PHYSICAL REVIEW C **68**, 014314 (2003)

A nuclear vibron model applied to light and heavy nuclear molecules

Huitzilin Yépez-Martínez and Peter O. Hess*
Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México Circuito Exterior, C.U., Apartado Postal 70-543, 04510 México D.F., México

Şerban Mişicu†
Institut für Theoretische Physik, J.W.v.-Goethe Universität, Robert-Mayer Str. 8-10, 60325 Frankfurt am Main, Germany and National Institute for Nuclear Physics, Bucharest, P.O. Box MG6, Romania

(Received 12 February 2003; published 29 July 2003)

A nuclear vibron model for nuclear molecules consisting of two clusters with inner structure is investigated. The Hamiltonian model has a $U_{C_1}(6)\otimes U_{C_2}(6)\otimes U_R(4)\supset SU_{C_1}(3)\otimes SU_{C_2}(3)\otimes SU_R(3)$ dynamical symmetry. Applying a geometrical mapping, the relation of the parameter of the coherent state to the relative distance of the two clusters is deduced. The Hamiltonian model exhibits a minimum at relative distances different from zero. It is discussed how to deduce the potential, knowing the spectrum, and how to deduce the spectrum, knowing the potential. As a classical example the system $^{12}C+^{12}C$ is taken, where the spectrum is known and the internuclear potential can be obtained. This system serves as a consistency check of the method. Afterwards, the heavy system $^{96}Sr+^{146}Ba$, playing a role as a subsystem of a possible three cluster molecule, is investigated and the possible structure of the spectrum is deduced. We show that in order to obtain a Hamiltonian consistent with a geometrical picture, the structure of this Hamiltonian is restricted. Ambiguities of the structure of the spectrum still exist but can be ordered into different classes.

DOI: 10.1103/PhysRevC.68.014314 PACS number(s): 21.60.Ev, 21.60.Fw, 21.60.Gx

I. INTRODUCTION

Nuclear molecules were observed for the first time in 1960 [1] in the dispersion of $^{12}C+^{12}C$. Since then, several new molecular systems were discovered (see the compilation of Ref. [2]). On the theoretical side, there exist numerous models to describe the formation of nuclear molecules. For example, in Ref. [3] the system is described by a two-center harmonic oscillator, which merges, in case of fusion, to a single harmonic oscillator, as a function of an adiabatic distance parameter. In Ref. [4] the double-resonance mechanism was used to describe the formation of a nuclear molecule and in Ref. [5] the band-crossing model was introduced. A complete overview of the advances in the last decades is given in Ref. [6].

Later, in Ref. [7] an algebraic model (the vibron model) is presented and successfully applied to the $^{12}C+^{12}C$ system [8]. No internal structure of the clusters was taken into account. The relative motion of the clusters is described by an $U_R(4)$ group, where the dynamical symmetry chain $U_R(4)\supset SO_R(4)$ was used (the index R refers to the relative motion). This chain produces a minimum in the relative potential [9], which is believed to be not the case for the $U_R(3)$ dynamical symmetry, which produces in general an anharmonic oscillator. In Ref. [10] the same system was investigated within the vibron model and in Ref. [11] within the nuclear Semimicroscopic Algebraic Cluster Model, taking into account the Pauli principle. There, it was found that the $U_R(3)$ dynamical chain is more appropriate for the description of the relative motion, a result that is very important for our procedure.

In Refs. [12,13] the nuclear vibron model with internal structure of the clusters was introduced for the description of spectra at low energy. After a general discussion, the model is restricted to one deformed cluster with the other participants being spherical (α clusters). The model is intended to describe the cluster structure of a nucleus at *low* energy, contrary to our intention to restrict to the molecular resonance sector only. The model [13] was successfully applied to various heavy nuclei [14]. Though, the application produces good agreement with the experiment, the Pauli Exclusion Principle should be important because of large overlap of the α particles with the core at low energy [15].

In Refs. [16,17] the Semimicroscopic Algebraic Cluster Model (SACM) was introduced. As an important feature, this model observes the *Pauli Exclusion Principle*. As a consequence, the number of relative oscillation quanta is limited from below. The model was applied successfully to various nuclei [11,18], encountering several systematic behaviors of the parameters [19]. Also the coexistence of different cluster structures within the same nucleus was investigated [20]. In Ref. [21] the SACM was mapped to a potential. Due to the lower limit in the relative oscillation quanta, a minimum at a value different from 0 is produced. One advantage of the SACM is that it describes within the same model the low and high energy part, for states of positive and negative parity. The high energy part can be related to nuclear molecules.

Recently, the study of nuclear molecules revived due to the possible observation of long living heavy systems with three clusters [22]. In Ref. [23] a geometrical model was used in order to deduce the structure of the molecular spectrum. A distinctive feature is that each cluster has an

---

*Email address: hess@nuclecu.unam.mx
†Email address: misicu@th.physik.uni-frankfurt.de

inner structure, i.e., a deformation, which plays an essential role. However, the molecular system is restricted to linear configurations and harmonic interactions, otherwise no analytical results can be obtained. In Ref. [24] a triangular configuration was considered without an inner structure of the clusters, and introducing deformation for the clusters leads to a complicated structure, difficult to solve, except numerically.

The difficulties encountered in the geometrical model lead to investigate algebraic models. The first attempts were restricted to spherical clusters [25,26]. Recently a complete description of the algebraic model was given [27], also restricted to spherical clusters (especially ^{12}C as composed by three α particles). As it seems, the algebraic model is more flexible in describing complicated configurations and anharmonic interactions of nuclear molecules. However, in most cases the clusters have deformation and their influence on the structure of the nuclear molecule should be important.

In order to study the introduction of deformation of the clusters, Ref. [26] investigated the system with two clusters. As shown there, the presence of deformation in clusters is important for the formation of a relative minimum. The Hamiltonian used did not belong to a dynamical symmetry chain and a diagonalization should be performed.

The objective of this paper is to present a nuclear vibron model for nuclear molecules, using a Hamiltonian within a dynamical symmetry, and to give a connection of this model to geometrical potentials, consistent with internuclear potentials obtained by double folding methods [28]. We will assume a small overlap between the clusters, implying that the *Pauli Exclusion Principle* plays a minor role [15]. Also to study the effects when *both* clusters are deformed is interesting on its own.

We will show that the $SO_R(4)$ dynamical symmetry is not the only one that produces a minimum in the relative potential but also does the $U_R(3)$ dynamical symmetry. For the construction of the relative potential, which will depend on the relative orientation and the deformation, the coherent state technique will be used [9,29–31].

Knowing the internuclear potential will also help reduce the number of ambiguity in the parameters, alternatively to the use of electromagnetic transition rates, not available in general.

The paper is organized as follows. In Sec. II a particular nuclear vibron model will be presented. In Sec. III the geometrical mapping is discussed. A relation will be derived between the parameters of the coherent state and the relative distance. In Sec. IV the model is applied first to ^{12}C+^{12}C. The results will be compared to the model introduced in Ref. [8]. Due to the assumption that the overlap of the two clusters is small, only the energy range where the nuclear molecules are located can be described by such a model. At lower energies the *Pauli Exclusion Principle* should be observed. Because we intend to apply the model later to heavy nuclear molecules, where the overlap is small, this procedure is justified. The ^{12}C+^{12}C system was also discussed within the SACM [11] and was able to describe the low and the high energy region at the same time. Here, the investigation of ^{12}C+^{12}C mainly serves as a consistency check, i.e., that fitting the spectra first and mapping afterwards to the potential is consistent with first deducing the parameter from a given internuclear potential and then determining the spectrum. The second system investigated is ^{96}Sr+^{146}Ba, which plays a role as a subsystem in a three-cluster molecule [22]. In Sec. V conclusions are drawn.

II. THE MODEL

The vibron model [7] is combined with the Interacting Boson Approximation (IBA) [32–34] in order to form the nuclear vibron model [12,13]. For light nuclei, the IBA-4 model is used [34,35], while for heavy nuclei the IBA-1 [32–34] has to be applied. Both approaches make use of the $U(6)$ group, whose generators are all possible combinations of a creation and annihilation operator of an s (spin 0) and/or a d boson (spin 2). In the IBA-4 model, there are besides the proton and neutron pair bosons also proton-neutron pair bosons. Each cluster will be represented by such a group. The relative motion is described by a $U_R(4)$ group, whose generators are composed by p bosons (spin 1) and an auxiliary s boson, different from that in the IBA, which introduces a cutoff when the total number of bosons $n_s+n_p=N_R$ is kept constant. The p bosons vary from 0 to the cutoff value. The large group is given by the direct product $G=U_{C_1}(6)\otimes U_{C_2}(6)\otimes U_R(4)$, where the index C_i refers to the ith cluster and R refers to the relative motion.

There are many possible subgroup chains, each corresponding to a dynamical symmetry. The general classification will be done elsewhere [36] and the method, presented in this contribution, can be applied to all other situations. Here, in particular, we will discuss the chain

$$\begin{aligned}
&U_{C_1}(6)\otimes U_{C_2}(6)\otimes U_R(4)\supset SU_{C_1}(3)\otimes SU_{C_2}(3)\otimes SU_R(3)\\
&\qquad\supset[N_1]\ \ [N_2]\ \ [N_R]\ \ (\lambda_1,\mu_1)\ \ (\lambda_2,\mu_2)(n_R,0)\\
&\qquad\supset SU_C(3)\otimes SU_R(3)\supset SU(3)\supset SO(3),\\
&\qquad\qquad\rho_c\ \ (\lambda_C,\mu_C)\ \ (n_R,0)(\lambda,\mu)\quad \kappa L \qquad (1)
\end{aligned}$$

where N_i gives the number of bosons in the IBA model, n_R in the total number of bosons in the relative motion, (λ_i,μ_i) denotes the $SU(3)$ representation of the ith cluster, (λ_C,μ_C) is the $SU(3)$ irrep (irreducible representation) to which the two clusters are coupled, (λ,μ) is the total $SU(3)$ irrep, L is the angular momentum, and ρ_C and κ are multiplicity indices. No multiplicity appears in the reduction of $SU_C(3)\otimes SU_R(3)$ to the total $SU(3)$ group, because the irrep of $SU_R(3)$ is symmetric. The κ value can be approximately related to the projection of the angular momentum L on the intrinsic z axis [37]. In the case of a symmetric system, the additional condition $(\lambda+\mu+n_R)=$even has to be observed [17]. Note that for symmetric systems, such as ^{12}C+^{12}C, where no inner structure is taken into account ($\lambda=\mu=0$), only $n_R=$even is allowed, which implies $L=$even and positive parity. However, when the inner structure is included, the final λ and μ values are, in general, different from 0. In this case n_R can be odd and, consequently, $L=$odd too, and negative parity is allowed.

