Harmonic hyperspherical basis for identical particles without permutational symmetry

M. Gattobigio,[1] A. Kievsky,[2] M. Viviani,[2] and P. Barletta[3]
[1]*INLN, Université de Nice-Sophia Antipolis, CNRS, 1361 route des Lucioles, 06560 Valbonne, France*
[2]*Istituto Nazionale di Fisica Nucleare, Largo Pontecorvo 3, 56100 Pisa, Italy*
[3]*Department of Physics and Astronomy, University College London, Gower Street, London WC1E_6BT, United Kingdom*
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The hyperspherical harmonic basis is used to describe bound states in an A-body system. The approach presented here is based on the representation of the potential energy in terms of hyperspherical harmonic functions. Using this representation, the matrix elements between the basis elements are simple, and the potential energy is presented in a compact form well suited for numerical implementation. The basis is neither symmetrized nor antisymmetrized, as required in the case of identical particles; however, after the diagonalization of the Hamiltonian matrix, the eigenvectors reflect the symmetries present in it and the identification of the physical states is possible, as it will be shown in specific cases. We have in mind applications to atomic, molecular, and nuclear few-body systems in which symmetry-breaking terms are present in the Hamiltonian; their inclusion is straightforward in the present method. As an example, we solve the case of three and four particles interacting through a short-range central interaction and Coulomb potential.

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I. INTRODUCTION

The harmonic hyperspherical (HH) method provides a systematic way to construct an expansion basis for a system of A particles. The N Jacobi vectors ($N=A-1$) are transformed to the hyper-radius ρ plus $3N-1$ hyperangular coordinates which are used to define the HH functions. These functions are the eigenfunctions of the hyperangular part of the Laplacian operator for a given number of particles (see Ref. [1] and references therein).

Applications of the HH method to describe bound states of $A=3,4$ nuclei are well documented in the literature (for a recent review, see Ref. [2]). In these applications, the HH basis elements extended to spin and isospin degrees of freedom have been combined in order to construct antisymmetric basis functions. In fact, the HH functions, as normally defined, do not have well-defined properties under particle permutation; this results from the selection of a particular ordering of the particles in the definition of the Jacobi coordinates and—as a consequence—of the hyperangular coordinates used to define the HH functions. Changing the ordering of the particles, it is possible to define a different set of Jacobi coordinates and, accordingly, HH functions depending on the hyperangular variables obtained from this different set. To be noticed, the HH functions defined using a particular choice of the Jacobi coordinates form a complete basis.

The HH functions defined in one set of Jacobi coordinates can be transformed to HH functions defined in another set. In this transformation (permutation) the grand angular quantum number K, which identifies a subset of HH functions, is conserved. For finite values of K, the dimension N_K of this subset is finite, and therefore a finite number of HH functions, having all the same value of K, is necessary to describe a HH function having the same value of K but defined in a different Jacobi set. The coefficients of the transformation can be collected in a matrix having the dimension N_K for each number of particles. For $A=3$ these matrix elements are the Raynal-Revai [3] coefficients. For $A>3$ the coefficients cannot be given in a close form, and a few methods have been devised for their calculations [4–7]. The knowledge of these coefficients allows for the construction of basis elements with well-defined permutational symmetry. In fact, each subset defined by K is invariant under particle permutation; as a consequence, the construction of basis elements with that property is performed as linear combinations of HH functions having the same value of K. Different schemes to construct hyperspherical functions with an arbitrary permutational symmetry are given in Refs. [6,8–11]. Recently, a procedure for constructing HH functions in terms of a single-particle basis has been proposed in Ref. [12].

In problems in which the A-body system is composed by identical particles, the wave function of the system has to be completely symmetric or antisymmetric in the case of bosons or fermions, respectively. Considering a Hilbert space extended to spin and isospin degrees of freedom, the construction of HH functions having well-defined permutational properties allows for a reduction in the large degeneracy of the basis. In general the completely symmetric or antisymmetric basis functions are a small part of the total Hilbert space. However, the difficulties of constructing HH functions with well-defined permutational symmetries increase with A and K; therefore, the preliminary step of constructing basis functions with well-defined permutational symmetry for A particles could be sometimes very difficult to carry out.

In the present paper, we investigate a different strategy. We intend to perform the description of a A-body system using the HH basis defined on one set of Jacobi coordinates, the reference set, and not having a well-defined behavior under particle permutation. We will loose the advantage of using a reduced part of the total Hilbert space; however, we will gain in simplicity in the calculation of the matrix elements. By including all HH basis elements up to a certain grand angular momentum K, the diagonalization of the Hamiltonian matrix will produce eigenvectors reflecting its symmetries. If the Hamiltonian commutes with the group of permutations of A objects S_A, in the case of nondegenerated eigenvalues, the eigenvectors will have a well-defined per-

mutation symmetry and can be organized in accordance with the irreducible representations of S_A. Therefore, identifying those eigenvectors with the desired symmetry, the corresponding energies can be considered variational estimates. In particular, it will be possible to identify a subset of eigenvectors and eigenvalues corresponding exactly to those that would be obtained performing the preliminary symmetrization of the states. The disadvantage of this method results in the large dimension of the matrices to be diagonalized. However, at present, different techniques are available to treat (at least partially) this problem.

For a system interacting through a two-body potential $V(i,j)$, the potential-energy operator results in a sum over pairs. Its matrix elements can be reduced to one term, let us say $V(1,2)$, times the number of pairs when symmetric or antisymmetric state functions are considered. When HH functions without well-defined permutation behavior are used, the calculation of the potential-energy operator cannot be reduced to the computation of one term. So we have to face the problem of computing the matrix elements of a general term $V(i,j)$ between HH functions defined in the reference set of Jacobi coordinates in which the distance r_{ij} between particles (i,j) has not a simple form.

The calculation of $V(i,j)$ in the reference set of Jacobi coordinates is performed in two steps. (i) First, we use a property of the HH basis which allows to expand a general function of the coordinates (i,j) in terms of a subset of the basis called the potential basis (PB) [1]; (ii) then, as for the case of a generic HH basis element, each PB element is transformed to the HH basis defined in the reference set of Jacobi coordinates. In the case of the PB, the transformation coefficients are known analytically for each value of K and for a general number of particles A. In this way, each term $V(i,j)$ of the potential energy can be first expanded in the PB and then transformed to HH functions defined in the reference set. So, after this procedure, the potential energy will be expressed in terms of HH functions. As we will see, the computation of the matrix elements of the potential energy is now very simple since it results in a combination of integrals of three HH functions. A compact form suitable for a numeric treatment of the problem will be given.

