Realization of the algebraic version of the resonating-group method for three-cluster systems*

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The harmonic-oscillator basis for the description of three-cluster systems is constructed in the Fock–Bargmann representation. The transformation of basis functions accompanying the nucleon permutation operation is found. The problem of constructing the allowed states is solved. An algorithm for calculation of the Hamiltonian matrix elements in the basis of allowed states is developed. The matrix elements of the kinetic- and potential-energy operators are obtained for the ^{6}He(^{4}He$+n+n$) system in the state with zero orbital angular momentum. © *1994 American Institute of Physics.*

1. INTRODUCTION

The microscopic theory of collisions of light nuclei that takes into account only binary entrance channels has proved its efficiency in a number of reaction calculations. Its realization, at least in simple cases, with the resonating-group method (RGM)[1–4] or its algebraic version,[5–7] does not now encounter any fundamental difficulties. However, the problem becomes much more complicated if one tries to include three-body exit channels.

There appeared, however, papers in which the three-cluster problems of the discrete[8–11] and the continuous[12] spectrum were successfully solved. But in each case the clusters were taken as structureless particles whose interaction was modeled by some effective *cluster–cluster* potential and the Pauli principle was taken into account only approximately. Of course, this made it possible to simplify the calculations, but if we try to take into account other possible cluster partitions of a nucleus (e.g., the channel $t+t$ together with ^{4}He$+n+n$ in ^{6}He), the number of effective potentials needed for the calculations apparently becomes excessive. Therefore, it is naturally desirable to solve problems of this sort by using the same *nucleon–nucleon* potential. The RGM algebraic version could provide this possibility.

In the present work we present the basic ideas of the generalization of the RGM algebraic version for the three-cluster systems, discuss the difficulties that occur, and outline ways to overcome them. The analytical results will be obtained for the simplest three-cluster system, ^{6}He (^{4}He$+n+n$), in the state with zero orbital angular momentum. Nevertheless, the ideas discussed below are applicable to any system of three s clusters.

Let us recall that this approach is based on the expansion of a nuclear wave function over the multiparticle harmonic-oscillator basis. We begin with the construction of an oscillator basis that: a) takes into account the intrinsic structure of the three clusters; b) reproduces the dynamics of their relative motion; c) has a certain permutation symmetry. The last restriction, due to the Pauli principle, causes the major part of the computational difficulties.

As is well known, in the case of binary channels, the Pauli principle excludes from the complete set of harmonic-oscillator basis states those which vanish when acted on by the antisymmetrization operator and, therefore, cannot be used in calculations (these states are called the *forbidden* states). In the case of three-body channels, a number of basis states are also forbidden, but their identification becomes more complicated.[13–15] If the number of oscillator quanta is not less than the minimal number allowed by the Pauli principle, the allowed states can be identified as the eigenvectors of a density matrix with nonzero eigenvalues, while the forbidden states correspond to its zero eigenvalues.

The realization of the RGM algebraic version is based on extensive use of *generalized coherent states* (GCS),[5,16,17] which are the generating functions of the harmonic-oscillator basis. The GCS also perform a transformation from the coordinate space to the so-called *Fock–Bargmann space*,[18–20] where the basis functions have a simpler form, making the derivations less cumbersome.

The main steps in the implementation of the approach remain the same as in the binary-channel case. First we construct the generating functions of the three-cluster oscillator basis. Then we calculate their overlap integral and perform its projection onto the basis states. In this step we also discuss the choice of the quantum numbers for the classification of basis states and calculate the transition matrices between different bases. After that we obtain the matrix elements of the kinetic- and potential-energy operators of the six-nucleon system between the generating invariants. Finally, we find the Hamiltonian matrix elements between the basis states. The analytical calculations are concluded with a discussion of the asymptotic behavior of the Fourier coefficients and a derivation of the dynamical equations of the RGM algebraic version.

2. GENERATING FUNCTIONS OF THE THREE-CLUSTER OSCILLATOR BASIS

We shall write the wave function of a system of $N_{\rm cl}$ clusters in a form that is traditional for the RGM:

$$\Psi(\{\mathbf{r}_i,\sigma_i,\tau_i\})=\mathscr{A}\{\varphi(1)\ldots\varphi(N_{\rm cl})f(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1})\}. \tag{1}$$

Here $\{\mathbf{r}_i,\sigma_i,\tau_i;\ i=1,\ldots,A\}$ are the spatial, spin, and isospin coordinates of the A nucleons; $\mathscr{A}$ is the antisymmetrization operator; $\varphi(1),\ldots,\varphi(N_{\rm cl})$ are the functions describing the in-

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ternal structure of each cluster, these functions being fixed; $f(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1})$ is the function describing the relative motion of the clusters, depending on a set of $N_{\rm cl}-1$ translationally invariant Jacobi vectors of an $N_{\rm cl}$-cluster system. The latter are the *dynamical variables*, and the wave function f depending on them must be found by solving the integro-differential equation obtained from the Schrödinger equation after substitution in it of the trial function of the above form and integration over the remaining Jacobi vectors (intrinsic cluster coordinates).

In the framework of the RGM algebraic version the relative function $f(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1})$ is expanded in the basis states of the multiparticle harmonic oscillator

$$f(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1})=\sum_{\{n\}} C_{\{n\}} f_{\{n\}}(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1}) \tag{2}$$

and the dynamical equations are reduced to a set of linear algebraic equations for the expansion coefficients $C_{\{n\}}$. Here $\{n\}$ is the set of quantum numbers characterizing the basis states. The basis functions $f_{\{n\}}(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1})$ can be written as certain linear combinations of products of $N_{\rm cl}-1$ single-particle oscillator functions,

$$f_{nlm}(\mathbf{q}) = (-1)^n \sqrt{\frac{2n!}{r_0\Gamma(n+l+3/2)}}\, x^l e^{-x^2/2} L_n^{l+1/2} \times (x^2) Y_{lm}(\Omega_q), \tag{3}$$

where $x=q/r_0$, r_0 is the oscillator length, the parameter of the basis, $L_n^k(x)$ are the Laguerre polynomials, and $Y_{lm}(\Omega_q)$ are the spherical functions. The exact form of these linear combinations and the selection of the quantum numbers $\{n\}$ will be discussed in Sec. 3.

The expansion (2) of f is equivalent to the following expansion of Ψ:

$$\Psi(\{r_i,\sigma_i,\tau_i\})=\sum_{\{n\}} C_{\{n\}}\Psi_{\{n\}}(\{r_i,\sigma_i,\tau_i\}), \tag{4}$$

where the basis states $\Psi_{\{n\}}$ are introduced in analogy with (1):

$$\Psi_{\{n\}}(\{r_i,\sigma_i,\tau_i\})=\mathscr{A}\{\varphi(1)\ldots\varphi(N_{\rm cl}) f_{\{n\}} \times(\mathbf{q}_1,\ldots,\mathbf{q}_{N_{\rm cl}-1})\}. \tag{5}$$

As has already been mentioned, the idea of using the generating functions in work with the oscillator basis turned out to be very productive for calculations of nuclear processes involving binary channels (see the reviews of Refs. 5–7 and 3,4). A well-known example of a generating function is that of the Hermite polynomials:[21]

$$e^{2xt-t^2}=\sum_{n=0}^{\infty}\frac{t^n}{n!}H_n(x).$$

In our case, the generating functions for the basis states (3) are a generalization of the above function. They are constructed as Slater determinants composed of single-particle Brink orbitals:[22]

$$\varphi(\mathbf{R}_k,\mathbf{r})=\exp\{-\tfrac{1}{2}\mathbf{r}^2+\sqrt{2}\mathbf{R}_k\mathbf{r}-\tfrac{1}{2}\mathbf{R}_k^2\}\zeta(\sigma,\tau), \quad k=1,\ldots,N_{\rm cl}. \tag{6}$$

Here $\zeta(\sigma,\tau)$ are the spin–isospin functions, and $\mathbf{R}_k$ ($k=1,\ldots,N_{\rm cl}$) are the generating parameters. The generating function

$$\Phi(\{\mathbf{R}_k\},\{\mathbf{r}_i,\sigma_i,\tau_i\})=\det\|\varphi(\mathbf{R}_k,\mathbf{r}_i)\| \tag{7}$$

is not translationally invariant, but it allows an easy separation of the factor describing the center-of-mass motion (see Ref. 23)

$$\Phi(\{\mathbf{R}_k\},\{\mathbf{r}_i,\sigma_i,\tau_i\}) = \varphi(\{\mathbf{Q}_k\},\{\mathbf{r}_i,\sigma_i,\tau_i\})\Phi_{\rm CM}(\mathbf{R}_{\rm CM},\mathbf{r}_{\rm CM}) \tag{8}$$

by introducing the Jacobi vectors $\{\mathbf{q}_k\}$ and the corresponding generating coordinates $\{\mathbf{Q}_k\}$ ($k=1,\ldots,N_{\rm cl}-1$). It can be shown that the function $\varphi(\{\mathbf{Q}_k\},\{r_i,\sigma_i,\tau_i\})$ has a form similar to (1):

$$\varphi(\{\mathbf{Q}_k\},\{\mathbf{r}_i,\sigma_i,\tau_i\})=\mathscr{A}\{\varphi(1)\ldots\varphi(N_{\rm cl})f(\{\mathbf{Q}_k\},\{\mathbf{q}_k\})\}, \tag{9}$$

where

$$\varphi(k)=\exp\{-\tfrac{1}{2}\rho_k^2\}\zeta_k, \quad \rho_k^2=\sum_{i\in A_k}(\mathbf{r}_i-\mathbf{R}_k^{\rm CM})^2,$$

$$\zeta_k=\prod_{i\in A_k}\zeta(\sigma_i,\tau_i) \tag{10}$$

(the summation and the multiplication run over the coordinates of the nucleons belonging to the kth cluster) and

$$f(\{\mathbf{Q}_k\},\{\mathbf{q}_k\})=\prod_{k=1}^{N_{\rm cl}-1}\exp\{-\tfrac{1}{2}\mathbf{q}_k^2+\sqrt{2}\mathbf{Q}_k\mathbf{q}_k-\tfrac{1}{2}\mathbf{Q}_k^2\}. \tag{11}$$

The function $\varphi(\{\mathbf{Q}_k\},\{\mathbf{r}_i,\sigma_i,\tau_i\})$ which we have just constructed is a generalized coherent state[5,16,17] for the nuclear system under consideration. In this sense it is a wave packet generating the harmonic-oscillator basis describing the dynamics of the cluster relative motion. Indeed, it can be shown that the function in the product in Eq. (11) is the generating function for the basis states (3):

$$\exp\left\{-\frac{1}{2}\mathbf{q}^2+\sqrt{2}\mathbf{Q}\mathbf{q}-\frac{1}{2}\mathbf{Q}^2\right\} = \sum_{nlm}\left[\frac{\pi^3 2^{-2n-l+1}}{n!\Gamma(n+l+3/2)}\right]^{1/2} Q^{2n+l}Y_{lm}^*(\Omega_Q)f_{nlm}(\mathbf{q}). \tag{12}$$

Furthermore, the function $\varphi(\{\mathbf{Q}_k\},\{r_i,\sigma_i,\tau_i\})$ is the kernel of an integral transformation which maps the wave function in the coordinate space into the Fock–Bargmann space,[18–20] where it depends only on $N_{\rm cl}-1$ vector generating parameters (as we have already mentioned, the intrinsic cluster functions are fixed in this approach).

Below, using the generating function (9), we shall find the Fock–Bargmann images of the Pauli-allowed basis states and, remaining in the Fock–Bargmann space, calculate all

the necessary matrix elements. Special attention will be paid to the overlap integral of generating functions with different generating parameters, since this makes it possible to obtain comprehensive information on the harmonic-oscillator basis for a three-cluster system.

Although the expressions for the basis functions will be obtained in the Fock–Bargmann space, this does not hinder our main objective, which is to obtain the Schrödinger equation in the harmonic-oscillator representation.