Note that one can also substitute the $U_{C_i}(6)$ groups by the microscopic $SU_{C_i}(3)$ groups, i.e., instead of working in a vibron model we can work in a *Fermion Algebraic Cluster Model*. The procedure presented in this contribution has a larger range of applicability.

A possible Hamiltonian corresponding to dynamical chain (1) can be, up to second order in the generators of the groups, given by

$$\begin{aligned}H=&\chi_1 C_2(SU_{C_1}(3))+\chi_2 C_2(SU_{C_2}(3))+\chi_{12}C_2(SU_C(3))\\&+\chi_\omega n_R+\chi_R C_2(SU_R(3))+\chi_T C_2(SU(3))\\&+\chi_N[C_2(SU_C(3))-\langle C_2(SU_C(3))\rangle_{\theta_0}]n_R+aL^2+cK^2,\end{aligned}\tag{2}$$

where χ_ω is the parameter of n_R and the other χ values give the strength of the different quadrupole-quadrupole interactions, L^2 is the angular momentum operator, and K^2 is the operator introduced in Ref. [37] whose eigenvalue κ^2 is approximately the square of the projection of the angular momentum onto the intrinsic symmetry axis. The second order Casimir operators are a function of the angular momentum operators and the quadrupole operators. The n_R in the first line in Eq. (2) is the number operator of the relative oscillation quanta. The significance of the term proportional to χ_N will be explained later on. It will allow us to reproduce the correct position of the minimum in a cut through the potential at a given relative orientation, different from that at the absolute minimum. The expression $\langle\cdots\rangle$ contains geometric information and we will show below that to obtain a suitable Hamiltonian, geometric information is indispensable, otherwise inconsistencies with the calculated internuclear potential appears. For example, the minimum of the mapped potential at inclination angles different from 0 would be far off the correct position and the number of relative quanta at the equilibrium position would not be that of the lowest state of the molecular system.

The Hamiltonian in Eq. (2) is an extension of that proposed by Daley and Iachello [13], where only one deformed and one spherical clusters were considered. Some new terms are, e.g., the K^2 and the χ_N term. Surely, the Hamiltonian in Eq. (2) is not the most general one and further terms should be added in order to get a complete description of two-cluster molecules. However, our intention is to keep as simple the Hamiltonian as possible. Furthermore, as will be seen later on, the Hamiltonian proposed can already reproduce sufficiently the mean features of the structure of nuclear molecules and the internuclear potential. One possible reason is that the Hamiltonian in Eq. (2) renders the quadrupole-quadrupole interaction as the dominant one, which is a reasonable assumption for large extended and deformed systems, as the nuclear molecule.

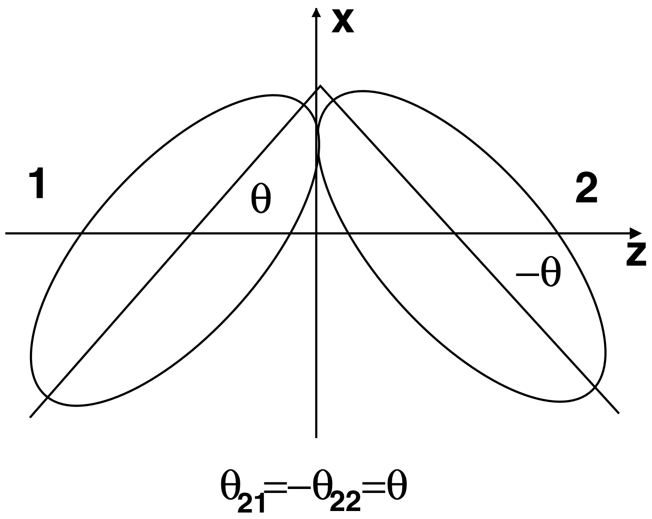

FIG. 1. The intrinsic system of the nuclear molecule. The z axis connects the two centers of masses. For prolate deformed nuclei, the diagonal lines indicate the symmetry axes. For oblate deformed nuclei, the symmetry axes are perpendicular to the diagonal lines.

For the cluster quadrupole operators we have [32,34]

$$Q_{\mathrm{IBA}-i,m}=[d^\dagger_{im}\tilde{s}+s^\dagger\tilde{d}_{im}]\pm\sqrt{\frac{7}{4}}\,[d^\dagger\otimes\tilde{d}]^2_m,\tag{3}$$

where the positive sign refers to oblate and the negative sign refers to prolate nuclei. The index i in Eq. (3) refers to the number of the cluster and m is the magnetic component of the quadrupole operator.

The eigenvalue of Hamiltonian (2) with respect to the basis defined by dynamical group chain (1) is given up to a constant by

$$\begin{aligned}E=&\chi_1[\lambda_1^2+\mu_1^2+\lambda_1\mu_1+3(\lambda_1+\mu_1)]+\chi_2[\lambda_2^2+\mu_2^2+\lambda_2\mu_2\\&+3(\lambda_2+\mu_2)]+\chi_{12}[\lambda_C^2+\mu_C^2+\lambda_C\mu_C+3(\lambda_C+\mu_C)]\\&+\chi_\omega n_R+\chi_R(n_R^2+3n_R)+\chi_T[\lambda^2+\mu^2+\lambda\mu+3(\lambda+\mu)]\\&+\chi_N\{[\lambda_C^2+\mu_C^2+\lambda_C\mu_C+3(\lambda_C+\mu_C)]\\&-\langle C_2(SU_C(3))\rangle_{\theta_0}\}n_R+aL^2+cK^2.\end{aligned}\tag{4}$$

The question remains, if this dynamical symmetry exhibits a minimum in the relative potential. To show it, the geometrical mapping will be discussed in the following section.

III. THE GEOMETRICAL MAPPING

First, we consider the relative motion, using the coherent state technique [9,29,31]. It is sufficient to consider the system with respect to the molecular system defined as follows (see Fig. 1): The molecular z axis is along the vector connecting the centers of masses of each cluster. In this system, there are only p_0 bosons in the relative motion. The coherent state is given by

$$|N_R,\alpha_R\rangle=\frac{(s^\dagger+\alpha_R p_0^\dagger)^{N_R}}{\sqrt{N_R!(1+\alpha_R^2)^{N_R}}}|0\rangle, \tag{5}$$

where α_R is the parameter of the normalized coherent state.

The parameter α_R has to be related to the relative distance r of the two clusters. We start from the definition of the physical relative distance operator, before the auxiliary s boson was introduced, quantized with respect to the harmonic oscillator with frequency ω_r:

$$\boldsymbol{r}_m=\sqrt{\frac{\hbar}{2\mu\omega_r}}(p_m^\dagger+p_m). \tag{6}$$

Due to the artificial introduction of a cutoff (N_R), having added an additional s-boson operator, the relative distance operator has to be modified such that N_R is conserved and for large cutoff values $(N_R\to\infty)$ both operators have the same matrix elements, save a contribution from $n_s=s^\dagger s$ (see below). Therefore, we define the algebraic distance operator [9] by

$$\boldsymbol{r}_m^a=\sqrt{\frac{\hbar}{2\mu\omega_r}}(p_m^\dagger s+s^\dagger p_m), \tag{7}$$

and

$$r_m=\frac{\langle \boldsymbol{r}_m^a\rangle}{\sqrt{\langle s^\dagger s\rangle}} \tag{8}$$

as the distance variable, where $\langle s^\dagger s\rangle$ is the expectation value of $s^\dagger s$ with respect to the coherent state. The upper index "a" refers to "algebraic" and m is the spherical component. Because the two nuclei are connected via the r_0 (z) axis, only r_0 will be important and is equal to the internuclear distance r. The variation of the algebraic operator has to be calculated too. If the variation is small compared to the expectation value, the distance variable gives the approximated distance of the two clusters. The variation is proportional to $1/N_R$, which is very small for large N_R, as will be the case here. For very small distances the variation is of the same order of the expectation value and the interpretation of r_m as a distance is inaccurate. For the situation discussed here, the distance is always large (small overlap). The definition of the relative distance is consistent with the Generator Coordinate Method (GCM) in the Gaussian overlap approximation without the contribution from the zero point motion [38]. In this approximation the collective potential is given by the expectation value of the Hamiltonian. Other observables are determined through their expectation value with respect to the trial state. In this sense it deviates from other definitions of the relative coordinate [9,34,39].

With this in mind, calculating the expectation value of algebraic distance operator (7) with respect to coherent state (4) we obtain for the absolute value r of the distance variable

$$\frac{r}{b\sqrt{2N_R}}=\frac{\alpha_R}{\sqrt{(1+\alpha_R^2)}}, \tag{9}$$

where $b=\sqrt{\hbar/\mu\omega_r}$ is the oscillator length.

Because the variable α_R ranges from 0 to ∞, r varies from 0 to a maximum value $b\sqrt{2N_R}$. In order to describe a nuclear molecule, the values of b and N_R have to be such that r ranges from 0 up to several fm above the distance where the two clusters are barely touching, defined as $R_{01}+R_{02}$ where R_{0i} is the nuclear radius of cluster i $(i=1,\ 2)$ in the direction of the molecular z axis. This implies a large N_R and thus a correct interpretation of r as the internuclear distance. As will be shown below, for large N_R the potential will depend explicitly only on the oscillator length b, and not on N_R.

