed in the actual microscopic calculation where the number N is chosen finite.

We applied the procedure to two simple systems. In the first one ($^{16}\mathrm{O}+\alpha$) both clusters have defomation zero and the corresponding Hamiltonian is particularly simple. The calculated value r_0 is consistent with the assumption that the minimum of the nuclear molecular potential should be approximately at the touching distance of the two clusters (assuming a box distribution in mass). We also estimated the position of the first excited 1^- state. This was possible because the anharmonic contribution in the relative distance turned out to be very small. The result of 7.024 MeV is of qualitative and order of magnitude agreement with the experimental observed one which is at 5.785 MeV. In the second case ($^{12}\mathrm{C}+\alpha$) one cluster is strongly oblate deformed ($\beta_C=-0.66$ [17]) and the other one (the α particle) is spherical. Also in this case the Hamiltonian is simple, though more complicated than in the first case. The potential depends now also on the deformation of the carbon nucleus and on its orientation with respect to the molecular z axis, which is defined to be along the vector connecting both clusters [20]. The minimum corresponds to the situation where the α particle approaches the ^{12}C nucleus along to the symmetry axis of the ^{12}C nucleus. This is in agreement with the algebraic considerations [19] and with the calculation of the potential energy surface in related cluster systems [18]. The estimated position of the first excited 1^- state is at 6.926 MeV compared to the experimental one, which is 7.117 MeV. The agreement is surprisingly good and is partly accidental. This positive result is also due to the new, standardized parametrization of the model Hamiltonian [14], allowing a consistent description of neighboring core$+\alpha$ systems. The results may change slightly when the deformation variables are treated dynamically.

Comparing also the calculated $r_0=3.45$ fm with the estimation of the touching distance, it agrees qualitatively with it. The overlap with the ^{12}C nucleus is larger than in the case with ^{16}O. Of course, the assumption of a box distribution of the mass, which entered in the estimation, is quite rough and, therefore, the deduced value of r_0 can be considered to be consistent with this estimation.

The method, presented in this paper, is able to give a relation of the semimicroscopic algebraic cluster model to a geometrical picture. With it the results can be, at least qualitatively, compared with other procedures where potential energy surfaces are deduced (or fitted). In fact, our method can also be used in order to propose starting potentials (estimations). It can also be applied in a systematic study where one is interested in how nuclear molecular potentials can be formed and how it depends on the underlying cluster structure.

ACKNOWLEDGMENTS

We acknowledge fruitful discussions with R. Bijker and A. Frank (ICN-UNAM). This work is supported by CONACyT-MTA Collaboration Grant No. E120-550/95 and the OTKA Project No. T014321.

APPENDIX A: NUCLEAR MOLECULAR DEGREES OF FREEDOM

In Ref. [20] the degrees of freedom of a nuclear molecule are discussed. There is the relative distance of the two clusters and two internal deformation variables of each nucleus. Additionally there are seven angular degrees of freedom. Two of them describe the orientation of the relative distance vector in the laboratory frame. Defining as in Ref. [20] the z axis of the molecular intrinsic frame along the relative distance vector, the orientation of one cluster is described by two Euler angles, the first is a rotation along the y axis (arbitrarily defined) and the second a rotation around the z axis of the intrinsic system of the *nucleus*. The orientation of the second cluster is then given by three Euler angles defined with respect the molecular axis.

The situation simplifies significantly when one cluster is spherical (e.g., the second cluster) and the other is axially symmetric. For example, in a spherical nucleus no Euler angles are needed and in an axially symmetric nulceus a rotation of its intrinsic z axis does not affect the nucleus. Also an axially symmetric nucleus has only one intrinsic deformation variable, i.e., β, which is negative for oblate nuclei. For the cases discussed in this paper, this is the situation we encounter. Therefore, we only have to deal with *three* degrees of freedom (apart from the two angles describing the orientation of the relative distance vector to the laboratory frame). These are the relative distance of the clusters, the deformation variable β, and the orientation angle of the intrinsic z axis of the deformed nucleus with respect to the molecular z axis (the deformation variable γ is implicitly present in the sign of β).

