Cluster model with breathing clusters: Dynamical distortion effects in ^{6}Li

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Distortion effects in an assembly of clusters are studied by using a trial wave function in which—in addition to the intercluster separations—the size parameters of individual clusters appear as generator coordinates. An application to the nucleus ^{6}Li, which is described as a bound alpha + deuteron system, shows that these new degrees of freedom, which can lead to compressional vibrations, are indeed important. We find that the deuteron cluster is compressed, whereas the size and the compressibility of the alpha cluster are unchanged with respect to the free case.

I. INTRODUCTION

The nuclear cluster model[1] provides a convenient framework for the description of those states in nuclei which may be interpreted in terms of the collective motion of an assembly of clusters. Because of the Pauli principle, the internal structure of the clusters is different[2–4] from that of the free clusters. In addition, the specific distortion of the clusters at close distances because of their mutual interaction has been clearly demonstrated by many authors.[5–12] In most of these studies, distortion effects are treated by one of the following two methods: (i) If there are clusters which are not tightly bound, it is plausible to assume that new clusters may be formed by transferring nucleons between them. This consideration led Mihailović and his collaborators[8–10] to study the interplay of different cluster structures in light nuclei. In these calculations, however, the simplifying assumption of equal oscillator parameters for all clusters has been adopted. (ii) As for the second method, one usually assumes that the clusters in a nucleus preserve more or less their identity (of course, Pauli distortion is always present), but that their internal structure is different from that of the free clusters. This point of view has been adopted by Tang and his collaborators[5,7,11] and by other groups.[6,12] Here one describes the internal wave function of a distorted cluster by a superposition of its undisturbed ground state wave function and a few square-integrable (distortion) functions. The wave functions of relative motion of the clusters are allowed to be different for the various intrinsic functions and are determined variationally. However, as Thompson and Tang[5] point out in their study of the alpha+deuteron system, "it would be more desirable to let the deuteron parameters be a function of the cluster separation. However, we should point out that this will be a very difficult way of studying the specific distortion effects."

In our model, we use the parameters which describe the internal structure of the clusters as generator coordinates. The wave function of the nucleus is thus assumed as a superposition of various cluster configurations with an amplitude which depends on the separations of the shell model potentials as well as on the internal parameters of each individual cluster. In this way, we avoid the above mentioned difficulties which are related to the adoption of a nonlinear variational procedure. Thus, in our calculation, the mathematical ease of a linear variational principle is preserved, while at the same time we may employ trial functions of great flexibility. If we assume, for instance, that the clusters may change their size but otherwise preserve their shape, we may describe compressional vibrations of individual clusters in the nucleus in addition to their moleculelike collective motion.

We should mention that the generator coordinate method (GCM) has already been applied to describe compressional vibrations of doubly magic nuclei. Flocard and Vautherin[13] and Abgrall and Caurier[14] calculated monopole and quadrupole vibrations in ^{4}He, ^{16}O, and ^{40}Ca using Skyrme's interaction. The method was extended by Krewald *et al.*[15] who employed single-particle wave functions obtained from a constrained Hartree-Fock calculation.

In our present investigation, the model with breathing clusters is applied to the nucleus ^{6}Li. The bound alpha+deuteron system is especially suited for our purpose because its constituent clusters exhibit two different features: The tightly bound α particle shows a breathing mode[16,17] at an excitation energy of 20.1 MeV. The ground state correlations related to this degree of freedom might be of importance also in the bound α cluster. On the other hand, because of its weak binding, the deuteron cluster is known to become appreciably distorted in the nucleus ^{6}Li.[11] In addition, we expect distortion effects to be more pronounced in the bound nucleus than in a scattering event where, at least at high energies, the clusters will be close together only for a relatively short time.

The special case of the $A=6$ system has also been studied extensively[18,19] by an approach which differs essentially from the one presented in this work: This is the exact three-body theory (undistorted α particle plus two nucleons, αNN). Using suitably chosen αN and NN interactions, good agreement[20] with the low energy data is obtained.

In the next section, we give a description of the GC trial function for a multicluster system. Here our main interest is in describing the methods of projecting the

center-of-mass momentum, angular momentum, and parity and in demonstrating how the calculation of complicated internal structures of clusters may recursionally be reduced to that of simple ones. In Sec. III, we discuss the results for the bound $\alpha+\mathrm{d}$ system, beginning with a study of the separate α and deuteron clusters. Finally, in Sec. IV, we summarize the results of this investigation.

II. THE GENERATOR COORDINATE TRIAL WAVE FUNCTION

A. The basis of the generator coordinate wave function

In order to describe states in a nucleus with A nucleons which may be interpreted in terms of the collective motion of the nucleons in individual clusters and/or moleculelike vibrations and rotations of an assembly of clusters, we start with single-particle wave functions ($\vec{x}_i$ is the spatial coordinate of particle i)

$$\varphi_i(\vec{x}_i)=\varphi(\vec{x}_i-\vec{S}_i,\beta_i,n_i,l_i,m_i)\ , \tag{2.1}$$

which describe the motion of a nucleon in a harmonic oscillator well centered at the point $\vec{S}_i$ with width parameter β_i. The quantum numbers n_i, l_i, and m_i denote the radial excitation, the orbital angular momentum, and its z component. Introducing the spin and isospin wave functions χ_i of each nucleon, we form A-particle Slater-determinant wave functions ϕ. As an intermediate step, we assume that each nucleon occupies its own harmonic oscillator orbit $(\vec{S}_i,\beta_i)$, but restricts the quantum numbers to the values $[nlm]=0$

$$\phi([\vec{x}\vec{S}\beta],[nlm]=0)=\mathscr{A}\prod_{i=1}^{A}[\varphi(\vec{x}_i-\vec{S}_i,\beta_i,n_i=l_i=m_i=0)\chi_i]\ , \tag{2.2}$$

where $\mathscr{A}$ is the antisymmetrization operator. A set of quantities such as $\vec{S}_1,\ldots,\vec{S}_A$ is denoted by $[\vec{S}]$. A Slater determinant with nucleons in arbitrary oscillator orbits may be obtained from the wave function (2.2) by repeated use of the following recurrence relations which may be easily derived from the properties[21] of the harmonic oscillator functions (2.1):

$$\phi([\vec{x}\vec{S}\beta],[n]=0,l,m,\ldots,l_i+1m_i,\ldots)=[\beta_i(l_i+1)/2]^{-1/2}\sum_{m'm''}(1m',l_im''\mid l_i+1m_i)\times\nabla_{m'}(\vec{S}_i)\phi([\vec{x}\vec{S}\beta],[n]=0,l,m,\ldots,l_im'',\ldots) \tag{2.3}$$

and

$$\phi([\vec{x}\vec{S}\beta]n,\ldots,n_i+1,\ldots,[lm])=[(n_i+1)(n_i+l_i+\tfrac{3}{2})]^{-1/2}(2\beta_i\partial/\partial\beta_i)\phi([\vec{x}\vec{S}\beta]n_1,\ldots,n_i,\ldots,[lm])+[n_i(n_i+l_i+\tfrac{1}{2})/(n_i+1)(n_i+l_i+\tfrac{3}{2})]^{1/2}\phi([\vec{x}\vec{S}\beta]n_1,\ldots,n_i-1,\ldots,[lm])\ . \tag{2.4}$$