Now we consider the construction of the generating functions and the calculation of their overlap integral for ^{6}He, which we regard as a system of three clusters, an alpha particle and two neutrons. For each cluster we introduce Brink orbitals with a corresponding generator parameter or, in more detail, four single-particle states for the alpha cluster,

$$|1\rangle \equiv \phi_1|p\uparrow\rangle, \quad |2\rangle \equiv \phi_1|p\downarrow\rangle, \quad |3\rangle \equiv \phi_1|n\uparrow\rangle,$$

$$|4\rangle \equiv \phi_1|n\downarrow\rangle, \tag{13}$$

and two states for the two neutron clusters,

$$|5\rangle \equiv \phi_2|n\uparrow\rangle; \quad |6\rangle \equiv \phi_3|n\downarrow\rangle, \tag{14}$$

where ϕ_k is the spatial part of $\phi(\mathbf{R}_k,\mathbf{r})$, and the spin–isospin functions are labeled in an obvious manner. We shall use also states with other generating parameters:

$$\tilde{\phi}_k\zeta(\sigma,\tau) = \phi(\tilde{\mathbf{R}}_k,\mathbf{r}), \quad k=1,2,3. \tag{15}$$

Now let

$$\Phi(\mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3;\{\mathbf{r}_i,\sigma_i,\tau_i\}) = \begin{vmatrix} \phi_1(\mathbf{r}_1)|p\uparrow\rangle & \phi_1(\mathbf{r}_2)|p\uparrow\rangle & \dots & \phi_1(\mathbf{r}_6)|p\uparrow\rangle \\ \phi_1(\mathbf{r}_1)|p\downarrow\rangle & \phi_1(\mathbf{r}_2)|p\downarrow\rangle & \dots & \phi_1(\mathbf{r}_6)|p\downarrow\rangle \\ \vdots & \vdots & & \vdots \\ \phi_3(\mathbf{r}_1)|n\downarrow\rangle & \phi_3(\mathbf{r}_2)|n\downarrow\rangle & \dots & \phi_3(\mathbf{r}_6)|n\downarrow\rangle \end{vmatrix}. \tag{16}$$

Then the overlap integral of two wave packets, Φ and $\tilde{\Phi}$, where

$$\tilde{\Phi} = \Phi(\tilde{\mathbf{R}}_1,\tilde{\mathbf{R}}_2,\tilde{\mathbf{R}}_3;\{\mathbf{r}_i,\sigma_i,\tau_i\}),$$

can be calculated as a determinant of single-particle overlaps:[24]

$$\langle\Phi|\tilde{\Phi}\rangle = \begin{vmatrix} \langle 1|\tilde{1}\rangle & \langle 1|\tilde{2}\rangle & \dots & \langle 1|\tilde{6}\rangle \\ \langle 2|\tilde{1}\rangle & \langle 2|\tilde{2}\rangle & \dots & \langle 2|\tilde{6}\rangle \\ \vdots & & & \vdots \\ \langle 6|\tilde{1}\rangle & \langle 6|\tilde{2}\rangle & \dots & \langle 6|\tilde{6}\rangle \end{vmatrix}. \tag{17}$$

Most of its elements vanish because of the orthogonality of the spin–isospin functions. Then

$$\langle\Phi|\tilde{\Phi}\rangle = \begin{vmatrix} \langle 1|\tilde{1}\rangle & 0 & 0 & 0 & 0 & 0 \\ 0 & \langle 2|\tilde{2}\rangle & 0 & 0 & 0 & 0 \\ 0 & 0 & \langle 3|\tilde{3}\rangle & \langle 3|\tilde{5}\rangle & 0 & 0 \\ 0 & 0 & \langle 5|\tilde{3}\rangle & \langle 5|\tilde{5}\rangle & 0 & 0 \\ 0 & 0 & 0 & 0 & \langle 4|\tilde{4}\rangle & \langle 4|\tilde{6}\rangle \\ 0 & 0 & 0 & 0 & \langle 6|\tilde{4}\rangle & \langle 6|\tilde{6}\rangle \end{vmatrix}$$

$$= \langle 1|\tilde{1}\rangle\langle 2|\tilde{2}\rangle \times \begin{vmatrix} \langle 3|\tilde{3}\rangle & \langle 3|\tilde{5}\rangle \\ \langle 5|\tilde{3}\rangle & \langle 5|\tilde{5}\rangle \end{vmatrix} \begin{vmatrix} \langle 4|\tilde{4}\rangle & \langle 4|\tilde{6}\rangle \\ \langle 6|\tilde{4}\rangle & \langle 6|\tilde{6}\rangle \end{vmatrix}. \tag{18}$$

Thus, the generating overlap integral has a multiplicative form. Calculating the overlaps of the Brink orbitals

$$\langle\phi(\mathbf{R})|\tilde{\phi}(\tilde{\mathbf{R}})\rangle = \exp(\mathbf{R}\tilde{\mathbf{R}}),$$

where the constant factor $\pi^{3/2}$ is dropped, we obtain the overlap integral of the generating wave packets:

$$\begin{aligned} \langle\Phi|\tilde{\Phi}\rangle = {} & \exp\{4\mathbf{R}_1\tilde{\mathbf{R}}_1 + \mathbf{R}_2\tilde{\mathbf{R}}_2 + \mathbf{R}_3\tilde{\mathbf{R}}_3\} \\ & - \exp\{3\mathbf{R}_1\tilde{\mathbf{R}}_1 + \mathbf{R}_1\tilde{\mathbf{R}}_2 + \mathbf{R}_2\tilde{\mathbf{R}}_1 + \mathbf{R}_3\tilde{\mathbf{R}}_3\} \\ & - \exp\{3\mathbf{R}_1\tilde{\mathbf{R}}_1 + \mathbf{R}_2\tilde{\mathbf{R}}_2 + \mathbf{R}_1\tilde{\mathbf{R}}_3 + \mathbf{R}_3\tilde{\mathbf{R}}_1\} \\ & + \exp\{2\mathbf{R}_1\tilde{\mathbf{R}}_1 + \mathbf{R}_1\tilde{\mathbf{R}}_2 + \mathbf{R}_2\tilde{\mathbf{R}}_1 + \mathbf{R}_1\tilde{\mathbf{R}}_3 + \mathbf{R}_3\tilde{\mathbf{R}}_1\}. \end{aligned} \tag{19}$$

In the calculations we used generating functions with fixed total isospin of the system, $T=1$, while with respect to the spin coordinates we have superposition of singlet and triplet states ($S=0,1$). Later on, we shall show how to separate basis functions with definite spin.

To separate the center-of-mass motion, we introduce new generating parameters, which we denote by $(\mathbf{a},\mathbf{b},\mathbf{R}_{CM})$ and $(\tilde{\mathbf{a}},\tilde{\mathbf{b}},\tilde{\mathbf{R}}_{CM})$:

$$\mathbf{a} = \frac{2}{\sqrt{3}}\left[\mathbf{R}_1 - \frac{1}{2}(\mathbf{R}_2+\mathbf{R}_3)\right],$$

$$\tilde{\mathbf{a}} = \frac{2}{\sqrt{3}}\left[\tilde{\mathbf{R}}_1 - \frac{1}{2}(\tilde{\mathbf{R}}_2+\tilde{\mathbf{R}}_3)\right],$$

$$\mathbf{b} = \frac{1}{\sqrt{2}}(\mathbf{R}_2-\mathbf{R}_3), \quad \tilde{\mathbf{b}} = \frac{1}{\sqrt{2}}(\tilde{\mathbf{R}}_2-\tilde{\mathbf{R}}_3),$$

$$\mathbf{R}_{CM} = \frac{1}{\sqrt{6}}(4\mathbf{R}_1+\mathbf{R}_2+\mathbf{R}_3),$$

$$\tilde{\mathbf{R}}_{CM} = \frac{1}{\sqrt{6}}(4\tilde{\mathbf{R}}_1+\tilde{\mathbf{R}}_2+\tilde{\mathbf{R}}_3). \tag{20}$$

After transformation to the new parameters, the overlap integral becomes

$$\langle\Phi|\tilde{\Phi}\rangle=\exp(\mathbf{R}_{\mathrm{CM}}\tilde{\mathbf{R}}_{\mathrm{CM}})\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle, \tag{21}$$

$$\begin{aligned}\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle=&\exp(\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}})\\&-\exp\{1/4\mathbf{a}\tilde{\mathbf{a}}+\sqrt{6}/4\mathbf{a}\tilde{\mathbf{b}}+\sqrt{6}/4\mathbf{b}\tilde{\mathbf{a}}+1/2\mathbf{b}\tilde{\mathbf{b}}\}\\&-\exp\{1/4\mathbf{a}\tilde{\mathbf{a}}-\sqrt{6}/4\mathbf{a}\tilde{\mathbf{b}}-\sqrt{6}/4\mathbf{b}\tilde{\mathbf{a}}+1/2\mathbf{b}\tilde{\mathbf{b}}\}\\&+\exp\{-1/2\mathbf{a}\tilde{\mathbf{a}}\},\end{aligned} \tag{22}$$

thus factoring out the center-of-mass motion. In the Fock–Bargmann space, the generating parameters, the vectors $\mathbf{a}$ and $\mathbf{b}(\tilde{\mathbf{a}},\tilde{\mathbf{b}})$, correspond to the Jacobi vectors of a three-body system in the coordinate space describing the relative position of two neutrons ($\mathbf{a}$) and the relative position of the alpha particle and the center of mass of the two neutrons ($\mathbf{b}$).

Let us now examine the calculation of the overlap integral from a different point of view, by explicitly considering the antisymmetrization operator $\mathscr{A}$. Among all $6!=720$ nucleon permutations composing $\mathscr{A}$ one must take into account only those that involve nucleons in the same spin–isospin state. There are four such permutations, the identity permutation, the transpositions P_{35} and P_{46}, and their product $P_{35}P_{46}$. The antisymmetrization operator becomes

$$\mathscr{A}=1-P_{35}-P_{46}+P_{35}P_{46}$$

and we have four terms in the overlap (19) corresponding to these permutations. If we write the first term (which is an overlap of nonantisymmetrized generating functions) as

$$\exp\{\mathbf{R}_1\tilde{\mathbf{R}}_1+\mathbf{R}_1\tilde{\mathbf{R}}_1+\mathbf{R}_1\tilde{\mathbf{R}}_1+\mathbf{R}_1\tilde{\mathbf{R}}_2+\mathbf{R}_1\tilde{\mathbf{R}}_2+\mathbf{R}_3\tilde{\mathbf{R}}_3\},$$

the other terms can be obtained from it by interchanging *one* of $\mathbf{R}_1$ with $\mathbf{R}_2$ or $\mathbf{R}_3$ or simultaneously *two* of $\mathbf{R}_1$ with $\mathbf{R}_2$ and $\mathbf{R}_3$.