Having defined the molecular z axis along the relative distance vector, which coincides with the direction of α_m, one finds that the variable α_m in the molecular frame is just $\alpha_0 = i\alpha$. The factor i is chosen in order to have the correct transformation properties with respect to complex conjugation, i.e., $\alpha^m = (-1)^{1-m}\alpha_{-m}$. As shown in Eq. (29) a typical interaction includes the coupling $[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[2]}_m$. It will now acquire the form

$$[\boldsymbol{\alpha}\times\boldsymbol{\alpha}]^{[2]}_m = -\sqrt{2/3}\alpha^2\delta_{m0}. \tag{A1}$$

With this and supposing that the first nucleus is deformed and axially symmetric, the last term in Eq. (29) can be rewritten as

$$-\frac{1}{2}\sqrt{\frac{5}{\pi}}NN_{0,1}\alpha^2\beta(1)[3\cos^2\theta_2(1)-1]. \tag{A2}$$

We have used that the deformation variable $\alpha_{20}(1)$ is given by [10]

$$\alpha_{20} = \tfrac{1}{2}\beta(1)[3\cos^2\theta_2(1)-1], \tag{A3}$$

where $\beta(1)$ is the deformation and $\theta_2(1)$ the orientation angle of the symmetry axis of the nucleus with respect to the molecular z axis.

When relation (27) is assumed, we get, for expression $(A2)$,

$$-\frac{1}{2}\left(\frac{m\omega}{2\hbar}\right)\sqrt{\frac{5}{\pi}}N_{0,1}\beta(1)[3\cos^2\theta_2(1)-1](r-r_0)^2. \tag{A4}$$

APPENDIX B: EXTENSION TO A SYMMETRIC SYSTEM

Up to now only asymmetric systems have been considered. In order to include symmetric systems one has to symmetrize the coherent trial state of Eq. (6) with respect to the parity transformation. Because the π boson changes its sign under this transformation, the state $|\boldsymbol{\alpha}\rangle$ changes to

$$|-\boldsymbol{\alpha}\rangle = \mathcal{N}_{Nn_0}[\sigma^\dagger - (\boldsymbol{\alpha}\cdot\boldsymbol{\pi}^\dagger)]^N|0\rangle. \tag{B1}$$

The new trial state has the form

$$|\boldsymbol{\alpha}) = \mathcal{N}(|\boldsymbol{\alpha}\rangle + |-\boldsymbol{\alpha}\rangle). \tag{B2}$$

The normalization constant $\mathcal{N}$ is given by

$$\mathcal{N}^{-2} = 2(\langle\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle + \langle\boldsymbol{\alpha}|-\boldsymbol{\alpha}\rangle) \tag{B3}$$

where we used that $\langle-\boldsymbol{\alpha}|-\boldsymbol{\alpha}\rangle = \langle\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle$ and $\langle-\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle = \langle\boldsymbol{\alpha}|-\boldsymbol{\alpha}\rangle$. The first term in Eq. (B3) was derived in the main text. The second one is obtained with the same methods. The result is

$$\langle\boldsymbol{\alpha}|-\boldsymbol{\alpha}\rangle = \frac{{}_2F_1(-n_0,-N;1;-(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})/[1-(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})])}{{}_2F_1(-n_0,-N;1;-(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})/[1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})])} \times\left[\frac{1-(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}{1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}\right]^N \to\left[\frac{1-(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}{1+(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})}\right]^N, \tag{B4}$$

where the arrow gives the limit of $N\to\infty$. Because of the appearence of the exponential N, we cannot neglect the $(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})$. Remember that the α_m is inversely proportional to $\sqrt{N}$. Therefore, using Eq. (27) the $[1\pm(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]$ is proportional to

$$[1\pm(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})]^N \approx\left[1\pm\left(\frac{m\omega}{2\hbar}\right)\frac{(r-r_0)^2}{N}\right]^N \to e^{\pm(m\omega/2\hbar)(r-r_0)^2}.$$

With this, the normalization factor acquires the form

$$\mathcal{N} = \frac{1}{[2(1+e^{-(m\omega/\hbar)(r-r_0)^2})]^{1/2}}. \tag{B5}$$

Now we consider the evaluation of the expectation value of

$$\mathbf{O}=\pi^{\dagger}_{m_1}\ldots\pi^{\dagger}_{m_k}\pi_{n_1}\ldots\pi_{n_k},$$

where the number of creation operators is equal to the number of annihilation operators. As in the main text we apply the creation operators to the left and the annihilation operators to the right. The expectation value of $\mathbf{O}$ with respect to the new trial state is given by

$$(\boldsymbol{\alpha}|\mathbf{O}|\boldsymbol{\alpha})=2\mathcal{N}(\langle\boldsymbol{\alpha}|\mathbf{O}|\boldsymbol{\alpha}\rangle+\langle\boldsymbol{\alpha}|\mathbf{O}|-\boldsymbol{\alpha}\rangle). \tag{B6}$$

(We used that $\langle-\boldsymbol{\alpha}|\mathbf{O}|\boldsymbol{\alpha}\rangle=\langle\boldsymbol{\alpha}|\mathbf{O}|-\boldsymbol{\alpha}\rangle$ and $\langle-\boldsymbol{\alpha}|\mathbf{O}|-\boldsymbol{\alpha}\rangle=\langle\boldsymbol{\alpha}|\mathbf{O}|\boldsymbol{\alpha}\rangle$.)