As can be seen from Eq. (9) the parameter α_R is approximately proportional to r for small values of α_R. However, in general, this is not the case and one has to take great care in *not identifying* α_R *directly with the distance* r.

There is another definition of the parameter of the coherent state, i.e., $\sim(\sqrt{(1-\delta_R^2)}s^\dagger+\delta_R p_0^\dagger)^{N_R}|0\rangle$ [9]. In this form the relative distance is directly proportional to the parameter δ_R. However, due to the square root the permitted range of δ_R is limited between 0 and 1. This results into the same constraint in r as given above.

Let us now turn our attention to the structure part of each cluster, described by the IBA-1 (for heavy clusters) or IBA-4 (for light clusters). We have to use the following coherent state [30]. (In the following section we will show that for light nuclei, where the IBA-4 model [34,35] has to be applied and there are proton-proton, neutron-neutron, and proton-neutron bosons, the distinction of the different bosons can be skipped for a particular representation.)

$$|N_i;\beta_i,\theta_{2i}\rangle=\frac{(\hat{s}^\dagger+\alpha_{i2}\hat{\boldsymbol{d}}_i^\dagger)^{N_i}}{\sqrt{N_i!(1+\alpha_i^2)^{N_i})}}|0\rangle, \tag{10}$$

where $\alpha_{i2}\hat{\boldsymbol{d}}_i^\dagger=\Sigma_m\alpha_{i2m}\hat{d}_{i2m}^\dagger$ and $\alpha_i^2=(\alpha_{i2}\cdot\alpha_{i2})$.

In general, the values of the coefficients α_{i2m} are given by the expression $\alpha_{i2m}=\Sigma_{m'}D_{mm'}^{(2)*}(\theta_i)a_{i2m'}$, [40] where in the intrinsic reference system of each one of the nuclei we have the usual relations: $a_{i20}=\beta_i^{\mathrm{IBA}}\cos\gamma_i$, $a_{i2\pm1}=0$, and $a_{i2\pm2}=(\beta_i^{\mathrm{IBA}}/\sqrt{2})\sin\gamma_i$, where the index IBA refers to the deformation variable used with the IBA model (see below).

We concentrate now our attention to axially symmetric nuclei only, i.e., $\gamma=0$ with $\beta^{\mathrm{IBA}}>0$ for prolate and $\beta^{\mathrm{IBA}}<0$ for oblate nuclei. For these cases, $\alpha_{i2\mu}$ are given by $\alpha_{i2m}=\beta_i^{\mathrm{IBA}}\,D_{m0}^2(\theta_{2i})$, implying $a_{i2\mu}=\beta_i^{\mathrm{IBA}}\delta_{\mu0}$.

We finally obtain, with respect to the molecular system, defined in Fig. 1, $\alpha_{i20}=\frac{1}{2}\beta_i^{\mathrm{IBA}}(3\cos^2\theta_{2i}-1)$, $\alpha_{i2\pm1}=\pm\sqrt{\frac{3}{8}}\beta_i^{\mathrm{IBA}}\sin(2\theta_{2i})$, and $\alpha_{i2\pm2}=\sqrt{\frac{3}{8}}\beta_i^{\mathrm{IBA}}\sin^2(\theta_{2i})$, where θ_{2i} is the inclination angle of the symmetry axis of cluster i with respect to the molecular z axis.

The complete coherent state is given by the direct product of coherent state of the relative motion (5) and the two coherent states related to inner structure (10). The expectation value of the Hamiltonian (2) with respect to this total coherent state is calculated for $L=0$, $K=0$ $(\kappa=1)$. We obtain, using V instead of $\langle H\rangle$ (for a short hand notation we use $\beta_i^{\mathrm{IBA}}=\beta_i$),

$$
\begin{aligned}
V=&(\chi_1+\chi_{12}+\chi_T)\left[10N_1+\frac{4N_1(N_1-1)\beta_1^2}{(1+\beta_1^2)^2}\left(2\pm\sqrt{2}\beta_1+\frac{1}{4}\beta_1^2\right)\right]+(\chi_2+\chi_{12}+\chi_T)\left[10N_2+\frac{4N_2(N_2-1)\beta_2^2}{(1+\beta_2^2)^2}\right.\\
&\left.\times\left(2\pm\sqrt{2}\beta_2+\frac{1}{4}\beta_2^2\right)\right]+(\chi_R+\chi_T)\left(\frac{2}{b^2}r^2+\frac{1}{4b^4}r^4\right)+\chi_\omega\frac{1}{2b^2}r^2+(\chi_{12}+\chi_T)\frac{8N_1N_2\beta_1\beta_2}{(1+\beta_1^2)(1+\beta_2^2)}\left(1\pm\frac{\beta_1}{2\sqrt{2}}\right)\left(1\pm\frac{\beta_2}{2\sqrt{2}}\right)\\
&\times[3\cos^2(\theta_{21}-\theta_{22})-1]+\sqrt{2}\chi_T\frac{1}{b^2}r^2\frac{N_1\beta_1}{1+\beta_1^2}\left(1\pm\frac{\beta_1}{2\sqrt{2}}\right)[3\cos^2(\theta_{21})-1]+\sqrt{2}\chi_T\frac{1}{b^2}r^2\frac{N_2\beta_2}{1+\beta_2^2}\left(1\pm\frac{\beta_2}{2\sqrt{2}}\right)[3\cos^2(\theta_{22})-1]\\
&+\chi_N\frac{1}{b^2}r^2\frac{4N_1N_2\beta_1\beta_2}{(1+\beta_1^2)(1+\beta_2^2)}\left(1\pm\frac{\beta_1}{2\sqrt{2}}\right)\left(1\pm\frac{\beta_2}{2\sqrt{2}}\right)\{[3\cos^2(\theta_{21}-\theta_{22})-1]-[3\cos^2(\theta_{21_0}-\theta_{22_0})-1]\},
\end{aligned}
\tag{11}
$$

where the upper (lower) sign refers to prolate (oblate) nuclei. The last term in the square bracket in the last line comes from the expectation value $\langle C_2(SU_C(3))\rangle$. The expectation value is taken at given angles of the orientation of the symmetry axes of the two clusters and guarantees that the minimum in the potential at these orientations is at the desired position. Otherwise, the structure of the Hamiltonian is too rigid and would produce a dependence in the orientation, which contradicts severely the calculated relative nuclear potential (see Sec. IV).

Note that for the case of zero deformation ($\beta_i=0,\ i=1,2$) only the terms proportional to r^2 and r^4 appear, which are all positive, except for the χ_ω term that can be negative. For $\chi_\omega\geqslant 0$ we obtain the known limit of the anharmonic oscillator. However, when the deformation parameters of the clusters are different from 0, we can obtain further the terms that depend on the relative distance variable r *and can be negative*, depending on the sign and absolute value of the χ parameters. Also if $\chi_\omega<0$ a minimum can be formed. This is a novel feature implying the formation of a deformed minimum in the limit of the dynamical symmetry $U_R(3)$ in *the relative motion*. In contrast to the usual procedure, where $\chi_\omega>0$ always and the lowest state is given by $n_R=0$, in our model χ_ω can be negative and the ground state will have a $n_R>0$.

The deformation parameters appearing in Eq. (11) are those as deduced in the coherent state. As shown in Ref. [30], they are not equal to the physical values but have to be corrected by a factor. Usually the $\beta=\beta^{\mathrm{iba}}$ value in the IBA model is by a factor 3–5 larger than the physical deformation β^{phys}. An approximate relation is [30]

$$\beta_i^{\mathrm{phys}}=1.18\left(\frac{2N_i}{A}\right)\beta_i^{\mathrm{IBA}}. \tag{12}$$

Due to additional factors, the corrections of $O(1/N_i)$ is small even for small values of N_i (up to 20%).

In Eq. (11) there is still a free scale parameter b, which was not present before in the Hamiltonian. As discussed above, the introduction of b was necessary in order to obtain the potential as a function in the relative distance, given in fm.

IV. APPLICATION TO ^{12}C+^{12}C AND ^{96}Sr+^{146}Ba

This section is divided into two parts: In Sec. IV A we investigate the light system ^{12}C+^{12}C. This system has been studied within the vibron model [8] and the nuclear vibron model [11]. The reason to do this again is that not only new experimental information about its spectrum is available here [2], but also the relative nuclear potential can be calculated, i.e., both the spectrum and the potential are known. This allows us to adjust the parameters of the algebraic model to the spectrum and deduce the relative potential, which, in turn, can be compared to the relative nuclear potential obtained by other means, e.g., double folding calculations [41]. In this way the ^{12}C+^{12}C system can be used as a test case in order to verify the validity of the result starting from a known relative nuclear potential and deduce the parameters of the algebraic Hamiltonian. It will become especially important for heavy systems where no experimental data are available and one depends strongly on theoretically determined nuclear potentials.

In the second part we will address our attention to the heavy nuclear molecule ^{96}Sr+^{146}Ba, which forms the part of a possible three-cluster nuclear molecule [22]. There are no available experimental data of the spectrum and the calculation will predict a possible structure of such a hypothetical nuclear molecule.

A. ^{12}C+^{12}C

The carbon nucleus has to be treated within the IBA-4. The appropriate group structure for the description of the nucleus ^{12}C within the IBA-4 is given by [34,35]:

$$U(36)\supset U_{ST}(6)\otimes U_{sd}(6), \tag{13}$$

where $U_{ST}(6)$ describes the isospin (T) and the spin (S) degrees of freedom.

One way to obtain the T and S labels is to reduce the $U_{ST}(6)$ group to its subgroups $SU_T(2)\otimes SU_S(2)$ of the isospin and spin groups, using as an intermediate stage of the group $SU(4)$, the Wigner supermultiplet group for bosons:

$$U(36)\supset U_{ST}(6)\otimes U_{sd}(6)\supset SU(4)\otimes U_{sd}(6)\supset (SU_T(2)\otimes SU_S(2))\otimes U_{sd}(6). \tag{14}$$

The presence of this group is expected because the six types of bosons $T=1$, $S=0$ and $T=0$ $S=1$ belong to a single representation of the group $SU(4)$, namely, the six-dimensional irrep (0,1,0).