The action of the antisymmetrization operator $\mathscr{A}$ in the space of the translationally invariant generating parameters $\mathbf{a}$ and $\mathbf{b}$ reduces to a certain linear transformation of $\mathbf{a}$ and $\mathbf{b}$. It can be shown (see Ref. 23) that the matrices of this transformation corresponding to the permutations P_{35}, P_{46}, and $P_{35}P_{46}$ are

$$T^{(1)}=\begin{pmatrix}\frac{1}{4} & \sqrt{\frac{3}{8}}\\ \sqrt{\frac{3}{8}} & \frac{1}{2}\end{pmatrix},$$

$$T^{(2)}=\begin{pmatrix}\frac{1}{4} & -\sqrt{\frac{3}{8}}\\ -\sqrt{\frac{3}{8}} & \frac{1}{2}\end{pmatrix},\quad T^{(3)}=\begin{pmatrix}-\frac{1}{2} & 0\\ 0 & 0\end{pmatrix}, \tag{23}$$

respectively. Then the overlap integral can be formally rewritten as a sum of four similar terms:

$$\begin{aligned}\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle=&\exp\{\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}}\}-\exp\{\bar{\mathbf{a}}\tilde{\mathbf{a}}+\bar{\mathbf{b}}\tilde{\mathbf{b}}\}-\exp\{\bar{\bar{\mathbf{a}}}\tilde{\mathbf{a}}+\bar{\bar{\mathbf{b}}}\tilde{\mathbf{b}}\}\\&+\exp\{+\bar{\bar{\bar{\mathbf{a}}}}\tilde{\mathbf{a}}+\bar{\bar{\bar{\mathbf{b}}}}\tilde{\mathbf{b}}\},\end{aligned} \tag{24}$$

where

$$\bar{\mathbf{a}}=\frac{1}{4}\mathbf{a}+\sqrt{\frac{3}{8}}\mathbf{b},\quad \bar{\mathbf{b}}=\sqrt{\frac{3}{8}}\mathbf{a}+\frac{1}{2}\mathbf{b}.$$

$$\bar{\bar{\mathbf{a}}}=\frac{1}{4}\mathbf{a}-\sqrt{\frac{3}{8}}\mathbf{b},\quad \bar{\bar{\mathbf{b}}}=-\sqrt{\frac{3}{8}}\mathbf{a}+\frac{1}{2}\mathbf{b}.$$

$$\bar{\bar{\bar{\mathbf{a}}}}=-\tfrac{1}{2}\mathbf{a},\quad \bar{\bar{\bar{\mathbf{b}}}}=0. \tag{25}$$

We see that to calculate the overlap integral we need only know the overlap of the nonantisymmetrized generating functions and the transformation of the generating parameters induced by the operation of nucleon permutation, i.e., the representation of the antisymmetrization operator $\mathscr{A}$ in the Fock–Bargmann space. This idea will be applied also to the calculation of the matrix elements of other operators, namely, the operators of kinetic and potential energy.

To clarify the subsequent transformations of the overlap integral $\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle$, let us recall some facts about the generating wave packets. The translationally invariant generating function φ introduced by (9) generates the harmonic-oscillator basis describing the dynamics of the relative motion of the clusters. On the other hand, as we have already mentioned, it is the kernel of the integral transformation

$$\begin{aligned}&\Psi(\mathbf{a},\mathbf{b})\\&=\int\ldots\int\varphi(\mathbf{a},\mathbf{b},\{\mathbf{r}_i,\sigma_i,\tau_i\})\Psi(\{\mathbf{r}_i,\sigma_i,\tau_i\})d\mathbf{r}_1\ldots d\mathbf{r}_6,\end{aligned} \tag{26}$$

which maps a wave function of the system in the coordinate space, $\Psi(\{\mathbf{r}_i,\sigma_i,\tau_i\})$, onto its image $\Psi(\mathbf{a},\mathbf{b})$ in the Fock–Bargmann space. Indeed,

$$\varphi(\mathbf{a},\mathbf{b},\{\mathbf{r}_i,\sigma_i,\tau_i\})=\sum_{\{n\}}\varphi(\{n\};\mathbf{a},\mathbf{b})\Psi^*_{\{n\}}(\{\mathbf{r}_i,\sigma_i,\tau_i\}), \tag{27}$$

where $\{\Psi_{\{n\}}\}$ are the orthonormalized harmonic-oscillator basis states (5), and $\varphi(\{n\};\mathbf{a},\mathbf{b})$ are their images. Therefore, the expansion (4) can be rewritten in the Fock–Bargmann space,

$$\Psi(\mathbf{a},\mathbf{b})=\sum_{\{n\}}C_{\{n\}}\varphi(\{n\};\mathbf{a},\mathbf{b}), \tag{28}$$

and we encounter the problem of constructing the image $\Psi(\mathbf{a},\mathbf{b})$ of wave functions in terms of their expansion coefficients $C_{\{n\}}$ and the subsequent return to the original wave functions

$$\Psi(\{\mathbf{r}_i,\sigma_i,\tau_i\})=\sum_{\{n\}}C_{\{n\}}\Psi_{\{n\}}(\{\mathbf{r}_i,\sigma_i,\tau_i\}).$$

Of course, the original wave function replaced by its image $\Psi(\mathbf{a},\mathbf{b})$ would be only an approximate solution of the Schrödinger equation. However, this solution gives us adequate information on nuclear phenomena that do not involve the process of alpha cluster decay.

The reason for introducing the image $\varphi(\{n\};\mathbf{a},\mathbf{b})$ is its simplicity and clarity of representation compared with the original $\Psi_{\{n\}}$. Just compare the simplest oscillator function in the coordinate space [Eq. (3)] and its Fock–Bargmann image [extracted from (12)]:

$$a_{nl}Q^{2n+l}Y_{lm}(\Omega_Q),$$

where

$$a_{nl}=\left[\frac{\pi^3 2^{-2n-l+1}}{n!\Gamma(n+l+3/2)}\right]^{1/2}.$$

For the three-cluster system, the image is a function of two vectors which can be written explicitly for most cases, whereas $\Psi_{\{n\}}(\{r_i,\sigma_i,\tau_i\})$ depends on all Jacobi vectors and spin–isospin variables of the coordinate space and is a rather complicated construction. Various features of the latter become clear after its image is found. Working with the basis $\varphi(\{n\};\mathbf{a},\mathbf{b})$ effectively reduces our six-particle problem to a three-particle one, thus making it possible to use some techniques developed for the three-body problem.[25–27]

So far we have not yet shown an algorithm for constructing the basis functions $\varphi(\{n\};\mathbf{a},\mathbf{b})$, although we have obtained an expression for $\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle$ which permits us to formulate such an algorithm.

From the expansion (27) and the orthonormality of the basis functions $\Psi_{\{n\}}$ it follows that

$$\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle=\sum_{\{n\}}\varphi(\{n\};\mathbf{a},\mathbf{b})\varphi(\{n\};\tilde{\mathbf{a}},\tilde{\mathbf{b}}), \tag{29}$$

i.e., the overlap integral (22) can be written as a convolution of the basis functions to be found. This fact will be used later, when we shall obtain expressions for $\varphi(\{n\};\mathbf{a},\mathbf{b})$ for the states with zero orbital angular momentum.

3. ON THE CHOICE OF THE OSCILLATOR BASIS

Having determined our objective as the derivation of the Schrödinger equation for a three-cluster system in the representation of the oscillator basis states $\{\Psi_{\{n\}}\}$, we must specify what classification of the basis states will be used. Among the quantum numbers labeling the basis state there are two evident ones, the total number of oscillator excitation quanta, n, and the orbital angular momentum of the cluster relative motion, L. At first we shall restrict ourselves to the case $L=0$. Then only three dynamical degrees of freedom remain and, therefore, besides n, two other quantum numbers must be specified. Their choice is determined by the Pauli principle and the need to simplify as much as possible the calculations of Hamiltonian matrix elements between the basis states. The Pauli principle requires that the basis states be antisymmetric with respect to transposition of nucleons. Therefore, it is desirable to have quantum numbers which—along with n—remain unchanged under nucleon permutations.

The choice of these quantum numbers is based on the classification of harmonic-oscillator basis states provided by the $SU(3)$ group.[28] It is known that the space spanned by the harmonic-oscillator basis states with a given n is a direct sum of the subspaces spanned by states with a fixed $SU(3)$ symmetry $(\lambda\mu)$. For $L=0$, the numbers n, λ, and μ must be even, so that the following pairs of indices are possible:

$$\lambda=n,\quad \mu=0;\quad \lambda=n-4,\quad \mu=2,;\ \ldots;$$

$$\lambda=n-4m,\quad \mu=2m;\ \ldots\ .$$

If n is fixed, only one of $(\lambda\mu)$ is independent, for instance, μ. Letting $\mu=2m$, we take m as the second quantum number of a basis function. It can take any integer value from 0 to $[n/4]$.

For the states with $(\lambda\mu)=(n-4m2m)$ we must also introduce a third quantum number, since there are $n-2m+1$ states for each fixed n and m, with the following n_1 and n_2:

$$n_1=2m,\quad n_2=n-2m;\quad n_1=2m+1,$$

$$n_2=n-2m-1;\ldots;n_1=n-2m,\quad n_2=2m.$$

This quantum number could be n_1 $(2m\leqslant n_1\leqslant n-2m)$ or n_2 $(2m\leqslant n_2\leqslant n-2m)$, but we choose another quantum number. For this purpose we consider the action of the antisymmetrization operator on the functions $|n_1n_2 2m\rangle$, which have no definite permutation symmetry but maintain a simple algorithm for calculation of the potential-energy matrix elements. We shall work with the basis functions $|n_1n_2 2m\rangle$ in the Fock–Bargmann representation:

$$\langle abt|n_1n_2 2m\rangle=\Psi(n_1,n_2,2m;a,b,t), \tag{30}$$

where $a=|\mathbf{a}|$, $b=|\mathbf{b}|$, and t is the cosine of the angle between $\mathbf{a}$ and $\mathbf{b}$. The exact expressions for the functions $\Psi(n_1,n_2,2m;a,b,t)$ can be found in Sec. 4; for now we only say that these functions are proportional to a^{n_1}, b^{n_2}, and $|[\mathbf{ab}]|^{2m}$.

Let us list the most important features of the basis functions (30). First, the matrix elements of the potential-energy operator in this basis have a comparatively simple form (they reduce to double sums; see Sec. 6). Second, the transformation of these functions under nucleon permutations is also simple, so that it is not difficult to find linear combinations of the functions (30) which are eigenvectors of the antisymmetrization operator. As regards the third quantum number of the antisymmetric basis functions, it is convenient to identify it with the eigenvalue of the antisymmetrization-operator matrix in the space of the basis functions (30).

This is not the only possible classification of the oscillator basis states. Another choice, used in Ref. 23, is based on the quantum numbers of two single-particle oscillators $\{n_1,l_1,n_2,l_2,L,M\}$ with their angular momenta coupled to the total angular momentum L. This classification has a clearer physical interpretation, but the calculations with such a basis are more complicated

4. HARMONIC-OSCILLATOR BASIS STATES IN THE GENERATOR PARAMETER SPACE

The overlap integral (22) of generating wave packets is a natural way of constructing the harmonic-oscillator basis states in the Fock–Bargmann representation, i.e., in the space of the generator parameters $\mathbf{a}$, $\mathbf{b}$ $(\tilde{\mathbf{a}},\tilde{\mathbf{b}})$. In order to construct these states we first consider the expansion in powers of $\mathbf{a}$, $\mathbf{b}$ $(\tilde{\mathbf{a}},\tilde{\mathbf{b}})$ of the first term in the overlap integral:

$$\exp(\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}})=\sum_{n=0}^{\infty}\left(\sum_{n_1+n_2=n}\frac{1}{n_1!n_2!}(\mathbf{a}\tilde{\mathbf{a}})^{n_1}(\mathbf{b}\tilde{\mathbf{b}})^{n_2}\right). \tag{31}$$

Each term of this sum is a homogeneous polynomial in the components of the vectors $\mathbf{a}$, $\mathbf{b}$, $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$ of the same homogeneity degree n with respect to $\mathbf{a}$, $\mathbf{b}$ and with respect to $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$. This polynomial can be considered as an overlap integral of basis functions with n oscillator quanta. Naturally, the basis functions of states with different n are orthogonal. Moreover, the term in Eq. (31) corresponds to a convolution of basis states classified by the number of quanta. Meanwhile, our aim is to construct a basis having quantum numbers such as the total number n, the $SU(3)$ symmetry indices $(\lambda\mu)$, the orbital angular momentum L, and its projection M.