The derivation and implementation of the final expression for the potential energy in the calculation of bound states are the main subjects of the present paper. As a simple application, a system of three and four nucleons interacting through a central potential will be analyzed. Different symmetries will appear considering or not the Coulomb interaction between two protons. To be noticed when antisymmetrized basis functions are used to describe three or four nucleons, the presence of the Coulomb interaction implies that states with total isospin $T=1/2,3/2$ (for $A=3$), and $T=0,1,2$ (for $A=4$) have to be considered. The extension of the Hilbert space to include these terms increases the dimension of the problem resulting comparable to that one in which the antisymmetrization of the basis is not performed. Finally, we would like to stress that the present paper is a step in a program devoted to applications of the HH basis to systems with $A>4$ interacting through realistic potentials.

The paper is organized as follows. Section II is devoted to a brief description of the HH basis. In Sec. III the expression for the potential energy in terms of HH states is given. In Sec. IV the results for the examples proposed are shown. Section V includes a brief discussion of the results and the perspectives of the present work.

II. HARMONIC HYPERSPHERICAL BASIS

In this section we present a brief overview of the properties of the HH basis following Ref. [1]. We start with the following definition of the Jacobi coordinates for an A-body system:

$$\mathbf{x}_{N-j+1} = \sqrt{\frac{2m_{j+1}M_j}{(m_{j+1}+M_j)m}}(\mathbf{r}_{j+1}-\mathbf{X}_j), \quad j=1,\ldots,N, \quad (1)$$

where m is a reference mass, $N=A-1$, and we have defined

$$M_j = \sum_{i=1}^{j} m_i, \quad \mathbf{X}_j = \frac{1}{M_j}\sum_{i=1}^{j} m_i \mathbf{r}_i. \quad (2)$$

Let us note that if all the masses are equal $m_i=m$, Eq. (1) simplifies to

$$\mathbf{x}_{N-j+1} = \sqrt{\frac{2j}{j+1}}(\mathbf{r}_{j+1}-\mathbf{X}_j), \quad j=1,\ldots,N. \quad (3)$$

For a given set of Jacobi coordinates $\mathbf{x}_1,\ldots,\mathbf{x}_N$, the hyperradius ρ is defined as

$$\rho = \left(\sum_{i=1}^{N} x_i^2\right)^{1/2} = \left[2\sum_{i=1}^{A}(\mathbf{r}_i-\mathbf{X})^2\right]^{1/2} = \left[\frac{2}{A}\sum_{j>i}^{A}(\mathbf{r}_j-\mathbf{r}_i)^2\right]^{1/2}, \quad (4)$$

and the hyperangular coordinates Ω_N

$$\Omega_N = (\hat{x}_1,\ldots,\hat{x}_N,\phi_2,\ldots,\phi_N), \quad (5)$$

with the hyperangles ϕ_i defined via

$$\cos\phi_i = \frac{x_i}{\sqrt{x_1^2+\ldots+x_i^2}}, \quad i=2,\ldots,N. \quad (6)$$

The radial components of the Jacobi coordinates can be expressed in terms of the hyperspherical coordinates

$$\begin{aligned} x_N &= \rho\cos\phi_N \\ x_{N-1} &= \rho\sin\phi_N\cos\phi_{N-1} \\ &\vdots \\ x_i &= \rho\sin\phi_N\cdots\sin\phi_{i+1}\cos\phi_i \\ &\vdots \\ x_1 &= \rho\sin\phi_N\cdots\sin\phi_3\sin\phi_2. \end{aligned} \quad (7)$$

Using the above hyperspherical angles Ω_N, the surface element becomes

$$d\Omega_N = \sin\,\theta_1 d\theta_1 d\varphi_1 \prod_{j=2}^{N} \sin\,\theta_j d\theta_j d\varphi_j (\cos\,\phi_j)^2 (\sin\,\phi_j)^{3j-4} d\phi_j, \tag{8}$$

and the Laplacian operator

$$\Delta = \sum_{i=1}^{N} \nabla_{\mathbf{x}_i}^2 = \left(\frac{\partial^2}{\partial \rho^2} + \frac{3N-1}{\rho} \frac{\partial}{\partial \rho} + \frac{\Lambda_N^2(\Omega_N)}{\rho^2} \right), \tag{9}$$

where the $\Lambda_N^2(\Omega_N)$ is the generalization of the angular momentum and is called the grand angular operator.

The HH functions $\mathcal{Y}_{[K]}(\Omega_N)$ are the eigenvectors of the grand angular-momentum operator

$$[\Lambda_N^2(\Omega_N) + K(K+3N-2)]\mathcal{Y}_{[K]}(\Omega_N) = 0. \tag{10}$$

They can be expressed in terms of the usual harmonic functions $Y_{\mathrm{lm}}(\hat{x})$ and of the Jacobi polynomials $P_n^{a,b}(z)$. In fact, the explicit expression for the HH functions is

$$\mathcal{Y}_{[K]}(\Omega_N) = \left[\prod_{j=1}^{N} Y_{l_j m_j}(\hat{x}_j) \right] \left[\prod_{j=2}^{N} {}^{(j)}\mathcal{P}_{K_j}^{l_j, K_{j-1}}(\phi_j) \right], \tag{11}$$

where $[K]$ stands for the set of quantum numbers $l_1, \ldots, l_N, m_1, \ldots, m_N, n_2, \ldots, n_N$, the hyperspherical polynomial is

$${}^{(j)}\mathcal{P}_{K_j}^{l_j, K_{j-1}}(\phi_j) = \mathcal{N}_{n_j}^{l_j, K_j} (\cos\,\phi_j)^{l_j} (\sin\,\phi_j)^{K_{j-1}} P_{n_j}^{\nu_{j-1}, l_j + 1/2}(\cos 2\phi_j), \tag{12}$$

where the K_j quantum numbers are defined as

$$K_j = \sum_{i=1}^{j} (l_i + 2n_i), \quad n_1 = 0, \quad K \equiv K_N, \tag{13}$$

and the normalization factor

$$\mathcal{N}_{n_j}^{l_j, K_j} = \sqrt{\frac{2\nu_j \Gamma(\nu_j - n_j) n_j!}{\Gamma(\nu_j - n_j - l_j - 1/2)\Gamma(n_j + l_j + 3/2)}}, \tag{14}$$

with $\nu_j = K_j + 3j/2 - 1$. The quantum number K is also known as the grand angular momentum.