Here $\nabla_m(\vec{S}_i)$, $m=-1,0,1$, are the components of the gradient operator in a spherical representation[22] operating on the variable $\vec{S}_i$ and $(1m',l_im''\mid l_i+1m_i)$ is a Clebsch-Gordan coefficient.[22]

In most cases of physical interest, it is unnecessary to use a separate oscillator well for each particle. Instead one may form nucleon clusters like ^{2}H, ^{3}He, ^{4}He, etc., by choosing the same values of $\vec{S}_i$ and β_i for nucleons belonging to the same cluster. In our formulation, this has to be done after the differentiations in Eqs. (2.3) and (2.4) are carried out.

B. Projection of eigenstates of center-of-mass momentum

The center of mass of the nucleus represented by the A-center shell model wave function, Eqs. (2.2)—(2.4), is confined to a finite region in space. If we want to describe a physical state, with total linear momentum $\hbar\vec{k}$, we may use a projection method which is similar to that of Yoccoz.[23] To proceed, we introduce

$$\vec{S}=A^{-1}\sum_{i=1}^{A}\vec{S}_i\ , \tag{2.5}$$

the mean position of all A oscillator wells and

$$\vec{s}_i=\vec{S}_i-\vec{S},\quad (i=1,\ldots,A) \tag{2.6}$$

the vectors specifying the positions of the oscillator wells with respect to $\vec{S}$. Similarly, let

$$\vec{R}=A^{-1}\sum_{i=1}^{A}\vec{x}_i \tag{2.7}$$

and

$$\vec{\xi}_i=\vec{x}_i-\vec{R},\quad (i=1,\ldots,A) \tag{2.8}$$

denote the coordinate of the center of mass of the nucleus and the intrinsic coordinates, respectively. A particular term in the expansion of the Slater-determinant wave function with $[nlm]=0$, Eq. (2.2), will contain a product of orbital wave functions

$$\prod_{i=1}^{A}\exp[-\beta_{\alpha(i)}(\vec{x}_i-\vec{S}_{\alpha(i)})^2/2]=\exp[-\sum_{i=1}^{A}\beta_{\alpha(i)}(\vec{R}-\vec{S}+\vec{\xi}_i-\vec{s}_{\alpha(i)})^2/2]\ , \tag{2.9}$$

where $\alpha(i)$ denotes the ith element of the permutation α. If we integrate the functions (2.9) over $\vec{S}$, with the weight $\exp(i\vec{k}\cdot\vec{S})$, then the center-of-mass coordinate $\vec{R}$ factors out in the form $\exp(i\vec{k}\cdot\vec{R})$, appropriate for an eigenstate of linear momentum. For the remaining part, depending on intrinsic coordinates only, we find (up to a normalization constant)

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta],[nlm]=0)\equiv\exp\left\{-i\sum_{i=1}^{A}\bar{\beta}_{\alpha(i)}(\vec{s}_{\alpha(i)}-\vec{\xi}_i)\cdot\vec{k}-\sum_{j=1}^{A}\beta_{\alpha(j)}\left[(\vec{s}_{\alpha(j)}-\vec{\xi}_j)-\sum_{i=1}^{A}\beta_{\alpha(i)}(\vec{s}_{\alpha(i)}-\vec{\xi}_i)\right]^2/2\right\}, \tag{2.10}$$

where

$$\bar{\beta}_{\alpha(i)}=\beta_{\alpha(i)}\Big/\sum_{j=1}^{A}\beta_j\ . \tag{2.11}$$

Notice that the intrinsic wave function $\phi_\alpha^{(\mathrm{int})}$ still depends on the momentum $\vec{k}$. If some of the single-particle orbits have $l_i\neq 0$ and/or $n_i\neq 0$, we may use the recurrence relations (2.3) and/or (2.4) with $\nabla_m(\vec{S}_i)$ replaced by $\nabla_m(\vec{s}_i)$, together with the fact that the operations $\partial/\partial\beta_i$ and $\nabla_m(\vec{s}_i)$ commute with the integration $\int d^3S$.

C. Projection of eigenstates of angular momentum and parity

In two previous publications,[24,25] a method of projecting angular momentum and parity for two- and three-cluster wave functions was developed which is based on an analysis of their tensor properties in the space of the vectors $[\vec{s}]$ specifying the positions of the potential wells. Here we generalize this method to include cases where the orbital angular momenta of the single-particle orbits may be arbitrary and the number of clusters may be as large as the number of nucleons. In many practical problems it will be sufficient to consider the case $\vec{k}=0$ only, to which the following discussion is restricted.

To begin with, we define spherical differentiation operators $\nabla(l,m,\vec{s})$ via the recursion relations

$$\nabla(l+1,m,\vec{s})=\sum_{m'm''}(1m',lm''\,|\,l+1m)\times\nabla(1,m',\vec{s})\nabla(l,m'',\vec{s}),\quad(l\geq 1) \tag{2.12}$$

and

$$\nabla(1,m,\vec{s})=\nabla_m(\vec{s})\ . \tag{2.13}$$

Using the differential operators $\nabla(l,m,\vec{s})$ (which are spherical tensor operators of rank l) we find (with $\vec{k}=0$) from Eqs. (2.3) and (2.10) for the intrinsic part of the A-particle wave function

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta lm],[n]=0)=\left[\prod_{i=1}^{A}\nabla(l_{\alpha(i)},m_{\alpha(i)},\vec{s}_{\alpha(i)})\right]\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta],[nlm]=0)\ , \tag{2.14}$$

where we have again written only one term in the expansion of the Slater-determinant wave function and left out a normalization constant. The restriction to $[n]=0$ is not serious because by using Eq. (2.4) we may generate wave functions with arbitrary $[n]$ without affecting the angular momentum algebra. It is convenient to rewrite the product of differentiation operators in Eq. (2.14) in terms of the following set of operators which may be defined by the recursion relation:

$$\begin{aligned}\nabla([ll']lm[\vec{s}])&\equiv\nabla\left[\left[((\ldots(l_1l_2)l_3'l_3)l_4',\ldots)l_A'l_A\right]lm;\vec{s}_1,\ldots,\vec{s}_A\right]\\&=\sum_{m_Am_A'}\nabla((\ldots(l_{A-1}'l_{A-1})l_A'm_A';\vec{s}_1,\ldots,\vec{s}_{A-1})\nabla(l_A,m_A,\vec{s}_A)(l_A'm_A',l_Am_A\,|\,lm)\ ,\end{aligned} \tag{2.15}$$

