Hyperspherical functions with arbitrary permutational symmetry

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An algorithm is formulated for the construction of many-particle permutational symmetry adapted functions in hyperspherical coordinates. A recursive procedure is proposed, introducing hyperspherical coefficients of fractional parentage (hscfps). These coefficients are the eigenvectors of the transposition class sum of the symmetric group in an appropriate basis. Only the matrix element of the transposition of the last two particles has to be calculated in each step. This matrix element is obtained by using the hscfps calculated in the preceding step as well as the Raynal-Revai and the T coefficients. The results are applicable to the study of the atomic, molecular, and nuclear few-body problem.

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I. INTRODUCTION

The method of hyperspherical coordinates, along with the associated hyperspherical functions, was introduced in 1935 by Zernike and Brinkman [1]. Delves [2] and Smith [3] reintroduced this method in a different form 25 years later, and it was recently reviewed by Nikiforov *et al.* [4]. The hyperspherical functions were extensively used in recent years to study few-body problems in nuclear, atomic, and molecular physics [5].

In this method the internal degrees of freedom of an N-body system are reduced to a single hyperradial coordinate and a set of $3N-4$ angular coordinates. The hyperradius is invariant under particle permutations, making the hyperspherical coordinates very useful for rearrangement processes. A further convenient feature is that each hyperspherical basis function is separable into a product of a function of the hyperradius and a function of the hyperangular coordinates.

Since the total (space-spin) wave functions of a many-body system should be antisymmetric, the construction of permutational symmetry adapted hyperspherical functions has been considered extensively. Nevertheless, no generally valid efficient procedure, which is applicable for systems consisting of more than three particles, has been developed so far [6].

Four years ago, we introduced a recursive procedure for the construction of nonspurious harmonic oscillator functions with arbitrary permutational symmetry, in Jacobi coordinates [7]. According to this procedure, each symmetry-adapted N-particle harmonic oscillator function is written as a linear combination of angular-momentum coupled products of permutational symmetry adapted $(N-1)$-particle wave functions and an Nth-particle wave function, all members of the linear combination having the same N-particle harmonic oscillator energy. The coefficients of this linear combination are the harmonic oscillator coefficients of fractional parentage. These coefficients are the eigenvectors of the transposition class sum of the symmetric group, in the appropriate basis.

In the present article we use a variant of this recursive method to evaluate hyperspherical functions belonging to well defined irreducible representations (irreps) of the symmetric group. We diagonalize the transposition class sum of the symmetric group within invariant subspaces with respect to S_N, spanned by appropriate hyperspherical functions. Each of these functions is an angular momentum as well as hyperspherical angular momentum coupled product of an $(N-1)$-particle permutational symmetry adapted hyperspherical function with a single particle function. The eigenvalues that are obtained after the diagonalization uniquely identify the irreps of the symmetric group. The eigenvectors are the hyperspherical coefficients of fractional parentage (hscfps). In the actual computation only the matrix element of the transposition of the last two particles has to be evaluated.

The presentation is organized as follows: In Secs. II and III we introduce the hyperspherical coordinates and the hyperspherical Laplacian, respectively. The hyperspherical functions are presented in Sec. IV. In Sec. V we briefly review the Raynal-Revai and the T coefficients that are used in the subsequent sections. In Sec. VI we summarize the relevant part of the representation theory of the symmetric group. The permutational symmetry adapted hyperspherical basis is presented in Sec. VII for three particles and in Sec. VIII for N particles. The computational algorithm is given in Sec. IX. Some concluding remarks are made in Sec. X.

II. THE HYPERSPHERICAL COORDINATES

Several variants of hyperspherical coordinates have been used by different authors. They differ by both the choice of the underlying set of "single-particle," coordinates, the number (one or three) of spatial components specifying a "single-particle," and certain details concerning the definition of the angular and/or hyperangular coordinates [4,5].

We shall be using a version of the hyperspherical coordinates in which the center of mass motion of the system is removed, thereby obtaining a set of nonspurious basis functions. To introduce these hyperspherical coordinates we start from the center-of-mass coordinate $\mathbf{R} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i$ and the normalized Jacobi coordinates

$$\boldsymbol{\rho}_j = \sqrt{\frac{j-1}{j}}\left(\mathbf{r}_j - \frac{1}{j-1}(\mathbf{r}_1 + \mathbf{r}_2 + \cdots + \mathbf{r}_{j-1})\right), \qquad j = 2, 3, \ldots, N, \quad (1)$$

in which the jth particle is specified relative to the center of mass of particles 1 to $j-1$. $\boldsymbol{\rho}_j$ consists of a radial coordinate ρ_j and a pair of angular coordinates $\Omega_j \equiv (\theta_j, \phi_j)$.

A two-particle system is specified by the Jacobi coordinate $\boldsymbol{\rho}_2$ that consists of the radial coordinate $r_{(2)} \equiv \rho_2$ and of the angular coordinates $\Omega_2 = (\theta_2, \phi_2)$. For a three-particle system we transform the two radial coordinates ρ_2 and ρ_3 into a hyperradial coordinate $r_{(3)}$ and a hyperangular coordinate α_3 defined via

$$\begin{aligned} \rho_2 = r_{(2)} &= r_{(3)} \cos\alpha_3, \\ \rho_3 &= r_{(3)} \sin\alpha_3. \end{aligned} \quad (2)$$

The complete set of six coordinates consists of $r_{(3)}$, α_3, Ω_2, and Ω_3.

Adding the fourth particle we define the hyperradial coordinate $r_{(4)}$ and the hyperangular coordinate α_4 via

$$\begin{aligned} r_{(3)} &= r_{(4)} \cos\alpha_4, \\ \rho_4 &= r_{(4)} \sin\alpha_4. \end{aligned} \quad (3)$$

The internal coordinates for four particles are the two hyperangular coordinates α_3 and α_4, the six coordinates Ω_2, Ω_3, and Ω_4, and the hyperradial coordinate $r_{(4)}$.

In general, having defined the hyperradial coordinate $r_{(j-1)}$ we define $r_{(j)}$ and α_j so as to satisfy

$$\begin{aligned} r_{(j-1)} &= r_{(j)} \cos\alpha_j, \\ \rho_j &= r_{(j)} \sin\alpha_j, \end{aligned} \quad (4)$$

where

$$r_{(j)}^2 = r_{(j-1)}^2 + \rho_j^2 = \sum_{i=2}^{j} \rho_i^2 = \frac{1}{j} \sum_{\substack{i > i' \\ i = 2}}^{j} (\mathbf{r}_i - \mathbf{r}_{i'})^2. \quad (5)$$

Therefore, the hyperradial coordinate is symmetric with respect to permutations of the underlying single-particle coordinates.

The $3(N-1)$ internal coordinates for the N-particle system consist of the hyperradial coordinate $r_{(N)}$, the $N-2$ hyperangular coordinates $\alpha_{(N)} \equiv \{\alpha_3, \alpha_4, \ldots, \alpha_N\}$, and the $2(N-1)$ angular coordinates $\Omega_{(N)} \equiv \{\Omega_2, \Omega_3, \ldots, \Omega_N\}$. These coordinates depend on the set of Jacobi coordinates specified in Eq. (1). For a different ordering of particle indices a different set of hyperangular coordinates as well as a permuted set of angular coordinates is obtained. On the other hand, the hyperradial coordinate is independent of the order of the particle indices; cf. Eq. (5).

As was pointed out in the Introduction, in order to obtain the permutational symmetry-adapted linear combination of hyperspherical functions we have to evaluate the matrix elements of the transposition of the last two particles, i.e. $(N-1, N)$. This is conveniently done by constructing the N-particle hyperspherical coordinates in terms of the set of $N-3$ Jacobi coordinates corresponding to the first $N-2$ particles and the set consisting of the two Jacobi coordinates $\boldsymbol{\rho}_{N-1}$ and $\boldsymbol{\rho}_N$. This construction only involves the radial parts of the various Jacobi coordinates; the angular coordinates $\Omega_{(N)}$ are not affected. The hyperangular coordinates that are related to the Jacobi coordinates of the first $N-2$ particles, $\alpha_{(N-2)}$, also remain unchanged. However, instead of the two hyperangular coordinates α_{N-1} and α_N we have one hyperangular coordinate $\alpha_{N-1,N}$ which is obtained from the transformation

$$\begin{aligned} \rho_{N-1} &= r_{N-1,N} \cos\alpha_{N-1,N}, \\ \rho_N &= r_{N-1,N} \sin\alpha_{N-1,N}, \end{aligned} \quad (6)$$

and a second hyperangular coordinate α'_N which is obtained from the coordinates $r_{(N-2)}$ and $r_{N-1,N}$ by the relation

$$\begin{aligned} r_{(N-2)} &= r_{(N)} \cos\alpha'_N, \\ r_{N-1,N} &= r_{(N)} \sin\alpha'_N. \end{aligned} \quad (7)$$

Note that $r_{N-1,N} = \sqrt{\rho_{N-1}^2 + \rho_N^2}$ is *not* the distance between the particles $N-1$ and N. Note also that the hyperangular coordinate α'_N, defined in Eq. (7), is different from the hyperangular coordinate α_N defined in Eq. (4).

III. THE LAPLACE OPERATOR IN HYPERSPHERICAL COORDINATES

The internal kinetic energy operator for a two-particle system is given by the three-dimensional Laplace operator, expressed in terms of the relative motion Jacobi coordinate ρ_2 and the corresponding angular coordinates Ω_2,

$$\Delta_{(2)} = \Delta_{\boldsymbol{\rho}_2} = \Delta_{\rho_2} - \frac{1}{\rho_2^2}\hat{\ell}_2^2, \quad (8)$$

where the radial part is

$$\Delta_{\rho_2} = \frac{\partial^2}{\partial\rho_2^2} + \frac{2}{\rho_2}\frac{\partial}{\partial\rho_2} \quad (9)$$

and $\hat{\ell}_2^2$ is the angular momentum operator of the relative motion.