The states lowest in energy are those symmetric in $U_{sd}(6)$. Because the $U(36)$ irrep has to be symmetric, the $U_{ST}(6)$ irrep has to be symmetric too. This irrep of $U_{ST}(6)$ contains the $SU(4)$ irreps $(0,\sigma,0)$, with $\sigma=N,N-2,\ldots,1$, or 0. The T and S values, contained in a representation $(0,\sigma,0)$, are given by the condition $T+S=\sigma,\sigma-2,\ldots,1$, or 0.

In the case of ^{12}C the number of bosons for the irreps $[N]$ of $U_{sd}(6)$ results to be $[N]=[2]$, because there are two boson holes in the valence shell (four nucleon holes). In this case the problem reduces to as if treating only one kind of s and d bosons, which justifies the use of the coherent state as given in the last section.

Since $N=2$, σ can take the values $\sigma=0,2$, and the T and S content can be obtained using the standard procedure [34]. For the reduction of the $U_{sd}(6)$ to the $SU_{sd}(3)$ group we need to take into account that $N=2$ and the (λ,μ) irreps of $SU_{sd}(3)$ are given by

$$(\lambda,\mu)=(0,4)\oplus(2,0). \tag{15}$$

This defines the $SU(3)$ content of each cluster. For the single cluster the (0,4) irrep is the lowest in energy. According to Eq. (1) the two cluster irreps are coupled to the irreps $(\lambda_C,\mu_C)=(4,0)+(3,2)+(2,4)+(6,1)+(0,8)$ of $SU_C(3)$, where (4,0) is the most prolate one [42]. It is also the lowest one in energy as pointed out in Refs. [10,11].

The parameters of the model will be adjusted to the spectrum and the geometric potential deduced. The procedure is as follows: We require that the r_0 in $n_0=\langle n_R\rangle=r_0^2/2b^2$ is equal to the position of the minimum. The equilibrium distance can be estimated in various ways, one is to calculate the radius of the nuclei in the direction of the molecular axis, or via the slope of the ground state band as a function of $L(L+1)$, or taking as r_0 the position of the minimum as it results for the internuclear potential (see further below). The derivation of r_0 from the slope was used in Ref. [8] resulting in $r_0=6.75$ fm, which is quite large because taking as deformation for ^{12}C the value 0.5 (see Ref. [43] including the correction for largely deformed nuclei [40]) and determining the distance for the touching point, assuming that the two carbon nuclei touch each other at their bellies, we get $r_0=4.75$ fm. This estimation does not assume a smooth fall off of the nuclear density and might give a too low r_0. We, therefore, prefer to use the r_0 value as obtained for the internuclear potential, i.e., $r_0=5.75$ fm. We emphasize that it is only an estimation, which, however, should be in the correct range. r_0^2 depends on the number of oscillation quanta via the relation

$$r_0^2=2b^2n_0. \tag{16}$$

Equation (16) expresses the fact that for the construction of a wave function, whose dominant contribution is around r_0, one needs n_0 oscillation quanta and this value depends on the stiffness of the basis oscillator, expressed by the oscillator length.

The variable n_R also appears in the expression of energy (4). In order to have consistency, we have to require that $E(n_R)$ is minimal at $n_R=n_0$, where n_R is treated as a continuous variable. This condition gives the relation

$$n_0=-\frac{[3\chi_R+3\chi_T+\chi_\omega+\chi_T(2\lambda_C+\mu_C)]}{2(\chi_R+\chi_T)}-\frac{\chi_N[\lambda_C^2+\mu_C^2+\lambda_C\mu_C+3(\lambda_C+\mu_C)-\langle C_2(SU_C(3))\rangle_{\theta_0}]}{2(\chi_R+\chi_T)} \tag{17}$$

and we have to require that this value is the same as that in Eq. (16). It relates the oscillator length b with n_0. In Eq. (17) the expression $\langle C_2(SU_C(3))\rangle_{\theta_0}$ refers to the numerical value of the geometrical mapped Casimir operator of $SU_C(3)$ [see Eq. (11)] at $\theta=\theta_0$. The symmetry axis of a carbon nucleus (oblate deformed) is perpendicular to the molecular axis, which connects the two nuclei (see Fig. 1). When we imagine the line connecting the center of a cluster to the touching point, we can define for ^{12}C$+^{12}$C as the new inclination angle Θ via $\theta=90°+\Theta$, where the θ is the inclination angle of the symmetry axis of a cluster with respect to the molecular axis.

After this consideration, the relative motion for the ground state is given by the irrep $(n_0,0)$ of $SU_R(3)$. When (4,0) is the lowest irrep of $SU_C(3)$ then the lowest irrep in energy is given by $(n_0+4,0)$.

In order to proceed, an assumption has to be made about the structure of the spectrum at low energy. We assume that the lowest 0^+ states are the band heads with all the same n_0 but different (λ_C,μ_C), which seems to be an *ad hoc* assumption. A different choice is to assume that these states have the same (λ_C,μ_C) but different n_0. With the first choice, however, we obtain a better agreement with the experiment, as will be seen below. (We will come back to this point when the spectrum is deduced starting from a known potential.) The relevant quantum numbers of the lowest bands are listed in Table I. The remaining χ parameters are adjusted to the lowest 0^+ states, with the above assumption of the bands at low energy. The a and c parameters are adjusted, respectively, to the moment of inertia $(a=\hbar^2/2\mu r_0^2)$ and to the position of the second 2^+ of the first total $SU(3)$ irreps

TABLE I. Irreducible representations used for the fit of the energy spectrum of the system $^{12}C+^{12}C$.

n_R	C_1 C_2	C_{12}	C_{12R}	κ	L		$C_2(SU(3)_T)$
n_0	(0,4) (0,4)	(0,8)	$(n_0,8)$	8	$L=8,9,\ldots,n_0+8$		$n_0^2+11n_0+88$
				6	$L=6,7,8,\ldots,n_0+6$		
				4	$L=4,5,\ldots,n_0+4$		
				2	$L=2,3,\ldots,n_0+2$		
				0	$L=0$ or $1,\ldots,n_0-2,n_0$		
n_0	(0,4) (0,4)	(0,8)	$(n_0-1,7)$	7	$L=7,8,\ldots,n_0+6$		$(n_0+4)^2+45$
				5	$L=5,6,\ldots,n_0+4$		
				3	$L=3,4,\ldots,n_0+2$		
				1	$L=1,2,\ldots,n_0$		
n_0	(0,4) (0,4)	(0,8)	$(n_0-2,6)$	6	$L=6,7,8,\ldots,n_0+4$		$n_0^2+5n_0+40$
				4	$L=4,5,\ldots,n_0+2$		
				2	$L=2,3,\ldots,n_0$		
				0	$L=0$ or $1,\ldots,n_0-4,n_0-2$		
n_0	(0,4) (0,4)	(1,6)	$(n_0+1,6)$	6	$L=6,7,8,\ldots,n_0+7$	not allowed by symmetry when $n_0=$even	
				4	$L=4,5,\ldots,n_0+5$		
				2	$L=2,3,\ldots,n_0+3$		
				0	$L=0$ or $1,\ldots,n_0-1,n_0+1$		
n_0	(0,4) (0,4)	(1,6)	$(n_0-1,7)$	7	$L=7,8,\ldots,n_0+6$		$(n_0+4)^2+45$
				5	$L=5,6,\ldots,n_0+4$		
				3	$L=3,4,\ldots,n_0+2$		
				1	$L=1,2,\ldots,n_0$		
n_0	(0,4) (0,4)	(1,6)	$(n_0-2,6)$	6	$L=6,7,8,\ldots,n_0+4$		$n_0^2+5n_0+40$
				4	$L=4,5,\ldots,n_0+2$		
				2	$L=2,3,\ldots,n_0$		
				0	$L=0$ or $1,\ldots,n_0-4,n_0-2$		
n_0	(0,4) (0,4)	(2,4)	$(n_0+2,4)$	4	$L=4,5,\ldots,n_0+6$		$n_0^2+11n_0+46$
				2	$L=2,3,\ldots,n_0+4$		
				0	$L=0$ or $1,\ldots,n_0,n_0+2$		
n_0	(0,4) (0,4)	(2,4)	$(n_0,5)$	5	$L=5,6,\ldots,n_0+5$	not allowed by symmetry when $n_0=$even	
				3	$L=3,4,\ldots,n_0+3$		
				1	$L=1,2,\ldots,n_0+1$		
n_0	(0,4) (0,4)	(2,4)	$(n_0-2,6)$	6	$L=6,7,8,\ldots,n_0+4$		$n_0^2+5n_0+40$
				4	$L=4,5,\ldots,n_0+2$		
				2	$L=2,3,\ldots,n_0$		
				0	$L=0$ or $1,\ldots,n_0-4,n_0-2$		
n_0	(0,4) (0,4)	(3,2)	$(n_0+3,2)$	2	$L=2,3,\ldots,n_0+5$	not allowed by symmetry when $n_0=$even	
				0	$L=0$ or $1,\ldots,n_0+1,n_0+3$		
n_0	(0,4) (0,4)	(3,2)	$(n_0+1,3)$	3	$L=3,4,\ldots,n_0+4$		$(n_0+4)^2+9$
				1	$L=1,2,\ldots,n_0+2$		
n_0	(0,4) (0,4)	(3,2)	$(n_0-1,4)$	4	$L=4,5,\ldots,n_0+3$	not allowed by symmetry when $n_0=$even	
				2	$L=2,3,\ldots,n_0+1$		
				0	$L=0$ or $1,\ldots,n_0-3,n_0-1$		
n_0	(0,4) (0,4)	(4,0)	$(n_0+4,0)$	0	$L=0$ or $1,\ldots,n_0+2,n_0+4$		$n_0^2+11n_0+28$
n_0	(0,4) (0,4)	(4,0)	$(n_0+2,1)$	1	$L=1,2,\ldots,n_0+3$	not allowed by symmetry when $n_0=$even	
n_0	(0,4) (0,4)	(4,0)	$(n_0,2)$	2	$L=2,3,\ldots,n_0+2$		$n_0^2+5n_0+10$
				0	$L=0$ or $1,\ldots,n_0-2,n_0$		

TABLE II. Energy spectrum of the system $^{12}C+^{12}C$, in our model with inner structure $[U_R(3)=U(3)]$ compared to experiment (Exp.) and the $SO_R(4)[=SO(4)]$ model [8].