The HH functions are normalized

$$\int d\Omega_N [\mathcal{Y}_{[K']}(\Omega_N)]^* \mathcal{Y}_{[K]}(\Omega_N) = \delta_{[K],[K']}, \tag{15}$$

moreover, the HH basis is complete

$$\sum_{[K]} [\mathcal{Y}_{[K]}(\Omega_N)]^* Y_{[K]}(\Omega_N') = \delta^{3N-1}(\Omega_N' - \Omega_N). \tag{16}$$

With the above definitions, the HH functions do not have well-defined total orbital angular momentum L and z projection M. It is possible to construct HH functions having well-defined values of LM by coupling the functions $Y_{l_j m_j}(\hat{x}_j)$. This can be achieved using different coupling schemes. Accordingly, we can define the following HH function:

$$\mathcal{Y}_{[K]}^{LM}(\Omega_N) = [Y_{l_1}(\hat{x}_1) \otimes \ldots \otimes Y_{l_N}(\hat{x}_N)]_{LM} \left[\prod_{j=2}^{N} {}^{(j)}\mathcal{P}_{K_j}^{l_j, K_{j-1}}(\phi_j) \right], \tag{17}$$

having well-defined values of LM, although the particular coupling scheme is not indicated. The set of quantum numbers $[K]$ now includes the values of LM plus $N-2$ intermediate l values instead of the N magnetic numbers m_j. When necessary, the explicit coupling scheme of the above HH function will be given.

A. Potential basis

If we have a function which depends only on the difference of two-particle positions $f(\mathbf{r}_1 - \mathbf{r}_2)$, we can use a subset of the HH's to expand that function called the PB [1]. Let us use the Jacobi coordinates such that $\mathbf{x}_N = \mathbf{r}_1 - \mathbf{r}_2$; then the PB subset is defined by the following condition [$\Omega_{12} \equiv (\hat{x}_N, \phi_N)$ and $\Omega_N = (\Omega_{N-1}, \hat{x}_N, \phi_N)$]:

$$\Lambda_{N-1}^2(\Omega_{N-1}) \mathcal{P}_{2n+l}^{l,m}(\Omega_{12}) = 0, \tag{18}$$

where $(n,l,m) \equiv (n_N, l_N, m_N)$, and by

$$\Lambda_N^2(\Omega_N) \mathcal{P}_{2n+l}^{l,m}(\Omega_{12}) = -K(K+3N-2) \mathcal{P}_{2n+l}^{l,m}(\Omega_{12}), \tag{19}$$

with $K = l + 2n$. Thus, the PB is a subset of the HH's which depends only on $(\hat{x}_N, \phi_N)$ variables, and which is specified by only three quantum numbers n,l,m, instead of the $3N-1$. The PB basis element has well-defined angular momentum l and projection m. The expression of the PB elements is

$$\mathcal{P}_{2n+l}^{l,m}(\Omega_{12}) = Y_{lm}(\hat{x}_N)(\cos\,\phi_N)^l P_n^{3(N-1)/2-1, l+1/2}(\cos 2\phi_N) \times Y_{[0]}(D-3), \tag{20}$$

where $(D = 3N)$

$$Y_{[0]}(D-3) = \left[\frac{\Gamma[(D-3)/2]}{2\pi^{(D-3)/2}} \right]^{1/2} \tag{21}$$

is the normalization verifying

$$\int [Y_{[0]}(D-3)]^2 d\Omega_{N-1} = 1. \tag{22}$$

The surface element is conveniently written as

$$d\Omega_N = d\Omega_{N-1} d\Omega_{12} = d\Omega_{N-1} d\hat{x}_N d\phi_N (\cos\,\phi_N)^2 (\sin\,\phi_N)^{3N-4}. \tag{23}$$

We can extend the definition of the PB elements to depend on the coordinates of a general pair (i,j) as $\mathcal{P}_{2n+l}^{l,m}(\Omega_{ij})$. The coordinates $\Omega_{ij} \equiv (\hat{x}_N, \phi_N)$ are now defined by a different ordering of the particles entering in the Jacobi coordinates such that $\mathbf{x}_N = \mathbf{r}_i - \mathbf{r}_j$. One important property of the PB elements is the following. When a PB element is defined in the space spanned by the coordinates Ω_{ij}, its expression in terms of HH functions defined in the reference set Ω_N corresponding to the ordering of the particles $1,2,\ldots,N$ is known and results

$$\mathcal{P}^{l,m}_{2n+l}(\Omega_{ij}) = \sum_{[K'=2n+l]} {}^{(N)}C^{n,l}_{[K']}(\varphi^{ij})\mathcal{Y}^{lm}_{[K']}(\Omega_N), \tag{24}$$

where the coefficients ${}^{(N)}C^{n,l}_{[K']}(\varphi^{ij})$ are given by the following relation:

$${}^{(N)}C^{n,l}_{[K']}(\varphi^{ij}) = \left\{ {}^{(N)}\mathcal{P}^{l,0}_{2n+l}(0)\sqrt{\frac{\Gamma(3(N-1)/2)}{2\pi^{3(N-1)/2}}}\right\}^{-1} \times \int d\hat{x} Y^*_{lm}(\hat{x})\mathcal{Y}^{lm}_{[K']}(\Omega^{ij}_z). \tag{25}$$

The angles $\varphi^{ij}=\{\varphi^{ij}_N,\ldots,\varphi^{ij}_2\}$ defined from the following kinematic rotation vector:

$$\mathbf{z}(\varphi^{ij}) = \mathbf{x}_N \cos\varphi^{ij}_N + \mathbf{x}_{N-1}\sin\varphi^{ij}_N\cos\varphi^{ij}_{N-1} + \cdots + \mathbf{x}_1 \sin\varphi^{ij}_N \sin\varphi^{ij}_{N-1}\cdots\sin\varphi^{ij}_2 \tag{26}$$

are chosen to verify $\mathbf{z}(\varphi^{ij})=\mathbf{r}_j-\mathbf{r}_i$. The hyperangles Ω^{ij}_z are defined as $\Omega^{ij}_z \equiv \{\hat{x},\ldots\hat{x},\varphi^{ij}_N,\ldots,\varphi^{ij}_2\}$, with $\hat{x}$ repeated N times. The particular form of the HH function $\mathcal{Y}^{lm}_{[K']}(\Omega^{ij}_z)$ produces the coefficients of Eq. (25) to be independent of m. In Eq. (24), the sum over all quantum numbers $[K']$ is limited by the condition $2n+l=K'$, showing that a PB basis element depending on Ω_{ij} can be given as a linear combination of HH basis elements having the same value of grand angular quantum number but depending on Ω_N. A generic function $f(\mathbf{r}_i-\mathbf{r}_j)$ can be expanded in terms of the PB as

$$f(\mathbf{r}_i-\mathbf{r}_j) = \sum_{nlm} f_{nlm}(\rho)\mathcal{P}^{l,m}_{2n+l}(\Omega_{ij}), \tag{27}$$

with

$$f_{nlm}(\rho) = \int d\Omega_{ij} f(\mathbf{r}_i-\mathbf{r}_j)\int d\Omega_{N-1}[\mathcal{P}^{l,m}_{2n+l}(\Omega_{ij})]^* = \frac{1}{Y_0(D-3)}\int d\Omega_{ij} Y^*_{lm}(\cos\phi_N)^l \times P^{3(N-1)/2-1,l+1/2}_n(\cos 2\phi_N) f(\mathbf{r}_i-\mathbf{r}_j). \tag{28}$$