The internal kinetic energy of a three-particle system is described by the six-dimensional Laplace operator which is a sum over the three-dimensional Laplace operators that act on the coordinates $\boldsymbol{\rho}_2$ and $\boldsymbol{\rho}_3$ separately,

$$\Delta_{(3)} = \Delta_{\boldsymbol{\rho}_2} + \Delta_{\boldsymbol{\rho}_3} = \Delta_{\rho_2} + \Delta_{\rho_3} - \frac{1}{\rho_2^2}\hat{\ell}_2^2 - \frac{1}{\rho_3^2}\hat{\ell}_3^2. \quad (10)$$

Using Eq. (2) we can transform the two radial coordinates ρ_2 and ρ_3 into the hyperradial coordinate $r_{(3)}$ and the hyperangular coordinate α_3, in terms of which

$$\Delta_{(3)} = \Delta_{r_{(3)}} - \frac{1}{r_{(3)}^2}\hat{K}_3^2. \quad (11)$$

The radial part in Eq. (11) depends only on the hyperradial coordinate $r_{(3)}$, i.e.,

$$\Delta_{r_{(3)}} = \frac{\partial^2}{\partial r_{(3)}^2} + \frac{5}{r_{(3)}}\frac{\partial}{\partial r_{(3)}}. \quad (12)$$

The hyperspherical angular-momentum operator $\hat{K}_3^2$ is expressed in terms of the hyperangular coordinate α_3 and the two angular momentum operators $\hat{\ell}_2^2$ and $\hat{\ell}_3^2$ as follows:

$$\hat{K}_3^2 = -\frac{\partial^2}{\partial\alpha_3^2} - 4\cot(2\alpha_3)\frac{\partial}{\partial\alpha_3} + \frac{1}{\cos^2\alpha_3}\hat{\ell}_2^2 + \frac{1}{\sin^2\alpha_3}\hat{\ell}_3^2. \quad (13)$$

The internal angular-momentum operator of the three-particle system is $\hat{\mathbf{L}}_3 = \hat{\boldsymbol{\ell}}_2 + \hat{\boldsymbol{\ell}}_3$. Note that $\hat{L}_3^2$ and $\hat{L}_{3_z}$ commute with $\Delta_{(3)}$, $\hat{\ell}_2^2$, $\hat{\ell}_3^2$ and $\hat{K}_3^2$.

The $3(N-1)$-dimensional Laplace operator, describing the internal kinetic energy of the N-particle system, is a sum over the three-dimensional Laplace operators that act on the coordinates $\boldsymbol{\rho}_2, \boldsymbol{\rho}_3, \ldots, \boldsymbol{\rho}_N$,

$$\Delta_{(N)} = \sum_{i=2}^{N}\Delta_{\boldsymbol{\rho}_i} = \sum_{i=2}^{N}\left(\Delta_{\rho_i} - \frac{1}{\rho_i^2}\hat{\ell}_i^2\right). \quad (14)$$

This N-particle Laplace operator can be expressed by means of the recurrence relation

$$\Delta_{(N)} = \Delta_{(N-1)} + \Delta_{\boldsymbol{\rho}_N} = \Delta_{r_{(N-1)}} + \Delta_{\rho_N} - \frac{1}{r_{(N-1)}^2}\hat{K}_{N-1}^2 - \frac{1}{\rho_N^2}\hat{\ell}_N^2. \quad (15)$$

We can apply Eq. (4) and transform the coordinates $r_{(N-1)}$ and ρ_N into the hyperradial coordinate $r_{(N)}$ and the hyperangular coordinate α_N. In this case the $3(N-1)$ dimensional Laplace operator, Eq. (14), can be written in the form

$$\Delta_{(N)} = \Delta_{r_{(N)}} - \frac{1}{r_{(N)}^2}\hat{K}_N^2, \quad (16)$$

where the radial part is

$$\Delta_{r_{(N)}} = \frac{\partial^2}{\partial r_{(N)}^2} + \frac{3N-4}{r_{(N)}}\frac{\partial}{\partial r_{(N)}}. \quad (17)$$

$\hat{K}_N^2$, the N-particle hyperspherical angular-momentum operator, can be expressed in terms of $\hat{K}_{N-1}^2$ and $\hat{\ell}_N^2$ as follows [8]:

$$\hat{K}_N^2 = -\frac{\partial^2}{\partial\alpha_N^2} + \frac{3N-9-(3N-5)\cos(2\alpha_N)}{\sin(2\alpha_N)}\frac{\partial}{\partial\alpha_N} + \frac{1}{\cos^2\alpha_N}\hat{K}_{N-1}^2 + \frac{1}{\sin^2\alpha_N}\hat{\ell}_N^2, \quad (18)$$

where we define $\hat{K}_2^2 \equiv \hat{\ell}_2^2$. The internal N-particle angular-momentum operator is $\hat{\mathbf{L}}_N = \hat{\mathbf{L}}_{N-1} + \hat{\boldsymbol{\ell}}_N$. The operators $\hat{K}_{N-1}^2$, $\hat{\ell}_N^2$, $\hat{K}_N^2$, $\hat{L}_N^2$, and $\hat{L}_{N_z}$ commute with each other.

In the final paragraph of the preceding section we constructed the set of N-particle hyperspherical coordinates in terms of the hyperspherical coordinates corresponding to the first $N-2$ particles, and the hyperspherical representation of the Jacobi coordinates of the last two particles, $\boldsymbol{\rho}_{N-1}$ and $\boldsymbol{\rho}_N$. In this scheme the N-particle Laplace operator has to be expressed in terms of the Laplace operators corresponding to the two subsets of particles specified.

Applying Eq. (15) twice and using Eqs. (6) and (7) we obtain the following expression for the N-particle Laplace operator:

$$\begin{aligned}\Delta_{(N)} &= \left\{\Delta_{r_{(N-2)}} - \frac{1}{r_{(N-2)}^2}\hat{K}_{N-2}^2\right\} + \left\{\left(\Delta_{\rho_{N-1}} - \frac{1}{\rho_{N-1}^2}\hat{\ell}_{N-1}^2\right) + \left(\Delta_{\rho_N} - \frac{1}{\rho_N^2}\hat{\ell}_N^2\right)\right\} \\ &= \left\{\Delta_{r_{(N-2)}} - \frac{1}{r_{(N-2)}^2}\hat{K}_{N-2}^2\right\} + \left\{\Delta_{r_{N-1,N}} - \frac{1}{r_{N-1,N}^2}\hat{K}_{N-1,N}^2\right\} = \Delta_{r_{(N)}} - \frac{1}{r_{(N)}^2}\hat{K}_N'^2 .\end{aligned} \quad (19)$$

The structure of the operator $\Delta_{r_{N-1,N}}$ is analogous to that of $\Delta_{r_{(3)}}$ [Eq. (12)], substituting $r_{N-1,N}$ for $r_{(3)}$. The expression for the hyperspherical angular-momentum operator $\hat{K}_{N-1,N}^2$ is similar to the expression for $\hat{K}_3^2$ [Eq. (13)], where the hyperangular coordinate is $\alpha_{N-1,N}$ and the two angular-momentum operators are referred to the Jacobi coordinates $\boldsymbol{\rho}_{N-1}$ and $\boldsymbol{\rho}_N$, i.e.,

$$\hat{K}_{N-1,N}^2 = -\frac{\partial^2}{\partial\alpha_{N-1,N}^2} - 4\cot(2\alpha_{N-1,N})\frac{\partial}{\partial\alpha_{N-1,N}} + \frac{1}{\cos^2(\alpha_{N-1,N})}\hat{\ell}_{N-1}^2 + \frac{1}{\sin^2(\alpha_{N-1,N})}\hat{\ell}_N^2. \quad (20)$$

The expression finally obtained for the N-particle hyperspherical angular-momentum operator is

$$\hat{K}_N'^2 = -\frac{\partial^2}{\partial \alpha_N'^2} + \frac{3N-9-(3N-5)\cos(2\alpha_N')}{\sin(2\alpha_N')}\frac{\partial}{\partial \alpha_N'} + \frac{1}{\cos^2\alpha_N'}\hat{K}_{N-2}^2 + \frac{1}{\sin^2\alpha_N'}\hat{K}_{N-1,N}^2, \tag{21}$$

where α_N' was defined in Eq. (7). Note that this expression is similar to Eq. (18) where α_N, $\hat{K}_{N-1}$, and $\hat{\ell}_N$ are replaced by α_N', $\hat{K}_{N-2}$, and $\hat{K}_{N-1,N}$, respectively. Actually, comparing Eq. (16) and Eq. (19) we note that $\hat{K}_N'^2$ and $\hat{K}_N^2$ are expressions for the same operator in terms of different sets of coordinates.

IV. THE HYPERSPHERICAL FUNCTIONS

The angular part of the internal state for two particles is described by the spherical harmonic $Y_{\ell_2,m_2}(\Omega_2)$. While permutational symmetry adaptation will only concern us in Sec. VII, we point out in passing that the two-particle state belongs to the irrep **[2]** of the symmetric group S_2 if ℓ_2 is even and to **[11]** if ℓ_2 is odd. Adding one more particle belonging to the state $Y_{\ell_3,m_3}(\Omega_3)$ we form the three-particle state $\Phi_{L_3M_3;\ell_2\ell_3}(\Omega_{(3)})$, which is an eigenstate of the operators $\hat{\ell}_2^2$, $\hat{\ell}_3^2$, $\hat{L}_3^2$, and $\hat{L}_{3_z}$. This three-particle state is obtained by conventional angular-momentum coupling of the states $Y_{\ell_2,m_2}(\Omega_2)$ and $Y_{\ell_3,m_3}(\Omega_3)$,

$$\Phi_{L_3M_3;\ell_2\ell_3}(\Omega_{(3)}) = \sum_{m_2,m_3}\langle \ell_2 m_2 \ell_3 m_3 | L_3 M_3\rangle \times Y_{\ell_2,m_2}(\Omega_2) Y_{\ell_3,m_3}(\Omega_3), \tag{22}$$

in which only the single-particle angular coordinates Ω_2 and Ω_3 are involved. Recall that $\Omega_{(3)} \equiv \{\Omega_2, \Omega_3\}$.

