Shell model approach to construction of a hyperspherical basis for A identical particles: Application to hydrogen and helium isotopes

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A new method to construct hyperspherical functions basis for A identical particles, beyond the minimal approximation, is presented. This method is based on the link between the hyperspherical function method (HSFM) and the oscillator no-core shell model and uses a Slater determinant representation of the hyperspherical functions. It is shown that, because of this representation, the HSFM matrix elements are related to the inverse Laplace transforms of the oscillator shell model matrix elements, on the condition that the center-of-mass motion and the hyperradial excitations are removed from the shell model states. The applicability of the proposed method is demonstrated for the case of the $^{3-7}$ H and $^{4-10}$ He isotopes.

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I. INTRODUCTION

One of the possible ways to solve the many-body problem for a system of A identical particles is to introduce the hyperspherical coordinates and to expand the wave function of this system in the hyperspherical functions basis. Because the hyperspherical functions form a complete orthonormal set, such an expansion should provide a solution of the many-body problem. This idea forms the foundation of the hyperspherical functions method (HSFM), in which a manybody wave function is represented as a sum of products of the hyperradial and the hyperspherical functions. The HSFM and its advanced modifications have been reviewed, for example, in Refs. [1–3].

The hyperspherical expansion has been shown to converge for three- and four-nucleon bound systems providing comparable results for binding energies and root mean squared radii to other few-body methods [3-9]. For A > 4, the number of the hyperspherical harmonics becomes very large and no studies of convergence have been done within the traditional formulation of the HSFM. However, in Refs. [10,11] some *p*-shell nuclei have been studied within two modified versions of the HSFM. In Ref. [10], a method combining the Faddeev approach and the pair-correlated hyperspherical harmonic method has been used to study ⁶Li, ⁸Be, and ¹²C. In Ref. [11], the effective interaction method, traditionally used in the framework of the harmonic oscillator basis, has been applied to the hyperspherical formalism of the A = 3-6 nuclei. Both works report that, for the nucleonnucleon (NN) interactions chosen, convergence was achieved with a relatively small number of hyperspherical functions.

The application of either a simple version of the HSFM, or its advanced modifications, requires a knowledge of how to construct the matrix elements of the *NN* interaction for a system of identical particles. Three approaches to calculate these matrix elements are known.

(1) The transformation coefficients between the hyperspherical functions constructed with different sets of Jacobi coordinates can be used to calculate the *NN* matrix elements. For a three-body case, these coefficients, known as RaynalRevai coefficients [12], can be easily calculated. For A > 3, a number of methods to calculate these coefficients have been proposed over the last thirty years. The most recent ones can be found in Refs. [13,14] together with the references to earlier works. However, numerical applications to the solution of the physical problems using this technique have been published only for A = 4 (see, for example, Ref. [9]) and no calculations for A > 4 are known to the author.

(2) The matrix elements of the NN potential can be calculated easily using two-particle coefficients of fractional parentage (CFP) introduced in Refs. [15,16]. A general recursive procedure to construct the HSFM one- and two-particle CFPs has been described in Ref. [2] about 25 years ago. It has also been shown that the hyperspherical CFPs (HCFPs) can be related to those of the translation-invariant shell model (TISM) [15]. The HCFPs for A=3 and $K \le 4$ have been tabulated in Ref. [15]. However, no numerical calculations of the HCFPs for A > 4 were done at that time. Recently, a new recursive procedure, which provides the hyperspherical states with well-defined orthogonal and permutational symmetry, has been worked out and encoded [17]. This technique has been used to calculate the HCFPs and NN matrix elements for the A = 3-6 nuclei and ⁸Be and ¹²C in Refs. [10,11].