The functions $f_{nlm}(\rho)$ are the hyper-radial multipoles. Using the transformation of Eq. (24) in the above expressions, it is possible to write a general function $f(\mathbf{r}_i-\mathbf{r}_j)$ in terms of HH functions given in the reference set. We will use this property for the potential energy of an A-body system.

III. POTENTIAL ENERGY IN TERMS OF HH FUNCTIONS

A local two-body interaction can be put in the form

$$V(i,j) = \sum_l [A_l(i,j)\otimes Y_l(\hat{r}_{ij})]_0 V_l(r_{ij}), \tag{29}$$

where we use the compact notation

$$[A_{l_1}(i,j)\otimes Y_{l_2}(\hat{r}_{ij})]_{LM} = \sum_{m_1 m_2}(l_1 m_1 l_2 m_2|LM)A_{l_1 m_1}(i,j)Y_{l_2 m_2}(\hat{r}_{ij}). \tag{30}$$

$A_{lm}(i,j)$ is an operator independent of the coordinates $\mathbf{r}_{ij}$, and the coupling with the spherical harmonics to zero in Eq. (29) shows that the potential is a scalar in total space. We can use the PB elements to expand each l term of the expansion,

$$V(i,j) = \sum_{ln}[A_l(i,j)\otimes\mathcal{P}^l_{2n+l}(\Omega_{ij})]_0 V^l_n(\rho), \tag{31}$$

where the functions $V^l_n(\rho)$ are obtained from the following integral in the hyperangular space:

$$V^l_n(\rho) = \int d\Omega_{ij} V_l(r_{ij})Y_{lm}(\hat{r}_{ij})\int d\Omega_{N-1}[\mathcal{P}^{l,m}_{2n+l}(\Omega_{ij})]^* = \frac{1}{Y_0(D-3)}\int d\phi_N(\cos\phi_N)^{2+l} \times(\sin\phi_N)^{3N-4}P^{3(N-1)/2-1,l+1/2}_n(\cos 2\phi_N)V_l(r_{ij}). \tag{32}$$

The complete potential energy is

$$\sum_{i<j}V(i,j) = \sum_{i<j}\sum_{ln}[A_l(i,j)\otimes\mathcal{P}^l_{2n+l}(\Omega_{ij})]_0 V^l_n(\rho). \tag{33}$$

It would be convenient to have the potential energy expressed in the coordinates defined by Ω (in the following we drop the suffix N for the reference set). To this end, we transform the PB elements obtaining

$$\sum_{i<j}V(i,j) = \sum_{ln}V^l_n(\rho)\sum_{[K'=2n+l]}\sum_{i<j}{}^{(N)}C^{n,l}_{[K']}(\varphi^{ij}) \times[A_l(i,j)\otimes\mathcal{Y}^l_{[K']}(\Omega)]_0 = \sum_{ln}V^l_n(\rho)\mathcal{G}^l_n(\Omega), \tag{34}$$

where we have defined

$$\mathcal{G}^l_n(\Omega) = \sum_{[K'=2n+l]}\left[\sum_{i<j}{}^{(N)}C^{n,l}_{[K']}(\varphi^{ij})\right][A_l(i,j)\otimes\mathcal{Y}^l_{[K']}(\Omega)]_0. \tag{35}$$

The final form of Eq. (34) gives a general expression for the potential energy in terms of the HH basis elements. In the case of central potentials $l=0$ and $A_{lm}=1$, and the above expressions reduce to (omitting the indices $l=0$, $m=0$)

$$\sum_{i<j}V(i,j) = \sum_{i<j}\sum_n\left[\sum_{[K'=2n]}{}^{(N)}C^n_{[K']}(\varphi^{ij})\mathcal{Y}_{[K']}(\Omega)\right]V_n(\rho) = \sum_n V_n(\rho)\sum_{[K'=2n]}\left[\sum_{i<j}{}^{(N)}C^n_{[K']}(\varphi^{ij})\right]\mathcal{Y}_{[K']}(\Omega) = \sum_n V_n(\rho)\mathcal{G}_n(\Omega), \tag{36}$$

with

$$\mathcal{G}_n(\Omega) = \sum_{[K'=2n]}\left[\sum_{i<j}{}^{(N)}C^n_{[K']}(\varphi^{ij})\right]\mathcal{Y}_{[K']}(\Omega) = \sum_{i<j}\mathcal{P}_{2n}(\Omega_{ij}). \tag{37}$$

The matrix elements of the potential energy between two different HH basis elements result

$$\langle \mathcal{Y}^{L_1M_1}_{[K_1]}|\sum_{i<j} V(i,j)|\mathcal{Y}^{L_2M_2}_{[K_2]}\rangle_\Omega = \sum_{nl} V^l_n(\rho)\langle \mathcal{Y}^{L_1M_1}_{[K_1]}|\mathcal{G}^l_n(\Omega)|\mathcal{Y}^{L_2M_2}_{[K_2]}\rangle_\Omega. \tag{38}$$

The above expression represents an integral in the hyperangular space and shows the tensor-product form between the hyper-radius and the hyperangular coordinates which is typical using the HH basis. The matrix elements of the operators $\mathcal{G}^l_n(\Omega)$ are independent of the potential

$$\langle \mathcal{Y}^{L_1M_1}_{[K_1]}|\mathcal{G}^l_n(\Omega)|\mathcal{Y}^{L_2M_2}_{[K_2]}\rangle_\Omega = \sum_{[K'=2n+l]} \sum_{i<j} {}^{(N)}C^{n,l}_{[K']}(\varphi^{ij}) \sum_m \frac{(-1)^{l-m}}{\sqrt{2l+1}} A_{l-m}(i,j) \times \int d\Omega [\mathcal{Y}^{L_1M_1}_{[K_1]}(\Omega)]^* \mathcal{Y}^{lm}_{[K']}(\Omega) \mathcal{Y}^{L_2M_2}_{[K_2]}(\Omega). \tag{39}$$