$L=0$			$L=2$			$L=4$			$L=6$			$L=8$		
Exp.	$SO(4)$	$U(3)$	Exp.	$SO(4)$	$U(3)$	Exp.	$SO(4)$	$U(3)$	Exp.	$SO(4)$	$U(3)$	Exp.	$SO(4)$	$U(3)$
3.17	3.44	3.17	3.75	3.90	3.79	4.46	4.96	5.26	6.49	6.63	7.56	9.65	8.91	10.70
3.35	4.4	3.49	4.62	4.86	4.12	5.77	5.92	5.58	7.55	7.59	7.88	9.84	9.87	11.02
4.25	5.2	4.25	4.88	5.66	4.61	5.96	6.72	6.07	8.86	8.39	8.37	10.30	10.67	11.51
5.80	5.84	5.80	5.00	6.3	4.88	6.85	7.36	6.34	9.05	9.03	8.64	10.63	11.31	11.78
5.97	6.32	5.97	5.37	6.78	5.37	7.30	7.84	6.83	9.33	9.51	9.13	10.90	11.79	12.27
	6.64	6.42	5.64	7.1	5.84	7.45	8.16	7.30	9.98	9.83	9.60	11.20	12.11	12.74
	6.8		5.80	7.26	6.43	7.71	8.32	7.54	10.45	9.99	9.84	11.38	12.27	12.98
			6.01		6.60	7.90		7.89			10.19	11.90		13.33
			6.25		6.82	8.26		8.06			10.36	12.36		13.50
			6.63		6.92	8.45		8.28			10.58	12.98		13.72
			7.05		7.05			8.30			10.60			13.74
					7.09			8.38			10.68			13.82
								9.67			11.41			13.78
								9.85			11.59			13.96

where both values λ and μ are different from zero and even. The deduced values are

$$\chi_R=0.828\,66 \ \ \text{MeV},$$

$$\chi_T=-0.0412 \ \ \text{MeV},$$

$$\chi_{12}=0.164\,38 \ \ \text{MeV},$$

$$\chi_\omega=-15.4202 \ \ \text{MeV},$$

$$\chi_N=-0.0132 \ \ \text{MeV},$$

$$n_0=8,$$

$$a=0.104 \ \ \text{MeV},$$

$$c=0.1225 \ \ \text{MeV},$$

$$b=1.437 \ \ \text{fm}. \tag{18}$$

The numerical energy values of our theoretical calculation are listed in Table II [column $U_R(3)$]. These can be compared to the experimental values given by Refs. [2,8]. The theoretical energy values as obtained by the model of Ref. [8], without inner structure of the clusters, are given in column $SO_R(4)$ of Table II. In the $SO_R(4)$ model only those states are listed, which have a corresponding interpretation in the experiment. In Fig. 2 the spectrum within our model is depicted (middle panel) and compared to the experimental one (left panel). In the right panel the spectrum as obtained in the $SO_R(4)$ model is depicted.

When one compares the spectrum of our model and the $SO_R(4)$ model to the experiment, we observe a qualitative agreement of our model while the spectrum of the $SO_R(4)$ model does not reproduce as good the characteristic structure of the experimental result. In the theory there are some states not present in the experiment and also the inverse observation can be made. One has to keep in mind that not all states listed in Refs. [2,8] are completely verified experimentally; however, it is difficult to decide which ones are not real states (molecular resonances) of the system [44]. There might also be more states than reported in the experiment.

Note that only positive parity states are listed. In Ref. [8] there are only positive parity states because the clusters have no structure (see discussion in Sec. II). In our model, however, negative parity states and thus also odd spins exist. In the reaction channel $^{12}C+^{12}C$ negative parity states cannot be populated but maybe they can be reached in exciting the ^{24}Mg nucleus. In this way one could discriminate between different models. To measure electromagnetic transition rates is also recommendable. Of course, these states are very difficult to measure but experiments are planed [45].

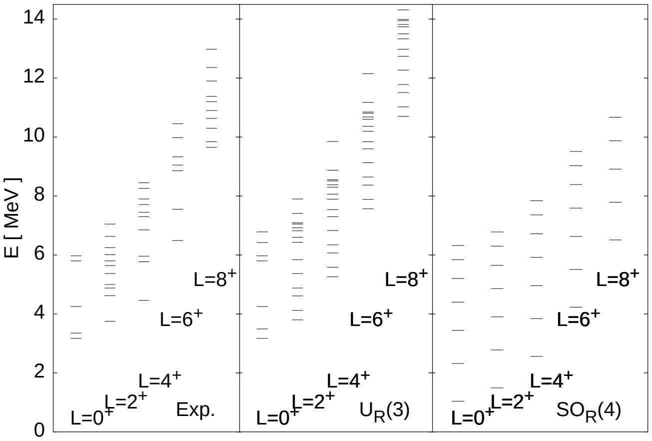

FIG. 2. Energy spectrum of a nuclear molecule $^{12}C+^{12}C$, for the model with inner structure of the clusters. The left panel shows the experiment and the middle one shows the theory. In the right panel the spectrum of the $SO_R(4)$ model is depicted [8].

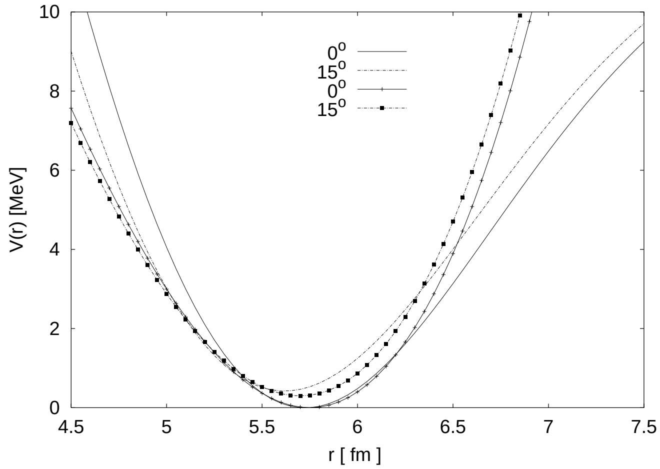

FIG. 3. Mapped geometrical potential for $^{12}C+^{12}C$ as obtained in the model with inner structure of the clusters, after having adjusted the experimental spectrum.

An alternative is given by the requirement to reproduce the internuclear potential as obtained in a double folding calculation.

Having obtained a satisfactory fit for the spectrum we can now use the obtained parameter set in order to deduce the relative potential of the two carbon nuclei as a function of the relative inclination angle. Below we will show that our potential is consistent with that obtained in double folding calculations [41]. The result is depicted in Fig. 3. Note that the potential, as obtained by adjusting the energies, is remarkably well reproduced. Though, r_0 was fixed by hand, the stiffness of the geometrical potential comes out without any further fitting.

Now we proceed to get information about the spectrum of the nuclear molecule, *starting from the knowledge of the relative nuclear potential only*. The potential can be obtained using double folding techniques [28]. We use the procedure described in Ref. [41]. In order to deduce the model parameters, some conditions have to be fulfilled.

(1) The position of the minimum should agree to the calculated one, i.e.,

$$\left.\frac{\partial V}{\partial r}\right|_{r_0,\Theta_0}=0, \tag{19}$$

where r_0 is the position of the minimum at the equilibrium orientation Θ_0.

(2) The stiffness C_r at the minimum, as obtained in the double folding calculation, i.e., for r_0 and at the equilibrium orientation angle Θ_0, should be the same

$$\left.\frac{\partial^2 V}{\partial r^2}\right|_{r_0,\Theta_0}=C_r. \tag{20}$$

(3) The slope of the potential at the minimum position r_0 for a different orientation than the equilibrium one (C_{r,Θ_1}) should be reproduced or somehow given, i.e.,

$$\left.\frac{\partial V}{\partial r}\right|_{r_0\Theta_1}=C_{r,\Theta_1}, \tag{21}$$

(this condition can also be substituted by requiring that the position of the minimum at Θ_1 is reproduced). C_{r,Θ_1} is chosen such that the minimum at Θ_1 is near the calculated one. (In general, adjusting the exact position of the minimum at Θ_1 is difficult to achieve, which led us to this approximation.)

(4) The expectation value of $\langle n_R\rangle$ is proportional to r_0^2, which gives

$$r_0^2=2b^2n_0. \tag{22}$$

(5) The energy as a function of n_R, the number of relative oscillation quanta, has to give *the same* value of n_0

$$E(n_0)=\text{minimal}, \tag{23}$$

where we assumed that the lowest irreducible representation (irrep) is at the maximal coupling, i.e., $(\lambda,\mu)=(\lambda_C+n_0,\mu_C)$ of the cluster irrep with the relative motion, where (λ_C,μ_C) is obtained by a coupling of the individual cluster states. The indices Θ_0 and Θ_1 refer to the orientation angle at equilibrium and another angle, respectively.