(3) The two approaches mentioned above use an explicit representation of the hyperspherical functions by the usual spherical functions and the Jacobi polynomials. Such a representation may not be necessary if the link between the HSFM and TISM is used to calculate the matrix elements. This link has been previously investigated in Refs. [18-20,15,2]. In particular, it has been shown that for the minimum possible value of the hyperangular momentum (or in the so-called minimal or lowest order approximation) a hyperspherical function can be related to a linear combination of oscillator shell model Slater determinants [18–20]. In this case, the HSFM matrix elements of the minimal approximation can be derived from the $0\hbar\omega$ oscillator shell model matrix elements with the help of the inverse Laplace transform [20]. The shell model technique made it possible to perform the HFSM calculations for a wide range of the A >4 nuclei in the minimal approximation. Numerical calculations with this technique using different effective *NN* interactions have been performed for the 0*p*-shell nuclei, the oxygen isotopes, and ⁴⁰Ca, ⁵⁶Ni, ^{90,92}Zr, ¹⁷⁶Yb, ¹²⁰Sn, ²⁰⁸Pb, and ²⁴⁴Pu nuclei [1,2,21–24]. The binding energies of the 0*p*-shell nuclei obtained in the minimal approximation of the HSFM have been compared to the no-core $0\hbar\omega$ shell model calculations [2]. It was shown that when $\hbar\omega$ is chosen in such a way that the overlap between the HSFM and the oscillator shell model hyperradial wave functions is maximal, the binding energies obtained in these two methods are very close to each other.

Beyond the minimal approximation, a general procedure to construct the hyperspherical functions with the help of the Slater determinants has been proposed in Ref. [18]. However, this procedure leads to highly complicated expressions for the HSFM matrix elements [19] in which the analogy with the shell model is obscured [25]. A straightforward way to calculate these matrix elements using the method of Ref. [20], in which the link to the shell model is clear, requires matrix elements of many-body operators to be calculated. An approach proposed in Ref. [25], which aims to avoid such operators, still looks very complicated and in 30 years it has generated only one practical application, namely, the calculation of the ¹⁶O binding energy in the $K_{max} = K_{min} + 2$ approximation [26].

An alternative way to construct the hyperspherical basis with the help of the Slater determinants has been discussed in Ref. [27]. In this work, an optimal subset originating from the product of the total interaction and the hyperspherical function of the minimal order has been generated. However, no numerical HSFM calculations have been performed with this technique for A > 4 beyond the minimal approximation.

The possibility to construct the hyperspherical basis using the link to the shell model looks very attractive because it could exploit the huge experience accumulated by shell model calculations over many years. In this paper, I present a new method to construct the hyperspherical basis beyond the minimal approximation, with the help of the Slater determinant representation. This method is a further development of the ideas of Refs. [18–20,25], leading to an improved version of the formalism proposed by these papers, which is much more suitable for computational purposes. I show that, after a proper selection of the linear combinations of the Slater determinants, the HSFM matrix elements can be simply related to the inverse Laplace transforms of the matrix elements of the no-core oscillator shell model. In Sec. II the HSFM is described, in Sec. III the Slater determinant representation of the hyperspherical functions is introduced, while in Sec. IV the HSFM and the shell model matrix elements for arbitrary values of the hyperangular momentum are related. In Sec. V some examples of the numerical calculations are shown and the results are discussed in Sec. VI.

II. MANY-BODY HYPERSPHERICAL FUNCTIONS METHOD

A wave function of an *A*-body system is a function of *A* -1 Jacobi coordinates $\xi_i = \sqrt{i/(i+1)}(\Sigma_{j=1}^i r_j/i - r_{i+1})$. The 3A - 3 components of these coordinates can be considered as the components of a single vector $\boldsymbol{\rho}$ in a 3(A-1) dimensional space and the hyperspherical coordinates $(\rho, \hat{\rho})$ can be introduced in this space. Then the square of the length of $\boldsymbol{\rho}$, called the hyperradius, is

$$\rho^{2} = \sum_{i=1}^{A-1} \boldsymbol{\xi}_{i}^{2} = \sum_{i=1}^{A} \boldsymbol{r}_{i}^{2} - \boldsymbol{R}_{A}^{2} = \frac{1}{A} \sum_{i < j}^{A} (\boldsymbol{r}_{i} - \boldsymbol{r}_{j})^{2}, \qquad (1)$$

where $\mathbf{R}_A = (\sum_{i=1}^{A} \mathbf{r}_i)/\sqrt{A}$ is the normalized coordinate of the center-of-mass and \mathbf{r}_i is the individual coordinate of the *i*th nucleon. The set of 3A-4 hyperangles $\hat{\rho} = \{\theta_1, \theta_2, \dots, \theta_{3A-4}\}$ can be related to the 3A-3 Cartesian coordinates ξ_i in a following way [28]:

$$\xi_{1} = \rho \sin \theta_{3A-4} \cdots \sin \theta_{2} \sin \theta_{1},$$

$$\xi_{2} = \rho \sin \theta_{3A-4} \cdots \sin \theta_{2} \cos \theta_{1},$$

$$\vdots$$

$$\xi_{3A-4} = \rho \sin \theta_{3A-4} \cos \theta_{3A-5},$$

$$\xi_{2A-2} = \rho \cos \theta_{2A-4},$$

(2)