Each $\mathcal{G}^l_n$ is a combination of HH functions with grand orbital momentum $K'=2n+l$; therefore its matrix elements follow a triangular relation. In fact, given K_1 and K_2, the values of n,l to be considered in the sum of Eq. (38) are limited by the relation $|K_1-K_2|\leq 2n+l\leq K_1+K_2$. A triangular relation is also verified by the orbital angular momenta $|L_1-L_2|\leq l \leq L_1+L_2$. Furthermore, the matrix elements of $\mathcal{G}^l_n$ include the computation of integrals of three HH basis elements,

$$\int d\Omega [\mathcal{Y}^{L_1M_1}_{[K_1]}(\Omega)]^* \mathcal{Y}^{lm}_{[K']}(\Omega) \mathcal{Y}^{L_2M_2}_{[K_2]}(\Omega). \tag{40}$$

These integrals factorize in products of one-dimensional integrals consisting of either three hyperspherical polynomials or three spherical harmonics that can be obtained analytically or very efficiently using quadratures.

As shown in Eq. (35), each function $\mathcal{G}^l_n(\Omega)$ is symmetric in the particle indices; therefore its corresponding eigenvectors will have well-defined symmetry under particle permutations. For example, when $A_{lm}(i,j)=1$, $K_1=K_2=K$, $l=0$, implying $(L_1,M_2)=(L_2,M_2)=(L,M)$, and $2n=2K$, the following elements:

$$\langle \mathcal{Y}^{LM}_{[K]}|\mathcal{G}_K(\Omega)|\mathcal{Y}^{LM}_{[K]}\rangle_\Omega = \langle \mathcal{Y}^{LM}_{[K]}|\sum_{i<j} \mathcal{P}_{2n}(\Omega_{ij})|\mathcal{Y}^{LM}_{[K]}\rangle_\Omega, \tag{41}$$

form a matrix by varying all the quantum numbers in $[K]$ with fixed values of K and L,M. The dimension of the matrix is given by all HH functions with grand angular quantum number K coupled to L,M. Its eigenvectors, which are combinations of this family of HH functions, will have well-defined permutational symmetry. This reflects the fact that each K subset is invariant under particle permutations. Therefore, the diagonalization of the above matrix is a way to construct basis elements with well-defined permutational symmetry using HH functions with fix values of K and L.

IV. APPLICATION TO SYSTEMS WITH $A=3,4$

In the description of bound states in an A-body system, it is common to use basis elements having the required symmetry: symmetric states for bosons or antisymmetric states for fermions. In the present section, we will analyze the use of the HH basis without the initial symmetrization or antisymmetrization of the basis. Although the basis elements have not the required symmetry, the eigenvectors of the Hamiltonian will have a well-defined symmetry reflecting the symmetries appearing in the Hamiltonian. Therefore, among all eigenvectors and eigenvalues, the physical states have to be identified.

By taking opportune linear combinations of the HH basis elements, specific symmetries under particle permutation can be constructed for fixed values of K. Therefore two calculations, one in which all HH states up to a maximum value of K are considered and the other in which states with a particular symmetry up to the same value of K are considered, produce the same eigenvectors and eigenvalues. Of course, in the first calculation eigenvectors and eigenvalues will appear belonging to other symmetries not present in the second calculation. The simplification of avoiding the initial basis symmetrization is counterbalanced by the larger dimension of the Hamiltonian matrix.

Limiting the discussion to central potentials, Eq. (38) is well suited for a direct application of the HH basis. Let us present the following orthonormal basis element:

$$\langle \rho\Omega|m[K]\rangle = \left[\beta^{(\alpha+1)/2}\sqrt{\frac{m!}{(\alpha+m)!}}L^{(\alpha)}_m(\beta\rho)e^{-\beta\rho/2}\right]\mathcal{Y}^{LM}_{[K]}(\Omega), \tag{42}$$

where $L^{(\alpha)}_m(\beta\rho)$ is a Laguerre polynomial with $\alpha=3N-1$ and β a variational nonlinear parameter. We will discuss the case $L=0$ for $A=3,4$. The HH basis elements are

$$\mathcal{Y}_{[K]}(\Omega) = {}^{(2)}\mathcal{P}^{l,K_1}_K(\phi)[Y_l(\hat{x}_1)\otimes Y_l(\hat{x}_2)]_0 \tag{43}$$

for $A=3$, and

$$\mathcal{Y}_{[K]}(\Omega) = {}^{(2)}\mathcal{P}^{l_2,K_1}_{K_2}(\phi_2)\,{}^{(3)}\mathcal{P}^{l_3,K_2}_K(\phi_3) \times [[Y_{l_1}(\hat{x}_1)\otimes Y_{l_2}(\hat{x}_2)]_{l_3}\otimes Y_{l_3}(\hat{x}_3)]_0 \tag{44}$$

for $A=4$. The corresponding matrix elements of the Hamiltonian are

$$\langle m'[K']|H|m[K]\rangle = \langle m'[K']|T+V|m[K]\rangle. \tag{45}$$

The matrix elements of the potential energy corresponding to the Ω space have been discussed in Sec. III. Integrating also on ρ space, they result

$$\langle m'[K']|V|m[K]\rangle = \sum_n \langle m'|V_n(\rho)|m\rangle_\rho \langle [K']|\mathcal{G}_n(\Omega)|[K]\rangle_\Omega \equiv \sum_n (V^n_{m'm})(\mathcal{G}^n_{[K'][K]}). \tag{46}$$

The matrix elements of the kinetic energy are the following:

$$T_{K'm';Km} = \langle m'[K'] | - \frac{\hbar^2}{m} \sum_{i=1}^{N} \nabla^2_{\mathbf{x}_i} | m[K] \rangle$$
$$= -\frac{\hbar^2}{m} \langle m'[K'] | \frac{\partial^2}{\partial \rho^2} + \frac{N-1}{\rho} \frac{\partial}{\partial \rho} + \frac{\Lambda^2_N(\Omega)}{\rho^2} | m[K] \rangle$$
$$= -\frac{\hbar^2 \beta^2}{m} \delta_{[K],[K']} T^K_{m',m}$$
$$= -\frac{\hbar^2 \beta^2}{m} \delta_{[K],[K']} [T^{(1)}_{m'm} - K(K+3N-2) T^{(2)}_{m'm}], \quad (47)$$

with

$$T^{(1)}_{m'm} = \frac{1}{4} \delta_{m,m'} + \sqrt{\frac{m'!}{(\alpha+m')!}} \sqrt{\frac{m!}{(\alpha+m)!}} \int_0^\infty x^\alpha e^{-x} dx L^{(\alpha)}_{m'}(x)$$
$$\times \left[\left(-\frac{\alpha+2m}{2x} - \frac{m}{x^2} \right) L^{(\alpha)}_m(x) + \frac{m+\alpha}{x^2} \right.$$
$$\left. \times L^{(\alpha)}_{m-1}(x)(1-\delta_{m,0}) \right], \quad (48)$$

and

$$T^{(2)}_{m'm} = \sqrt{\frac{m'!}{(\alpha+m')!}} \sqrt{\frac{m!}{(\alpha+m)!}} \int_0^\infty x^\alpha e^{-x} dx L^{(\alpha)}_{m'}(x) \left(\frac{1}{x^2} \right)$$
$$\times L^{(\alpha)}_m(x). \quad (49)$$

Using the properties of the Laguerre polynomials, these integrals can be calculated analytically.