The eigenfunctions of $\hat{K}_3^2$, Eq. (13), are functions of the hyperangular coordinate α_3 [Eq. (2)] and depend on the value of the quantum number K_3 as well as on the values of ℓ_3 and $K_2(\equiv \ell_2)$, as follows [8]:

$$\Psi_{K_3;\ell_3\ell_2}(\alpha_3) = \mathcal{N}_3(K_3;\ell_3\ell_2)\,(\sin\alpha_3)^{\ell_3}(\cos\alpha_3)^{\ell_2} \times P_{\mu_3}^{\ell_3+\frac{1}{2},\ell_2+\frac{1}{2}}\big(\cos(2\alpha_3)\big)\,, \tag{23}$$

where $P_{\mu_3}^{\ell_3+\frac{1}{2},\ell_2+\frac{1}{2}}$ is the Jacobi polynomial, μ_3 is a nonnegative integer and

$$K_3 = 2\mu_3 + \ell_2 + \ell_3\,. \tag{24}$$

The normalization constant is [8]

$$\mathcal{N}_3(K_3;\ell_3\ell_2) = \left[\frac{(2K_3+4)\mu_3!\Gamma(\mu_3+\ell_3+\ell_2+2)}{\Gamma(\mu_3+\ell_3+\frac{3}{2})\Gamma(\mu_3+\ell_2+\frac{3}{2})}\right]^{\frac{1}{2}}. \tag{25}$$

The eigenvalues of $\hat{K}_3^2$ corresponding to the eigenfunctions (23) are $K_3(K_3+4)$, where $K_3 \geq \ell_2+\ell_3 \geq 0$ and has the same parity as $\ell_2+\ell_3$ [cf. Eq. (24)].

The hyperspherical function for three particles, which is an eigenfunction of $\hat{K}_3^2$ as well as of $\hat{L}_3^2$, is obtained by multiplying the function (23) by the function (22),

$$\mathcal{Y}_{[K_3]}(\Omega_{(3)}\alpha_3) = \Psi_{K_3;\ell_3\ell_2}(\alpha_3)\Phi_{L_3M_3;\ell_2\ell_3}(\Omega_{(3)}). \tag{26}$$

The symbol $[K_3]$ stands for the aggregate of five good quantum numbers K_3, L_3, M_3, ℓ_2, and ℓ_3, which completely label the state since there are five (internal) coordinates, i.e., $\Omega_2 = (\theta_2, \phi_2)$, $\Omega_3 = (\theta_3, \phi_3)$, and α_3.

The construction of basis functions that belong to well-defined irreps of the symmetric group S_3 will require the formation of linear combinations of the functions (26) with common values of K_3, L_3, and M_3. For ℓ_2 and ℓ_3 we will have to allow all values that are consistent with the values of K_3 and L_3 specified, and such that ℓ_2 is either always even or always odd (i.e., all the two-particle states belong to the same irrep of S_2). Consequently, K_3, L_3, and M_3 remain good quantum numbers after the permutational symmetry adaptation, but instead of ℓ_2 and ℓ_3 we have the Yamanouchi symbol Y_3 as well as the additional multiplicity label, β_3. This step will be discussed in detail in Sec. VII, but it is convenient to think about $[K_3]$ as standing for $K_3, L_3, M_3; \ell_2, \ell_3$ before the permutational symmetry adaptation and for $K_3, L_3, M_3; Y_3, \beta_3$ following it. From the point of view of the present section, $\mathcal{Y}_{[K_3]}$ in either sense is suitable as a parent state for constructing the four-particle hyperspherical functions.

In view of the fact that for two-particle states the angular momentum $\hat{\boldsymbol{\ell}}_2$ and the hyperspherical angular momentum $\hat{\mathbf{K}}_2$ coincide, the discussion presented above does not exhibit the generic characteristics of the recursive construction of hyperspherical functions in general. We therefore proceed to describe the formation of the four-particle hyperspherical functions.

Starting from any three-particle function corresponding to a given set of quantum numbers K_3 and L_3 we construct a four-particle hyperspherical function by coupling that function to the function $Y_{\ell_4,m_4}(\Omega_4)$. This is done in the following three steps. First, by using the O(3) Clebsch-Gordan coefficients we couple the angular momenta L_3 and ℓ_4 and obtain

$$\Phi_{L_4M_4;K_3L_3\ell_4}(\Omega_{(4)}\alpha_3) = \sum_{M_3,m_4}\langle L_3M_3\ell_4m_4|L_4M_4\rangle \times \mathcal{Y}_{[K_3]}(\Omega_{(3)}\alpha_3)Y_{\ell_4,m_4}(\Omega_4). \tag{27}$$

This function has seven (internal) coordinates, i.e., $\Omega_2 = (\theta_2, \phi_2)$, $\Omega_3 = (\theta_3, \phi_3)$, α_3 and $\Omega_4 = (\theta_4, \phi_4)$.

As a second step we use the transformation (3) and construct the eigenfunctions of the hyperangular momentum operator $\hat{K}_4^2$ [Eq. (18) for $N=4$] [8],

$$\Psi_{K_4;\ell_4K_3}(\alpha_4) = \mathcal{N}_4(K_4;\ell_4K_3)(\sin\alpha_4)^{\ell_4}(\cos\alpha_4)^{K_3} \times P_{\mu_4}^{\ell_4+\frac{1}{2},K_3+2}\big(\cos(2\alpha_4)\big), \tag{28}$$

where $P_{\mu_4}^{\ell_4+\frac{1}{2},K_3+2}$ is the Jacobi polynomial, μ_4 is a nonnegative integer, and

$$K_4 = 2\mu_4 + K_3 + \ell_4 \,. \tag{29}$$

The normalization constant $\mathcal{N}_4(K_4;\ell_4 K_3)$ is [8]

$$\mathcal{N}_4(K_4;\ell_4 K_3) = \left[\frac{(2K_4+7)\mu_4!\Gamma(\mu_4+\ell_4+K_3+\frac{7}{2})}{\Gamma(\mu_4+\ell_4+\frac{3}{2})\Gamma(\mu_4+K_3+3)}\right]^{\frac{1}{2}} . \tag{30}$$

The eigenvalues of $\hat{K}_4^2$ corresponding to the eigenfunctions (28) are $K_4(K_4+7)$ where $K_4 \geq K_3+\ell_4 \geq 0$ and has the same parity as $K_3+\ell_4$ [cf. Eq. (29)].

Having obtained the functions $\Phi_{L_4M_4;K_3L_3\ell_4}$ (27) and $\Psi_{K_4;\ell_4K_3}$ (28) we can construct the functions $\mathcal{Y}_{[K_4]}$ as the products of these two functions,

$$\mathcal{Y}_{[K_4]}(\Omega_{(4)}\alpha_{(4)}) = \Psi_{K_4;\ell_4K_3}(\alpha_4)\Phi_{L_4M_4;K_3L_3\ell_4}(\Omega_{(4)}\alpha_3), \tag{31}$$

where $[K_4]$ stands for K_4, L_4, M_4, K_3, L_3, ℓ_4, as well as either ℓ_2 and ℓ_3 or Y_3 and β_3, depending on the three-particle function we started from.

Assuming that permutational symmetry adapted $\mathcal{Y}_{[K_3]}$'s were used, we can now symmetry-adapt to S_4. This is achieved by forming appropriate linear combinations of $\mathcal{Y}_{[K_4]}$'s with common values of K_4, L_4, M_4, and Y_3 but summing over the remaining quantum numbers. When this is completed $[K_4]$ should be interpreted to stand for K_4, L_4, M_4, Y_4, and β_4, where Y_4 is the S_4 Yamanouchi symbol and β_4 is the further multiplicity label.

To formulate the general recursive procedure for the construction of the N-particle hyperspherical function let us assume that the $(N-1)$-particle functions $\mathcal{Y}_{[K_{N-1}]}$ are already available. These functions possess well defined hyperspherical angular momentum K_{N-1}, total angular momentum L_{N-1}, and z-component M_{N-1}. Assuming that they have been symmetry adapted to S_{N-1}, they have as additional quantum numbers the Yamanouchi symbol Y_{N-1} and the multiplicity label β_{N-1}, but these are for the time being irrelevant. The functions $\mathcal{Y}_{[K_{N-1}]}$ depend on the set of single-particle angular coordinates $\Omega_{(N-1)}$ as well as on the set of hyperangular coordinates $\alpha_{(N-1)}$.

The N-particle hyperspherical function $\mathcal{Y}_{[K_N]}$ is now obtained in the following three steps. First, we couple the function $\mathcal{Y}_{[K_{N-1}]}$ and the function $Y_{\ell_N,m_N}(\Omega_N)$ to obtain the function $\Phi_{L_NM_N;K_{N-1}L_{N-1}\ell_N}$,

$$\Phi_{L_NM_N;K_{N-1}L_{N-1}\ell_N}(\Omega_{(N)}\alpha_{(N-1)}) = \sum_{M_{N-1},m_N} \langle L_{N-1}M_{N-1}\ell_N m_N|L_NM_N\rangle \mathcal{Y}_{[K_{N-1}]}(\Omega_{(N-1)}\alpha_{(N-1)})Y_{\ell_N,m_N}(\Omega_N). \tag{32}$$

Second, using the transformation (4) in the subspace of the coordinates $(r_{(N-1)}\ ,\ \rho_N) \equiv (r_{(N)}\ ,\ \alpha_N)$, we construct the orthonormalized eigenfunctions of the hyperspherical angular-momentum operator $\hat{K}_N^2$ (18),

$$\Psi_{K_N;\ell_NK_{N-1}}(\alpha_N) = \mathcal{N}_N(K_N;\ell_NK_{N-1})(\sin\alpha_N)^{\ell_N}(\cos\alpha_N)^{K_{N-1}}P_{\mu_N}^{\ell_N+\frac{1}{2},K_{N-1}+\frac{3N-8}{2}}\big(\cos(2\alpha_N)\big), \tag{33}$$

where μ_N is a non-negative integer,

$$K_N = 2\mu_N + K_{N-1} + \ell_N \ , \tag{34}$$

and the normalization coefficient is [8]

$$\mathcal{N}_N(K_N;\ell_NK_{N-1}) = \left[\frac{(2K_N+3N-5)\mu_N!\Gamma(\mu_N+K_{N-1}+\ell_N+\frac{3N-5}{2})}{\Gamma(\mu_N+\ell_N+\frac{3}{2})\Gamma(\mu_N+K_{N-1}+\frac{3N-6}{2})}\right]^{\frac{1}{2}} . \tag{35}$$

The appropriate eigenvalues of the operator $\hat{K}_N^2$ (18) for the eigenfunctions (33) are

$$K_N(K_N+3N-5), \tag{36}$$

where $K_N \geq K_{N-1}+\ell_N \geq 0$ and has the same parity as $K_{N-1}+\ell_N$.