In the HSFM, a wave function of nucleus A with the total spin J, projection M_J , and parity π is represented as [1,2]

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$$\Psi_{A}^{J\pi M_{J}} = \rho^{-(3A-4)/2} \sum_{K\gamma} \chi_{K\gamma}^{J\pi}(\rho) Y_{K\gamma}^{JM_{J}}(\hat{\rho}), \qquad (3)$$

where the antisymmetric functions $Y_{K\gamma}^{JM_J}(\hat{\rho})$ are the eigenfunctions of the angular part of the multidimensional Laplacian $\Delta_{\hat{\rho}}$,

$$\Delta_{\hat{\rho}} Y_{K\gamma}^{JM_J}(\hat{\rho}) = -K(K+3A-5)Y_{K\gamma}^{JM_J}(\hat{\rho}).$$
(4)

They form a full set of orthonormal functions in the 3A-4 angular and 2A spin-isospin spaces. The quantum number $K = K_{min}^{J\pi}$, $K_{min}^{J\pi} + 2$, $K_{min}^{J\pi} + 4$,... is a hyperangular momentum and the index γ denotes the set of all other possible quantum numbers. The value $K_{min}^{J\pi}$ is state dependent and is greater than or equal to the minimum possible value $\sum_{i=1}^{A} (2n_i + l_i)$ of the oscillator shell model allowed by the Pauli principle. In the present paper, this value is denoted by K_{min}^{0} .

The hyperradial functions $\chi_{K\gamma}^{J\pi}(\rho)$ are found from the solution of the coupled set of differential equations

$$\left(\frac{d^2}{d\rho^2} - \frac{\mathcal{L}_K(\mathcal{L}_K+1)}{\rho^2} - \frac{2m}{\hbar^2} [E + V_{K\gamma,K\gamma}^{J\pi}(\rho)]\right) \chi_{K\gamma}^{J\pi}(\rho)$$
$$= \frac{2m}{\hbar^2} \sum_{K'\gamma' \neq K\gamma} V_{K\gamma,K'\gamma'}^{J\pi}(\rho) \chi_{K'\gamma'}^{J\pi}(\rho), \tag{5}$$

where $\mathcal{L}_K = K + (3A - 6)/2$, *m* is the nucleon mass, and the hyperradial potentials $V_{K\gamma,K'\gamma'}^{I\pi}(\rho)$ are the matrix elements of the *NN* interactions

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$$V_{K\gamma,K'\gamma'}^{J\pi}(\rho) = \langle Y_{K\gamma}^{JM_{j}}(\hat{\rho}) | \sum_{i < j} V_{ij}(\boldsymbol{r}_{i} - \boldsymbol{r}_{j}) | Y_{K'\gamma'}^{JM_{j}}(\hat{\rho}) \rangle, \quad (6)$$

which contain contributions from the central, spin-orbit, tensor, Coulomb, and any other *NN* forces. Three-body forces can also be included if necessary.

In what follows, the quantum numbers J, M_J , and π are omitted.

III. A SHELL MODEL APPROACH TO CONSTRUCTION OF THE HYPERSPHERICAL BASIS

In the case of the harmonic oscillator, the internal translation-invariant Hamiltonian of the *A*-body system in the hyperspherical coordinates is [15,2]

$$H = -\frac{\hbar^2}{2m} \left[\frac{1}{\rho^{n-1}} \frac{\partial}{\partial \rho} \left(\rho^{n-1} \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \Delta_{\hat{\rho}} \right] + \frac{1}{2} m \omega^2 \rho^2,$$
(7)

where n=3A-3 is the dimension of the space formed by the translation-invariant coordinates and ω is the oscillator frequency. Since in this Hamiltonian the spatial and angular variables are separated, its eigenfunctions corresponding to the energy eigenvalues of $(2\kappa + K + n/2)\hbar\omega$ are factorized as

$$\Psi_{NK\gamma}(\rho,\hat{\rho}) = R_{\kappa K}(\rho) Y_{K\gamma}(\hat{\rho}), \qquad (8)$$

where $N = 2\kappa + K$ is the total number of oscillator quanta. The hyperradial wave function $R_{\kappa K}(\rho)$ is [15,2]

$$R_{\kappa K}(\rho) = b^{-(K+n/2)} \left(\frac{2\kappa!}{\Gamma(\kappa+K+n/2)}\right)^{1/2} \left(\frac{\rho}{b}\right)^{K} e^{-\rho^{2}/2b^{2}} \times L_{\kappa}^{K+(n-2)/2}(\rho^{2}/b^{2}),$$
(9)

where $b = \sqrt{\hbar/m\omega}$ is the oscillator radius.