The following important relation gives us a key to solving the problem of constructing the basis states with the required quantum numbers:

$$(\mathbf{a}\tilde{\mathbf{a}})^{n_1}(\mathbf{b}\tilde{\mathbf{b}})^{n_2}=\sum_{m=0}^{\min(n_1/2,n_2/2)} B_m^2(n_1,n_2)a^{n_1-m}b^{n_2-m}|[\mathbf{ab}]|^m \times I(n_1,n_2,m)\tilde{a}^{n_1-m}\tilde{b}^{n_2-m}|[\tilde{\mathbf{a}}\tilde{\mathbf{b}}]|^m, \quad (32)$$

where the normalizing coefficients

$$B_m^2(n_1,n_2)=\frac{(n_1+n_2+1-2m)!n_1!n_2!}{m!(n_1+n_2+1-m)!(n_1-m)!(n_2-m)!} \quad (33)$$

determine the weight of the overlap integrals

$$I(n_1,n_2,m)=\langle n_1n_2(n_1+n_2-2mm)|\overline{n_1n_2(n_1+n_2-2mm)}\rangle \quad (34)$$

of wave packets $(\lambda\mu)=(n_1+n_2-2mm)$ of the $SU(3)$ irreducible representations when these integrals form the product $(\mathbf{a}\tilde{\mathbf{a}})^{n_1}(\mathbf{b}\tilde{\mathbf{b}})^{n_2}$. The overlap integrals (34) are normalized so that when t ($\tilde{t}$), the cosine of the angle between $\mathbf{a}$ and $\mathbf{b}$ ($\tilde{\mathbf{a}}$ and $\tilde{\mathbf{b}}$), is equal to 1, they take the well-known form first introduced by Elliott:[28]

$$I(n_1,n_2,m)=d_{11}^{n_1+n_2-2m}d_{33}^m, \quad (35)$$

where d_{33} is the cosine of the angle between the normals to the planes passing through $\mathbf{a}$, $\mathbf{b}$ and $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$ (these normals coincide with the axes ζ and $\tilde{\zeta}$ of the intrinsic coordinate frames spanned by the vectors $\mathbf{a}$, $\mathbf{b}$ and $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$, respectively), and d_{11} is the cosine of the angle between the axes ξ and $\tilde{\xi}$ of these coordinate frames.

In the present paper (as in Ref. 29) we restrict ourselves to consideration of states with $L=0$, reserving the generalization to the case of arbitrary L for the next paper. The $L=0$ states contain only the terms with even powers in the expansion (31). Retaining only these terms and denoting the others by dots, we rewrite (31) as

$$\exp(\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}})=\sum_{n=0}^{\infty}\sum_{n_1+n_2=2n}\frac{1}{n_1!n_2!}(\mathbf{a}\tilde{\mathbf{a}})^{n_1}(\mathbf{b}\tilde{\mathbf{b}})^{n_2}+\ldots$$

$$=\sum_{n=0}^{\infty}\sum_{n_1+n_2=2n}N^2(n_1,n_2;2m)a^{n_1-2m}b^{n_2-2m}\times[\mathbf{ab}]^{2m}\Phi(n_1,n_2,2m;t)\tilde{a}^{n_1-2m}\tilde{b}^{n_2-2m}\times|[\tilde{\mathbf{a}}\tilde{\mathbf{b}}]|^{2m}\Phi(n_1,n_2,2m;\tilde{t})+\ldots, \quad (36)$$

where

$$N^2(n_1,n_2;2m)=\frac{1}{n_1!n_2!}B_{2m}^2(n_1,n_2)C_{2m}^2(n_1,n_2),$$

$$C_{2m}^2(n_1,n_2)=\frac{\Gamma(\frac{1}{2}(n_1+n_2)-m+1)\Gamma(\frac{1}{2}(n_1+n_2)-2m+\frac{1}{2})\Gamma(m+\frac{1}{2})}{2\sqrt{\pi}m!\Gamma(\frac{1}{2}(n_1+n_2)-2m+1)\Gamma(\frac{1}{2}n_1+n_2)-m+\frac{3}{2})}. \quad (37)$$

The functions $\Phi(n_1,n_2,2m;t)$ are the eigenfunctions of the second-order Casimir operator of the $SU(3)$ group. They were obtained in Refs. 30 and 31. For even n_1 and n_2,

$$\Phi(n_1,n_2,2m;t)=F(-n_1/2+m,-n_2/2+m;-(n_1+n_2)/2+2m+1/2;1-t^2), \quad (38)$$

where $F(\alpha,\beta;\gamma;z)$ is the hypergeometric function.[21] For odd n_1 and n_2,

$$\Phi(n_1,n_2,2m;t)=tF(-(n_1-1)/2+m,-(n_2-1)/2+m;-(n_1+n_2)/2+2m+1/2;1-t^2). \quad (39)$$

Thus, the basis functions are chosen in the form

$$\Psi(n_1,n_2;2m)=N(n_1,n_2;2m)a^{n_1-2m}b^{n_2-2m}\times[\mathbf{ab}]^{2m}\Phi(n_1,n_2,2m;t). \quad (40)$$

They are the orthonormalized basis functions $|n_1n_22m\rangle$ in the Fock–Bargmann representation discussed in Sec. 3. Their $SU(3)$ symmetry is (n_1+n_2-4m2m), and the angular momentum is $L=0$. In addition, we now have a new expansion for the first term of the overlap integral (22), since it is found that terms of this expansion (polynomials of homogeneity degree n) can be written as a convolution of basis functions

$$\frac{(\mathbf{a}\tilde{\mathbf{a}})^{n_1}(\mathbf{b}\tilde{\mathbf{b}})^{n_2}}{n_1!n_2!}=\sum_{m=0}^{\min(n_1/2,n_2/2)}\Psi(n_1,n_2,2m;a,b,t)\times\Psi(n_1,n_2,2m;\tilde{a},\tilde{b},\tilde{t})+\ldots, \quad (41)$$

where the dots indicate states with $L\neq 0$.

Under the operation of nucleon permutation the basis states (40), as well as $|n_1n_22m\rangle$, are subjected to a linear transformation that preserves their $SU(3)$ symmetry and mixes only functions with different values of n_1-n_2 but not n_1+n_2 and m. The transformation of states (40) is induced by a linear transformation of $\mathbf{a}$ and $\mathbf{b}$. The states (40) therefore do not have fixed permutation symmetry, so that our next task is to find linear combinations of them that have permutation symmetry satisfying the Pauli principle (allowed states) and to eliminate the other (forbidden) states. In order to do that, we expand the last three terms of the overlap integral $\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle$ [Eq. (22)] in powers of the vector generating parameters. Then in a polynomial of even homogeneity degree (n) we retain only the terms with $L=0$ and fixed m. In this case, we obtain the following bilinear form in the basis functions (40):

$$\sum_{n_1+n_2=n}[\Psi(n_1,n_2,2m;\bar{\bar{a}},\bar{\bar{b}},\bar{\bar{t}})-\Psi(n_1,n_2,2m;\bar{a},\bar{b},\bar{t})$$
$$-\Psi(n_1,n_2,2m;\bar{\bar{a}},\bar{\bar{b}},\bar{\bar{t}})$$
$$+\Psi(n_1,n_2,2m;\bar{\bar{\bar{a}}},\bar{\bar{\bar{b}}},\bar{\bar{\bar{t}}})]\Psi(n_1,n_2,2m;\tilde{a},\tilde{b},\tilde{t}). \quad (42)$$

Since $\bar{\bar{\bar{b}}}=0$, the term with triple-barred a,b,t vanishes for $m\neq 0$; its contribution for $m=0$ is

$$\left(-\frac{1}{2}\right)^n N(n,0,0)a^n N(n,0,0)\tilde{a}^n.$$

In order to find the transformation of the basis functions under nucleon permutation we first consider the transformation of the basis functions induced by an arbitrary linear transformation of **a** and **b** given by the matrix $\|\alpha\|$:

$$\begin{pmatrix}\tilde{\mathbf{a}}\\ \tilde{\mathbf{b}}\end{pmatrix}=\begin{pmatrix}\alpha_{11} & \alpha_{12}\\ \alpha_{21} & \alpha_{22}\end{pmatrix}\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\end{pmatrix}.$$

This transformation, obtained in Ref. 32, is not very complicated:

$$\Psi(\tilde{n}_1,\tilde{n}_2,2m;\tilde{a},\tilde{b},\tilde{t})$$
$$=\sum_{n_1+n_2=\tilde{n}_1+\tilde{n}_2}\langle n_1n_22m|\alpha|\tilde{n}_1\tilde{n}_22m\rangle$$
$$\times\Psi(n_1,n_2,2m;a,b,t), \quad (43)$$

$$\langle n_1n_22m|\alpha|\tilde{n}_1\tilde{n}_22m\rangle$$
$$=(\det\alpha)^{2m}\frac{N(\tilde{n}_1,\tilde{n}_2,2m)}{N(n_1,n_2,2m)}$$
$$\times\sum_k\frac{(\tilde{n}_1-2m)!(\tilde{n}_2-2m)!}{k!(n_1-2m-k)!(\tilde{n}_1-2m-k)!(n_2-\tilde{n}_1+k)!}$$
$$\times(\alpha_{11})^k(\alpha_{21})^{n_1-2m-k}(\alpha_{12})^{\tilde{n}_1-2m-k}(\alpha_{22})^{n_2-\tilde{n}_1+k}. \quad (44)$$

Applying these results to the three matrices $T^{(p)}$ given by Eq. (23), we obtain the matrix of the antisymmetrization operator,

$$\|\langle n_1n_22m|\mathscr{A}|\tilde{n}_1\tilde{n}_22m\rangle\|,=\|\langle n_1n_22m|1-T^{(1)}-T^{(2)}+T^{(3)}|\tilde{n}_1\tilde{n}_22m\rangle\|, \quad (45)$$

which gives us the expression for the overlap integral (42):

$$\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle=\sum_{n_1+n_2=n}\sum_{\tilde{n}_1+\tilde{n}_2=n}\Psi(n_1,n_2,2m;a,b,t)$$
$$\times\langle n_1n_22m|\mathscr{A}|\tilde{n}_1\tilde{n}_22m\rangle$$
$$\times\Psi(\tilde{n}_1,\tilde{n}_2,2m;a,b,t). \quad (46)$$

Later, the transformation (43) of the basis functions will be used to obtain the matrix elements of the potential-energy operator.

Now we can return to the problem of separating the singlet and triplet spin states. The matrix (45) is symmetric, and it has a block-diagonal structure with two blocks corresponding to even and odd values of $n_1,n_2,\tilde{n}_1,\tilde{n}_2$. Basis functions with odd n_1,n_2 are antisymmetric with respect to transpositions of the spatial coordinates of the neutron clusters and therefore belong to the singlet spin state. The spin of a neutron pair is an integral of the motion, and the Hamiltonian does not mix triplet and singlet states.

Some examples of the matrices (45) for simple cases are as follows:

For $n=n_1+n_2=\tilde{n}_1+\tilde{n}_2=2$, $m=0$

$$\begin{array}{c}\\ \langle 200|\\ \langle 020|\end{array}\begin{array}{c}\begin{array}{cc}|200\rangle & |020\rangle\end{array}\\ \begin{pmatrix}\frac{9}{8} & -\frac{3}{4}\\ -\frac{3}{4} & \frac{1}{2}\end{pmatrix}\end{array}. \quad (47)$$

For $n=4$, $m=0$

$$\begin{array}{c}\\ \langle 400|\\ \langle 220|\\ \langle 040|\end{array}\begin{array}{c}\begin{array}{ccc}|400\rangle & |220\rangle & |040\rangle\end{array}\\ \begin{pmatrix}\frac{135}{128} & -\frac{3\sqrt{6}}{64} & -\frac{9}{32}\\ -\frac{3\sqrt{6}}{64} & \frac{5}{16} & -\frac{3\sqrt{6}}{16}\\ -\frac{9}{32} & -\frac{3\sqrt{6}}{16} & \frac{7}{8}\end{pmatrix}\end{array}. \quad (48)$$

The diagonalization of the matrix (45) solves the problem of eliminating the forbidden states and constructing the orthonormalized basis of allowed states, which are obtained as linear combinations of basis functions $\Psi(n_1,n_2,m;a,b,t)$.

The problem of forbidden states in many-cluster systems, in its general features, has already been studied in Refs. 13 and 14, where some important results have been obtained. The next task is to construct the basis of allowed states and to find the Hamiltonian matrix elements in this basis. However, first we shall clarify the relations between the basis of allowed states and its generating functions.