Finally, we construct the functions $\mathcal{Y}_{[K_N]}$. These are the N-particle hyperspherical functions which are coupled to a total angular momentum L_N. They are products of the two functions $\Phi_{L_NM_N;K_{N-1}L_{N-1}\ell_N}$, Eq. (32), and $\Psi_{K_N;\ell_NK_{N-1}}$, Eq. (33),

$$\mathcal{Y}_{[K_N]}(\Omega_{(N)}\alpha_{(N)}) = \Psi_{K_N;\ell_NK_{N-1}}(\alpha_N)\Phi_{L_NM_N;K_{N-1}L_{N-1}\ell_N}(\Omega_{(N)}\alpha_{(N-1)}), \tag{37}$$

where $[K_N]$ stands for K_N, L_N, M_N, K_{N-1}, L_{N-1}, ℓ_N and Y_{N-1}, β_{N-1}. The hyperspherical functions $\mathcal{Y}_{[K_N]}$ defined in Eq. (37) form a complete and orthonormal set of functions that satisfy [9]

$$\langle\mathcal{Y}_{[K_N]}|\mathcal{Y}_{[K_N']}\rangle = \delta_{[K_N],[K_N']} = \delta_{K_N,K_N'}\delta_{L_N,L_N'}\delta_{M_N,M_N'}\delta_{K_{N-1},K_{N-1}'}\delta_{L_{N-1},L_{N-1}'}\delta_{\ell_N,\ell_N'}\delta_{Y_{N-1},Y_{N-1}'}\delta_{\beta_{N-1},\beta_{N-1}'}. \tag{38}$$

The construction of many-particle hyperspherical functions can be represented by using the "tree" diagrams introduced in Ref. [10]. The sequential coupling scheme formulated above is presented in Fig. 1. Each segment in this "tree" connects two nodes, except the top segments which connect single-particle nodes with Cartesian components of the corresponding Jacobi coordinate. Each segment is called a propagator, and with each node we associate an angle. A propagator that extends to the right (left) upward from a node corresponds to the cosine (sine) of the angle. The components of the Jacobi coordinates in the "tree" are obtained by taking the product of $r_{(N)}$, Eq. (5), with *all* the appropriate cosine and sine functions, starting from the vertex at the bottom of the diagram. Further, the quantum number associated with each node is presented. The rules for obtaining the hyperspherical functions from the "tree" are given in Ref. [10].

The sequential scheme described above is one of many available routes for constructing the eigenfunctions of $\hat{K}_N^2$. In Sec. III we described the alternative route, in which the last two Jacobi coordinates are grouped together, separately from the first $N-3$ Jacobi coordinates. The eigenfunctions of the hyperspherical angular-momentum operator $\hat{K}^2_{N-1,N}$ [defined in Eq. (20)] are

$$\Psi_{K_{N-1,N};\ell_N\ell_{N-1}}(\alpha_{N-1,N})$$

$$= \mathcal{N}_{N-1,N}(K_{N-1,N};\ell_N\ell_{N-1}) \times(\sin\alpha_{N-1,N})^{\ell_N}(\cos\alpha_{N-1,N})^{\ell_{N-1}} \times P_{\mu_{N-1,N}}^{\ell_N+\frac{1}{2},\ell_{N-1}+\frac{1}{2}}\big(\cos(2\alpha_{N-1,N})\big), \quad (39)$$

where $K_{N-1,N}=2\mu_{N-1,N}+\ell_N+\ell_{N-1}$ and $\mu_{N-1,N}$ is a non-negative integer. These functions are similar to the functions (23) where α_3, K_3, μ_3, ℓ_3, and ℓ_2, are replaced by $\alpha_{N-1,N}$, $K_{N-1,N}$, $\mu_{N-1,N}$, ℓ_N, and ℓ_{N-1}, respectively. Using these substitutions we obtain the normalization constant $\mathcal{N}_{N-1,N}(K_{N-1,N};\ell_N\ell_{N-1})$ from the expression for $\mathcal{N}_3(K_3;\ell_3\ell_2)$ [Eq. (25)].

The hyperspherical functions for N particles, that are the eigenfunctions of the hyperspherical angular-momentum operator $\hat{K}_N'^2$ $(=\hat{K}_N^2)$ [cf. Eq. (21)], are constructed from the hyperspherical functions of the first $N-3$ Jacobi coordinates, $\Psi_{K_{N-2};\ell_{N-2}K_{N-3}}(\alpha_{N-2})$, and the functions of the last two coordinates $\Psi_{K_{N-1,N};\ell_N\ell_{N-1}}(\alpha_{N-1,N})$ [Eq. (39)] as follows:

$$\Psi_{K_N;K_{N-1,N}K_{N-2}}(\alpha'_N)$$

$$= \mathcal{N}_N(K_N;K_{N-1,N}K_{N-2}) \times(\sin\alpha'_N)^{K_{N-1,N}}(\cos\alpha'_N)^{K_{N-2}} \times P_{\mu'_N}^{K_{N-1,N}+2,K_{N-2}+\frac{3N-11}{2}}\big(\cos(2\alpha'_N)\big), \quad (40)$$

where $K_N=2\mu'_N+K_{N-2}+K_{N-1,N}$ and μ'_N is a non-negative integer. This expression is similar to Eq. (33), replacing α_N, μ_N, ℓ_N, and K_{N-1} by α'_N, μ'_N, $K_{N-1,N}$, and K_{N-2}, respectively. Using these substitutions we obtain the normalization constant $\mathcal{N}_N(K_N;K_{N-1,N}K_{N-2})$ from the expression for $\mathcal{N}_N(K_N;\ell_N K_{N-1})$ [Eq. (35)]. In addition to these substitutions, the correct form of the Jacobi polynomial and of the normalization constant in Eq. (40) require the addition of the constant $\frac{3}{2}$ to $K_{N-1,N}$ and its subtraction from K_{N-2} [8]. The "tree" structure corresponding to this hyperspherical coupling scheme is presented in Fig. 2.

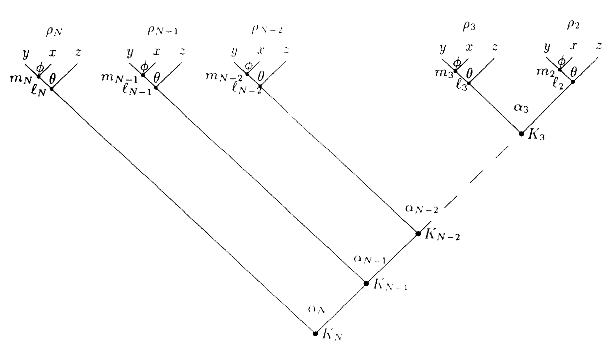

FIG. 1. The "tree" structure that represents the scheme for constructing the eigenfunctions of the hyperspherical angular-momentum operator $\hat{K}_N^2$. The particles are added sequentially.

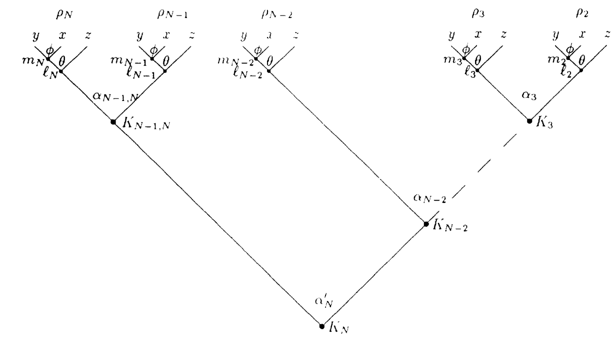

FIG. 2. The "tree" structure that represents the scheme for constructing the eigenfunctions of the hyperspherical angular-momentum operator $\hat{K}_N'^2$. The last two particles are coupled to one another before they are coupled to the rest of the system.

V. THE RAYNAL-REVAI AND THE T COEFFICIENTS

The hyperspherical functions, as constructed in the preceding section, depend on the choice of the Jacobi coordinates, Eq. (1), as well as on the order chosen for coupling the various single-particle functions. In subsection A of the present section we consider the transformation of the set of hyperspherical functions which results from transforming between different sets of Jacobi coordinates. This transformation is effected by means of the Raynal-Revai coefficients [11–13]. In subsection B we discuss the transformation between the two sets of hyperspherical functions corresponding to two different coupling schemes, that is effected by means of the T coefficients [14,15].

A. The Raynal-Revai coefficients

To enable the transformation between the sets of hyperspherical functions obtained for the same physical system using different choices of Jacobi coordinates we use the Raynal-Revai coefficients. These coefficients are needed in the present context in order to apply particle permutations to the hyperspherical functions. Such permutations give rise to transformations of the Jacobi coordinates that can equivalently be described in terms of appropriate rotations.

As was pointed out at the bottom of Sec. III the N-particle hyperspherical angular-momentum operator $\hat{K}_N^2$ is independent of the set of the angular coordinates $\Omega_{(N)}$ and of the choice of single-particle ordering or of groupings of subsets of particles assumed in the construction of the Jacobi coordinates.