where the notation is chosen such as to indicate the order of coupling of angular momenta. For example, we couple l_1 and l_2 to a resultant angular momentum l_3', then couple l_3' and l_3 to give l_4', etc. To keep the notation as simple as possible, we use the letter l to denote the total orbital angular momentum. It should not be confused with $[l]$ which stands for the set $l_1,\ldots,l_A$ of the intrinsic orbital angular momenta of all clusters. Using these generalized ∇ operators, we derive

$$\begin{aligned}\prod_{i=1}^{A}\nabla(l_{\alpha(i)},m_{\alpha(i)},\vec{s}_{\alpha(i)})=\sum_{[l'm']lm}&(l_{\alpha(1)}m_{\alpha(1)},l_{\alpha(2)}m_{\alpha(2)}\,|\,l_3'm_3')(l_3'm_3',l_{\alpha(3)}m_{\alpha(3)}\,|\,l_4'm_4')\\&\cdots(l_A'm_A',l_{\alpha(A)}m_{\alpha(A)}\,|\,lm)\nabla([ll']lm[\vec{s}])\ .\end{aligned} \tag{2.16}$$

Next we expand $\phi_\alpha^{(\mathrm{int})}$, Eq. (2.14), in terms of A-polar spherical harmonics ($[n]=0$ is omitted for brevity)

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta lm])=\sum_{[LL']LM}\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta lm]LM)B^*([LL']LM[\hat{s}])\ . \tag{2.17}$$

The A-polar spherical harmonics $B([LL']LM[\hat{s}])$ are spherical tensors of rank L; they obey the same recursion relation, Eq. (2.15), as the ∇ operators. For $A=2$, these harmonics reduce to the well-known bipolar harmonics.[26] The complex conjugate of the tensor B is denoted by B^* and the symbol $\hat{}$ is used to denote unit vectors.

If we let the operators (2.15) act upon the wave function $\phi_\alpha^{(\mathrm{int})}$ with $[lm]=0$, we obtain eigenfunctions of the total internal orbital angular momentum l and its z component m of all clusters

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta ll']lm)=\nabla([ll']lm[\vec{s}])\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta],[lm]=0)\ , \tag{2.18a}$$

where $[l']$ denotes the set of intermediate orbital angular momenta, defined in Eq. (2.15). We should stress that in Eq. (2.18a), the orbital angular momenta $[l]$ are those with respect to the centers of the oscillator wells and may differ from those used for instance in the resonating group method (RGM). The latter ones are defined with respect to the centers of mass of the clusters. If we expand the function (2.18a) in terms of A-polar harmonics, as we did in Eq. (2.17),

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}\vec{s}\beta ll']lm)=\sum_{[LL']LM}\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta ll']lmLM)B^*([LL']LM[\hat{s}])\ , \tag{2.18b}$$

then a theorem proved in the Appendix shows that the functions

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta ll'](lL)\lambda M_\lambda)=\sum_{mM}(lm,LM\mid\lambda M_\lambda)\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta ll']lmLM)\ ,\quad (M_\lambda=-\lambda,\ldots,\lambda) \tag{2.19}$$

form a spherical tensor of rank λ with respect to the intrinsic coordinates $[\vec{\xi}]$. Equation (2.19) is the basic result of our projection method. In order to make it more transparent, let us summarize what has been achieved: Assume for the moment that none of the clusters carries an intrinsic orbital angular momentum, i.e., $[l]=0$. In order to project the orbital angular momentum of the multicluster wave function it is then sufficient to analyze its dependence on the set of vectors $[\vec{s}]$ specifying the centers of the oscillator wells. This analysis is performed by expanding the wave function in terms of spherical harmonics $Y_{LM}(\hat{s})$, bipolar harmonics $B(L_1L_2LM\hat{s}_1\hat{s}_2)$, etc. for a system with two, three, etc. clusters. If some of the clusters carry an intrinsic orbital angular momentum, we first apply the generalized gradient operator $\nabla([ll']lm[\vec{s}])$, Eq. (2.15), to the wave function with $[l=0]$. As this function is usually taken as a Gaussian function, the result can be written analytically. The next step is then an expansion in terms of $Y_{LM}(\hat{s})$, $B(L_1L_2LM\hat{s}_1\hat{s}_2)$, etc. Finally, eigenfunctions of the total orbital angular momentum λ and z component M_λ of the system are formed by coupling l and L to λM_λ.

Because of $[\vec{s}]$ being just a set of parameters, it is advantageous to perform the study of the dependence of the wave function on $[\vec{s}]$ in the relevant matrix elements rather than in the wave functions itself. Finally, we should mention that the set of orbital angular momenta $[L]$ is related to the motion of the oscillator wells. Again our method is different from that employed in the RGM where the angular momenta related to the intercluster motion are introduced. Examples of such a study, for two- and three-cluster systems, may be found in Refs. 24 and 25.

It remains to construct eigenstates of the total angular momentum. This may be simplified by coupling the spins of all nucleons belonging to the same cluster to the spin of the corresponding free cluster only. Upon coupling the spins of all clusters to the total spin (IM_I) and by coupling I and the orbital angular momentum λ to the total angular momentum (JM_J), we end up with the following wave function:

$$\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta ll'II']((lL)\lambda I)JM_J)=\sum_{M_\lambda M_I}(\lambda M_\lambda,IM_I\mid JM_J)\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta ll'II'](lL)\lambda M_\lambda,IM_I)\ , \tag{2.20}$$

where $[I]$ stands for the set of all spins of individual clusters, while $[I']$ denotes the set of intermediate spins which result from coupling the spins of the clusters to the total spin (IM_I). The order of coupling of angular momenta is indicated by using the same notation as in Eq. (2.15).

The form of the wave function (2.19) is very convenient for a study of its properties under the parity transformation $[\vec{\xi}]\rightarrow[-\vec{\xi}]$. We see from Eq. (2.10) that (with $\vec{k}=0$)

$$\phi_\alpha^{(\mathrm{int})}([-\vec{\xi}\vec{s}\beta],[nlm]=0)=\phi_\alpha^{(\mathrm{int})}([\vec{\xi}-\vec{s}\beta],[nlm]=0)\ . \tag{2.21}$$

Making use of the parity relations

$$B([LL']LM[-\hat{s}])=\left[\prod_i(-)^{L_i}\right]B([LL']LM[\hat{s}]) \tag{2.22}$$

and

$$\nabla([ll']lm[-\vec{s}])=\left[\prod_i(-)^{l_i}\right]\nabla([ll']lm[\vec{s}])\ , \tag{2.23}$$

we find from Eqs. (2.18) and (2.19)

$$\phi_\alpha^{(\mathrm{int})}([-\vec{\xi}LL's\beta ll'](lL)\lambda M_\lambda)=\left[\prod_i(-)^{l_i}\right]\left[\prod_i(-)^{L_i}\right]\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta ll'](lL)\lambda M_\lambda)\ . \tag{2.24}$$