In this paper, Eq. (8) is used to construct a full set of hyperspherical functions $Y_{K\gamma}$. For this purpose, a full set of functions $\Psi_{NK\gamma}$ of fixed N and K, and therefore κ , should be generated and then divided by hyperradial functions $R_{\kappa K}$. Although for a fixed K the values of N and κ are arbitrary, the most sensible choice is N=K and $\kappa=0$ because, in this case, (i) the number of oscillator quanta of the wave function $\Psi_{NK\gamma}$ is minimal and (ii) the hyperradial function R_{0K} does not have any nodes and can be safely used in a denominator.

The wave functions $\Psi_{NK\gamma}$ times the 0s center-of-mass wave function $\Phi_{000}(\mathbf{R}_A)$ can be represented by some linear combinations of the Slater determinants $D_i^N(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$ with a total number of oscillator quanta of *N*. Therefore,

$$\Psi_{NK\gamma}(\rho,\hat{\rho}) = \Phi_{000}^{-1}(\boldsymbol{R}_A) \sum_i \tilde{C}_i^{NK\gamma} D_i^N(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_A),$$
(10)

where the individual coordinates r_i are chosen in an arbitrary fixed coordinate system that is not related to the center-ofmass motion. Here, $\tilde{C}_i^{NK\gamma}$ are some unknown yet coefficients. With $\kappa = 0$ one can get from Eqs. (8) and (10) an explicit expression for the hyperspherical function $Y_{K\gamma}(\hat{\rho})$,

$$Y_{K\gamma}(\hat{\rho}) = [\Phi_{000}(\mathbf{R}_{A})R_{0K}(\rho)]^{-1}\sum_{i} C_{i}^{K\gamma}D_{i}^{K}(\mathbf{r}_{1},\mathbf{r}_{2},\ldots,\mathbf{r}_{A}),$$
(11)

where $C_i^{K\gamma} \equiv \tilde{C}_i^{KK\gamma}$. Since both the functions $\Phi_{000}(\mathbf{R}_A)$ and $R_{0K}(\rho)$ are symmetrical with respect to the permutation of nucleons, the hyperspherical functions constructed in this way are antisymmetric. They do not depend on the choice of the origin of the coordinate system or on the oscillator radius *b*. If the linear combinations of the Slater determinants are chosen in such a way that the functions $\Psi_{NK\gamma}$ possesses well-defined orbital momenta, spin, isospin, and permutational symmetry, then the hyperspherical functions $Y_{K\gamma}$, obtained from Eq. (11), will have the same properties.

The expansion coefficients $C_i^{K\gamma}$ can be calculated in the following way. First, we construct all possible n(K) linear combinations of the Slater determinants $D^K(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$ with the total number of oscillator quanta equal to K, which provide the required set of quantum numbers α and contain only 0s motion of the center of mass,

$$\Phi_{K\alpha}(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_A) = \sum_i c_i^{K\alpha} D_i^K(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_A).$$
(12)

Here, the coefficients $c_i^{K\alpha}$ are the eigenvectors of the matrix R_A^2 of the center-of mass radius squared, corresponding to the minimum possible eigenvalues $\frac{3}{2}b^2$. The basis states $\Phi_{K\alpha}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$ obtained in such a way will have a welldefined value of the hypermoment only for the minimal value of the oscillator quanta associated with the chosen set of the quantum numbers α . In the general case, these states contain an admixture $\Phi'_{\kappa K'\beta}$ of the states = $\Phi_{000}(\mathbf{R}_A) R_{\kappa \kappa'}(\rho) Y_{\kappa'\beta}(\hat{\rho})$ with hypermoment K' < K and with hyperradial excitations $\kappa \neq 0$,

$$\Phi_{K\alpha}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = \sum_{\substack{\kappa, K' \beta \\ (2\kappa + K' = K)}} A_{\kappa K' \beta, K\alpha} \Phi'_{\kappa K' \beta}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A).$$
(13)