We have chosen as a generating function the wave packet $\Phi(\mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3;\{\mathbf{r}_i,\sigma_i,\tau_i\})$ constructed as a Slater determinant composed of six one-particle Brink orbitals [see Eq. (7)]. In the center-of-mass system we have already introduced the generating function

$$\varphi(\mathbf{a},\mathbf{b};\{\mathbf{r}_i,\sigma_i,\tau_i\}),$$

and now we introduce the corresponding nonantisymmetrized function φ_0

$$\varphi(\mathbf{a},\mathbf{b};\{\mathbf{r}_i,\sigma_i,\tau_i\})=\mathscr{A}\varphi_0(\mathbf{a},\mathbf{b};\{\mathbf{r}_i,\sigma_i,\tau_i\}). \quad (49)$$

It is also a generating function, but, unlike φ, it generates a basis of nonantisymmetrized functions $\{|n\gamma\rangle\}$, which contains both allowed and forbidden states:

$$\varphi_0(\mathbf{a},\mathbf{b};\{\mathbf{r}_i,\sigma_i,\tau_i\})=\sum_{n,\gamma}\varphi_0(n,\gamma;\mathbf{a},\mathbf{b})|n\gamma\rangle. \quad (50)$$

Here n is the number of oscillator excitation quanta, γ is the set of additional quantum numbers, and $\varphi(n,\gamma;\mathbf{a},\mathbf{b})$ is the Fock–Bargmann image of the basis states $|n\gamma\rangle$.

We cannot content ourselves with the basis $\{|n\gamma\rangle\}$ and construct the Hamiltonian matrix elements in it immediately for the Schrödinger equation, since this basis contains forbidden states. Each of the functions $|n\gamma\rangle$ has no permutation symmetry and, in general, is a superposition of allowed and forbidden states. The transition from the basis $\{|n\gamma\rangle\}$ to the orthonormalized basis of allowed states (i.e., states which satisfy the Pauli principle) is an orthogonal transformation of the basis $\{|n\gamma\rangle\}$:

$$|n\nu\rangle=\sum_{\gamma}|n\gamma\rangle\langle n\gamma|n\nu\rangle. \tag{51}$$

Now we list the order of the procedures necessary to construct the Schrödinger equation

$$\sum_{n',\nu'}[\langle n\nu|\hat{H}|n'\nu'\rangle-E\delta_{n'\nu'}]C_{n'\nu'}=0 \tag{52}$$

in the representation of the allowed states of the harmonic-oscillator basis $\{|n\nu\rangle\}$ for the general case. We recall that $\{|n\gamma\rangle\}$ is the basis of states with no definite permutation symmetry, and γ denotes all quantum numbers other than n. On the other hand, $\{|n\nu\rangle\}$ is the basis of allowed states (here the quantum numbers additional to n are denoted by ν). For $L=0$

$$|n\gamma\rangle=|n_1n_2 2m\rangle$$

$$|n\nu\rangle=|n_1 2m;\lambda^3_\nu\rangle \quad \text{and} \quad |n\nu\rangle=|n_1 2m;\lambda^1_\nu\rangle$$

$$\nu=1,2,\ldots,$$

where the indices 1 and 3 of λ correspond to singlet and triplet spin states.

1. First, the overlap integral of *nonantisymmetrized* generating functions $\langle\varphi_0|\tilde{\varphi}_0\rangle$ is calculated, and the basis states $\{|n\gamma\rangle\}$ in the Fock–Bargmann representation $[\varphi_0(n,\gamma;\mathbf{a},\mathbf{b})]$ are extracted:

$$\langle\varphi_0|\tilde{\varphi}_0\rangle=\exp(\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}})$$

$$=\sum_{n,\gamma}\varphi_0^*(n,\gamma;\mathbf{a},\mathbf{b})\varphi_0(n,\gamma;\tilde{\mathbf{a}},\tilde{\mathbf{b}}). \tag{53}$$

2. The overlap integral of *antisymmetrized* generating functions $\langle\varphi|\tilde{\varphi}\rangle$ is calculated and then diagonalized in the basis $\{\varphi_0(n,\gamma;\mathbf{a},\mathbf{b})\}$,

$$\langle\varphi|\tilde{\varphi}\rangle=\sum_{n,\gamma,\tilde{\gamma}}\varphi_0^*(n,\gamma;\mathbf{a},\mathbf{b})\langle n\gamma|\mathscr{A}|n\tilde{\gamma}\rangle\varphi_0(n,\tilde{\gamma};\tilde{\mathbf{a}}\tilde{\mathbf{b}}), \tag{54}$$

and is written as

$$\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle=\sum_{n,\nu}\lambda_\nu\varphi^*(n,\nu;\mathbf{a},\mathbf{b})\varphi(n,\nu;\tilde{\mathbf{a}},\tilde{\mathbf{b}}), \tag{55}$$

where λ_ν are the eigenvalues of the matrix $\langle n\gamma|\mathscr{A}|n\tilde{\gamma}\rangle$. The transition matrix from the $\{|n\gamma\rangle\}$ to the $\{|n\nu\rangle\}$ basis,

$$\varphi(n,\nu;\mathbf{a},\mathbf{b})=\sum_{\gamma}\langle n\gamma|n\nu\rangle\varphi_0(n,\gamma;\mathbf{a},\mathbf{b}), \tag{56}$$

is found by the diagonalization procedure. Note that $\lambda_\nu(n)=0$ for the forbidden states, and therefore these states drop out in the expansion (55), although they are present in the expansion (53).

3. After that, the Hamiltonian matrix elements between the generating functions

$$\varphi_0(\mathbf{a},\mathbf{b};\{\mathbf{r}_i,\sigma_i,\tau_i\}) \quad \text{and} \quad \varphi_0(\tilde{\mathbf{a}},\tilde{\mathbf{b}};\{\mathbf{r}_i,\sigma_i,\tau_i\})$$

are calculated, and they are projected onto the basis states $\varphi_0(n,\gamma;\mathbf{a},\mathbf{b})$ and $\varphi_0(\tilde{n},\tilde{\gamma};\tilde{\mathbf{a}},\tilde{\mathbf{b}})$:

$$\langle\varphi_0|\hat{H}|\tilde{\varphi}_0\rangle=\sum_{n\gamma}\sum_{\tilde{n}\tilde{\gamma}}\varphi_0^*(n,\gamma;\mathbf{a},\mathbf{b})$$

$$\times\langle n\gamma|\hat{H}|\tilde{n}\tilde{\gamma}\rangle\varphi_0(\tilde{n},\tilde{\gamma};\tilde{\mathbf{a}},\tilde{\mathbf{b}}), \tag{57}$$

which yields the matrix elements $\langle n\gamma|\hat{H}|\tilde{n}\tilde{\gamma}\rangle$.

4. Finally, the Hamiltonian matrix elements in the basis $\{|n\nu\rangle\}$ are found:

$$\langle n\nu|\hat{H}|\tilde{n}\tilde{\nu}\rangle=\sum_{\gamma}\sum_{\tilde{\gamma}}\langle n\nu|n\gamma\rangle\langle n\gamma|\hat{H}|\tilde{n}\tilde{\gamma}\rangle\langle\tilde{n}\tilde{\gamma}|\tilde{n}\tilde{\nu}\rangle. \tag{58}$$

Of course, it is simpler to extract the Hamiltonian matrix elements from $\langle\varphi_0|\hat{H}|\tilde{\varphi}_0\rangle$ than from $\langle\varphi|\hat{H}|\tilde{\varphi}\rangle$.

Now we shall show how to implement this procedure for the specific case of the system ^{4}He$+n+n$ and states with $L=0$.

We start with the determination of the allowed states. This problem is solved by diagonalization of the symmetric matrix (45) given above. We denote the matrix eigenvalues and eigenvectors for the singlet states by

$$\lambda^1_\nu(n,2m), \quad \text{and} \quad \Phi^1_\nu(n,2m) \quad \nu=1,2,\ldots,n/2-2m+1,$$

and those for the triplet states by

$$\lambda^3_\nu(m,2m), \quad \text{and} \quad \Phi^3_\nu(n,2m) \quad \nu=1,2,\ldots,n/2-2m+1.$$

Then, instead of (46), we get

$$\langle\mathbf{ab}|\tilde{\mathbf{a}}\tilde{\mathbf{b}}\rangle=\sum_{\nu}\lambda_\nu(n,2m)\Phi_\nu(n,2m)\Phi_\nu(n,2m). \tag{59}$$

The terms with zero eigenvalues λ_ν drop out in this sum; they correspond to forbidden states.

The simplest examples of singlet eigenvalues and eigenfunctions are:

$$\lambda^1_1(2,0)=\tfrac{13}{8},$$

$$\Phi^1_1(2,0)=\frac{3}{\sqrt{13}}|200\rangle-\frac{2}{\sqrt{13}}|020\rangle$$

$$=\frac{1}{\sqrt{78}}(3a^2-2b^2), \tag{60}$$

where $\Phi^1_1(2,0)$ is the image of the ^{6}He shell-model ground-state function, and

$$\lambda^1_1(4,0)=0.936,$$

$$\Phi_1^1(4,0)=0.706|400\rangle-0.499|220\rangle+0.502|040\rangle; \tag{61}$$

$$\lambda_2^1(4,0)=1.306,$$

$$\Phi_2^1(4,0)=0.671|400\rangle-0.245|220\rangle+0.699|040\rangle. \tag{62}$$

The transition from the basis $\Psi(n_1,n_2,2m)$ to the basis $\Phi_\nu(n,2m)$ is carried out by means of the matrix $\langle n_1 n_2 2m|n2m\nu\rangle$:

$$\Phi_\nu(n,2m)=\sum_{n_1+n_2=n}\Psi(n_1,n_2,2m)\langle n_1 n_2 2m|n2m\nu\rangle. \tag{63}$$

The matrix elements of $\hat{H}$ in the new basis are calculated by means of the same matrix:

$$\langle n2m\nu|\hat{H}|\tilde{n}2\tilde{m}\tilde{\nu}\rangle=\sum_{n_1+n_2=n}\sum_{\tilde{n}_1+\tilde{n}_2=\tilde{n}}\langle n2m\nu|n_1n_2 2m\rangle \times\langle n_1 n_2 2m|\hat{H}|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle \times\langle n_1 n_2 2m|n2m\nu\rangle. \tag{64}$$

Then the Schrödinger equation in the representation $\{|n2m\nu\rangle\}$ becomes

$$\sum_{\tilde{n},\tilde{m},\tilde{\nu}}\langle n,2m,\nu|\hat{H}-E|\tilde{n},2\tilde{m},\tilde{\nu}\rangle C(\tilde{n},2\tilde{m},\tilde{\nu})=0. \tag{65}$$

To conclude this section we note two important points:

1. Forbidden states correspond to zero eigenvalues of the antisymmetrization-operator matrix. They are absent if $m\neq 0$. If $m=0$, then for each n there are two forbidden states, one singlet and one triplet. Eigenvectors of forbidden states cannot be realized, since they vanish after the antisymmetrization. One discovers that by obtaining $\lambda_\nu=0$.

2. Allowed states correspond to λ_ν which are not equal to unity in the general case. Although all the λ_ν of the allowed states are close to unity, they lie between ~ 1.25 and ~ 0.9375, even if $n\to\infty$. Thus, we see that the action of the Pauli principle results not only in the emergence of forbidden states, but also in a change of the normalization factors of the allowed states in the Fock–Bargmann space. These factors differ from the ones which would have been obtained if only the orthogonality of the allowed and forbidden states were required (i.e., the normalization factors extracted from the overlap integral $\langle\varphi_0|\tilde{\varphi}_0\rangle$).