D. The Hill-Wheeler variational equation

A (discretized) GC trial function with linear momentum $\vec{k}=0$, angular momentum (JM_J), and parity π may be constructed by superimposing the functions (2.20)

$$\psi^{(\mathrm{int})}([\vec{\xi}I]JM_J\pi)=\sum_{[LL's\beta nll'I']lL\lambda I\alpha}\epsilon_\alpha f([LL's\beta nll'II']lL\lambda IJM_J\pi)\phi_\alpha^{(\mathrm{int})}([\vec{\xi}LL's\beta nll'II'](lL)\lambda I)JM_J)\ , \tag{2.25}$$

where ϵ_α is the signature of the permutation α. The sum over the set of orbital angular momenta $[Ll]$ in Eq. (2.25) is restricted by the parity relation

$$\left[\prod_i(-)^{l_i}\right]\left[\prod_i(-)^{L_i}\right]=\pi\ , \tag{2.26}$$

which follows from Eq. (2.24). The GC amplitude f in Eq. (2.25) is determined by solving the Hill-Wheeler (HW) variational equation

$$\delta E=\delta[\langle\psi^{(\mathrm{int})}\mid H\mid\psi^{(\mathrm{int})}\rangle/\langle\psi^{(\mathrm{int})}\mid\psi^{(\mathrm{int})}\rangle]=0\ , \tag{2.27}$$

where the Hamiltonian H has the form

$$H=(-\hbar^2/2m)\sum_i\nabla_i^2+\sum_{i<j}V_{ij}\ . \tag{2.28}$$

Here V_{ij} stands for the nucleon-nucleon interaction which in our calculations is approximated by the effective nuclear potential number 2 of Volkov.[27] The Coulomb interaction is neglected. For the mass m of the nucleon, appearing in the kinetic energy operator, we use

$$m=938.926\ \mathrm{MeV}/c^2\ . \tag{2.29}$$

In practical calculations, a knowledge of the relevant degrees of freedom and quantum numbers of the individual clusters, e.g., size, shape, sensitivity to changes in size and shape, spin and orbital angular momenta, etc., will lead to considerable simplifications. The great flexibility of the trial wave function (2.25) allows us to select those sets of parameters which are expected to play a dominant role also in the assembly of clusters. This will be demonstrated in the next section for the case of the bound $\alpha+$d system.

III. APPLICATION TO THE BOUND ALPHA+DEUTERON SYSTEM

The main purpose of this work is to investigate in overlapping clusters the effects of distortion, or more precisely, the effects which are related to changes in the size of the clusters. It is therefore necessary to begin with a study of the size and (for the α particle) also of the sensitivity to changes in the size of the separate clusters.

A. The clusters as separate nuclei

Dealing with a single cluster with nucleon number $A\leq4$, we restrict the GC trial function to contain orbits with $[nlm]=0$ only. In addition, we assume that all single-particle orbits are characterized by a common oscillator parameter β which is used as generator coordinate. In this case, the HW equation for the GC amplitude $f(\beta,E)$ is given by

$$\sum_{i=1}^{N}f(\beta_i,E)(\beta_i+\beta_j)^{3(1-A)/2}[\,3(A-1)\hbar^2\beta_i\beta_j/2m(\beta_i+\beta_j)+A(A-1)/2$$
$$\times\{V_a[1+4/\alpha^2(\beta_i+\beta_j)]^{-3/2}+V_r[1+4/\rho^2(\beta_i+\beta_j)]^{-3/2}\}-E]=0,\quad(j=1,\ldots,N) \tag{3.1}$$

where N is the number of discrete values of the generator coordinate β. The parameters V_a, V_r, α, and ρ specify the strength and range of the effective nucleon-nucleon interaction. Notice that using translational invariant states ($\vec{k}=0$), the energy E is the intrinsic energy.

1. The alpha particle

The HW equation (3.1) for the α particle is solved using the set of $N=8$ oscillator parameters β_α which are equidistantly distributed over the interval

$$0.1\leq\beta_\alpha\leq0.8\ \mathrm{fm}^{-2}\ . \tag{3.2a}$$

The energy of the ground state

$$(E_\alpha)_{\mathrm{g.s.}}=-29.391\ (-28.296)\ \mathrm{MeV}\ , \tag{3.3a}$$

while the excitation energy of the first excited state

$$(E_\alpha)_{\mathrm{ex}}=24.979\ (20.1)\ \mathrm{MeV} \tag{3.4a}$$

(Throughout this paper, experimental values are given in parentheses.) The reliability of these results may be confirmed by repeating the above calculation with a larger set of parameters. If we add the two parameters

$$\beta_\alpha=0.9\ \text{and}\ \beta_\alpha=1.0\ \mathrm{fm}^{-2} \tag{3.2b}$$

to the set (3.2a), we obtain

$$(E_\alpha)_{\mathrm{g.s.}}=-29.402\ \mathrm{MeV} \tag{3.3b}$$

and

$$(E_\alpha)_{\mathrm{ex}}=24.979\ \mathrm{MeV}\ , \tag{3.4b}$$

which is in satisfactory agreement with the results (3.3a) and (3.4a).

In our model, it is tempting to interpret the first excited state as a breathing mode, i.e., a compressional vibration of the α particle. In order to study this degree of freedom

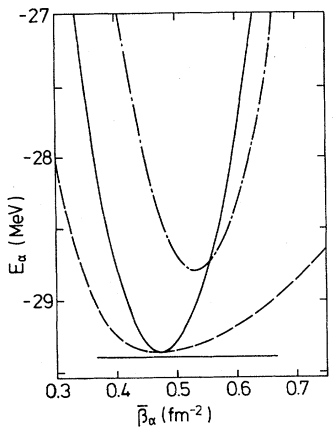

FIG. 1. Ground state energy E_α of the α particle. The broken curve shows the lowest eigenvalue of the (3×3) Hill-Wheeler (HW) equation as a function of the mean value $\bar{\beta}_\alpha$ of the set $\bar{\beta}_\alpha,\bar{\beta}_\alpha\pm0.05$ fm^{-2} of generator coordinates. The full curve represents the expectation value of the Hamiltonian, calculated with the GC amplitude for the minimum of the broken curve for different values of $\bar{\beta}_\alpha$. The dash-dotted curve shows the dependence of the energy on $\bar{\beta}_\alpha$, when only one value of the generator coordinate ($\bar{\beta}_\alpha$) is chosen. The result of an (8×8) HW equation, using the set of equidistantly chosen generator coordinates, $\beta_\alpha=0.1, 0.2, \ldots, 0.8$ fm^{-2}, is indicated by a straight line.

which is related to the nuclear compressibility[17] in more detail, we calculate the intrinsic energy E_α of the α particle for different size parameters β_α. The results are summarized in Fig. 1. The dash-dotted curve shows the ground state energy of the α particle as a function of the oscillator parameter β_α. (For this curve the quantity $\bar{\beta}_\alpha$ shown in Fig. 1 is equal to β_α.) The equilibrium value

$$(\beta_\alpha)_{\rm eq}=0.53 \text{ fm}^{-2} \tag{3.5}$$

determines the rms radius of the charge distribution

$$r=\{1.5[(1-1/A)/\beta_{\rm eq}+a_{\rm p}^2]\}^{1/2} , \tag{3.6}$$

where $a_{\rm p}$ corrects for the finite size of the proton.[25] With

$$a_{\rm p}^2=0.43 \text{ fm}^{-2} \tag{3.7}$$

we obtain

$$r_\alpha=1.66\ (1.674\pm0.015) \text{ fm} , \tag{3.8}$$

where the experimental value is taken from Ref. 28.