Therefore, the matrix elements of the Hamiltonian are sums of tensor products of two matrices: one calculated on ρ space, depending on indices m, m', and one calculated on Ω space, depending on the indices $[K], [K']$,

$$\langle m'[K'] | H | m[K] \rangle = -\frac{\hbar^2 \beta^2}{m} [T^{(1)}_{m'm} - K(K+3N-2) T^{(2)}_{m'm}]$$
$$\times \delta_{[K'][K]} + \sum_n (V^n_{m'm})(\mathcal{G}^n_{[K'][K]}). \quad (50)$$

Defining the diagonal matrix D such that $\langle [K'] | D | [K] \rangle = \delta_{[K],[K']} K(K+3N-2)$ and the identity matrix I in K space, we can rewrite the Hamiltonian schematically as

$$H = -\frac{\hbar^2 \beta^2}{m} (I \otimes^{(1)} T + D \otimes^{(2)} T) + \sum_n \mathcal{G}_n \otimes V_n, \quad (51)$$

in which the tensor-product character of the expression is explicitly given. A scheme to diagonalize such a matrix is given in the Appendix.

In the following, we give results for nucleon systems with $A=3,4$ using the Volkov potential

$$V(r) = V_R e^{-r^2/R_1^2} + V_A e^{-r^2/R_2^2} \quad (52)$$

with $V_R = 144.86$ MeV, $R_1 = 0.82$ fm, $V_A = -83.34$ MeV, and $R_2 = 1.6$ fm. The nucleons are considered to have the same mass chosen to be equal to the reference mass m and corresponding to $\hbar^2/m = 41.47$ MeV fm^{-2}. With this parametrization of the potential, the two-nucleon system has a binding energy of 0.54592 MeV.

TABLE I. Lowest Volkov-energy eigenvalues of each irreducible representations of S_4 for the $N=4$ case, with $m_{\max}=0$, $K_{\max}=6$, and $\beta=2$ fm^{-1}. The multiplets are further identified as being symmetric or antisymmetric under permutation of particles 1 and 2.

Irreps.		Eigenvalues (MeV)	Sym. (1 and 2)	Antisym. (1 and 2)
[4]		−25.794	−25.794	
[2^2]		27.680	27.680	
		27.680		27.680
[3 1]		28.430	28.430	
		28.430	28.430	
		28.430		28.430
[21^2]		102.85	102.85	
		102.85		102.85
		102.85		102.85
⋮	⋮	⋮	⋮	⋮
[1^4]		199.56		199.56
⋮	⋮	⋮	⋮	⋮

This potential has been used several times in the literature making its use very useful to compare different methods [11,13–15]. The results will be obtained after a direct diagonalization of the Hamiltonian matrix of Eq. (50) including $m_{\max}+1$ Laguerre polynomials with a fix value of β and all HH states corresponding to maximum value of the grand angular momentum $K_{\max}$. The scale parameter β can be used as a nonlinear parameter to study the convergence in the index $m=0,1,\ldots,m_{\max}$, with $m_{\max}$ the maximum value considered. In the present analysis, the convergence will be studied with respect to the index $K_{\max}$; therefore, the number of Laguerre polynomials at each step $m_{\max}+1$ will be sufficiently large to guarantee independence from β of the physical eigenvalues and eigenvectors.

In Table I we show the different symmetries of the eigenvectors and the corresponding eigenvalues, for $A=4$, in the particular case in which the Hamiltonian matrix has been diagonalized for $m_{\max}=0$, $\beta=2$ fm^{-1}, and $K_{\max}=6$. In this case, the total dimension of the matrix is 56 with 32 "even" elements, corresponding to even values of l_3, and 24 "odd" elements corresponding to odd values of l_3. In particular, there are six totally symmetric states irreducible representation [4] using the Yamagouchi symbol, two totally antisymmetric states [1^4], eight states belonging to the three-dimensional irreducible representation [3 1], six states belonging to the two-dimensional irreducible representation [2^2], and four states belonging to the three-dimensional irreducible representation [2 1^2]. The lowest eigenvalue of each irreducible representation is given in the table. In the last two columns of the table, the eigenvalues are reported considering separately even- and odd-basis elements. Symmetric

TABLE II. Results for the Volkov's potential, as a function of K_{max} using 30 Laguerre's polynomials, and $\beta=3$ fm^{-1} for the three-body case. In the last column, the results including the Coulomb potential are given.

K_{max}	N_{HH}	E (MeV)	
0	1	7.7075	6.9926
10	12	8.4157	7.7083
20	36	8.4623	7.7566
30	72	8.4647	7.7693
40	121	8.4649	7.7694
SVM[a]	30	8.46	

[a]Reference [13].

states are formed exclusively by even-basis element, whereas antisymmetric states are formed exclusively by odd-basis elements. The three mixed symmetries, one two dimensional and the other two three dimensional, show degenerate eigenvalues. In order to distinguish between the two three-dimensional mixed symmetries, we observe that the three degenerate eigenvalues divide differently in even and odd elements. The mixed symmetry [3 1] is twice degenerate when the expansion basis is restricted to even states, whereas the mixed symmetry [2 1^2] is not. Therefore by performing two different diagonalizations, one using a restricted basis considering only even states and one considering only odd states, all the symmetries can be identified.

Furthermore, we can see from Table I that a bound state appears in correspondence to a symmetric state. The fact that only one spatial symmetry is present in the bound state is a direct consequence of using a central potential. The final antisymmetrization of the state, as required in the case of four nucleons, is performed by multiplying the spatial symmetric wave function by the corresponding spin functions, singlet spin states $S_{12}=0$ for the two protons labeled (1,2), and $S_{34}=0$ for the two neutrons labeled (3,4). In the case of using the isospin formalism, the spatial symmetric state is multiplied by a four-nucleon antisymmetric spin-isospin function having total spin $S=0$ and total isospin $T=0$.