The coefficients $A_{\kappa K'\beta,K\alpha} = \langle \Phi_{K\alpha} | \Phi'_{\kappa K'\beta} \rangle$, which measure the weights of the states with the hyperradial excitations κ in the function $\Phi_{K\alpha}$ and which will be calculated later, determine also the inverse expansion

$$\Phi_{\kappa K'\beta}'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_A) = \sum_{\alpha} A_{\kappa K'\beta,K\alpha} \Phi_{K\alpha}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_A).$$
(14)

If the contribution of the states with hyperradial excitations $\kappa \neq 0$ is subtracted both from the left- and right-hand sides of Eq. (13), the remainder will not contain any hyperradial excitation. Therefore, using Eqs. (13) and (14) one can intro-

duce a set of new states $\tilde{\Phi}_{K\alpha}$ that are the eigenfunctions of the angular part of the multidimensional Laplacian corresponding to the eigenvalue -K(K+3A-5),

$$\Phi_{K\alpha}(\mathbf{r}_{1},\mathbf{r}_{2},\ldots,\mathbf{r}_{A}) = \Phi_{K\alpha}(\mathbf{r}_{1},\mathbf{r}_{2},\ldots,\mathbf{r}_{A})$$
$$-\sum_{\substack{\kappa\neq 0, K'\beta\\(2\kappa+K'=K)}} A_{\kappa K'\beta,K\alpha} \Phi_{\kappa K'\beta}'(\mathbf{r}_{1},\mathbf{r}_{2},\ldots,\mathbf{r}_{A})$$
$$=\sum_{\alpha'} B_{\alpha\alpha'} \Phi_{K\alpha'}(\mathbf{r}_{1},\mathbf{r}_{2},\ldots,\mathbf{r}_{A}),$$
(15)

where

$$B_{\alpha\alpha'} = \delta_{\alpha\alpha'} - \sum_{\substack{\kappa \neq 0, K' \beta \\ (2\kappa + K' = K)}} A_{\kappa K' \beta, K \alpha} A_{\kappa K' \beta, K \alpha'}.$$
(16)

However, this set is overcomplete. If $d(K_i)$ is the dimension of the subspace, spanned by the set of the hyperspherical functions with the hypermoment $K_i < K$, then the dimension of the subspace, spanned by n(K) states $\Phi_{K\alpha}$, is d(K) $= n(K) - d(K-2) - d(K-4) - \cdots - d(K_{min})$. To construct the orthonormal basis for this subspace, a singular value decomposition $B = U[\operatorname{diag}(w_j)]V^T$, where $j = 1, \ldots, n(K)$, of the matrix $B \equiv B_{\alpha\alpha'}$ can be found. From the numerical point of view [29], this procedure is more stable than the Gram-Schmidt orthogonalization. In this procedure, d(K) is equal to the rank of the matrix **B** and the d(K) linear independent basis states $\Phi_{K\gamma}^0$ are the range of the matrix **B**. They can be constructed from the γ columns of the matrix **U** corresponding to nonzero w_i 's,

$$\Phi^{0}_{K\gamma}(\boldsymbol{r}_{1},\boldsymbol{r}_{2},\ldots,\boldsymbol{r}_{A}) = \sum_{\alpha} u_{\alpha\gamma} \Phi_{K\alpha}(\boldsymbol{r}_{1},\boldsymbol{r}_{2},\ldots,\boldsymbol{r}_{A}).$$
(17)

Therefore, taking into account Eq. (12), the expansion coefficients $C_i^{K\gamma} = \langle D_i^K | \Phi_{K\gamma}^0 \rangle$ can be found as a part of the product of the matrices U and $\{c_i^{K\alpha}\}$,

$$C_i^{K\gamma} = \sum_{\alpha} u_{\alpha\gamma} c_i^{K\alpha}.$$
 (18)

Thus, the problem of constructing the hyperspherical basis in the Slater determinants representation is solved if the coefficients $A_{\kappa K'\beta,K\alpha}$, which determine the matrix **B**, are known.