5. MATRIX ELEMENTS OF THE KINETIC-ENERGY OPERATOR

For the kinetic-energy operator in the center-of-mass system

$$\hat{T}=-\frac{\hbar^2}{2Mr_0^2}\sum_{i=1}^{A}\nabla_i^2-\frac{\hbar^2}{2AMr_0^2}\nabla_{\mathrm{CM}}^2 \tag{66}$$

(M is the nucleon mass, and r_0 is the oscillator length) we first calculate the matrix elements of the single-particle operator $(\hbar^2/2Mr_0^2)\nabla^2$ between the Brink orbitals (7):

$$\left\langle\phi(\mathbf{R})\left|\frac{\hbar^2}{2Mr_0^2}\nabla^2\right|\phi(\tilde{\mathbf{R}})\right\rangle =\pi^{3/2}\frac{\hbar^2}{2Mr_0^2}[3-(\mathbf{R}-\tilde{\mathbf{R}})^2]\exp(\mathbf{R}\tilde{\mathbf{R}}). \tag{67}$$

After some transformations, dropping the factor $\pi^{3/2}$, we obtain the matrix elements of the operator (66) between the nonantisymmetrized generating functions φ_0 and $\tilde{\varphi}_0$ for the case of ^{6}He:

$$\langle\varphi_0|\hat{T}|\tilde{\varphi}_0\rangle=\frac{h^2}{2Mr_0^2}[15-(\mathbf{a}-\tilde{\mathbf{a}})^2 -(\mathbf{b}-\tilde{\mathbf{b}})^2]\exp(\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}}). \tag{68}$$

Then for the diagonal matrix elements between the basis functions we get

$$\langle n_1 n_2 2m|\hat{T}|n_1 n_2 2m\rangle=\frac{h^2}{4Mr_0^2}(2n_1+2n_2+15) =\frac{h^2}{4Mr_0^2}(2n+15). \tag{69}$$

There are eight different nondiagonal matrix elements, but it is sufficient to write here only four of them, which are contained in the following identities:

$$\begin{aligned}a^2\Psi(n_1,n_2,2m;a,b,t) &=\frac{N(n_1,n_2,2m)}{N(n_1+2,n_2,2m)}\times\Psi(n_1+2,n_2,2m;a,b,t)\\ &+\frac{N(n_1,n_2,2m)}{N(n_1+2,n_2,2m+2)}\times\frac{(n_2-2m-1)(n_2-2m)}{(n_1+n_2-4m-1)(n_1+n_2-4m+1)}\\ &\times\Psi(n_1+2,n_2,2m+2;a,b,t);\end{aligned} \tag{70}$$

$$\begin{aligned}b^2\Psi(n_1,n_2,2m;a,b,t) &=\frac{N(n_1,n_2,2m)}{N(n_1,n_2+2,2m)}\times\Psi\Big((n_1,n_2+2,2m;a,b,t)\\ &+\frac{N(n_1,n_2,2m)}{N(n_1,n_2+2,2m+2)}\times\frac{(n_1-2m-1)(n_1-2m)}{(n_1+n_2-4m-1)(n_1+n_2-4m+1)}\\ &\times\Psi(n_1,n_2+2,2m+2;a,b,t).\end{aligned} \tag{71}$$

It is evident now that

$$\langle n_1+2n_2 2m|\hat{T}|n_1 n_2 2m\rangle=-\frac{\hbar^2}{4Mr_0^2}\frac{N(n_1,n_2,2m)}{N(n_1+2,n_2,2m)}; \tag{72}$$

$$\langle n_1 n_2+22m|\hat{T}|n_1 n_2 2m\rangle = -\frac{\hbar^2}{4Mr_0^2}\frac{N(n_1,n_2,2m)}{N(n_1,n_2+2,n_2,2m)}; \tag{73}$$

$$\langle n_1+2n_2 2m+2|\hat{T}|n_1 n_2 2m\rangle = -\frac{\hbar^2}{4Mr_0^2}\frac{N(n_1,n_2,2m)}{N(n_1+2,n_2,2m+2)} \times\frac{(n_2-2m-1)(n_2-2m)}{(n_1+n_2-4m-1)(n_1+n_2-4m+1)}; \tag{74}$$

$$\langle n_1 n_2+22m+2|\hat{T}|n_1 n_2 2m\rangle = -\frac{\hbar^2}{4Mr_0^2}\frac{N(n_1,n_2,2m)}{N(n_1,n_2+2,2m+2)} \times\frac{(n_1-2m-1)(n_1-2m)}{(n_1+n_2-4m-1)(n_1+n_2-4m+1)}. \tag{75}$$

The matrix elements (72)–(75) are obtained as a result of the raising operators (a^2 and b^2) applied to the basis states $|n_1 n_2 2m\rangle$ (these operators add two to the total number of oscillator quanta). Similarly, the other four matrix elements correspond to the action of the lowering operators ($\tilde{a}^2$ and $\tilde{b}^2$).

The transition to the matrix elements

$$\langle n2m\nu|\hat{T}|\tilde{n}2\tilde{m}\tilde{\nu}\rangle \tag{76}$$

is carried out by using the rules formulated in the previous section.

The basis $|n2m\nu\rangle$ of allowed states is, however, not very convenient for the study of the continuum states of three-cluster systems. The classification of basis states optimal for constructing wave functions with the asymptotic behavior characteristic of the continuous spectrum is that provided by the basis of hyperspherical harmonics.[25,33–36] The hypermomentum quantum number K is unchanged under the kinetic-energy operator, and therefore for the basis functions $|nK\kappa\rangle$ (κ is the additional quantum number of the hyperspherical basis) one gets

$$\hat{T}|nK\kappa\rangle = \langle n+2K\kappa|\hat{T}|nK\kappa\rangle|n+2K\kappa\rangle + \frac{\hbar^2}{4Mr_0^2}(2n+15)|nK\kappa\rangle + \langle n-2K\kappa|\hat{T}|nK\kappa\rangle|n-2K\kappa\rangle. \tag{77}$$

The transition from the basis $|n2m\nu\rangle$ to the basis $|nK\kappa\rangle$ is carried out by means of the orthogonal transformation

$$|nK\kappa\rangle = \sum_{m,\nu}|n2m\nu\rangle\langle n2m\nu|nK\kappa\rangle. \tag{78}$$

The transition matrix $\langle n2m\nu|nK\kappa\rangle$ must be determined in the final stage of constructing the Schrödinger equation in the representation of the hyperspherical harmonic oscillator:

$$\sum_{\tilde{n}\tilde{K}\tilde{\kappa}}\langle nK\kappa|\hat{H}-E|\tilde{n},\tilde{K}\tilde{\kappa}\rangle C(\tilde{n},\tilde{K}\tilde{\kappa}) = 0. \tag{79}$$

6. MATRIX ELEMENTS OF THE POTENTIAL-ENERGY OPERATOR

For the nucleon–nucleon potential with a Gaussian spatial dependence

$$V(\mathbf{r}_1-\mathbf{r}_2) = V_0\exp\left\{-\frac{(\mathbf{r}_1-\mathbf{r}_2)^2}{s^2}\right\} \tag{80}$$

the calculation of the matrix elements between the generating functions begins with the evaluation of the integral

$$J = \int \exp\left\{-r_1^2-r_2^2+\sqrt{2}(\mathbf{R}_1+\tilde{\mathbf{R}}_1,\mathbf{r}_1) + \sqrt{2}(\mathbf{R}_2+\tilde{\mathbf{R}}_2,\mathbf{r}_2)-\tfrac{1}{2}(R_1^2+S_1^2+R_2^2+S_2^2) - \frac{2r_0^2}{s^2}\left(\frac{\mathbf{r}_1-\mathbf{r}_2}{\sqrt{2}}\right)^2\right\}d\mathbf{r}_1 d\mathbf{r}_2. \tag{81}$$

After introducing the new vectors

$$\mathbf{r} = \frac{1}{\sqrt{2}}(\mathbf{r}_1-\mathbf{r}_2), \quad \mathbf{q} = \frac{1}{\sqrt{2}}(\mathbf{r}_1+\mathbf{r}_2), \quad d\mathbf{r}_1 d\mathbf{r}_2 = d\mathbf{r}d\mathbf{q}, \tag{82}$$

taking into account the relations

$$\mathbf{r}_1^2+\mathbf{r}_2^2 = \mathbf{r}^2+\mathbf{q}^2;$$

$$\sqrt{2}(\mathbf{R}_1+\tilde{\mathbf{R}}_1,\mathbf{r}_1)+\sqrt{2}(\mathbf{R}_2+\tilde{\mathbf{R}}_2,\mathbf{r}_2) = (\mathbf{R}_1+\tilde{\mathbf{R}}_1+\mathbf{R}_2+\tilde{\mathbf{R}}_2,\mathbf{q})+(\mathbf{R}_1+\tilde{\mathbf{R}}_1-\mathbf{R}_2-\tilde{\mathbf{R}}_2,\mathbf{r}),$$

the integrand is factorized and the integral can be easily calculated:

$$J = \pi^3 z^{3/2}\exp\{\tfrac{1}{2}(\mathbf{R}_1+\mathbf{R}_2,\tilde{\mathbf{R}}_1+\tilde{\mathbf{R}}_2)+\tfrac{1}{2}z(\mathbf{R}_1-\mathbf{R}_2,\tilde{\mathbf{R}}_1-\tilde{\mathbf{R}}_2) + \tfrac{1}{4}(z-1)[(\mathbf{R}_1-\mathbf{R}_2)^2+(\tilde{\mathbf{R}}_1-\tilde{\mathbf{R}}_2)^2]\}, \tag{83}$$

where $z=(1+2r_0^2/s^2)^{-1}$. (Below, we shall omit the factor π^3, as we have been doing for the overlap integral.)

The generating matrix element can be obtained easily after some transformation of the overlap integral (19). Considering first only the spatial dependence of the nucleon–nucleon potential (80), we discuss the transformation of the first term in (19). For the matrix elements corresponding to the interaction of nucleons belonging to the alpha cluster, this transformation reduces to the product of the exponential, the intensity V_0 of the Gaussian potential, the number of nucleon pairs, and the factor $z^{3/2}$. Denoting the nonantisymmetrized generating function before separation of the center-of-mass motion by Φ_0 ($\Phi=\mathscr{A}\Phi_0$), for the six nucleon pairs of the alpha particle we get

$$\langle\Phi_0|\hat{U}_{11}|\tilde{\Phi}_0\rangle = 6z^{3/2}V_0\exp\{4\mathbf{R}_1\tilde{\mathbf{R}}_1+\mathbf{R}_2\tilde{\mathbf{R}}_2+\mathbf{R}_3\tilde{\mathbf{R}}_3\} = 6z^{3/2}V_0\exp\{\mathbf{R}_{CM}\tilde{\mathbf{R}}_{CM}+\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}}\}. \tag{84}$$

The calculation of matrix elements corresponding to the interaction of nucleons belonging to different clusters is more complicated. Again, it is necessary to determine how many nucleon pairs there are and to take into account the integral

J. Then in the case of the interaction of nonalpha neutrons [corresponding to generating vectors $\mathbf{R}_2$ and $\mathbf{R}_3$ ($\tilde{\mathbf{R}}_2$ and $\tilde{\mathbf{R}}_3$)] we have

$$\begin{aligned}\langle\Phi_0|\hat{U}_{23}|\tilde{\Phi}_0\rangle &= z^{3/2}V_0\ \exp\{4\mathbf{R}_1\tilde{\mathbf{R}}_1\}\exp\{\tfrac{1}{2}(\mathbf{R}_2+\mathbf{R}_3,\tilde{\mathbf{R}}_2+\tilde{\mathbf{R}}_3)\\ &\quad+\tfrac{1}{2}z(\mathbf{R}_2-\mathbf{R}_3,\tilde{\mathbf{R}}_2-\tilde{\mathbf{R}}_3)\\ &\quad+\tfrac{1}{4}(z-1)[(\mathbf{R}_2-\mathbf{R}_3)^2+(\tilde{\mathbf{R}}_2-\tilde{\mathbf{R}}_3)^2]\}\\ &= z^{3/2}V_0\ \exp\{\mathbf{R}_{CM}\tilde{\mathbf{R}}_{CM}+\mathbf{a}\tilde{\mathbf{a}}+z\mathbf{b}\tilde{\mathbf{b}}\\ &\quad+\tfrac{1}{2}(z-1)(b^2+\tilde{b}^2)\}. \end{aligned}\tag{85}$$