Condition (1) with (4) leads to

$$\frac{r_0^2}{2b^2}=-\frac{[4(\chi_R+\chi_T)+\chi_\omega+\chi_T\Gamma]}{2(\chi_R+\chi_T)} \tag{24}$$

and condition (2) leads to

$$C_r=8(\chi_R+\chi_T)\frac{r_0^2}{2b^4}, \tag{25}$$

where Γ is defines as (note that $\theta=90°+\Theta$)

$$\Gamma=\sqrt{8}\frac{N_1\beta_1}{1+\beta_1^2}\left(1\pm\frac{\beta_1}{2\sqrt{2}}\right)[3\cos^2(\theta_{21_0})-1]+\sqrt{8}\frac{N_2\beta_2}{1+\beta_2^2}\left(1\pm\frac{\beta_2}{2\sqrt{2}}\right)[3\cos^2(\theta_{22_0})-1]. \tag{26}$$

The last equation relates the value n_0, as obtained in Eq. (23), with that in Eq. (22). The result is

$$\frac{r_0^2}{2b^2}=n_0=-\frac{[3\chi_R+3\chi_T+\chi_\omega+\chi_T(2\lambda_C+\mu_C)]}{2(\chi_R+\chi_T)}-\frac{\chi_N[\lambda_C^2+\mu_C^2+\lambda_C\mu_C+3(\lambda_C+\mu_C)-\langle C_2(SU_C(3))\rangle_{\Theta_0}]}{2(\chi_R+\chi_T)}. \tag{27}$$

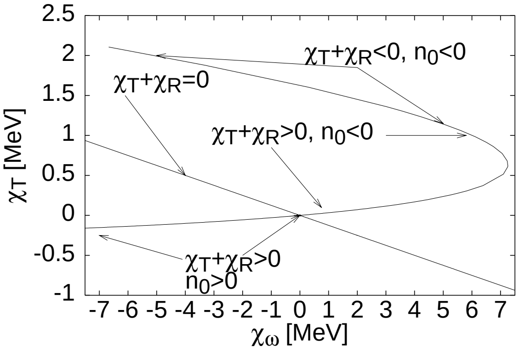

FIG. 4. Dependence of the parameter χ_T on χ_ω, for ^{12}C $+{}^{12}$C. The physical and unphysical branches are indicated. The lines indicate the positions that fulfill all conditions.

Substituting Eqs. (22) and (27) into Eqs. (24) and (25) we arrive at

$$C_r=\frac{2[4(\chi_R+\chi_T)+\chi_\omega+\chi_T\Gamma]^2}{r_0^2(\chi_R+\chi_T)} \tag{28}$$

and

$$\begin{aligned}(\chi_R+\chi_T)=&\chi_T[\Gamma-(2\lambda_C+\mu_C)]-\chi_N[\lambda_C^2+\mu_C^2+\lambda_C\mu_C\\&+3(\lambda_C+\mu_C)-\langle C_2(SU_C(3))\rangle_{\Theta_0}].\end{aligned} \tag{29}$$

Finally, we use the condition given in Eq. (21), to obtain

$$\begin{aligned}C_{r,\Theta_1}=&\frac{r_0^2}{2b^2}[2(\Gamma'-\Gamma)\chi_T]\\&+\chi_N[\langle C_2(SU_C(3))\rangle_\Theta-\langle C_2(SU_C(3))\rangle_{\Theta_0}],\end{aligned} \tag{30}$$

where $\Gamma'=\Gamma$ $(\Theta=\Theta_1)$. Using Eqs. (28), (29), and (30) we finally obtain a relation between χ_T and χ_ω of the form $f(\chi_\omega,\chi_T)=0$ and $\chi_R=\chi_R(\chi_\omega,\chi_T)$.

For these equations we obtain an infinite number of values (χ_ω,χ_T) that satisfy all the conditions that we are considering; however, we need that $(\chi_R+\chi_T)>0$ and $n_0>0$. In Fig. 4 χ_T is plotted as a function of χ_ω and the lines indicate the points that fulfill all conditions. There are several branches but only one is of physical significance. One branch corresponds to a negative n_0, while another one (the straight line) corresponds to $(\chi_T+\chi_R)=0$. This implies a degeneracy in all n_0 as can be deduced from the form of the energy [Eq. (4)] in terms of $\Delta n=n_R-n_0$, which is $E=E(n_0)+c(\chi_T+\chi_R)\Delta n^2$, where c is a numerical factor. The only branch of interest is that with negative χ_ω (a result that depends on the particular system considered).

As a consequence, all parameters of the model can be determined as a function of $\chi_\omega<0$, reflecting the remaining ambiguity. In Fig. 5 χ_T, $\chi_R+\chi_T$, $\chi_{12}+\chi_T$, and $\chi_{12}+\chi_T+n_0\chi_N$ are plotted. The last determines the scale of excitation of different irreps (λ_C,μ_C), where a negative value favors the largest dimensional irrep at low energy, while a positive value results in the lowest dimensional irrep at low energy. $\chi_R+\chi_T$ gives the scale of excitation in the relative motion. Large positive values imply a big difference between different radial excitations, while small values imply a dense excitation spectrum in the radial degree of freedom.

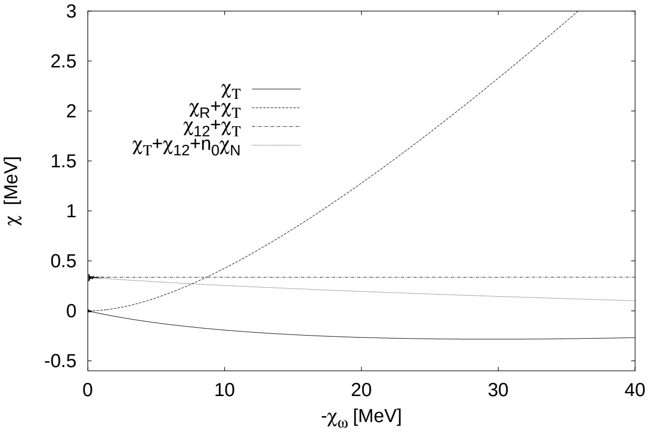

FIG. 5. Some χ parameters and combinations of them as a function of $-\chi_\omega$, for the physical branch of the system ^{12}C$+{}^{12}$C.

All choices of χ_ω will give potentials of equivalent form, i.e., the main differences are at large r. However, the spectrum changes from small values of $-\chi_\omega$ to large ones. For small values, the spectrum is dense and the radial excitations are very near together, while for larger $-\chi_\omega$ values the spectrum gets less dense and the radial excitations are farther away.

There are two distinct regions: (i) $(-\chi_\omega)$ greater than approximately 5.4 and (ii) $(-\chi_\omega)$ lower than approximately 5.4. The first region corresponds to small n_0 and there lies the solution, which we obtained adjusting the energy spectrum. However, it is clear now that this was not the only choice. For comparison, we choose a point in the second region, leading to the χ values:

$$\begin{gathered}\chi_R=0.101\ \text{MeV},\\ \chi_T=-0.066\ \text{MeV},\\ \chi_{12}=0.396\ \text{MeV},\\ \chi_\omega=-2.5\ \text{MeV},\\ \chi_N=-6.0\times10^{-4}\ \text{MeV},\\ n_0=40,\\ a=0.103\ \text{MeV},\\ c=0\ \text{MeV},\\ b=0.64\ \text{fm},\end{gathered} \tag{31}$$

where c could not be deduced from the potential and we put it equal to 0. The value of c can only be determined knowing the spectrum. The a parameter can be estimated, assuming a moment of inertia μr_0^2, with μ as the reduced mass and r_0

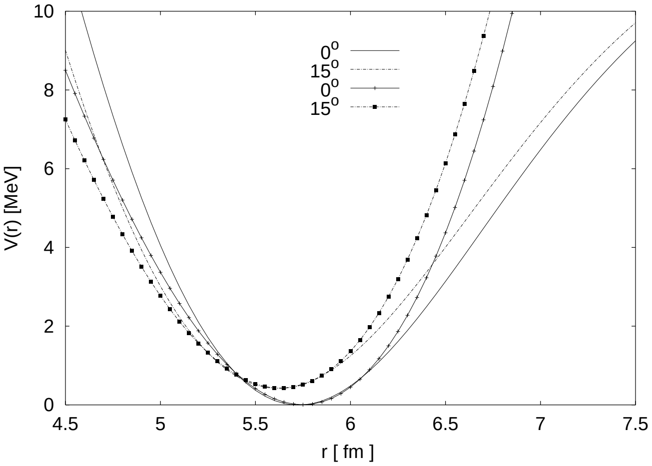

FIG. 6. Adjustment of the geometrically mapped potential to that as obtained in a double folding calculation.

the position of the minimum in the relative motion. The fitted potential is shown in Fig. 6, which is comparable to that as obtained fitting first the energy spectrum (Fig. 3).

The spectrum is depicted in Fig. 7. As can be seen, the quality of the spectrum is comparable to the former one. This shows that there exist an ambiguity in which χ_ω value to choose. When we go to even larger values of $-\chi_\omega$ the spectrum gets more stretched, leading to a low density of states per unit energy interval.

The interpretation of the structure of the spectrum is also different in the two regions. While for $(-\chi_\omega) \geqslant 5.4$ all low lying 0^+ bands correspond to the same $n_R = n_0$ but different (λ_C, μ_C), for $(-\chi_\omega) < 5.4$ the low lying 0^+ bands have the same (λ_C, μ_C) but different $n_R = n_0$, $n_0 \pm 2$, etc.

The results of this subsection do imply the following. (1) It is not sufficient to propose for the Hamiltonian just a linear combination of second order Casimir operators. The resulting potential may be wrong. (2) Geometrical information is essential in order to propose a consistent Hamiltonian. (3) The potential, as obtained in a double folding calculation, is not sufficient to pin down the structure of the spectrum, but one can discuss at least distinct scenarios.

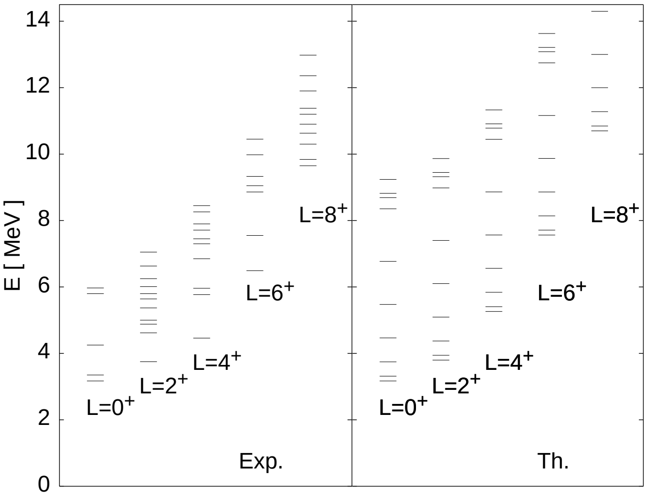

FIG. 7. The deduced energy spectrum of the molecular resonances of ^{12}C+^{12}C as obtained from adjusting to the double folding potential.