The coefficients $A_{\kappa K'\beta,K\alpha} = \langle \Phi_{K\alpha} | \Phi'_{\kappa K'\beta} \rangle$ can be found using the following procedure. Let us expand the functions $\Phi'_{\kappa K'\beta}$ in the Slater determinant basis

$$\Phi_{\kappa K'\beta}'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_A) = \Phi_{000}(\mathbf{R}_A)R_{\kappa K'}(\rho)Y_{K'\beta}(\hat{\rho})$$
$$= \sum_i a_i^{\kappa K'\beta}D_i^K(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_A).$$
(19)

Then, using the recurrence relations for the hyperradial functions $R_{\kappa \kappa}(\rho)$,

$$R_{\kappa K}(\rho) = \left(2\kappa - 2 + K + \frac{n}{2} - \frac{\rho^2}{b^2}\right) \left[\kappa \left(\kappa + K + \frac{n}{2} - 1\right)\right]^{-1/2}$$
$$\times R_{\kappa - 1K}(\rho) - \left(\kappa - 2 + K + \frac{n}{2}\right)$$
$$\times \left(\frac{\kappa - 1}{\kappa \left(\kappa + K + \frac{n}{2} - 1\right) \left(\kappa + K + \frac{n}{2} - 2\right)}\right)^{1/2}$$
$$\times R_{\kappa - 2K}(\rho), \qquad (20)$$

we can obtain for the coefficients $a_i^{\kappa K'\beta} = \langle D_i^K | \Phi'_{\kappa K'\beta} \rangle$,

$$a_{i}^{\kappa K'\beta} = -\frac{\left[\kappa\left(\kappa + K + \frac{n}{2} - 1\right)\right]^{-1/2}}{b^{2}}$$
$$\times \langle D_{i}^{K} | \rho^{2} | \Phi_{000}(\mathbf{R}_{A}) R_{\kappa-1K'}(\rho) Y_{K'\beta}(\hat{\rho}) \rangle. \tag{21}$$

Here we use $\langle D_i^K | \Phi_{000} R_{\kappa-1K'} Y_{K'\beta} \rangle = 0$ and $\langle D_i^K | \Phi_{000} R_{\kappa-2K'} Y_{K'\beta} \rangle = 0$. Now, with the help of Eqs. (19), (21), and (1), we can rewrite Eq. (21) as

$$a_{i}^{\kappa K'\beta} = -\frac{\left[\kappa\left(\kappa + K + \frac{n}{2} - 1\right)\right]^{-1/2}}{b^{2}}$$

$$\times \sum_{i'} a_{i'}^{\kappa - 1K'\beta} \langle D_{i'}^{K-2} | \frac{1}{A} \sum_{i_{1} < i_{2}}^{A} (\mathbf{r}_{i_{1}} - \mathbf{r}_{i_{2}})^{2} | D_{i}^{K} \rangle$$
(22)

and get the coefficients $A_{\kappa K'\beta,K\alpha}$,

$$A_{\kappa K'\beta,K\alpha} = \sum_{i} c_{i}^{K\alpha} a_{i}^{\kappa K'\beta}.$$
 (23)

Therefore, the coefficients $A_{\kappa K'\beta,K\alpha}$ can be constructed recursively using the fact that for $K = K_{min}$ the functions $\Phi_{K\alpha}$ already have a well-defined value of the hypermoment K_{min} and that $C_i^{K_{min}\gamma} = c_i^{K_{min}\gamma} = a_i^{0K_{min}\gamma}$.

IV. MATRIX ELEMENTS IN THE HYPERSPHERICAL FUNCTIONS BASIS

Due to the Slater determinant representation of hyperspherical functions (11), the matrix elements $O_{K\gamma,K'\gamma'}(\rho) = \langle Y_{K\gamma}(\hat{\rho}) | \hat{O}(\rho,\hat{\rho}) | Y_{K'\gamma'}(\hat{\rho}) \rangle$ of an arbitrary operator $\hat{O}(\rho,\hat{\rho})$ can be related to those calculated in the oscillator shell model. Using the integral representation of an arbitrary function f(x),

$$f(z) = \frac{1}{\pi i} \int_0^\infty dx x f(x) \int_{-i\infty}^{i\infty} ds e^{-s(x^2 - z^2)},$$
 (24)

where the integration path bypasses the origin in the counterclockwise direction, we can express a quantity $\rho^{K+K'+n-2}O_{K\gamma,K'\gamma'}(\rho)$ as

$$\rho^{K+K'+n-2}O_{K\gamma,K'\gamma'}(\rho)$$

$$=\frac{1}{\pi i}\int_{-i\infty}^{i\infty} ds e^{s\rho^2}\int_0^{\infty} d\tilde{\rho}\tilde{\rho}^{K+K'+n-1}e^{-s\tilde{\rho}^2}$$

$$\times \int d\hat{\rho}Y_{K\gamma}(\hat{\rho})\hat{O}(\tilde{\rho},\hat{\rho})Y_{K'\gamma'}(\hat{\rho}). \qquad (25)$$