Let us consider the two Jacobi coordinates $\boldsymbol{\rho}_{N-1}$ and $\boldsymbol{\rho}_N$. The hyperspherical functions constructed from these two Jacobi coordinates are uniquely specified by the quantum numbers ℓ_{N-1}, ℓ_N, $K_{N-1,N}$, $L_{N-1,N}$, and $M_{N-1,N}$ (as was explained in the preceding section). These hyperspherical functions can be expressed in terms of the hyperspherical functions depending on two different Jacobi coordinates $\boldsymbol{\rho}'_{N-1}$ and $\boldsymbol{\rho}'_N$, that are related to the first two by means of a rotation by an angle γ, by using the Raynal-Revai coefficients [11–13], as follows:

$$|\ell_{N-1}\ell_N K_{N-1,N}L_{N-1,N}M_{N-1,N}\rangle = \sum_{\ell'_{N-1}\ell'_N} \langle \ell_{N-1}\ell_N|\gamma|\ell'_{N-1}\ell'_N\rangle_{K_{N-1,N}L_{N-1,N}} |\ell'_{N-1}\ell'_N K_{N-1,N}L_{N-1,N}M_{N-1,N}\rangle \,, \tag{41}$$

where the sum is restricted by the relation $|\ell'_{N-1}-\ell'_N| \leq L_{N-1,N} \leq \ell'_{N-1}+\ell'_N \leq K_{N-1,N}$ such that $\ell'_{N-1}+\ell'_N$ has the same parity as $K_{N-1,N}$. Note that the quantum numbers $K_{N-1,N}$ and $L_{N-1,N}$ (as well as $M_{N-1,N}$) are common to both sets of hyperspherical functions, as was explained above.

The Raynal-Revai coefficients defined by Eq. (41) can be expressed in terms of the harmonic-oscillator Talmi-Moshinsky brackets [12]. Using this relation, an analytic expression for the transformation brackets for hyperspherical functions was obtained by Raynal and Revai for three particles [11,12]. A generalization to four particles was studied in Ref. [13]. This generalization is not required in our present context.

B. The T coefficients

The T coefficients are the recoupling coefficients that enable the expression of a hyperspherical function obtained by coupling of three subsystems in a particular order in terms of the set of hyperspherical functions describing the same composite system, obtained using a different coupling order [14,15].

According to the sequential scheme specified in the preceding section the functions of the Nth particle are coupled to appropriate $(N-1)$-particle hyperspherical functions, Eq. (33). The alternative scheme, in which we couple the hyperspherical functions of the last two particles to suitable $(N-2)$-particle sequentially coupled hyperspherical functions, results in a different set of N-particle hyperspherical functions, Eqs. (39) and (40). The transformation between these two coupling schemes is the case which is relevant to our present problem. In other words, we are interested in the transformation from the "tree" structure in Fig. 1 to the "tree" structure in Fig. 2. This transformation is effected by means of the T coefficients (of type F) introduced in Ref. [14]. The transformation is presented in Fig. 3 which is the figure of case F in Ref. [14]; Only the relevant parts of the two "trees" are plotted.

Let us assume that the hyperspherical functions presented by Figs. 1 and 2 have been constructed from the same $(N-2)$-particle hyperspherical function, which had been symmetry adapted to S_{N-2}. Therefore, both hyperspherical functions have the same quantum numbers K_{N-2}, L_{N-2}, the Yamanouchi symbol Y_{N-2}, and the multiplicity label β_{N-2}. All the relevant angular momenta, i.e., ℓ_{N-1}, ℓ_N, and L_N are also the same for both hyperspherical functions. In this case we can express the hyperspherical function of Fig. 1 in terms of those of Fig. 2 by using the appropriate T coefficients, as follows:

$$|K_{N-2}L_{N-2}Y_{N-2}\beta_{N-2};\ell_{N-1}K_{N-1}L_{N-1};\ell_N K_N L_N M_N\rangle$$
$$= \sum_{K_{N-1,N}} \langle K_{N-1,N}|K_N;\ell_N,\ell_{N-1},K_{N-2}|K_{N-1}\rangle |K_{N-2}L_{N-2}Y_{N-2}\beta_{N-2};(\ell_{N-1}\ell_N)K_{N-1,N};K_N L_N M_N\rangle. \tag{42}$$

The summation over $K_{N-1,N}$ is subject to the restriction $(\ell_N+\ell_{N-1}) \leq K_{N-1,N} \leq (K_N-K_{N-2})$, where the parities of $K_{N-1,N}$, (K_N-K_{N-2}) and $(\ell_N+\ell_{N-1})$ should be the same.

The two intermediate quantum numbers, which differ in the two parts of Fig. 3, appear in the "bra" and the "ket" of the T coefficient in Eq. (42). Between the "bra" and the "ket" we write the quantum number that appears

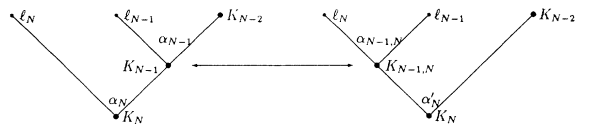

FIG. 3. A schematic representation of the T coefficient between the "tree" of Fig. 1 and the "tree" of Fig. 2. Only the relevant parts of the two "trees" are plotted. The two-headed arrow points to the two different intermediate quantum numbers.

in the vertex of both "trees", K_N, followed by the three quantum numbers of the three subsystems, ℓ_N, ℓ_{N-1}, and K_{N-2}. The analytic expression for this particular T coefficient is given in Ref. [15].

VI. PERMUTATIONAL SYMMETRY ADAPTATION

In the present section we consider the construction of spatial wave functions with arbitrary permutational symmetry. Symmetry adaptation with respect to the symmetric group S_N is achieved by diagonalization of the transposition class sum, $[(2)]_N$, which is defined below, within an appropriate invariant subspace with respect to S_N [16]. In all variants of this procedure one applies the fact that $[(2)]_N$ commutes with the N-particle angular-momentum operator $\hat{L}^2_{(N)}$ and with its z-component $\hat{L}_{(N)z}$, as well as with the center of the symmetric subgroup S_{N-1}. This allows the construction of invariant subspaces with respect to S_N, each of which is specified by a given Yamanouchi symbol Y_{N-1} with respect to the group-subgroup chain $S_{N-1} \supset S_{N-2} \supset \cdots \supset S_2$. These labels are not sufficient to specify a finite invariant subspace. This is a consequence of the fact that angular-momentum coupling allows a given N-particle angular momentum to be obtained starting from arbitrarily high values of the $(N-1)$-particle angular momentum, provided that the Nth particle coupled to it has a sufficiently high angular momentum.

In the conventional shell-model approach the N-particle invariant subspace is kept finite by allowing the single-particle angular momentum to obtain a given unique value, or at most a small set of values corresponding to the shells which are allowed to be occupied [16].

In the harmonic oscillator basis one uses the fact that the Hamiltonian commutes with the N-particle total angular momentum as well as with the elements of S_N. Consequently, any subspace specified by a specific eigenvalue of the harmonic oscillator Hamiltonian is invariant with respect to S_N. These subspaces are finite dimensional [7].

In the hyperspherical basis it is the specification of the quantum number K_N, corresponding to the N-particle hyperspherical angular momentum, which provides finite-dimensional N-particle invariant subspaces with respect to S_N. This is due to the fact that the hyperspherical angular momentum, like the total energy and unlike the total spatial angular momentum, cannot decrease upon addition of a particle.

As long as particles with spin $\frac{1}{2}$ are considered we could confine our attention to irreps of the symmetric group with at most two columns, as these can be coupled with corresponding spin functions belonging to the adjoint irrep (in which columns are turned into rows) to obtain total wave functions which are properly antisymmetric. Since we gain very little by making this restriction we shall consider the most general case.

The central idea is that we obtain the N-particle symmetry adapted wave function starting from an $(N-1)$-particle wave-function that is characterized by means of a Yamanouchi symbol Y_{N-1}, or, in other words, that belongs to a sequence of irreps $\Gamma_2, \Gamma_3, \ldots, \Gamma_{N-1}$ of $S_2 \subset S_3 \subset \cdots \subset S_{N-1}$. Such a function is fully characterized by being a common eigenfunction of the transposition class sums $[(2)]_2$, $[(2)]_3$, $\ldots$, $[(2)]_{N-1}$ where

$$[(2)]_j = \sum_{\substack{i > i' \\ i = 2}}^{j} (i, i'). \tag{43}$$

This is a consequence of the following two facts:

a. The irreps of the symmetric group S_N are simply subducible with respect to the sequence $S_N \supset S_{N-1} \supset \cdots \supset S_2$.

b. The eigenvalue of $[(2)]_N$ is sufficient to characterize the irrep to which a function belongs, given that it belongs to some definite irrep of S_{N-1}.

The eigenvalue of $[(2)]_N$ corresponding to a given irrep of S_N, which is represented by the Young diagram Γ_N, can be written in the following two equivalent ways:

$$[(2)]_N\Big|_{\Gamma_N} = \begin{cases} \frac{1}{2}\sum_i \lambda_i(\lambda_i - 2i + 1) \\ \text{or} \\ \sum_{i,j\in\Gamma_N} (j - i), \end{cases} \tag{44}$$

where i and j are the row and column indices of the N boxes of the irrep Γ_N and λ_i is the number of boxes in the ith row.

Starting from a given irrep of S_{N-1}, represented by the Young diagram Γ_{N-1}, and adding one box we obtain Young diagrams Γ_N corresponding to distinct eigenvalues of the transposition class sum; cf. Eq. (44). In fact, the eigenvalues corresponding to the Young diagrams Γ_{N-1} and Γ_N differ by the "content" of the box which was added to Γ_{N-1} in order to form Γ_N; the "content" being the difference $j - i$ between the column index j and the row index i of that box.

The actual symmetry adaptation will take place by diagonalizing $[(2)]_N$ within a finite invariant subspace with respect to S_N, which consists of functions that belong to a given Yamanouchi symbol Y_{N-1} and that are coupled into some total angular momentum L_N and some total hyperspherical angular momentum K_N.

The calculation of the matrix elements of the operator $[(2)]_N$ within this set of states reduces to the calculation of the matrix elements of the transposition $(N-1, N)$.