If we adopt the phenomenological model[17] of the nuclear breathing mode, the excitation energy is simply related to the compressibility K_α of the α particle and thus to the curvature of the dash-dotted curve in Fig. 1 at $\beta_{\rm eq}$:

$$K_\alpha=\left[\beta_\alpha^2\frac{d^2E_\alpha}{d\beta_\alpha^2}\right]_{\rm eq} , \tag{3.9}$$

$$(E_\alpha)_{\rm ex}=[K_\alpha\hbar^2/m]^{1/2}/r_\alpha . \tag{3.10}$$

Using the result

$$\left[\frac{d^2E_\alpha}{d\beta_\alpha^2}\right]_{\rm eq}=210 \text{ MeV fm}^2 , \tag{3.11}$$

we find

$$K_\alpha=58.99 \text{ MeV} \tag{3.12}$$

and

$$(E_\alpha)_{\rm ex}=29.80 \text{ MeV} , \tag{3.13}$$

which is considerably larger than our previous result for the excitation energy, Eq. (3.4b).

As far as the ground state is concerned, we notice from Fig. 1 that using a trial function of the GC-type (with eight β_α values) lowers the energy by 0.6 MeV as compared to the model with a single β_α [at $\beta_\alpha=(\beta_\alpha)_{\rm eq}$]. We may improve this model by choosing a few values of β_α in the neighborhood of an average $\bar{\beta}_\alpha$ and solving the corresponding HW equation. For our purposes, it is sufficient to choose the three values

$$\beta_\alpha=\bar{\beta}_\alpha,\ \beta_\alpha=\bar{\beta}_\alpha\pm0.05 \text{ fm}^{-2} . \tag{3.14}$$

The ground state energy which results from solving the 3×3 HW equation for different $\bar{\beta}_\alpha$ is given by the dashed line in Fig. 1. For the equilibrium

$$(\bar{\beta}_\alpha)_{\rm eq}=0.475 \text{ fm}^{-2} , \tag{3.15}$$

the rms radius which may approximately be obtained from Eq. (3.6),

$$r=1.74 \text{ fm} , \tag{3.16}$$

is slightly larger than the previous one, Eq. (3.8). The corresponding ground state energy

$$E_\alpha(\bar{\beta}_\alpha)_{\rm eq}=-29.360 \text{ MeV} \tag{3.17}$$

is almost the same as that obtained by solving the HW equation with the set (3.2a). The curvature of the dashed line in Fig. 1 at $\bar{\beta}_\alpha=(\bar{\beta}_\alpha)_{\rm eq}$ must not be related, however, to the compressibility K_α, Eq. (3.9). The reason is that performing completely independent HW calculations for each $\bar{\beta}_\alpha$, we allow the α particle to readjust itself in a way that goes beyond a simple change in a coordinate scale factor which is implicitly assumed in Eqs. (3.9) and (3.10). If we want to study the change in energy which results from a change in a coordinate scale factor, we may use the following procedure: First, we determine the GC amplitude $f_{\rm eq}(\beta_\alpha)$ for the equilibrium $(\bar{\beta}_\alpha)_{\rm eq}$. For nonequilibrium values of $\bar{\beta}_\alpha$, the energy E_α is then calculated as the expectation value of the Hamiltonian with the amplitude $f_{\rm eq}(\beta_\alpha)$. The result is represented by the solid curve in Fig. 1. The curvature at the equilibrium

$$\left[\frac{d^2E_\alpha}{d\bar{\beta}_\alpha^2}\right]_{\rm eq}=208 \text{ MeV fm}^2 \tag{3.18}$$

is close to that of the model with a single β_α, Eq. (3.11). If we use Eqs. (3.9), (3.10), and (3.16), we obtain for the compressibility and the excitation energy of the breathing mode

$$K_\alpha=46.93 \text{ MeV} , \tag{3.19}$$

$$(E_\alpha)_{\rm ex}=25.41 \text{ MeV} . \tag{3.20}$$

It is gratifying to notice that the excitation energy of the

breathing mode as calculated with our refined model is in excellent agreement with the excitation energy of the first excited state resulting from a fully microscopic GCM calculation, Eq. (3.4b). This fact encourages us to apply the same model to a study of the size and compressibility of the α cluster in the nucleus ^{6}Li.

2. The deuteron

The free deuteron is known to be less satisfactorily described by a simple central interaction such as employed in our calculations than the α particle. Solving the HW equation (3.1) for the case of the deuteron using the set of 14 oscillator parameters β_d which are equidistantly distributed over the interval

$$0.04 \leq \beta_d \leq 0.56 \text{ fm}^{-2} , \tag{3.21}$$

we obtain the ground state energy

$$(E_d)_{g.s.} = -0.600 \ (-2.23) \text{ MeV} . \tag{3.22}$$

From the fact that an exact solution[10] of the Schrödinger equation for the free deuteron with the same interaction gives -0.6 MeV for the ground state energy we conclude that our method of solving this equation is rather accurate and that the discrepancy between the calculated and experimental binding energy is due to the effective interaction. However, if we calculate the binding energy using a single β_d only, we find that the deuteron is unbound. In Fig. 2, this corresponds to the dash-dotted curve. The solution of the HW equation using the set

$$\beta_d = \bar{\beta}_d, \ \beta_d = \bar{\beta}_d \pm 0.05 \text{ fm}^{-2} \tag{3.23}$$

for different $\bar{\beta}_d$ is represented by the dashed line in Fig. 2. If we use Eq. (3.6), we find from the equilibrium value

$$(\bar{\beta}_d)_{eq} = 0.19 \text{ fm}^{-2} \tag{3.24}$$

the rms radius

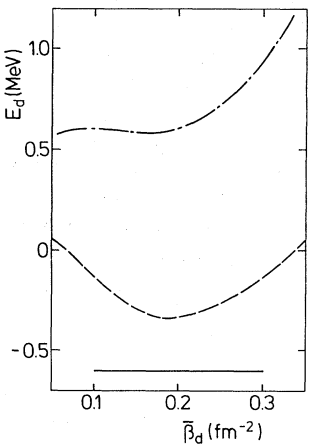

FIG. 2. Ground state energy of the deuteron. The dashed and dash-dotted curves are calculated in the same manner as those of Fig. 1. The result of a (14×14) HW equation, using the set of equidistantly chosen generator coordinates, $\beta_d = 0.04, 0.08, \ldots, 0.56$ fm^{-2}, is indicated by a straight line.

$$r_d = 2.12 \ (2.51 \pm 0.10) \text{ fm} . \tag{3.25}$$

Although the free deuteron is not accurately described by the central effective interaction used in our calculations, we still expect to get qualitative information on the change of the size of the deuteron in the bound α+d system.