Then we substitute $Y_{K\gamma}(\hat{\rho})$ by its representation (11) with $s = b^2$, multiply Eq. (25) by $\Phi_{000}^2(\mathbf{R}_A)$, integrate it over \mathbf{R}_A and, taking into account that

$$d\mathbf{R}_{A}d\tilde{\rho}d\hat{\rho} = d\mathbf{R}_{A}d\boldsymbol{\xi}_{1}d\boldsymbol{\xi}_{2}\cdots d\boldsymbol{\xi}_{A-1} = d\mathbf{r}_{1}d\mathbf{r}_{2}\cdots d\mathbf{r}_{A},$$
(26)

we find that the matrix elements $O_{K\gamma,K'\gamma'}(\rho)$ are the inverse Laplace transforms

$$O_{K\gamma,K'\gamma'}(\rho) = \frac{\left[\Gamma(K+n/2)\Gamma(K'+n/2)\right]^{1/2}}{\rho^{K+K'+n-2}} \frac{1}{2\pi i} \\ \times \int_{-i\infty}^{i\infty} ds e^{s\rho^2} s^{-(K+K'+n)/2} O_{K\gamma,K'\gamma'}(s)$$
(27)

of the usual oscillator shell model matrix elements $O_{K\gamma,K'\gamma'}(s)$ calculated with the oscillator radius $b = s^{-1/2}$,

$$O_{K\gamma,K'\gamma'}(s) = \sum_{ii'} C_i^{K\gamma} C_{i'}^{K'\gamma'} \int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_A$$
$$\times D_{i'}^{K'\dagger}(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_A) \hat{O} D_i^K(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_A).$$
(28)

In the case of $K = K_{min}^0$ the inverse Laplace transform representation (27)–(28) coincides with the one derived in Ref. [20], and for $K > K_{min}^0$ it still formally resembles the one from Ref. [20]. However, the difference is that for $K = K_{min}^0$ the expressions (27)–(28) are valid for any choice of the coefficients $C_i^{K_{min}^0\gamma}$ while for $K > K_{min}^0$ these expressions are only valid for specially selected coefficients $C_i^{K\gamma}$, namely, for those that guarantee that the center-of-mass motion and the hyperradial excitations are excluded from the shell model wave functions. On the other hand, for $K > K_{min}^0$, Eqs. (27)–(28) are much simpler than those derived in Refs. [19,25].

If the operator \hat{O} is a sum of the *NN* interaction potentials, $\hat{O}(\rho, \hat{\rho}) = \sum_{i < j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$, the shell model matrix elements $O_{K\gamma,K'\gamma'}(s)$ are just numbers that do not depend on spatial coordinates but depend on the oscillator radius as a parameter. By contrast, the hyperradial potentials $O_{K\gamma,K'\gamma'}(\rho)$ explicitly depend on a collective spatial coordinate, the hyperradius, and their shapes are determined by the shapes and strengths of the *NN* interactions. These potentials play the role of a self-consistent collective mean field. Unlike the self-consistent Hartree-Fock mean field that generates single-particle wave functions, the hyperspherical mean field generates the hyperradial wave functions that describe the collective motion of nucleons interacting with the chosen *NN* force.

In the particular case when the *NN* potential V(r) has a Gaussian shape, $V(r) \propto e^{-(r/\alpha)^2}$, the shell model matrix elements (28) are sums of the type $\sum_{\ell=0}^{\ell_{max}} C_{\ell} y^{3+2\ell}$, where $y = (1+2b^2/\alpha^2)^{-1/2}$ and ℓ is the relative orbital momentum between two nucleons. It is easy to show that in this case the HSFM matrix elements $V_{K\gamma,K'\gamma'}(\rho)$ can be obtained from the shell model ones by replacing everywhere $y^{3+2\ell}$ by

$$\frac{[\Gamma(K+n/2)\Gamma(K'+n/2)]^{1/2}}{\Gamma[(K+K'+n)/2]} {}_{1}F_{1}\left(\frac{3}{2}+\mathscr{N};\frac{K+K'+n}{2};-\frac{2\rho^{2}}{\alpha^{2}}\right),$$