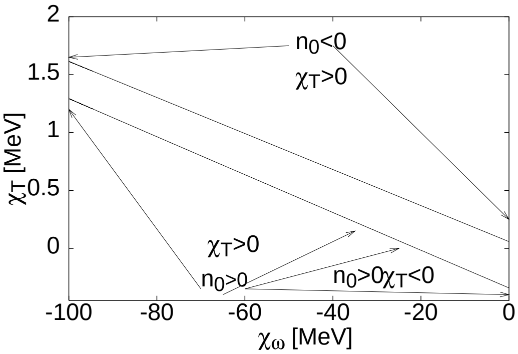

FIG. 8. Dependence of the parameter χ_T on χ_ω, for ^{96}Sr + ^{146}Ba. The physical and unphysical branches are indicated. The arrows indicate the range of validity of the limits associated to χ_T and n_0.

Fitting first the spectrum and afterwards mapping to a potential is, within a certain acceptance, consistent with first adjusting a potential and then calculating the spectrum. The ambiguities, which appear in the mapping, can be reduced to distinct classes of spectra. This gives us hope that one can deduce some characteristics of the spectrum of heavy nuclear molecules, where only a potential can be obtained and no experimental information is available yet. The relative nuclear potential, as obtained in a double folding calculation, is a good starting point.

The comparison to the $SO_R(4)$ model was also given. The spectrum of the $SO_R(4)$ model does not reflect the correct structure of the experimental spectrum.

B. ^{96}Sr+^{146}Ba

The description of such a system can be done, considering the algebraic $U_{C_i}(6)$ IBA-1 model [32–34], as one possibility, for the internal degrees of freedom of each nucleus and for the relative motion of the clusters a $U_R(4)$ group [33,34] is used.

The Hamiltonian that corresponds to dynamical chain (1) is shown in Eq. (2). The $SU_{C_i}(3)$ irreps are (18,0) and (14,0) for Sr and Ba, respectively. The coupled cluster irrep, which is lowest in energy, is $(\lambda_C, \mu_C) = (32,0)$, i.e., the most prolate one.

The geometrically mapped potential is given by Eq. (11). For the nuclei ^{96}Sr and ^{146}Ba (see Fig. 8), the deformations and N-values are $\beta(\text{Sr}) = \beta_1^{\text{phys}} = 0.338$, $\beta(\text{Ba}) = \beta_2^{\text{phys}} = 0.2$, $N(\text{Sr}) = N_1 = 9$, and $N(\text{Ba}) = N_2 = 7$, where the tables of Möller and Nix [46] were used in order to deduce the deformation values. They are transformed to the β^{iba} deformation values according to Eq. (12). With this, we obtain the values for the parameters β_i: $\beta_1 = 1.53$ and $\beta_2 = 1.77$.

We proceed in a similar way as for ^{12}C+^{12}C. Applying the conditions of the last subsection, we again arrive at the allowed range of $\chi_\omega < 0$. In Fig. 9 the χ_T and the same combinations as in Fig. 5 are plotted. Note that $\chi_R + \chi_T$,

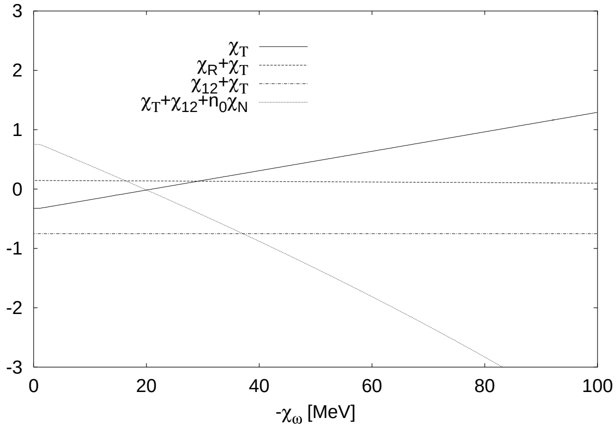

FIG. 9. Some χ parameters and combinations of them as a function of $-\chi_\omega$, for the physical branch. The system considered is ^{96}Sr+^{146}Ba.

responsible for the scale of the radial excitation, is nearly constant and small, which implies low lying radial excitations throughout the whole range of χ_ω, a stable feature not encountered in the previous example. The combination $\chi_T+\chi_{12}+n_0\chi_N$, giving the scale of the (λ_C,μ_C) excitations, and χ_T are small for $-\chi_\omega$ around 20 MeV and raise towards larger or lower $-\chi_\omega$, while their signs are opposite. χ_T determines if the largest irrep (λ_C+n_0,μ_C) is lowest in energy (when $\chi_T<0$) or the smallest one (when $\chi_T>0$). The crossing point from one situation to the other is at about $-\chi_\omega=20$ MeV.

The n_0 value and the oscillator length b do not change appreciably either over the indicated range of $-\chi_\omega$.

In Fig. 10 we plot the potential as obtained in the double folding calculation (solid line for $\theta=0°$ inclination of the symmetry axes and dashed-dotted line for $\theta=15°$) and as deduced from adjusting the parameters of the geometrically mapped potential. We had problems to shift the minimum at 15° to the right position, indicating a too stiff behavior of the algebraic model, i.e., probably further interaction terms are needed. However, without the χ_N term the minimum at 15° would be far off and contradictions appear related to the consistency requirements.

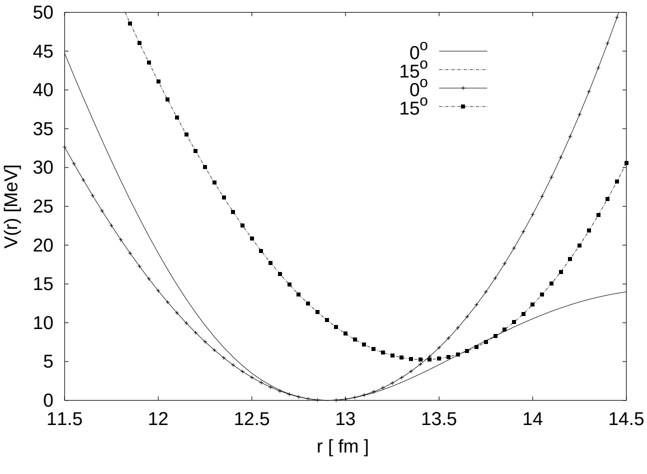

FIG. 10. The relative potential for $\theta=0°$ and 15°, as obtained by the mapping to the geometrical potential, compared to the double folding calculation. θ gives the inclination angle of the symmetry axis of the *now prolate* nuclei to the molecular z axis.

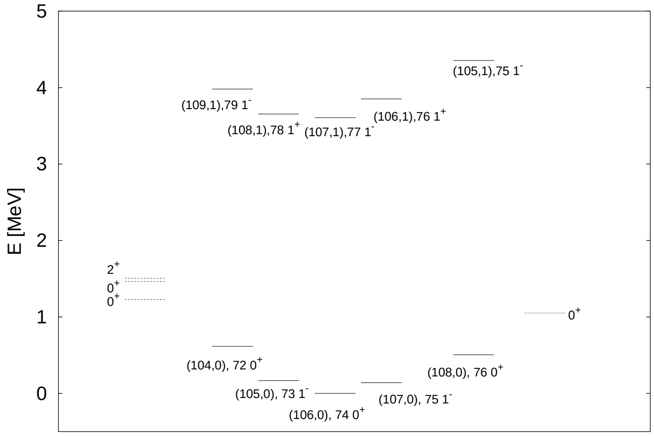

FIG. 11. Spectrum of the hypothetical heavy nuclear molecule ^{96}Sr+^{146}Ba. The dotted lines refer to excited bands on Sr (left) and Ba (right).

Finally, in Fig. 11 we plot the spectrum of the hypothetical nuclear molecule ^{96}Sr + ^{146}Ba for $-\chi_\omega=12.03$ MeV. Also in Fig. 11 the first vibrational β- and γ-band heads of the Sr and Ba nuclei are shown, as far as reported [47]. The parameter set, obtained by fitting to the double folding potential, is given by

$$
\begin{aligned}
\chi_R&=0.286\ \text{MeV},\\
\chi_T&=-0.146\ \text{MeV},\\
\chi_{12}&=-0.606\ \text{MeV},\\
\chi_\omega&=-12.03\ \text{MeV},\\
\chi_N&=0.014\ \text{MeV},\\
n_0&=74,\\
a&=0.0218\ \text{MeV},\\
c&=0\ \text{MeV},\\
b&=1.06\ \text{fm},
\end{aligned}
\tag{32}
$$

where, as in the carbon-carbon case, the c parameter can not be determined and it is put arbitrarily equal to 0.

The choice of the χ_ω value is also *ad hoc*, but it shows one particular property of the heavy nuclear molecule: The rotational bands are severely squeezed due to the large moment of inertia. The Coriolis effect is not strong enough in order to distort the rotational structure of the vibrational bands, as happened in the model for three-cluster nuclear molecules, proposed in Ref. [25]. The structure found here will prevail also for three-cluster molecule, i.e., also there the states within a rotational band are squeezed, showing that the large Coriolis effect seen in Ref. [25] is the result of the interaction used. It also indicates that one has to be very careful in choosing a Hamiltonian and the mapped potential has to be consistent.