B. The bound alpha+deuteron system

1. The full GC calculation

The bound α+d system is studied by using a single-particle basis with $[nlm]=0$ and taking into account the three generator coordinates β_α, β_d, and s, i.e., the oscillator parameters of the α particle and the deuteron and the separation of their oscillator wells. The following values for the generator coordinates are used:

$$\beta_\alpha = 0.3, \ 0.4, \ 0.5, \ 0.6 \text{ fm}^{-2} ,$$
$$\beta_d = 0.05, \ 0.15, \ 0.25, \ 0.35 \text{ fm}^{-2} , \tag{3.26}$$

$$s = 2, \ 3, \ 4, \ 5, \ 6, \ 7 \text{ fm} . \tag{3.27a}$$

Solving the corresponding (96×96) HW equation, we obtain the ground state energy

$$(E_{Li})_{g.s.} = -30.3 \ (-32.0) \text{ MeV} . \tag{3.28}$$

Thus there is a discrepancy of 1.7 MeV between the calculated and experimental binding energy. In order to gain some insight into possible deficiencies of the model space, we add a second component to our trial wave function and study its influence on the ground state energy. The second component differs from the first one only as far as the deuteron is concerned which is now described by a proton and a neutron in $n=0$, $l=1$ orbits coupled to zero orbital angular momentum. The corresponding many-body matrix elements are calculated from those with $[nlm]=0$ using the recursion relation (2.3). Also in the second component, we use the parameters β_α, β_d, and s as generator coordinates. However, with the sets (3.26) and (3.27a) of the GC coordinates, we find that adding the second component does not enlarge the model space. Thus, even with the restriction to the simplest set of quantum numbers $[nlm]=0$, our model wave function is shown to be already quite flexible.

In this context, it is instructive to compare our results with those obtained by Krivec and Mihailović[10] who developed two different cluster models for the nucleus ^{6}Li adopting the same effective interaction as we do in our calculations. If the nucleus ^{6}Li is described as an interplay of the two-cluster structures (α+d), (^{5}He+p), and (^{5}Li+n), by using the same oscillator parameter for all clusters, then the calculated ground state energy $E_{g.s.} = -28.3$ MeV. Similarly, when these authors describe ^{6}Li in terms of the three-cluster structure (α+p+n), again using a common β, they find $E_{g.s.} = -28.7$ MeV.

We conclude that the picture of breathing spherical clusters is a quite successful one within the limitations of our simple effective nuclear Hamiltonian. Although further extensions of the model space are conceivable, we

consider it more appropriate to include a noncentral term in the nucleon-nucleon interaction. Thus deformed clusters are expected to become favored. As our formalism is well suited to describe also this degree of freedom (which also includes shape vibrations of the clusters), such a study is planned for the near future.

2. *Restricted GC calculations*

In order to study distortion effects in the α particle and the deuteron when they come close enough to form a bound ^{6}Li nucleus, we restrict the set of parameters in the HW equation. We choose only three s points

$$s=\bar{s},\ s=\bar{s}\pm 1\ \text{fm}\ , \tag{3.27b}$$

but take the same set of coordinates β_α and β_d as in Eq. (3.26). The ground state energy which is obtained by solving the (48×48) HW equation for different values of the average distance $\bar{s}$ is shown by the full curve in Fig. 3. This curve exhibits a minimum at the equilibrium value

$$\bar{s}_{\text{eq}}=3.78\ \text{fm}\ . \tag{3.29}$$

This value is close to the result for the rms radius, $r_{\alpha d}=3.32$ fm, of the α+d relative wave function, found by Plattner *et al.*[29] in a model-independent analysis of α-d scattering data. The energy at the minimum

$$(E_{\text{Li}})_{\text{eq}}=-30.1\ \text{MeV} \tag{3.30}$$

differs only by 0.2 MeV from $(E_{\text{Li}})_{\text{g.s.}}$, Eq. (3.28), obtained by the full GC calculation. Therefore, it is reasonable to expect that the restriction to the set of parameters,

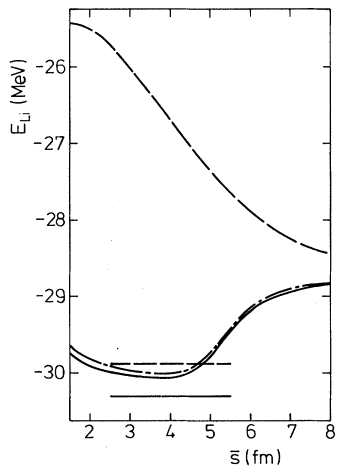

FIG. 3. Ground state energy of ^{6}Li. The full curve shows the result of the (48×48) HW calculation with the following set of generator coordinates: (i) $\beta_\alpha=0.3$, 0.4, 0.5, and 0.6 fm^{-2}; (ii) $\beta_d=0.05$, 0.15, 0.25, and 0.35 fm^{-2}; (iii) $s=\bar{s}$, $\bar{s}\pm 0.1$ fm, for different values of the intercluster distance $\bar{s}$. The dash-dotted and dashed curves are obtained by "switching off" the distortion of the α cluster and both the α and deuteron clusters, respectively. The energy resulting from a (96×96) HW calculation, using the sets (i) and (ii), and $s=2, 3, \ldots, 7$ fm of generator coordinates, is indicated by a straight line. The sum of the (intrinsic) energies of the separated α and deuteron clusters is given by a dashed straight line.

Eqs. (3.26) and (3.27b), is unlikely to affect seriously the resulting behavior of the α and d clusters in ^{6}Li.

In order to demonstrate in a qualitative way the importance (or unimportance) of distortion effects in a cluster, we simply "switch off" its distortion. For the α cluster, this is realized by the following ansatz for the GC amplitude:

$$f(\beta_\alpha,\beta_d,s)=f_\alpha^{(\text{free})}(\beta_\alpha)f(\beta_d,s)\ , \tag{3.31}$$

where $f_\alpha^{(\text{free})}(\beta_\alpha)$ is the GC amplitude obtained for the free α particle, while the remaining part of the GC amplitude, $f(\beta_d,s)$, is determined variationally. If we solve the HW equation for different values of $\bar{s}$, we obtain the dash-dotted curve in Fig. 3. As is seen, the distortion effects in the α particle are not important in the bound α+d system. For distances $\bar{s}>7$ fm, distortion effects in the α particle become completely negligible.