In Tables II and III, the convergence of the ground-state binding energies for $A=3,4$ is given as a function of K_{max}, respectively. In the last column, the point Coulomb interaction between the two protons labeled as particles (1,2) has been considered. In the case without the Coulomb potential, the spatial component of the ground state is completely symmetric. When the Coulomb potential is taken into account, this component is symmetric with respect to particles (1,2). For $A=4$, it is also symmetric with respect to the particles (3,4): the two neutrons. In this case, it is convenient to use the H-type Jacobi coordinates (for a recent application, see Ref. [16]),

$$\mathbf{x}_3 = \mathbf{r}_2 - \mathbf{r}_1$$

$$\mathbf{x}_2 = \frac{\mathbf{r}_4 + \mathbf{r}_3}{\sqrt{2}} - \frac{\mathbf{r}_2 + \mathbf{r}_1}{\sqrt{2}}$$

TABLE III. $A=4$ results for the Volkov's potential, using 25 Laguerre's polynomials, and $\beta=2$ fm^{-1}. Two different types of Jacobi coordinates have been used. In the last two columns, the results without and with Coulomb potential, using independently K-type or H-type Jacobi coordinates, are given, respectively. At a fixed value of K_{max}, the results, using either one or the other type of coordinates, coincide.

K_{max}	N_{HH} (K type)	N_{HH} (H type)	E (MeV)	
0	1	1	28.580	27.748
10	136	78	30.278	29.456
20	1547	819	30.416	29.596
30	7872	4056	30.420	29.599
SVM[a]	50		30.42	

[a]Reference [13].

$$\mathbf{x}_1 = \mathbf{r}_4 - \mathbf{r}_3, \tag{53}$$

and construct HH basis elements based on this type of coordinates. These HH functions are linear combinations of the HH function based on the K-type coordinates given in Eq. (3) and used in Secs. I–III at fixed values of the grand angular quantum number K. As an example, in Table III, the two different types of Jacobi coordinates have been considered. The dimension of the bases indicated corresponds to taking into account even-basis elements which are the only ones entering in the construction of the bound states. As stated before, for the K-type Jacobi coordinates this means to take even values of l_3. For the H-type, both l_1 and l_3 are taken as even. The dimension of the problem for obtaining the eigenvalue at $K_{max}=30$ results to be 72 for $A=3$ and 7872 (4056) for $A=4$, using the K type (H type). The use of the H-type Jacobi coordinates reduces the dimension of the problem by nearly a factor of 2.

The calculations corresponding to the two different types of coordinates differ in the set of angles φ^{ij} defined in Eq. (26), reflecting the different way of defining the interparticle distances in both cases. In the case in which the symmetric states are identified and constructed before diagonalization, the dimension is reduced to 27 for $A=3$ and around 600 for $A=4$. We observe a considerable reduction in the dimension of the eigenvalue problem for the symmetrized basis. However, the computational cost of constructing HH states with specific permutational symmetry has to be compared to the simplicity in constructing the matrix elements of $\mathcal{G}_n$ and in solving the system of Eq. (51). To be noticed, the results using the symmetrized HH basis of Refs. [8,14] coincide with the results presented here for each value of K_{max}. For the sake of comparison, the results using the stochastic variational method (SVM) [13] are shown in the table.

When the Coulomb potential between protons is included, the system can be treated as composed by two different species (the protons and the neutrons), having different interactions and slightly different masses. Using the complete HH basis, this causes no extra difficulties since the following term can be added to the Hamiltonian:

TABLE IV. Contributions to the bound-state energies, for $A=3,4$, of the different isospin components using antisymmetrized HH functions.

$A=3$			$A=4$		
$K_{\max}$	$T=1/2$	$T=1/2,3/2$	$K_{\max}$	$T=0$	$T=0,1,2$
0	6.9926	6.9926	0	27.748	27.748
10	7.7072	7.7083	10	29.453	29.456
20	7.7555	7.7566	20	29.594	29.596
30	7.7582	7.7593	30	29.596	29.599
40	7.7583	7.7594			

$$\sum_n (V^{c,n}_{m'm})(\mathcal{F}^n_{[K'][K]}), \tag{54}$$

where $V^{c,n}_{m'm}$ are the hyper-radial matrix elements of the Coulomb potential multipoles and $\mathcal{F}^n_{[K'][K]}$ is a matrix equivalent to $\mathcal{G}^n_{[K'][K]}$ with the only difference that the sum over (i,j) is limited to protons. This term has the tensor-product form and therefore the Hamiltonian reads as

$$H = I\otimes^{(1)}T + D\otimes^{(2)}T + \sum_n \mathcal{G}_n \otimes V_n + \sum_n \mathcal{F}_n \otimes V^c_n. \tag{55}$$

In the above equation, protons and neutrons are assumed to interact with the same short-range potential. For realistic potentials, this is not the case and this assumption can be relaxed dividing the potential energy in three parts: one for the interaction between protons, one for the interaction between neutrons, and one for the interaction between protons and neutrons. To be noticed, by using the complete HH basis the dimension of the problem does not change by distinguishing protons and neutrons or not. However, as a common procedure, it is possible to treat the system as composed by identical particles using the isospin formalism. The Coulomb potential breaks the isospin symmetry and the use of antisymmetric states requires the inclusion of different isospin components in the wave function. The $A=3$ bound state will have isospin $T=1/2,3/2$ components, whereas the $A=4$ bound state will have $T=0,1,2$ components. After including all these components, the two procedures—one using the complete HH basis and the other using antisymmetrized states—will produce the same eigenvalues. An example for this case is given in Table IV, in which the results for $A=3,4$ using antisymmetric basis states, including the different isospin components, are shown. For $A=3$, the $T=1/2$ component is by far the most important one; however, the exact result is obtained after including both components $T=1/2$ and 3/2. To be noticed, the dimension of the basis using antisymmetrized HH states with isospin components $T=1/2,3/2$ is the same of the complete HH states using even-basis elements. Therefore in this case, the preliminary antisymmetrization of the basis is not convenient. For $A=4$, the $T=0$ component is by far the most important; however, the exact result is obtained after including the three isospin components $T=0,1,2$. In this case, the dimension of the basis using even HH states up to $K_{\max}$ is greater than that using antisymmetrized basis elements, since in the symmetrization with respect to the two neutrons is not included automatically in the even HH states and has to be constructed by the diagonalization procedure. However, the difference in the dimension of the two cases is considerably reduced with respect to the case in which the Coulomb potential was not included.