This results from the recurrence relation

$$[(2)]_N = [(2)]_{N-1} + \sum_{i=1}^{N-1}(i,N), \tag{45}$$

since the basis functions are eigenfunctions of $[(2)]_{N-1}$, and the matrix element of the sum $\sum_{i=1}^{N-1}(i,N)$ can be expressed in terms of the matrix elements of $(N-1,N)$ using the relation obtained in Ref. [16],

$$\langle \Gamma_{N-1}|\sum_{i=1}^{N-1}(i,N)|\Gamma'_{N-1}\rangle = \delta_{\Gamma_{N-1},\Gamma'_{N-1}}\frac{N-1}{n_{\Gamma_{N-1}}}\sum_{Y_{N-2}\in\Gamma_N}\langle Y_{N-2}\Gamma_{N-1}|(N-1,N)|Y_{N-2}\Gamma_{N-1}\rangle. \tag{46}$$

The sum on the right-hand side of Eq. (46) ranges over all the Yamanouchi symbols Y_{N-2} which can give rise to Γ_{N-1} by adding a single box. $n_{\Gamma_{N-1}}$ is the dimension of the irrep Γ_{N-1}.

VII. PERMUTATIONAL SYMMETRY ADAPTED HYPERSPHERICAL BASIS FOR THREE PARTICLES

In Sec. IV we mentioned that the spherical harmonic functions $Y_{\ell_2,m_2}(\Omega_2)$ describe the angular part of the internal state for two particles. The angles $\Omega_2 = (\theta_2,\phi_2)$ correspond to the coordinate $\boldsymbol{\rho}_2 = \frac{1}{\sqrt{2}}(\mathbf{r}_2-\mathbf{r}_1)$, that changes sign when the transposition $(1,2)$ is applied. Therefore, when we apply the transposition $(1,2)$ to the function $Y_{\ell_2,m_2}(\Omega_2)$ it is multiplied by the phase $(-1)^{\ell_2}$. (Note that for two particles $\ell_2 = L_2 = K_2$.) Consequently, all the functions with even (odd) values of ℓ_2 belong to the symmetric (antisymmetric) irrep **[2]** (**[11]**). The two-particle states will be written as

$$|\ell_2 m_2 \Gamma_2\rangle \equiv |L_2 M_2 Y_2\rangle, \tag{47}$$

where Γ_2 is either **[2]** or **[11]** and the distinction between Γ_2 and Y_2 is formal.

The construction of three-particle hyperspherical functions that possess a well-defined permutational symmetry was alluded to in Sec. IV. Starting from two-particle functions that belong to a given Yamanouchi symbol Y_2 we couple the third particle, described by the function $Y_{\ell_3,m_3}(\Omega_3)$, and obtain states with total angular momentum L_3 as in Eq. (22). We then use the Jacobi polynomial and obtain three-particle states with good quantum numbers K_3 [see Eq. (23)]. In this way we construct three-particle states with the good quantum numbers K_3, L_3, M_3, and Y_2,

$$|(L_2;\ell_3)K_3L_3M_3Y_2\rangle\,. \tag{48}$$

While these states do not belong to an irrep of the symmetric group S_3, it follows from the fact that $\hat{K}_3^2$, $\hat{L}_3^2$, $\hat{L}_{3_z}$ and the class sums of the symmetric group algebra all commute, that the complete set of states with given eigenvalues K_3, L_3, M_3, and Y_2 form an invariant subspace with respect to S_3. It follows from Eq. (24) that this subspace is finite dimensional.

In order to construct three-particle states with well defined permutational symmetry we have to diagonalize the matrix of the transposition class sum $[(2)]_3 = (1,2)+(1,3)+(2,3)$ [see Eq. (43)] within that invariant subspace. All the states of interest are eigenstates of $[(2)]_2 = (1,2)$ with a common eigenvalue, 1 or -1 for the irreps **[2]** or **[11]**, respectively [Eq. (44)]. Therefore, the matrix element of the transposition $(1,2)$ is diagonal in our basis states and its expression is

$$\langle (L_2;\ell_3)K_3L_3M_3Y_2|(1,2)|(L_2';\ell_3')K_3L_3M_3Y_2\rangle = (-1)^{L_2}\delta_{L_2,L_2'}\delta_{\ell_3,\ell_3'}. \tag{49}$$

According to Eq. (46) only the matrix element of the transposition $(2,3)$ between the states (48) has to be calculated. This transposition acts on the Jacobi coordinates $\boldsymbol{\rho}_2$ and $\boldsymbol{\rho}_3$ [Eq. (1)] in the following manner [15]:

$$(2,3)\begin{pmatrix}\boldsymbol{\rho}_2\\ \boldsymbol{\rho}_3\end{pmatrix} = \begin{pmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ \frac{\sqrt{3}}{2} & \frac{1}{2}\end{pmatrix}\begin{pmatrix}\boldsymbol{\rho}_2\\ -\boldsymbol{\rho}_3\end{pmatrix}. \tag{50}$$

This operation is actually a rotation by the angle $\frac{\pi}{3}$ in addition to a reflection of the coordinate $\boldsymbol{\rho}_3$. The rotation of the coordinates for hyperspherical functions is achieved by using the Raynal-Revai coefficients (41) whereas the reflection of the coordinate $\boldsymbol{\rho}_3$ yields the phase $(-1)^{\ell_3'}$. Therefore, the matrix element of the transposition $(2,3)$ in the basis states (48) is

$$\Big\langle (L_2;\ell_3)K_3L_3M_3Y_2|(2,3)|(L_2';\ell_3')K_3L_3M_3Y_2\Big\rangle = (-1)^{\ell_3'}\left\langle \ell_2\ell_3\left|\frac{\pi}{3}\right|\ell_2'\ell_3'\right\rangle_{K_3L_3}. \tag{51}$$

The eigenvalues of the matrix that represents the class sum $[(2)]_3$ within the invariant subspace defined above assume the values 3, 0, and -3, corresponding to the S_3 irreps **[3]**, **[21]**, and **[111]**, respectively [see Eq. (44)]. Actually, if we start from the S_2 irrep **[2]**, adding one box will only provide the irreps **[3]** and **[21]**; starting from **[11]** we can only get the irreps **[21]** and **[111]**. Since the eigenvalues corresponding to different irreps are distinct, they identify the S_3 irreps uniquely. The eigenvectors are the hscfps, which are the coefficients in the linear combination of the states (48) that yield three-particle states belonging to an irrep of S_3,

$$|K_3L_3M_3Y_2\Gamma_3\beta_3\rangle = \sum_{L_2,\ell_3}[(L_2;\ell_3)K_3L_3Y_2|\}K_3L_3Y_3\beta_3] \times|(L_2;\ell_3)K_3L_3M_3Y_2\rangle. \tag{52}$$

The range of the summation indices is restricted by the requirements that L_2 has a well defined parity and that $L_2 + \ell_3 \leq K_3$. In fact, from Eq. (24) it follows that the parity of ℓ_3 is also well defined by the requirement that $L_2 + \ell_3$ and K_3 should have the same parity. Another restriction results from the coupling of the angular momenta ℓ_2 and ℓ_3 to L_3, i.e., $|\ell_2 - \ell_3| \leq L_3 \leq \ell_2 + \ell_3$. The label β_3 in Eq. (52) is needed for unique identification of the symmetrized three-particle hyperspherical states since the quantum numbers K_3, L_3, M_3, and Y_3 do not completely label these states.

VIII. PERMUTATIONAL SYMMETRY ADAPTED HYPERSPHERICAL BASIS FOR N PARTICLES

We now present the general recursive procedure for constructing N-particle hyperspherical functions, that possess a well-defined permutational symmetry. Suppose that a complete set of $(N-1)$-particle states have been obtained, each of which is characterized by a Yamanouchi symbol Y_{N-1}, specifying its permutational symmetry, as well as by the quantum numbers K_{N-1}, L_{N-1}, M_{N-1}. (We also need an additional label β_{N-1} in order to distinguish between states with common values of the quantum numbers mentioned above.)

Let us consider all the $(N-1)$-particle states with the same Yamanouchi symbol Y_{N-1}, i.e., $(N-1)$-particle states which are labeled by the sequence of Young diagrams $\Gamma_2, \Gamma_3, \ldots, \Gamma_{N-1}$ that correspond to the groups $S_2, S_3, \ldots, S_{N-1}$, respectively. As above, we add the Nth particle, which is described by the function $Y_{\ell_N, m_N}(\Omega_N)$, in two steps. First, using the O(3) Clebsch-Gordan coefficients we obtain states with total angular momentum L_N as in Eq. (32). In the second step we use the Jacobi polynomial and obtain N-particle states with good quantum numbers K_N [see Eq. (33)].

In this way we construct N-particle states with the good quantum numbers K_N, L_N, M_N, and Y_{N-1},

$$|(K_{N-1}L_{N-1}Y_{N-1}\beta_{N-1};\ell_N)K_N L_N M_N\rangle. \tag{53}$$

These states do not belong to an irrep of the symmetric group S_N, but they form an invariant subspace with respect to this group. By Eq. (34), this invariant subspace is finite dimensional. In order to obtain the linear combination of these states, that belongs to a well defined irrep Γ_N of S_N, we have to diagonalize the N-particle transposition class sum, $[(2)]_N$, Eq. (45).

Actually, according to Eq. (45), $[(2)]_N$ can be written as a sum of two terms. The first term, $[(2)]_{N-1}$, is diagonal in the basis states (53) because they belong to the same Young diagram Γ_{N-1}. The matrix element of this operator in the basis states (53) is

$$\langle(K_{N-1}L_{N-1}Y_{N-1}\beta_{N-1};\ell_N)K_N L_N M_N|[(2)]_{N-1}|(K'_{N-1}L'_{N-1}Y_{N-1}\beta'_{N-1};\ell'_N)K_N L_N M_N\rangle$$
$$= \delta_{K_{N-1},K'_{N-1}}\delta_{L_{N-1},L'_{N-1}}\delta_{\beta_{N-1},\beta'_{N-1}}\delta_{\ell_N,\ell'_N}\,[(2)]_{N-1}\Big|_{\Gamma_{N-1}}. \tag{54}$$

This equation is the generalization of Eq. (49) to N particles.