The matrix element of the interaction of alpha-cluster nucleons and the $\mathbf{R}_2$ neutron differs only in minor details:

$$\begin{aligned}\langle\Phi_0|\hat{U}_{12}|\tilde{\Phi}_0\rangle &= 4z^{3/2}V_0\ \exp\{3\mathbf{R}_1\tilde{\mathbf{R}}_1+\mathbf{R}_3\tilde{\mathbf{R}}_3\}\\ &\quad\times\exp\{\tfrac{1}{2}(\mathbf{R}_1+\mathbf{R}_2,\tilde{\mathbf{R}}_1+\tilde{\mathbf{R}}_2)+\tfrac{1}{2}z(\mathbf{R}_1-\mathbf{R}_2,\tilde{\mathbf{R}}_1\\ &\quad-\tilde{\mathbf{R}}_2)+\tfrac{1}{4}(z-1)[(\mathbf{R}_1-\mathbf{R}_2)^2+(\tilde{\mathbf{R}}_1-\tilde{\mathbf{R}}_2)^2]\}\\ &= 4z^{3/2}V_0\ \exp\{\mathbf{R}_{CM}\tilde{\mathbf{R}}_{CM}+\mathbf{a}'\tilde{\mathbf{a}}'+z\mathbf{b}'\tilde{\mathbf{b}}'\\ &\quad+\tfrac{1}{2}(z-1)(b'^2+\tilde{b}'^2)\}\ , \end{aligned}\tag{86}$$

where in order to simplify both the notation and the subsequent calculation the Jacobi vectors corresponding to another choice of the Jacobi tree are introduced:

$$\mathbf{a}'=\sqrt{\frac{5}{6}}\left(\mathbf{R}_3-\frac{4\mathbf{R}_1+\mathbf{R}_2}{5}\right),\quad \mathbf{b}'=\frac{2}{\sqrt{5}}(\mathbf{R}_1-\mathbf{R}_2).\tag{87}$$

These Jacobi vectors are obtained from the old ones by means of an orthogonal transformation:

$$\mathbf{a}'=-\sqrt{\frac{2}{5}}\,\mathbf{a}-\sqrt{\frac{3}{5}}\,\mathbf{b},\quad \mathbf{b}'=\sqrt{\frac{3}{5}}\,\mathbf{a}-\sqrt{\frac{2}{5}}\,\mathbf{b}.\tag{88}$$

The third set of Jacobi vectors

$$\mathbf{a}''=\sqrt{\frac{5}{6}}\left(\mathbf{R}_2-\frac{4\mathbf{R}_1+\mathbf{R}_3}{5}\right),\quad \mathbf{b}''=\frac{2}{\sqrt{5}}(\mathbf{R}_1-\mathbf{R}_3);\tag{89}$$

$$\mathbf{a}''=-\sqrt{\frac{2}{5}}\,\mathbf{a}+\sqrt{\frac{3}{5}}\,\mathbf{b},\quad \mathbf{b}''=\sqrt{\frac{3}{5}}\,\mathbf{a}+\sqrt{\frac{2}{5}}\,\mathbf{b}\tag{90}$$

is introduced for the calculation of the matrix elements corresponding to the interaction of alpha-cluster nucleons and the neutron $\mathbf{R}_3$:

$$\begin{aligned}\langle\Phi_0|\hat{U}_{12}|\tilde{\Phi}_0\rangle &= 4z^{3/2}V_0\ \exp\{\mathbf{R}_{CM}\tilde{\mathbf{R}}_{CM}+\mathbf{a}''\tilde{\mathbf{a}}''\\ &\quad+(\tfrac{3}{8}+\tfrac{5}{8}z)\mathbf{b}''\tilde{\mathbf{b}}''+\tfrac{5}{16}(z-1)(b''^2+\tilde{b}''^2)\}. \end{aligned}\tag{91}$$

(The tilded vectors $\tilde{\mathbf{a}}',\tilde{\mathbf{b}}',\tilde{\mathbf{a}}'',\tilde{\mathbf{b}}''$ are expressed similarly in terms of $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{b}}$.)

The functions Φ_0 and $\tilde{\Phi}_0$ are products of single-particle orbitals, so that the matrix elements between them are calculated easily. Since

$$\langle\Phi_0|\hat{U}_{kl}|\tilde{\Phi}_0\rangle=\exp\{\mathbf{R}_{CM}\tilde{\mathbf{R}}_{CM}\}\langle\varphi_0|\hat{U}_{kl}|\tilde{\varphi}_0\rangle,\tag{92}$$

the expression for the matrix elements $\langle\varphi_0|U_{kl}|\tilde{\varphi}_0\rangle$ follows immediately from Eqs. (84)–(86) and (91).

The generalization to the case of central exchange forces with components $V_{2S+1,2T+1}$ (S and T are the total spin and isospin of an interacting nucleon pair) is shown separately for each of the four terms in Eqs. (84)–(86) and (91):

$$\langle\varphi_0|\hat{U}_{11}|\tilde{\varphi}_0\rangle=z^{3/2}(3V_{31}+3V_{13})\exp\{\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}}\};\tag{93}$$

$$\begin{aligned}\langle\varphi_0|\hat{U}_{23}|\tilde{\varphi}_0\rangle &= z^{3/2}\tfrac{1}{2}(V_{33}+V_{13})\exp\{\mathbf{a}\tilde{\mathbf{a}}+B_{23}\mathbf{b}\tilde{\mathbf{b}}\\ &\quad+D_{23}(\mathbf{b}^2+\tilde{\mathbf{b}}^2)\}\\ &\quad-z^{3/2}\tfrac{1}{2}(V_{33}+V_{13})\exp\{\mathbf{a}\tilde{\mathbf{a}}-B'_{23}\mathbf{b}\tilde{\mathbf{b}}\\ &\quad+D_{23}(\mathbf{b}^2+\tilde{\mathbf{b}}^2)\}; \end{aligned}\tag{94}$$

$$\begin{aligned}\langle\varphi_0|\hat{U}_{12}|\tilde{\varphi}_0\rangle &= z^{3/2}\tfrac{1}{4}(9V_{33}+3V_{31}+3V_{13}+V_{11})\\ &\quad\times\exp\{\mathbf{a}'\tilde{\mathbf{a}}'+B_{12}\mathbf{b}'\tilde{\mathbf{b}}'+D_{12}(\mathbf{b}'^2+\tilde{\mathbf{b}}'^2)\}\\ &\quad-z^{3/2}\tfrac{1}{4}(5V_{33}+3V_{31}+3V_{13}+V_{11})\\ &\quad\times\exp\{\mathbf{a}'\tilde{\mathbf{a}}'+B'_{12}\mathbf{b}'\tilde{\mathbf{b}}'+D_{12}(\mathbf{b}'^2+\tilde{\mathbf{b}}'^2)\}; \end{aligned}\tag{95}$$

$$\begin{aligned}\langle\varphi_0|\hat{U}_{13}|\tilde{\varphi}_0\rangle &= z^{3/2}\tfrac{1}{4}(9V_{33}+3V_{31}+3V_{13}+V_{11})\\ &\quad\times\exp\{\mathbf{a}''\tilde{\mathbf{a}}''+B_{13}\mathbf{b}''\tilde{\mathbf{b}}''+D_{13}(\mathbf{b}''^2+\tilde{\mathbf{b}}''^2)\}\\ &\quad-z^{3/2}\tfrac{1}{4}(5V_{33}+3V_{31}+3V_{13}+V_{11})\\ &\quad\times\exp\{\mathbf{a}''\tilde{\mathbf{a}}''+B_{13}\mathbf{b}''\tilde{\mathbf{b}}''+D_{13}(\mathbf{b}''^2+\tilde{\mathbf{b}}''^2)\}. \end{aligned}\tag{96}$$

Here

$$B_{23}=z,\quad B'_{23}=-z,\quad D_{23}=(z-1)/2,\tag{97}$$

$$\begin{aligned}&B_{12}=(3+5z)/8,\quad B'_{12}=(3-5z)/8,\\ &D_{12}=5(z-1)/16,\end{aligned}\tag{98}$$

$$B_{13}=B_{12},\quad B'_{13}=B'_{12},\quad D_{13}=D_{12}.\tag{99}$$

The generating matrix element of the potential-energy operator of a six-nucleon system $\hat{U}$ between the functions φ_0 and $\tilde{\varphi}_0$ is a sum of the four matrix elements given above:

$$\begin{aligned}\langle\varphi_0|\hat{U}|\tilde{\varphi}_0\rangle &= \langle\varphi_0|\hat{U}_{11}|\tilde{\varphi}_0\rangle+\langle\varphi_0|\hat{U}_{23}|\tilde{\varphi}_0\rangle+\langle\varphi_0|\hat{U}_{12}|\tilde{\varphi}_0\rangle\\ &\quad+\langle\varphi_0|\hat{U}_{13}|\tilde{\varphi}_0\rangle. \end{aligned}\tag{100}$$

Now we turn to the final stage of our calculations, the projection of the generating matrix elements $\langle\varphi_0|\hat{U}|\tilde{\varphi}_0\rangle$ onto the basis states $\Psi(n_1n_22m)$ and $\tilde{\Psi}(\tilde{n}_1\tilde{n}_22\tilde{m})$ and the subsequent extraction of the matrix elements $\langle n_1n_22m|\hat{U}|\tilde{n}_1\tilde{n}_22\tilde{m}\rangle$ of the three-cluster potential-energy operator.

We start by writing Eq. (36) as

$$\exp\{\mathbf{a}\tilde{\mathbf{a}}+\mathbf{b}\tilde{\mathbf{b}}\}=\sum_{n_1n_2m}\Psi(n_1,n_2,2m)\tilde{\Psi}(\tilde{n}_1,\tilde{n}_2,2\tilde{m})+\ldots,\tag{101}$$

where the terms with $L\neq 0$ are omitted and the $\Psi(n_1,n_2,2m)$ are given by Eq. (40); $\tilde{\Psi}(\tilde{n}_1,\tilde{n}_2,2\tilde{m})$ depends on the tilded generating parameters **a** and **b**.

The exponential

$$\exp\{\mathbf{a}\tilde{\mathbf{a}}+B\mathbf{b}\tilde{\mathbf{b}}+D(\mathbf{b}^2+\tilde{\mathbf{b}}^2)\} \tag{102}$$

is the basic block for all the matrix elements of the potential-energy operator. After being projected onto the basis states $\psi(n_1n_22m)$ and $\tilde{\psi}(\tilde{n}_1\tilde{n}_22\tilde{m})$, the expansion of this block in powers of $\mathbf{a},\mathbf{b},\tilde{\mathbf{a}},\tilde{\mathbf{b}}$ takes the form

$$\begin{aligned}&\exp\{\mathbf{a}\tilde{\mathbf{a}}+B\mathbf{b}\tilde{\mathbf{b}}+D(\mathbf{b}^2+\tilde{\mathbf{b}}^2)\}\\&=\sum_{n_1n_2m}\sum_{\tilde{n}_1\tilde{n}_2\tilde{m}}\Psi(n_1,n_2,2m)\\&\times\langle n_1n_22m|u_{23}(B,D)\\&\times|\tilde{n}_1\tilde{n}_22\tilde{m})\rangle\tilde{\Psi}(\tilde{n}_1,\tilde{n}_2,2\tilde{m})+\ldots\end{aligned} \tag{103}$$

and our task is to find the matrix elements

$$\langle n_1n_22m|u_{23}(B,D)|\tilde{n}_1\tilde{n}_22\tilde{m}\rangle, \tag{104}$$

which give us expressions for the matrix elements of all the terms of the nucleon–nucleon interaction potential-energy operator for different clusters.