As for the d cluster, we may switch off its distortion by using the ansatz

$$f(\beta_\alpha,\beta_d,s)=f_\alpha^{(\text{free})}(\beta_\alpha)f_d^{(\text{free})}(\beta_d)f(s)\ , \tag{3.32}$$

where $f_d^{(\text{free})}(\beta_d)$ is the GC amplitude for the free deuteron and $f(s)$ is again determined variationally. [The use of $f_\alpha^{(\text{free})}(\beta_\alpha)$ is justified by the unimportance of distortion effects in the α cluster.] The ground state energy calculated with the GC amplitude (3.32) for different $\bar{s}$ is shown by the dashed curve in Fig. 3. Here one sees that, up to a distance of 8 fm, the distortion of the deuteron cluster drastically affects the energy of the α+d system.

3. *Size of the deuteron cluster in ^{6}Li*

There is evidence from both theoretical[30,31] and experimental[32,33] investigations that the deuteron cluster in ^{6}Li has a somewhat shorter tail than a free deuteron. We may study this effect with our model by restricting the set of GC parameters:

$$\begin{aligned}&\beta_\alpha=\bar{\beta}_\alpha,\ \bar{\beta}_\alpha\pm 0.05\ \text{fm}^{-2}\ ,\\ &\beta_d=\bar{\beta}_d,\ \bar{\beta}_d\pm 0.05\ \text{fm}^{-2}\ ,\\ &s=\bar{s},\ \bar{s}\pm 1\ \text{fm}\ .\end{aligned} \tag{3.33}$$

By solving the (27×27) HW equation for different values of $\bar{\beta}_\alpha$, $\bar{\beta}_d$, and $\bar{s}$ we determine the minimum of the ground state energy of ^{6}Li

$$(E_{\text{Li}})_{\text{eq}}=-29.85\ \text{MeV}\ , \tag{3.34}$$

which is close to the result (3.28) obtained by solving the full (96×96) HW equation. This indicates that the restriction to the set (3.33) of GC parameters is not a severe one. The minimum of the energy is found for the following average GC parameters:

$$\begin{aligned}&(\bar{\beta}_\alpha)_{\text{eq}}=0.475\ \text{fm}^{-2}\ ,\\ &(\bar{\beta}_d)_{\text{eq}}=0.24\ \text{fm}^{-2}\ ,\end{aligned} \tag{3.35}$$

and

$$(\bar{s})_{\text{eq}}=3.8\ \text{fm}\ .$$

If we compare this result with the equilibrium parameters

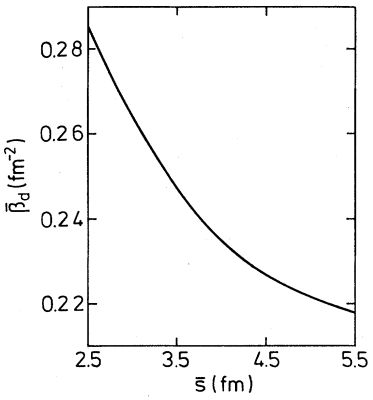

FIG. 4. Size of the deuteron cluster in ^{6}Li. The curve shows the dependence of the size parameter of the deuteron $\bar{\beta}_d$, obtained for the minimum of the energy of ^{6}Li as a function of the average intercluster distance $\bar{s}$.

of the free clusters, Eqs. (3.15) and (3.24), we find that the size of the α cluster is unchanged whereas that of the deuteron cluster is smaller.

It is also of interest to study the size of the deuteron cluster for nonequilibrium values of the average cluster separation $\bar{s}$. For this we solve the (27×27) HW equation for a range of parameters $\bar{\beta}_d$ and $\bar{s}$ [the use of $(\bar{\beta}_\alpha)_{eq}$ is justified by the unimportance of distortion effects in the α cluster] and determine the average oscillator parameter $\bar{\beta}_d$ corresponding to the minimum of energy for a given $\bar{s}$. The result is shown in Fig. 4. From this figure, one notes that $\bar{\beta}_d$ decreases with increasing $\bar{s}$. Thus, the shrinking of the deuteron cluster becomes weaker when the separation between the α and d clusters is increased. The same feature is exhibited in a more detailed way in Fig. 5, where the ground state energy of ^{6}Li is plotted in the vicinity of the equilibrium $(\bar{\beta}_d)_{eq}$ and $(\bar{s})_{eq}$. In this calculation, $\bar{\beta}_\alpha=(\bar{\beta}_\alpha)_{eq}$ and the GC amplitude

$$f(\beta_\alpha,\beta_d,s)=f_{eq}(\beta_\alpha,\beta_d,s)\ ,$$

obtained for the equilibrium configuration. This restriction is analogous to the one discussed in Sec. III A 1. Our result on the shrinking of the deuteron cluster in ^{6}Li is in accordance with calculations of the rms radius r_d of the deuteron cluster by Végh and Erö[31] who use the three-body wave function of Ref. 20. These authors find that r_d decreases considerably by increasing the momentum Q of the α particle relative to the deuteron.

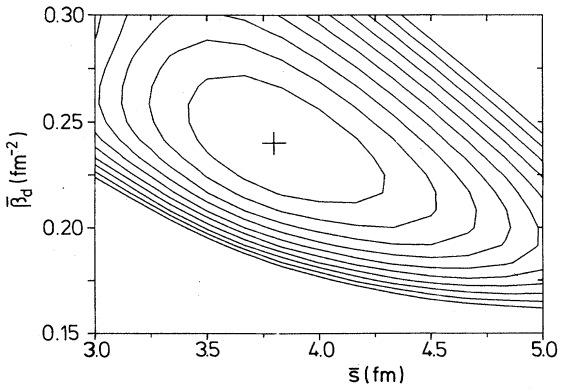

FIG. 5. Contour plot of the ground state energy of ^{6}Li in the $\bar{\beta}_d$, $\bar{s}$ parameter space. The energy increases from the minimum (+) with $E=-29.85$ MeV in steps of 0.1 MeV per line.

4. *Compressibility of the alpha cluster in ^{6}Li*

In Sec. III A 1, we calculated the excitation energy of the breathing mode of the free α particle both from its compressibility and by an independent GC calculation. It is an interesting question to ask whether this breathing mode still exists as a collective excitation when the α and d clusters are bound together in ^{6}Li. To shed some light on this problem, we calculate the compressibility of the α particle in the bound $\alpha+$d system, adopting a similar procedure as for the free α particle.