IV. CONCLUSION

In this paper we used an algebraic nuclear vibron model for nuclear molecules with inner structure of both clusters. We discussed the dynamical symmetry $U_{C_1}(6)\otimes U_{C_2}(6)\otimes U_R(4)\supset SU_{C_1}(3)\otimes SU_{C_2}(3)\otimes SU_R(3)$. The geometrical mapping of the corresponding Hamiltonian was investigated using the coherent state method. The trial state depends on a parameter α_R, which we relate to the distance r between the clusters. An important point is to note that the parameter α_R of the coherent state is not proportional to the inter cluster distance r and in addition is restricted from above via the cutoff N_R in the relative number of quanta.

We showed that the dynamical symmetry has a minimum in the relative distance at values different from 0, i.e., the $SU_R(3)$ dynamical symmetry is *not always related to the harmonic limit*. With a negative and sufficiently large χ_ω a minimum at $r\neq 0$ can already be obtained.

The model was first applied to the light system ^{12}C $+^{12}$C, where a lot of experimental information is available. The spectrum was adjusted satisfactorily to the experiment. The agreement of the $SO_R(4)$ model to the experiment was less satisfactorily, the spectrum being too sparse. Our procedure gives the correct stiffness at the minimum ($r=r_0$ and $\Theta_0=0°$), which is by no means trivial. One sees that geometrical information (position of r_0 and comparing the geometrically mapped potential to informations obtained via, e.g., the double folding calculation) is essential in order to guarantee that the algebraic Hamiltonian makes sense or not. The pure adjustment to energy (and also to a limited set of transition elements) is not sufficient. It also shows that the requirement, to reproduce the internuclear potential, may help pin down the structure of the Hamiltonian, as electromagnetic transitions do (the latter are extremely difficult to measure).

For heavy nuclear molecules no information about their spectrum is available yet. The model relies heavily on the double folding results for the potential. Using the information of the structure of the individual clusters, it permits to deduce the Hamiltonian of the nuclear molecule. In this way, the structure of the spectrum of such a nuclear molecule can be estimated.

We applied the model to the heavy system ^{96}Sr$+^{146}$Ba. The parameters of the model were adjusted to the potential obtained in a double folding calculation. The moment of inertia in the model (related to a) was defined via μr_0^2. The parameter in front of K^2 could not be determined due to missing information. A spectrum was given, showing no distortion of a large Coriolis force. While the scale of the radial excitations remains stable over a large range of χ_ω, χ_T and $\chi_{12}+\chi_T+n_0\chi_N$ vary appreciably, resulting in different scales for the excitation to different couplings of (λ_C,μ_C).

We showed that the geometrical mapping applied is able to give a consistent relation of the algebraic model and its geometrical interpretation. The potentials obtained are in remarkable agreement with those from double folding calculations.

The next step would be to investigate again three-cluster molecules. In Ref. [25] a strong Coriolis force was predicted, generating no squeezed rotational bands except for the ground state band. Whether this is still the case for another Hamiltonian, as that proposed in this contribution, has to be found out. However, the results of this contribution suggest that in the dynamical symmetry chosen this is not the case.

ACKNOWLEDGMENTS

The authors acknowledge very fruitful discussions with J. Cseh and G. Lévai from the ATOMKI (Debrecen, Hungary). This work was supported by the CONACyT-MTA and CSIC-MTA exchange programs and by the CONACyT. H.Y.M. acknowledges financial support from DGEP-UNAM. The Isotope Explorer, used for this publication, is supported by the Nuclear Physics division of the U.S. Department of Energy under Contract No. DE-AC03-765F00098. Financial help from DGAPA, Project No. IN119002, is also acknowledged. Ş. Mişicu acknowledges the financial support from the European Community through a Marie Curie fellowship.

---

[1] D.A. Bromley, J.A. Kuehner, and E. Almqvist, Phys. Rev. Lett. **4**, 365 (1960).
[2] U. Abbondanno, Report INFBM/BE-91/11 1991.
[3] D. Scharnweber, W. Greiner, and U. Mosel, Nucl. Phys. **A164**, 257 (1971).
[4] W. Scheid, W. Greiner, and R. Lemmer, Phys. Rev. Lett. **25**, 176 (1970).
[5] Y. Abe, Prog. Theor. Phys. **63**, 722 (1980); Y. Abe, Y. Kondo, and T. Matsuse, Suppl. Prog. Theor. Phys. **68**, 303 (1980).
[6] W. Greiner, J. Y. Park, and W. Scheid, *Nuclear Molecules* (World Scientific, Singapore 1995).
[7] F. Iachello, Phys. Rev. C **23**, 2778 (1981).
[8] K.A. Erb and D.A. Bromley, Phys. Rev. C **23**, 2781 (1981).
[9] O. S. Roosmalen, Ph.D. thesis, University of Groningen (Netherlands), 1982.
[10] J. Cseh, Phys. Rev. C **31**, 692 (1985); J. Cseh and J. Suhonen, *ibid.* **33**, 1553 (1986).
[11] J. Cseh, G. Lévai, and W. Scheid, Phys. Rev. C **48**, 1724 (1993).
[12] F. Iachello, Nucl. Phys. **A421**, 97c (1984).
[13] H.J. Daley and F. Iachello, Ann. Phys. (N.Y.) **167**, 73 (1986).
[14] H.J. Daley and B.R. Barrett, Nucl. Phys. **A449**, 256 (1986).
[15] K. Wildermuth and Y. C. Tang, *A Unified Theory of the Nucleus* (Academic, New York, 1977).
[16] J. Cseh, Phys. Lett. B **281**, 173 (1992).
[17] J. Cseh and G. Lévai, Ann. Phys. (N.Y.) **230**, 165 (1994).
[18] G. Lévai and J. Cseh, Phys. Rev. C **44**, 152 (1991); **44**, 166 (1991).

[19] G. Lévai and J. Cseh, Phys. Lett. B **381**, 1 (1996).

[20] J. Cseh, G. Lévai, A. Ventura, and L. Zuffi, Phys. Rev. C **58**, 2144 (1998).

[21] P.O. Hess, G. Lévai, and J. Cseh, Phys. Rev. C **54**, 2345 (1996).

[22] A.V. Hamilton, J.K. Hwang, J.H. Hamilton, A. Sandulescu, A. Florescu, G.M. Ter-Akopian, A.V. Daniel, Yu.Ts. Oganessian, G.S. Popeko, W. Greiner, J.D. Cole, and GANDS95 Collaboration, Phys. Rev. Lett. **81**, 947 (1998).

[23] P.O. Hess, W. Scheid, and W. Greiner, J. Phys. G **25**, L139 (1999); Ş. Mişicu, P.O. Hess, A. Sandulescu, and W. Greiner, *ibid.* **25**, L147 (1999); P.O. Hess, Ş. Mişicu, W. Greiner, and W. Scheid, *ibid.* **26**, 957 (2000).

[24] Ş. Mişicu, P.O. Hess, and W. Greiner, Phys. Rev. C **63**, 054308 (2001).

[25] R. Bijker, P.O. Hess, and Ş. Mişicu, Heavy Ion Phys. **13**, 89 (2001); P.O. Hess, R. Bijker, and Ş. Mişicu, Rev. Mex. Fis. **47**, 52 (2001).

[26] H. Yépez, P.O. Hess, and Ş. Mişicu, Heavy Ion Phys. **16**, 19 (2002).

[27] R. Bijker and F. Iachello, Phys. Rev. C **61**, 067305 (2000); R. Bijker and F. Iachello, Ann. Phys. (N.Y.) **298**, 334 (2002).

[28] M. Seiwert, W. Greiner, and W.T. Pinkston, J. Phys. G **11**, L21 (1985); E. Uegaki and Y. Abe, Prog. Theor. Phys. **90**, 615 (1993).

[29] J.N. Ginocchio and M.W. Kirson, Phys. Rev. Lett. **44**, 1744 (1980).

[30] J.N. Ginocchio and M.W. Kirson, Nucl. Phys. **A350**, 31 (1980).

[31] K. T. Hecht, *The Vector Coherent State Method and its Applications to Physical Problems of Higher Symmetries*, Lecture Notes in Physics Vol. 290 (Springer-Verlag, Heidelberg, 1987).

[32] F. Iachello and A. Arima, *The Interacting Boson Model* (Cambridge University Press, Cambridge, 1987).

[33] A. Frank and P. van Isacker, *Algebraic Methods in Molecular and Nuclear Structure* (Wiley Intersciences, New York, 1994).

[34] D. Bonatsos, *The Interacting Boson Models of Nuclear Structure* (Oxford Science Publications, Oxford, 1988).

[35] J.P. Elliot and A. Evans, Phys. Lett. B **101**, 216 (1981).

[36] J. Cseh, G. Lévai, H. Yépez, and P. O. Hess (unpublished).

[37] H. Naqvi and J.P. Draayer, Nucl. Phys. **A516**, 351 (1990).

[38] P. Ring and P. Schuck, *The Nuclear Many Body Problem* (Springer-Verlag, Heidelberg, 1980).

[39] S. Levit and U. Smilansky, Nucl. Phys. **A389**, 56 (1982).

[40] J. M. Eisenberg and W. Greiner *Nuclear Theory I: Nuclear Models* (North-Holland, Amsterdam, 1987).

[41] Ş. Mişicu, A. Sandulescu, F. Carstoiu, M. Rizea, and W. Greiner, Nuovo Cimento Soc. Ital. Fis., A **112A**, 313 (1999).

[42] O. Castaños, J.P. Draayer, and Y. Leschber, Z. Phys. A **329**, 33 (1988).

[43] S. Raman, C.H. Malarkey, W.T. Milner, C.W. Netsor, and P.H. Stelson, At. Data Nucl. Data Tables **36**, 1 (1987).

[44] N. Cindro (private communication).

[45] F. Haas, Procedings of the Symposium on Nuclear Clusters, Rauischholzhausen, Germany, 2002.

[46] P. Möller, J.R. Nix, W.D. Myers, and W.J. Swiatetecki, At. Data Nucl. Data Tables **59**, 185 (1995).

[47] C. Y. Cha, N. Nordberg, R. B. Firestone, and L. P. Ekström, computer code ISOTOPE EXPLORER, Version 2.23.