The second term in Eq. (45) requires the calculation of all the matrix elements of the transpositions (i, N), where $i = 1, 2, \ldots, N-1$. However, according to Eq. (46) it is sufficient to calculate the matrix element of the transposition $(N-1, N)$. This operator acts on the Jacobi coordinates $\boldsymbol{\rho}_{N-1}$ and $\boldsymbol{\rho}_N$ as follows [15]:

$$(N-1,N)\begin{pmatrix}\boldsymbol{\rho}_{N-1}\\ \boldsymbol{\rho}_N\end{pmatrix} = \begin{pmatrix}\frac{1}{N-1} & -\frac{\sqrt{N^2-2N}}{N-1}\\ \frac{\sqrt{N^2-2N}}{N-1} & \frac{1}{N-1}\end{pmatrix}\begin{pmatrix}\boldsymbol{\rho}_{N-1}\\ -\boldsymbol{\rho}_N\end{pmatrix}. \tag{55}$$

This transformation is equivalent to a rotation by an angle $\arccos\left(\frac{1}{N-1}\right)$, preceded by a reflection of the coordinate $\boldsymbol{\rho}_N$, which yields the phase factor $(-1)^{\ell'_N}$.

In order to calculate the matrix element of the transposition $(N-1, N)$ in the basis states (53) it is necessary to separate the last two particles, i.e., the $(N-1)$th and the Nth particle, from the first $N-2$ particles. This is carried out in the following steps (steps 2–4 have already been discussed in Ref. [15]):

(1) We use the $(N-1)$-particle hscfps in order to write the $(N-1)$-particle permutational symmetry adapted function as a linear combination of functions, each of which is an eigenfunction of $\hat{K}^2_{N-2}$, $\hat{L}^2_{N-2}$, and $\hat{\ell}^2_{N-1}$ in addition to being an eigenfunction of $\hat{K}^2_{N-1}$, $\hat{L}^2_{N-1}$, $\hat{\ell}^2_N$, and being coupled with the Nth particle function into an N-particle function which is an eigenfunction of $\hat{K}^2_N$ and $\hat{L}^2_N$.

(2) Using the $6j$ symbol we recouple the angular momenta, starting from the scheme in which L_{N-2} is coupled with ℓ_{N-1} to L_{N-1}, that is then coupled with ℓ_N to L_N, into the scheme in which ℓ_{N-1} and ℓ_N are coupled to $L_{N-1,N}$, that is then coupled with L_{N-2} to L_N.

(3) The initial hyperspherical angular-momentum scheme, in which we have K_{N-2}, K_{N-1}, and K_N as good quantum numbers is recoupled into the scheme in which the good quantum numbers are K_{N-2}, $K_{N-1,N}$, and K_N. The transformation of the "tree" structure is effected by

using the T coefficients (42) as presented schematically in Fig. 3.

(4) Using the Raynal-Revai coefficients we apply the rotation (55) on the coordinates $\boldsymbol{\rho}_{N-1}$ and $\boldsymbol{\rho}_N$ and multiply the resulting expression by the phase factor $(-1)^{\ell'_N}$. Using the orthogonality of the N-particle states (38) we finally obtain the matrix element of the transposition $(N-1,N)$ in the form

$$
\begin{aligned}
&\langle (K_{N-1}L_{N-1}Y_{N-1}\beta_{N-1};\ell_N)K_NL_NM_N|(N-1,N)|(K'_{N-1}L'_{N-1}Y_{N-1}\beta'_{N-1};\ell'_N)K_NL_NM_N\rangle \\
&\quad = (-1)^{\ell'_N}\left(2L_{N-1}+1)(2L'_{N-1}+1)\right)^{\frac{1}{2}} \\
&\quad\times \sum_{K_{N-2},L_{N-2},\beta_{N-2}} \sum_{\ell_{N-1},\ell'_{N-1}} [(K_{N-2}L_{N-2}Y_{N-2}\beta_{N-2};\ell_{N-1})K_{N-1}L_{N-1}|\}K_{N-1}L_{N-1}Y_{N-1}\beta_{N-1}] \\
&\quad\times [(K_{N-2}L_{N-2}Y_{N-2}\beta_{N-2};\ell'_{N-1})K'_{N-1}L'_{N-1}|\}K'_{N-1}L'_{N-1}Y_{N-1}\beta'_{N-1}] \\
&\quad\times \sum_{L_{N-1,N}} (2L_{N-1,N}+1)\begin{Bmatrix} \ell_N & \ell_{N-1} & L_{N-1,N} \\ L_{N-2} & L_N & L_{N-1}\end{Bmatrix}\begin{Bmatrix} \ell'_N & \ell'_{N-1} & L_{N-1,N} \\ L_{N-2} & L_N & L'_{N-1}\end{Bmatrix} \\
&\quad\times \sum_{K_{N-1,N}} \langle K_{N-1,N}|K_N;\ell_N,\ell_{N-1},K_{N-2}|K_{N-1}\rangle\langle K_{N-1,N}|K_N;\ell'_N,\ell'_{N-1},K_{N-2}|K'_{N-1}\rangle \\
&\quad\times \langle \ell_{N-1}\ell_N|\arccos\left(\frac{1}{N-1}\right)|\ell'_{N-1}\ell'_N\rangle_{K_{N-1,N}L_{N-1,N}}\ .
\end{aligned}
\tag{56}
$$

The T coefficients and the Raynal-Revai coefficients used in this equation were presented in Sec. V. The summation is carried out over all the hyperspherical functions which belong to the irrep Γ_{N-2} and which constitute the symmetrized hyperspherical functions for $N-1$ particles, for the "bra" and the "ket" states of Eq. (56). The summation over the quantum number $L_{N-1,N}$ is subject to the following three restrictions:

$$
\begin{aligned}
&|\ell_N-\ell_{N-1}| \le L_{N-1,N} \le \ell_N+\ell_{N-1}, \\
&|\ell'_N-\ell'_{N-1}| \le L_{N-1,N} \le \ell'_N+\ell'_{N-1}, \\
&|L_N-L_{N-2}| \le L_{N-1,N} \le L_N+L_{N-2}.
\end{aligned}
\tag{57}
$$

Similarly, the sum over $K_{N-1,N}$ is subject to the three restrictions that result from the properties of the Jacobi polynomials [see the explanation to Eqs. (39) and (40)], which can be written as a single condition,

$$
\max\{(\ell_N+\ell_{N-1}),(\ell'_N+\ell'_{N-1})\} \le K_{N-1,N} \le (K_N-K_{N-2}). \tag{58}
$$

In addition, the parity of $K_{N-1,N}$, $\ell_N+\ell_{N-1}$, $\ell'_N+\ell'_{N-1}$, and K_N-K_{N-2} should be the same. (This is an additional condition on the values of ℓ_{N-1} and ℓ'_{N-1}).

Inspection of the expressions for the matrix elements in Eqs. (54) and (56) suggests that for N particles the hscfps depend on the given Young diagrams Γ_N and Γ_{N-1} but not on the complete sequence of diagrams $\Gamma_2, \Gamma_3, \ldots, \Gamma_{N-2}$. Therefore, the Yamanouchi symbols Y_{N-2} and Y_{N-1} in the hscfps in Eq. (56) can be replaced by the Young diagrams Γ_{N-2} and Γ_{N-1}, respectively. Moreover, the sum over Y_{N-2} in Eq. (46) is drastically simplified by replacing it by a sum over the Young diagrams Γ_{N-2} obtained from the given Young diagram Γ_{N-1} by deleting a box, and multiplying each term by $n_{\Gamma_{N-2}}$—the degeneracy of the irrep Γ_{N-2} in S_{N-2}.

By using Eqs. (46), (54), and (56) we obtain the matrix representing the transposition class sum (45) in the basis set specified in Eq. (53). Its eigenvalues (44) uniquely specify the Young diagrams Γ_N that can be obtained from the Young diagram Γ_{N-1} by adding one box. The eigenvectors are the hscfps; they are the coefficients in the linear combinations of N-particle hyperspherical functions (53) that belong to well-defined irreps of S_N,

$$
\begin{aligned}
|K_NL_NM_NY_N\beta_N\rangle = &\sum_{K_{N-1},L_{N-1},\beta_{N-1},\ell_N} [(K_{N-1}L_{N-1}\Gamma_{N-1}\beta_{N-1};\ell_N)K_NL_N|\}K_NL_N\Gamma_N\beta_N] \\
&\times |(K_{N-1}L_{N-1}Y_{N-1}\beta_{N-1};\ell_N)K_NL_NM_N\rangle.
\end{aligned}
\tag{59}
$$

The summation in Eq. (59) is carried out subject to the condition that all the $(N-1)$-particle states belong to the irrep Γ_{N-1}. Since μ_N in Eq. (34) is a non-negative integer we obtain that $K_{N-1}+\ell_N \le K_N$ where K_N and $K_{N-1}+\ell_N$ have the same parity. Furthermore, $|L_N-\ell_N| \le L_{N-1} \le L_N-\ell_N$.