The equivalence of the last columns of Tables II and III with columns third and sixth of Table IV illustrates the simplicity of treating symmetry-breaking terms using the HH basis without the permutational symmetry.

V. CONCLUSIONS

In this work, we have presented a direct use of the HH basis in the description of a A-body system. The basis has neither been symmetrized nor antisymmetrized as required by a system of identical particles. However, the eigenvectors of the Hamiltonian have well-defined permutation symmetry. Among all the eigenvectors, the physical ones can be identified. The benefit of the direct use of the HH basis is based on a particular simple form used to represent the potential energy. Each term of the two-body potential $V(i,j)$ has been expanded in the potential basis and then expressed in terms of the HH basis defined in the reference set by using the corresponding transformation coefficients. These coefficients are known for each value of K and for a general number of particles A. Once the potential has been expressed in terms of the HH basis, it results in a sum of tensor-product terms originated from the separation of the hyper-radial and the hyperangular coordinates inherent to the method. Moreover, the kinetic energy can be put in a tensor-product form too. Therefore, the matrix representation of the Hamiltonian is expressed as a sum of tensor-product matrices, and this particular form can be diagonalized very efficiently using the technique given in the Appendix. As a test case, we have studied three and four nucleons interacting through a central potential (the Volkov potential) used many times in the literature. We have shown how the symmetries are present in the spectrum and can be identified. The symmetric and antisymmetric states appear as singlets, whereas the mixed symmetries appear as multiplets. We have identified all symmetries by dividing the spectrum in even and odd components. In the studied cases, only one bound state appears for $A=3$ and 4 corresponding to a symmetric state. To be noticed, if the potential depends on the spin-isospin degrees of freedom,

the Hamiltonian will still present the tensor-product form in the hyper-radial, hyperangular, spin, and isospin spaces.

For $A=4$, we have solved the problem using two different types of Jacobi coordinates, namely, the K-type corresponding to a $3+1$ configuration and the H-type corresponding to a $2+2$ configuration. The calculations using one or the other set differ in the values of the angles φ^{ij}, which can be considered as input parameters. Therefore, the method gives a systematic way of using the different types of Jacobi coordinates. The convenience of selecting one specific type is related to its capability to produce basis states having partially the required symmetry with a reduction in the total dimension of the problem. In the cases presented here, the $A=4$ bound state is constructed using basis elements based on the K-type Jacobi coordinates with even values of l_3 or based on the H-type with both l_1 and l_3 restricted to even values; the latter resulting in a basis with a dimension smaller by a factor of 2.

A further benefit of using the complete HH basis is obtained when symmetry-breaking terms are included in the Hamiltonian. The complete basis will generate eigenvectors having specific permutation symmetries reflecting the symmetries present in the Hamiltonian. The complexity of the numerical problem does not increase when these terms are present. This is not the case when symmetrized or antisymmetrized basis are used. For example, in the case of a nuclear system, the presence of charge symmetry-breaking terms requires the extension of the basis to include all the isospin components. As a specific example, here we have analyzed the case of the Coulomb interaction between protons. The results using the HH basis without well-defined permutation symmetry have been compared to the case in which antisymmetrized HH basis have been used. In the latter case, the different isospin components entering in the wave function have to be included, resulting in spatial components having more than one symmetry. Accordingly, the dimension of the basis increases. To this respect, the numerical effort to reduce the Hilbert space to subspaces with specific permutation symmetry is discussed in Ref. [8]. When one spatial symmetry is required, as, for example, a completely symmetric spatial state, the convenience of constructing symmetric HH state is obvious. When several spatial symmetries are present in the wave function, as in the case of an A-nucleus wave function, the convenience of constructing HH states with different spatial symmetries has to be compared to the capability of solving a large eigenvalue problem; for example, that one given in Eq. (51).

In Refs. [14,17,18]], the HH basis used to describe three- and four-nucleon bound states is antisymmetrized in the following way. The total wave function is expanded in angular-spin-isospin channels and, for each channel, it is written as a sum of Faddeev-type amplitudes; each of them antisymmetric in the pair (i,j). In this way, the total wave function results antisymmetric. Then, each (i,j) amplitude is expanded in the HH basis defined from Jacobi vectors corresponding to the different ordering of the particles. As a consequence, the amplitudes for the different channels are not orthogonal, resulting in a nonorthogonal basis. For large values of K, the nonorthogonality of the basis could causes numerical instabilities. In particular, for $A=4$, this problem is overcome by performing an orthonormalization of the basis using the Gram-Schmidt technique with quadruple precision in the numerical treatment of the process. Therefore, the extension to $A>4$ systems appears to be difficult. On the other hand, the direct use of the HH basis without antisymmetrization circumvents this problem. Therefore, the method presented here has to be considered as a step in a program devoted to the application of the HH basis to systems with $A>4$. Further works along this line are the extension of the method to treat realistic interactions and the numerical implementation of the Hamiltonian of Eq. (51) to systems with $A=5,6$. The extension of the method to treat three-nucleon interaction terms is also possible. In fact, the transformation of the spatial part of a three-nucleon interaction $W(i,j,k)$ in terms of HH functions constructed in the reference set can be performed using the algorithm developed for the "triplet basis" in Ref. [5].

APPENDIX: EFFICIENT MATRIX-VECTOR PRODUCT FOR TENSOR-PRODUCT MATRICES

The algorithm we used to diagonalize the Hamiltonian is an iterative one, namely, Lanczos's [19]. These kinds of algorithms are useful whenever an efficient matrix-vector product can be used, as in the case of sparse matrices; in the specific calculation, we have the product between a tensor-product matrix $M=A_1\otimes A_2$ and a vector $\mathbf{v}$,

$$\mathbf{w}=M\cdot\mathbf{v}=(A_1\otimes A_2)\cdot\mathbf{v}, \tag{A1}$$

with A_1 an $n\times n$ matrix, A_2 an $m\times m$ matrix, and $\mathbf{v}$ an $(n\cdot m)$-dimensional vector.

The product is done in three steps. (i) First, the vector $\mathbf{v}$ is reshaped in an $m\times n$ matrix V; (ii) then, the following matrix products are performed:

$$W=(A_1\cdot(A_2\cdot V)^T)^T, \tag{A2}$$

(iii) finally, the matrix W is reshaped into the $(n\cdot m)$-dimensional vector $\mathbf{w}$, which is the result of the multiplication. The above algorithm is easily generalized to tensor products of k matrices [20].

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