The first term is evaluated in the same way as for asymmetric systems while for the second we have to take into account that each application of an annihilation operator to the right gives an extra sign. With this we obtain finally

$$\begin{aligned}(\boldsymbol{\alpha}|\pi^{\dagger}_{m_1}\ldots\pi^{\dagger}_{m_k}\pi_{n_1}\ldots\pi_{n_k}|\boldsymbol{\alpha})&\\ =\frac{[1+(-1)^k e^{-(m\omega/\hbar)(r-r_0)^2}]}{[1+e^{-(m\omega/\hbar)(r-r_0)^2}]}&\\ \times\langle\boldsymbol{\alpha}|\pi^{\dagger}_{m_1}\ldots\pi^{\dagger}_{m_k}\pi_{n_1}\ldots\pi_{n_k}|\boldsymbol{\alpha}\rangle.&\end{aligned} \tag{B7}$$

Note that for $r=r_0$ this gives identical results as in the asymmetric case if $k=$even and it gives zero contribution if $k=$odd, all in the limit when $N\to\infty$. Away from $r=r_0$ there is a nonvanishing contribution also for $k=$odd, which approaches for r very far from r_0 the same result as for the asymmetric case.

[1] J. Cseh, Phys. Lett. B **281**, 173 (1992); J. Cseh and G. Lévai, Ann. Phys. (N.Y.) **230**, 165 (1994).
[2] F. Iachello and R. D. Levine, J. Chem. Phys. **77**, 3046 (1982).
[3] J. P. Elliott, Proc. R. Soc. London A **245**, 128 (1958); **245**, 562 (1958).
[4] K. Wildermuth and Y. C. Tang, *A Unified Theory of the Nucleus* (Academic Press, New York, 1977).
[5] R. Maass and W. Scheid, J. Phys. G **16**, 1359 (1990); R. Maass, J. Schmidt, and W. Scheid, Rev. Mex. Fís. **38**, Suppl. 2, 173 (1992).
[6] O. Castaños, J. P. Draayer, and Y. Leschber, Z. Phys. A **329**, 33 (1988).
[7] P. Ring and P. Schuck, *The Nuclear Many Body Problem* (Springer-Verlag, New York, 1980).
[8] M. W. Kirson *et al.*, Phys. Rev. Lett. **55**, 2846 (1985); A. Leviatan and M. W. Kirson, Ann. Phys. (N.Y.) **188**, 142 (1988).
[9] F. Iachello and A. Arima, *The Interacting Boson Model* (Cambridge Univeristy Press, Cambridge, England, 1987).
[10] J. M. Eisenberg and W. Greiner, *Nuclear Models I: Nuclear Theory*, 3rd ed. (North-Holland, Amsterdam, 1987).
[11] O. Castaños, P. O. Hess, J. P. Draayer, and P. Rochford, Phys. Lett. B **277**, 27 (1992).
[12] P. O. Hess, J. Schmidt, and W. Scheid, Ann. Phys. (N.Y.) **240**, 22 (1995).
[13] O. S. Roosmalen, Ph.D. thesis, Universtiy of Utrecht, 1982.
[14] G. Lévai and J. Cseh, Phys. Lett. B **381**, 1 (1996).
[15] J. Blomqvist and A. Molinari, Nucl. Phys. **A106**, 545 (1968).
[16] C. M. Lederer and V. S. Shirley, *Tables of Isotopes*, 7th ed. (Wiley, New York, 1978).
[17] K. Jones *et al.*, Phys. Rev. C **33**,17 (1986).
[18] G. Leander, S. E. Larson, Nucl. Phys. **A239**, 93 (1975).
[19] J. Cseh and W. Scheid, J. Phys. G **18**, 1419 (1992).
[20] P. O. Hess and W. Greiner, Nuovo Cimento A **83**, 76 (1984).