Since the hscfps are the orthogonal eigenvectors of a real symmetric matrix they satisfy the orthogonality relation

$$\sum_{K_{N-1},L_{N-1},\beta_{N-1},\ell_N} [(K_{N-1}L_{N-1}\Gamma_{N-1}\beta_{N-1};\ell_N)K_NL_N|\}K_NL_N\Gamma_N\beta_N]$$

$$\times[(K_{N-1}L_{N-1}\Gamma_{N-1}\beta_{N-1};\ell_N)K_NL_N|\}K_NL_N\Gamma'_N\beta'_N] = \delta_{\Gamma_N,\Gamma'_N}\delta_{\beta_N,\beta'_N}, \quad (60)$$

as well as the completeness relation

$$\sum_{\Gamma_N,\beta_N} [(K_{N-1}L_{N-1}\Gamma_{N-1}\beta_{N-1};\ell_N)K_NL_N|\}K_NL_N\Gamma_N\beta_N] \times [(K'_{N-1}L'_{N-1}\Gamma_{N-1}\beta'_{N-1};\ell'_N)K_NL_N|\}K_NL_N\Gamma_N\beta_N]$$

$$= \delta_{K_{N-1},K'_{N-1}}\delta_{L_{N-1},L'_{N-1}}\delta_{\beta_{N-1},\beta'_{N-1}}\delta_{\ell_N,\ell'_N}. \quad (61)$$

When states with a given Young diagram Γ_N can be obtained from more than one Young diagram Γ_{N-1}, our procedure leaves the relative phases of these states undetermined. However, the derivation of Eq. (46), based on the group theoretical orthogonality theorem, requires the following relation between states belonging to a particular irrep Γ_N, that originate from two different $(N-1)$-particle Young diagrams Γ_{N-1} and Γ'_{N-1} [17],

$$\langle K_NL_NM_NY_{N-2}\Gamma'_{N-1}\Gamma'_N\beta'_N|(N-1,N)|K_NL_NM_NY_{N-2}\Gamma_{N-1}\Gamma_N\beta_N\rangle = \frac{\sqrt{\sigma^2-1}}{|\sigma|}\delta_{\Gamma_N,\Gamma'_N}\delta_{\beta_N,\beta'_N}, \quad (62)$$

where σ is the difference between the "contents" (cf. Sec. VI) of the boxes in which the particles N and $N-1$ are placed in the Yamanouchi symbol $Y_N \equiv Y_{N-2}\Gamma_{N-1}\Gamma_N$. We note that the range of values of β_N for the given set of quantum numbers K_N, L_N, M_N depends *only* on Γ_N, and is common to all the states belonging to the different values of Y_{N-1} which are consistent with a given Γ_N.

By using the hscfps we can separate the N-particle states in both the bra and the ket of the matrix element (62). Then, by multiplying with the hscfp

$$[(K''_{N-1}L''_{N-1}\Gamma'_{N-1}\beta''_{N-1};\ell''_N)K_NL_N|\}K_NL_N\Gamma'_N\beta'_N]$$

on both sides of Eq. (62), summing over Γ'_N and β'_N and using the completeness relation (61), it follows that we can express *every* hscfp originating from $\Gamma'_{N-1} \in \Gamma_N$ as a sum over *all* the hscfps originating from $\Gamma_{N-1} \in \Gamma_N$ multiplied by appropriate matrix elements of the transposition $(N-1,N)$:

$$[(K'_{N-1}L'_{N-1}\Gamma'_{N-1}\beta'_{N-1};\ell'_N)K_NL_N|\}K_NL_N\Gamma_N\beta_N]$$

$$= \frac{|\sigma|}{\sqrt{\sigma^2-1}} \sum_{K_{N-1},L_{N-1},\beta_{N-1},\ell_N} [(K_{N-1}L_{N-1}\Gamma_{N-1}\beta_{N-1};\ell_N)K_NL_N|\}K_NL_N\Gamma_N\beta_N]$$

$$\times\langle(K'_{N-1}L'_{N-1}\Gamma'_{N-1}\beta'_{N-1};\ell'_N)K_NL_N|(N-1,N)|(K_{N-1}L_{N-1}\Gamma_{N-1}\beta_{N-1};\ell_N)K_NL_N\rangle. \quad (63)$$

There is only one difference between the matrix element of the transposition $(N-1,N)$ in Eq. (56) and that in Eq. (63). In the latter the two $(N-1)$-particle Young diagrams are different whereas in Eq. (56) they are the same. The expression for the matrix element in Eq. (63) is obtained by replacing Γ_{N-1} by Γ'_{N-1} in the appropriate places in Eq. (56).

In conclusion, whenever the Young diagram Γ_N originates from more than one $(N-1)$-particle Young diagram we keep after the diagonalization of $[(2)]_N$ only the set of hscfps that originate from one particular Γ_{N-1}. For definiteness we choose Γ_{N-1} to be the diagram obtained from Γ_n by deleting a box from the top row, i.e., with highest possible "content." The hscfps which originate from the other $(N-1)$-particle Young diagrams are constructed with consistent phases, using Eq. (63).

IX. THE COMPUTATIONAL ALGORITHM

In the preceding sections we described the method of diagonalizing the transposition class sum in the basis states (53) in order to obtain nonspurious symmetry-adapted N-particle hyperspherical functions. In this method we calculate the matrix element of the transposition $(N-1,N)$, Eq. (56), by using the hscfps for $N-1$ particles, that are assumed to have been calculated before.

To carry out the recursive algorithm systematically we choose some maximum value $K_{\max}$ for the hyperspherical angular momentum. The value of $K_{\max}$ chosen determines the size and quality of the hyperspherical set of functions constructed. Starting from two particles, we construct all the states (47) with a hyperspherical angular momentum not exceeding $K_{\max}$. In this case the allowed values of ℓ_2 are $0, 1, 2, \ldots, K_{\max}$. As we explained in Sec. V, the two-particle states with even ℓ_2 belong to the symmetric irrep **[2]** and the others to the antisymmetric irrep **[11]**. Consequently, only values of ℓ_2 $(= K_2 = L_2)$ with a parity that is consistent with the desired Y_2 have to be considered.

The three-particle states (48) are constructed from two-particle states that belong to a common permutational symmetry species. We add the third particle, which is described by the quantum number ℓ_3, and obtain three-particle states labeled by the quantum numbers K_3 and L_3 (see Sec. VII). The set of states with common K_3 and L_3 form an invariant subspace with respect to S_3, which is reduced by diagonalizing the transposition class sum to obtain three-particle states with good permutational symmetry, along with the corresponding hscfps.

From the relation $K_3 = 2\mu_3 + K_2 + \ell_3$ [Eq. (24)] where $\mu_3 = 0, 1, 2, \ldots, \lfloor \frac{K_3}{2} \rfloor$ we conclude that the parity of K_3 should be the same as that of $K_2 + \ell_3 = \ell_2 + \ell_3$ and that $K_2 \leq K_2 + \ell_3 \leq K_3$. In addition, we have $|\ell_2 - \ell_3| \leq L_3 \leq \ell_2 + \ell_3$ and therefore $L_3 \leq K_3$. Since the parities of K_3 and $\ell_2 + \ell_3$ are the same, the minimum value of $|\ell_2 - \ell_3|$, which is also the minimum value of L_3, is zero for even K_3 and 1 for odd K_3. Another consequence is that the possible values of ℓ_3 for given values for K_3, L_3, and ℓ_2 are $|L_3 - \ell_2| \leq \ell_3 \leq \min\{L_3 + \ell_2, K_3 - \ell_2\}$ where the parity of ℓ_3 is the same as that of $K_3 - \ell_2$, i.e., we have to consider either even or odd values of ℓ_3, but not both at the same time.

Based on the above discussion we obtain the following algorithm for constructing the three-particle hyperspherical functions (48), starting from the irrep Γ_2 (either **[2]** or **[11]**) of S_2:

(1) Consider *all* the possible values for K_3 within the range $\min\{K_2 = \ell_2\} \leq K_3 \leq K_{\max}$.

(2) For every given value of K_3 consider *all* the possible values for L_3 within the range (0 *or* 1) $\leq L_3 \leq K_3$.

(3) For any given selection of K_3 and L_3 consider *all* the values of ℓ_2 with the parity corresponding to Γ_2.

(4) Construct the states (48) by taking into account *all* the possible values of ℓ_3 as explained above.

(5) Having constructed the basis states (48) for given values of K_3 and L_3 diagonalize it as explained in Sec. VII and obtain the appropriate hscfps.

The rules for the possible values of K_3, L_3, ℓ_2, and ℓ_3 straightforwardly generalize to an arbitrary number of particles. From Eq. (34) it turns out that the minimum value of K_N is the same as the minimum value of K_{N-1} in the appropriate Γ_{N-1} irrep whereas the maximum value is the arbitrarily chosen $K_{\max}$. The values of L_N start from zero and cannot exceed the given value for K_N. This statement can be proved by induction: We have shown that $L_3 \leq K_3$. Assume that $L_{N-1} \leq K_{N-1}$. Then, for N particles we obtain from Eq. (34) and from angular-momentum coupling that $L_N \leq L_{N-1} + \ell_N \leq K_{N-1} + \ell_N \leq K_N$.

For every given K_N and L_N we should construct the complete set of states (53). We have to consider all the states, labeled by the quantum numbers K_{N-1}, L_{N-1}, and β_{N-1}, that belong to the Yamanouchi symbol Y_{N-1}. We add the Nth particle, with angular momentum ℓ_N, where $|L_N - L_{N-1}| \leq \ell_N \leq \min(L_N + L_{N-1}, K_N - K_{N-1})$. In addition, from relation (34) we conclude that for given values of K_N and K_{N-1} ℓ_N should have the same parity as $K_N - K_{N-1}$. Finally, we diagonalize with respect to $[(2)]_N$.

X. CONCLUSIONS

A systematic method for constructing hyperspherical functions that belong to well defined irreps of the symmetric group has been developed. We introduced the hyperspherical coefficients of fractional parentage (hscfps) which are the expansion coefficients of an N-particle hyperspherical function that belongs to the irrep Γ_N of S_N in terms of angular-momentum and hyperspherical angular-momentum coupled products of $(N-1)$-particle hyperspherical functions that belong to the irrep Γ_{N-1} of S_{N-1} with the hyperspherical functions for the Nth particle. This leads to a recursive calculation of the hscfps, each step involving a diagonalization of the transposition class sum of the symmetric group of appropriate order. It was noted that it is sufficient to calculate the matrix elements of the transposition of the last two particles in every step. These matrix elements are obtained by using the hscfps calculated in the preceding step as well as the Raynal-Revai and the T coefficients.

The permutational symmetry adapted hyperspherical functions are required for calculations in the L-S coupling scheme. The factorization method introduced by Jahn [18] facilitates the separation of the calculations for the orbital space and for the spin space. Since for spin σ particles the total spin function should belong to an irrep of the symmetric group labeled by a Young diagram with at most $2\sigma + 1$ rows, the hyperspherical functions should belong to an irrep of the symmetric group with a Young diagram that consists of at most $2\sigma + 1$ columns. Usually, $\sigma = \frac{1}{2}$.

The recursive procedure presented in this article is perfectly suitable for implementation on a computer. We expect that the computer code which we plan to develop for the calculation of the hscfps, based on this algorithm, will widely broaden the scope of feasible few-body calculations based on using the hyperspherical functions.

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