That is, we start from the solution of the (27×27) HW equation related to the set of GC parameters (3.33) where the average values are those of Eq. (3.35) for the equilibrium. Using the corresponding GC amplitude $f_{eq}(\beta_\alpha,\beta_d,s)$, we calculate the change in energy for nonequilibrium values of $\bar{\beta}_\alpha$. We obtain

$$(\partial^2 E_{Li}/\partial\bar{\beta}_\alpha^2)_{eq}=213\ \text{MeV fm}^2\ , \tag{3.36}$$

which is only slightly larger than the value 208 for the free α particle. If we use this result together with $(\bar{\beta}_\alpha)_{eq}$ from Eq. (3.35) in Eqs. (3.6), (3.9), and (3.10), we find for the α cluster the compressibility

$$K_{\alpha(Li)}=48.06\ \text{MeV} \tag{3.37}$$

and the excitation energy of the breathing mode

$$(E_{\alpha(Li)})_{ex}=25.72\ \text{MeV}\ . \tag{3.38}$$

Comparing these values with the result for the free α particle, Eqs. (3.19) and (3.20), we conclude that—in addition to its size—also the compressibility of the α cluster is rather insensitive to the presence of the d cluster in the nucleus ^{6}Li. These findings are of interest also in the context of three-body models[20] of ^{6}Li, where it is *a priori* assumed that the α cluster is undistorted.

IV. SUMMARY

Within the framework of the nuclear cluster model, we develop a formalism which allows one to treat the moleculelike vibrations of a multicluster system and various oscillations of the size and shape of individual clusters simultaneously. This is realized by using the separations between the clusters and the parameters which determine their size and shape as generator coordinates. It is the inclusion of the size parameters into the set of generator coordinates which (in our opinion) makes this model the most powerful method so far used for studying distortion effects within the framework of the cluster model.

The necessary formulae for projecting linear and angular momentum are worked out in detail. Recursion relations are derived which allow one to obtain many-body matrix elements which contain single-particle orbits with quantum numbers $[nlm]\neq0$ from those with $[nlm]=0$.

Thus our method is a very simple one, as it is sufficient to deal explicitly only with nucleon orbits with $[nlm]=0$. The tedious task of calculating matrix elements with more complicated orbits and the solution of the multidimensional HW equation is left to the computer.

The model is applied to the nucleus ^{6}Li which is treated as a bound $\alpha+$d system. Here it is demonstrated that the use of the size parameters of the α and d clusters (in addition to the intercluster separation) as generator coordinates leads to a rather flexible trial wave function which also allows one to study the properties of the clusters in the bound system. We find that the deuteron cluster is contracted as compared to the free deuteron. On the other hand, it turns out that the size and the compressibility of the α cluster are almost unchanged by the presence of the deuteron.

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APPENDIX

In this appendix we show that the wave functions (2.19) form a spherical tensor of rank λ with respect to the intrinsic coordinates $[\vec{\xi}]$. Referring to the usual definition[22] of a spherical tensor, we have to prove that the $2\lambda+1$ functions $\phi([\vec{\xi}LL's\beta ll'](lL)\lambda M_\lambda)$, $M_\lambda=-\lambda,\ldots,\lambda$, transform under a rotation $R_{[\vec{\xi}]}(\Omega)$ of the framework of intrinsic coordinates $[\vec{\xi}]$ in the following way:

$$R_{[\vec{\xi}]}(\Omega)\phi([\vec{\xi}LL's\beta ll'](lL)\lambda M_\lambda)=\sum_{M'}D^{\lambda}_{M'M_\lambda}(\Omega)\phi([\vec{\xi}LL's\beta ll'](lL)\lambda M') , \tag{A1}$$

where $D^{\lambda}_{M'M_\lambda}(\Omega)$ is the rotation matrix[22] related to the rotation $R(\Omega)$. Throughout this appendix, the abbreviation ϕ for the intrinsic wave function $\phi_\alpha^{(\mathrm{int})}$ is used.

We study the effect of a simultaneous rotation of the frame of reference of the coordinates $[\vec{s}]$ and $[\vec{\xi}]$ on the wave function (2.18a)

$$\begin{aligned}R_{[\vec{s}]}(\Omega)R_{[\vec{\xi}]}(\Omega)\phi([\vec{\xi}\vec{s}\beta ll']lm)&=R_{[\vec{s}]}(\Omega)\nabla([ll']lm[\vec{s}])R^{-1}_{[\vec{s}]}(\Omega)R_{[\vec{s}]}(\Omega)R_{[\vec{\xi}]}(\Omega)\phi([\vec{\xi}\vec{s}\beta],[lm]=0)\\&=\sum_{m'}D^{l}_{m'm}(\Omega)\nabla([ll']lm'[\vec{s}])\phi([\vec{\xi}\vec{s}\beta],[lm]=0)\\&=\sum_{m'}D^{l}_{m'm}(\Omega)\phi([\vec{\xi}\vec{s}\beta ll']lm') .\end{aligned} \tag{A2}$$

In deriving the first and third equation in this result, we used Eq. (2.18a). The second equation needs two steps: Firstly, we use the transformation properties[22] of the spherical tensor operator $\nabla([ll']lm[\vec{s}])$, Eq. (2.15). Secondly, we notice from Eq. (2.10) that a simultaneous rotation $R_{[\vec{s}]}(\Omega)R_{[\vec{\xi}]}(\Omega)$ does not change the function $\phi([\vec{\xi}\vec{s}\beta],[lm]=0)$. Alternatively we write Eq. (A2) in the form

$$R_{[\vec{\xi}]}(\Omega)\phi([\vec{\xi}\vec{s}\beta ll']lm)=\sum_{m'}D^{l}_{m'm}(\Omega)R^{-1}_{[\vec{s}]}(\Omega)\phi([\vec{\xi}\vec{s}\beta ll']lm') . \tag{A3}$$

If we now expand ϕ in Eq. (A3) in terms of A-polar harmonics,

$$\phi([\vec{\xi}\vec{s}\beta ll']lm)=\sum_{[LL']LM}\phi([\vec{\xi}LL's\beta ll']lmLM)B^*([LL']LM[\hat{s}]) \tag{A4}$$

and use

$$R^{-1}_{[\vec{s}]}(\Omega)B^*([LL']LM[\hat{s}])=\sum_{M'}D^{L}_{MM'}(\Omega)B^*([LL']LM'[\hat{s}]) , \tag{A5}$$

we find that

$$\begin{aligned}\sum_{[LL']LM}R_{[\vec{\xi}]}(\Omega)\phi([\vec{\xi}LL's\beta ll']lmLM)B^*([LL']LM[\hat{s}])\\=\sum_{[LL']LMM'm'}D^{l}_{m'm}(\Omega)D^{L}_{M'M}(\Omega)\phi([\vec{\xi}LL's\beta ll']lm'LM')B^*([LL']LM[\hat{s}]) .\end{aligned}$$

Equating the coefficient of $B^*([LL']LM[\vec{s}])$ on both sides of this equation, we obtain

$$R_{[\vec{\xi}]}(\Omega)\phi([\vec{\xi}LL's\beta ll']lmLM)=\sum_{M'm'}D^{l}_{m'm}(\Omega)D^{L}_{M'M}(\Omega)\phi([\vec{\xi}LL's\beta ll']lm'LM') . \tag{A6}$$

Finally, if we use the Clebsch-Gordan series[26] for the product of rotation matrices and introduce the functions (2.19), we find the desired result (A1).

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