We note first a simple consequence of the expansion (101) applied to the block (102):

$$\begin{aligned}&\exp\{\mathbf{a}\tilde{\mathbf{a}}+B\mathbf{b}\tilde{\mathbf{b}}+D(\mathbf{b}^2+\tilde{\mathbf{b}}^2)\}\\&=\sum_{n=0}^{\infty}\sum_{n_1+n_2=2n}\sum_{m=0}^{\min(n_1/2,n_2/2)}e^{Db^2}N(n_1,n_2,2m)\\&\times a^{n_1-2m}b^{n_2-2m}[\mathbf{ab}]^{2m}\Phi(n_1,n_2,2m;t)e^{D\tilde{b}^2}\\&\times B^{n_2}N(n_1,n_2,2m)\tilde{a}^{n_1-2m}\tilde{b}^{n_2-2m}[\tilde{\mathbf{a}}\tilde{\mathbf{b}}]^{2m}\\&\times\Phi(n_1,n_2,2m;\tilde{t})+\ldots\,.\end{aligned} \tag{105}$$

The constant B appears here to the power n_2 in each term of the expansion, as well as the moduli of the vectors **b** and $\tilde{\mathbf{b}}$. The next step is the expansion of $\exp\{D\mathbf{b}^2\}$ and $\exp\{D\tilde{\mathbf{b}}^2\}$ in powers of $\mathbf{b}^2$ and $\tilde{\mathbf{b}}^2$, respectively. Then the factors $\mathbf{b}^{2k}$ and $\tilde{\mathbf{b}}^{2k}$ appear in front of the basis functions. The products

$$\mathbf{b}^{2k}\Psi(n_1,n_2,2m)\quad\text{and}\quad\tilde{\mathbf{b}}^{2k}\tilde{\Psi}(n_1,n_2,2m)$$

can be represented as superpositions of the basis functions

$$\Psi(n_1,n_2+2k,2m+2l)\quad\text{and}\quad\tilde{\Psi}(n_1,n_2+2k,2m+2l)$$

with different l:

$$l=0,1,\ldots,\min\left(\frac{n_1}{2}-m,\ \frac{n_2}{2}+k-m\right).$$

This fact can be proved by using the Gauss recurrence relation for the hypergeometric functions,[21]

$$\begin{aligned}F(\alpha,\beta,\gamma;z)&=F(\alpha,\beta-1,\gamma-1;z)\\&+\frac{\alpha(\gamma-\beta)}{\gamma(\gamma-1)}zF(\alpha+1,\beta,\gamma+1;z),\end{aligned} \tag{106}$$

from which there follows the identity

$$\begin{aligned}&b^{2k}a^{n_1-2m}b^{n_2-2m}[\mathbf{ab}]^{2m}\Phi(n_1,n_2,2m;t)\\&=\sum_{l=0}^{\bar{n}}\frac{k!}{l!(k-l)!}\\&\times\frac{\Gamma(n_1/2-m+1)\Gamma(n_1/2-m+1/2)}{\Gamma(n_1/2-m-l+1)\Gamma(n_1/2-m-l+1/2)}\\&\times\frac{\Gamma(n/2+k-2m-2l+3/2)\Gamma(n/2-2m-l+1/2)}{\Gamma(n/2+k-2m-l+3/2)\Gamma(n/2-2m+1/2)}\\&\times a^{n_1-2m-2l}b^{n_2+2k-2m-2l}[\mathbf{ab}]^{2m+2l}\\&\times\Phi(n_1,n_2+2k,2m+2l;t)\\&=\sum_{l=0}^{\bar{n}}k!A(n_1,n_2,m;n_2+2k,m+l)\\&\times a^{n_1-2m-2l}b^{n_2+2k-2m-2l}\\&\times[\mathbf{ab}]^{2m+2l}\Phi(n_1,n_2+2k,2m+2l;t),\end{aligned} \tag{107}$$

where $\bar{n}=\min(n_1/2-m,n_2/2+k-m)$, $n=n_1+n_2$, and, by definition,

$$\begin{aligned}&A(n_1,\tilde{n}_2,\tilde{m};n_2,m)\\&=\frac{2^{-2(m-\tilde{m})}}{(m-\tilde{m})!\left(\dfrac{n_2-\tilde{n}_2}{2}-m+\tilde{m}\right)!}\frac{(n_1-2\tilde{m})!}{(n_1-2m)!}\\&\times\frac{\Gamma\left(\dfrac{n_1+\tilde{n}_2}{2}-m-\tilde{m}+\dfrac{1}{2}\right)\Gamma\left(\dfrac{n_1+n_2}{2}-2m+\dfrac{3}{2}\right)}{\Gamma\left(\dfrac{n_1+\tilde{n}_2}{2}-2\tilde{m}+\dfrac{1}{2}\right)\Gamma\left(\dfrac{n_1+n_2}{2}-m-\tilde{m}+\dfrac{3}{2}\right)}.\end{aligned} \tag{108}$$

Finally, we can now write the matrix element (104). It has the form of a double sum and can be expressed in terms of the coefficients $A(n_1,\tilde{n}_2,\tilde{m};n_2,m)$ and the normalization factors $N(n_1,n_2,2m)$:

$$\begin{aligned}&\langle n_1n_22m|u_{23}(B,D)|\tilde{n}_1\tilde{n}_22\tilde{m}\rangle\\&=\sum_{\tilde{n}_2=0}^{\min(n_2,\tilde{n}_2)}\sum_{\tilde{m}=0}^{\min(m,\tilde{m})}\\&\times\frac{N^2(n_1,\tilde{n}_2,2\tilde{m})}{N(n_1,n_2,2m)N(n_1,\tilde{n}_2,2\tilde{m})}B^{\tilde{n}_2}D^{(n_2+\tilde{n}_2)/2-\tilde{n}_2}\\&\times A(n_1,\tilde{n}_2,\tilde{m};n_2,m)A(n_1,\tilde{n}_2,\tilde{m};\tilde{n}_2,\tilde{m})\delta_{n_1\tilde{n}_1}.\end{aligned} \tag{109}$$

Two other matrix elements similar to (109) can be extracted from the same block (102) if the Jacobi vectors $\mathbf{a},\mathbf{b},\tilde{\mathbf{a}},\tilde{\mathbf{b}}$ are first replaced by $\mathbf{a}',\mathbf{b}',\tilde{\mathbf{a}}',\tilde{\mathbf{b}}'$ [see Eq. (88)] and then by $\mathbf{a}'',\mathbf{b}'',\tilde{\mathbf{a}}'',\tilde{\mathbf{b}}''$ [see Eq. (90)] and the following definitions are adopted:

$$\begin{aligned}&\exp\{\mathbf{a}'\tilde{\mathbf{a}}'+B\mathbf{b}'\tilde{\mathbf{b}}'+D(\mathbf{b}'^2+\tilde{\mathbf{b}}'^2)\}\\&=\sum_{n_1n_2m}\sum_{\tilde{n}_1\tilde{n}_2\tilde{m}}\psi(n_1n_22m)\end{aligned}$$

$$\times\langle n_1 n_2 2m|u'_{12}(B,D)$$
$$\times|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle\tilde{\Psi}(\tilde{n}_1,\tilde{n}_2,2\tilde{m})+\ldots, \quad (110)$$
$$\exp\{\mathbf{a}''\tilde{\mathbf{a}}''+B\mathbf{b}''\tilde{\mathbf{b}}''+D(\mathbf{b}''^2+\tilde{\mathbf{b}}''^2)\}$$

$$=\sum_{n_1 n_2 m}\sum_{\tilde{n}_1\tilde{n}_2\tilde{m}}\psi(n_1 n_2 2m)\langle n_1 n_2 2m|u'_{13}(B,D)$$
$$\times|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle\tilde{\Psi}(\tilde{n}_1,\tilde{n}_2,2\tilde{m})+\ldots . \quad (111)$$

To return to the basis of the initial Jacobi vectors $\mathbf{a},\mathbf{b},\tilde{\mathbf{a}},\tilde{\mathbf{b}}$, an orthogonal transformation of the matrices

$$\langle n_1 n_2 2m|u'_{12}(B,D)|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
and $\langle n_1 n_2 2m|u'_{13}(B,D)|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$

must be made. The matrices of this transformation,

$$\|\langle n_1 n_2 2m|\alpha'|n'_1 n'_2 2m\rangle\|$$
and $\|\langle n_1 n_2 2m|\alpha''|n'_1 n'_2 2m\rangle\|$,

are given by Eq. (44), where $\|\alpha'\|$ and $\|\alpha''\|$ are the matrices transforming $\mathbf{a},\mathbf{b}$ into $\mathbf{a}',\mathbf{b}'$ [Eq. (88)] and $\mathbf{a},\mathbf{b}$ into $\mathbf{a}'',\mathbf{b}''$ [Eq. (90)], respectively.

After the orthogonal transformation we get new matrices

$$\langle n_1 n_2 2m|u_{12}(B,D)|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$=\sum_{n'_1+n'_2=n_1+n_2}\sum_{\tilde{n}'_1+\tilde{n}'_2=\tilde{n}_1+\tilde{n}_2}\langle n_1 n_2 2m|\alpha'|n'_1 n'_2 2m\rangle$$
$$\times\langle n'_1 n'_2 2m|u'_{12}(B,D)|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$\times\langle\tilde{n}_1\tilde{n}_2 2\tilde{m}|\alpha'|\tilde{n}'_1\tilde{n}'_2 2\tilde{m}\rangle, \quad (112)$$
$$\langle n_1 n_2 2m|u_{12}(B,D)|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$=\sum_{n''_1+n''_2=n_1+n_2}\sum_{\tilde{n}''_1+\tilde{n}''_2=\tilde{n}_1+\tilde{n}_2}\langle n_1 n_2 2m|\alpha''|n''_1 n''_2 2m\rangle$$
$$\times\langle n''_1 n''_2 2m|u'_{12}(B,D)|\tilde{n}''_1\tilde{n}''_2 2\tilde{m}\rangle$$
$$\times\langle\tilde{n}_1\tilde{n}_2 2\tilde{m}|\alpha''|\tilde{n}''_1\tilde{n}''_2 2\tilde{m}\rangle. \quad (113)$$

Now, instead of the generating matrix elements [Eqs. (94)–(96)] we have the corresponding matrix elements between the basis functions:

$$\langle n_1 n_2 2m|\hat{U}_{23}|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$=z^{3/2}\{\tfrac{1}{2}(V_{31}+V_{13})\langle n_1 n_2 2m|u_{23}(B_{23},D_{23})|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$-\tfrac{1}{2}(V_{31}+V_{13}+V_{11})$$
$$\times\langle n_1 n_2 2m|u_{23}(B'_{23},D_{23})|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle\}; \quad (114)$$
$$\langle n_1 n_2 2m|\hat{U}_{12}|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$=z^{3/2}\{\tfrac{1}{4}(9V_{33}+3V_{31}+3V_{13}+V_{11})$$
$$\times\langle n_1 n_2 2m|u_{12}(B_{12},D_{12})|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle-\tfrac{1}{4}(5V_{33}+3V_{31}$$
$$+3V_{13}+V_{11})\langle n_1 n_2 2m|u_{12}(B'_{12},D_{12})|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle\}; \quad (115)$$
$$\langle n_1 n_2 2m|\hat{U}_{13}|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle$$
$$=z^{3/2}\{\tfrac{1}{4}(9V_{33}+3V_{31}+3V_{13}+V_{11})$$
$$\times\langle n_1 n_2 2m|u_{13}(B_{13},D_{13})|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle-\tfrac{1}{4}(5V_{33}+3V_{31}$$
$$+3V_{13}+V_{11})\langle n_1 n_2 2m|u_{13}(B'_{13},D_{13})|\tilde{n}_1\tilde{n}_2 2\tilde{m}\rangle\}. \quad (116)$$

This completes the derivation of the analytic formulas necessary for the construction of the Schrödinger equation.

7. CONCLUSION

Summarizing the investigation, we state the following basic results.

In the Fock–Bargmann space, the harmonic-oscillator basis for a three-cluster system with zero orbital angular momentum is constructed by using the technique of generating wave packets. The basis functions have the form of homogeneous polynomials in two Jacobi generator vectors and can be expressed in terms of the hypergeometric functions ${}_2F_1$. Their quantum numbers are the $SU(3)$ symmetry and the degree of homogeneity with respect to each Jacobi vector.

The rule of basis-function transformation induced by nucleon transpositions has been established. Linear combinations of basis states are found that do not vanish after antisymmetrization (the allowed states).

The matrix elements of the kinetic- and potential-energy operators between the generating wave packets have been obtained, and their projection onto the basis states has been performed. Explicit expressions for the Hamiltonian matrix elements in the basis of allowed states and the Schrödinger equation for a three-cluster system in the harmonic-oscillator representation have been obtained. In this procedure the Pauli principle has been taken into account accurately.

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