where ${}_{1}F_{1}$ is the confluent hypergeometrical function. For large ρ , asymptotic expressions can be used to calculate the hypergeometrical functions, which leads to the asymptotic inverse power expansion of the hyperradial potentials $V_{K\gamma,K'\gamma'}(\rho)$,

$$V_{K\gamma,K'\gamma'}(\rho) \approx V_{K\gamma,K'\gamma'}^{as}(\rho) = \sum_{\nu=0}^{r_{max}} v_{K\gamma,K'\gamma'}^{(\nu)} / \rho^{3+2\nu}.$$
 (29)

Equation (29) shows that the hyperradial potentials are strongly anharmonic and that at $\rho \rightarrow \infty$ they decrease as $1/\rho^3$. Such a slow decrease originates from the fact that two nucleons can still interact at small distances when some or all the other nucleons are far away from them. The wave functions generated by these potentials decrease asymptotically in a more realistic way as compared to the oscillator wave functions generated by the mean field parabolically increasing at large hyperradii.

V. APPLICATION TO THE HYDROGEN AND HELIUM ISOTOPES

This section illustrates the applicability of the approach described above and presents results of the numerical calculations of the ground state binding energies for hydrogen and helium isotopes with central and Coulomb *NN* interactions. The aim of these calculations is to investigate how far in hyperangular momentum one can go within the standard HSFM, using the shell model technique proposed in this paper.

The actual *NN* potential used in this work, was the Volkov V1 effective potential [30]. Its triplet even and singlet even components are equal, $V_{31}(r) = V_{13}(r) = 144.86e^{-(r/0.82)^2} - 83.34e^{-(r/1.6)^2}$ MeV, and the singlet and triplet odd components are related to the even ones as follows: $V_{33}(r) = V_{11}(r) = (1-2M)V_{31}(r)$, where *M* is the Majorana exchange parameter. In the present calculations, the standard value M = 0.6 was used. Also, $\hbar^2/m = 41.47$ MeV fm² was always used.

To construct the hyperspherical basis, the Slater determi-

nants of the oscillator shell model in the *ls*-coupling were used. The Slater determinants were made of the single particle oscillator wave functions with the quantum numbers $\{n, l, m, \sigma, \tau\}$, where σ and τ are the spin and isospin projections. Matrices of total orbital momentum L^2 , total spin S^2 , and total isospin T^2 have been diagonalized to find states with well-defined *LST* values and the matrix R_A^2 was diagonalized in order to remove the center-of-mass excitations. The hyperradial excitations were then excluded according to the algorithm described in Sec. III.

The basis states obtained in such a way do not generally possess any permutational or orthogonal symmetry. In the particular case of the Volkov force, mixing between the states with different permutational symmetries is absent. To get states with well-defined permutational symmetry, the second Casimir operator $\sum_{i < i'}^{A} (i, i')$ of the symmetric group has been diagonalized, as suggested in Ref. [17]. The eigenvalues of this operator, equal to $\frac{1}{2}\sum_i \gamma_i(\gamma_i - 2i + 1)$, are represented by the Young diagrams [f] with γ_i boxes in the *i*th row. In the present calculations, only the states corresponding to the largest eigenvalues were constructed, because such states have the lowest binding energies. At the present stage the hyperspherical basis has not been symmetrized with respect to the orthogonal group O_{A-1} . This leads to larger number of hyperradial functions to be coupled by a set of differential equations, many of which contribute negligibly to the binding energy.

The actual values of [f]LST for the ${}^{3-7}$ H and ${}^{4-10}$ He nuclei considered in this paper are: 3 H $[3](0\frac{1}{2}\frac{1}{2})$, 4 H [31](111), 5 H $[32](0\frac{1}{2}\frac{3}{2})$, 6 H [321](112), 7 H $[322](0\frac{1}{2}\frac{5}{2})$, 4 He [4](000), 5 He $[41](1\frac{1}{2}\frac{1}{2})$, 6 He [42](001), 7 He $[421](1\frac{1}{2}\frac{3}{2})$, 8 He [422](002), 9 He $[4221](1\frac{1}{2}\frac{5}{2})$, and 10 He [4222](003). With the currently available computer code, it was possible to go up to $\Delta K_{max} = 16$ for 3 H, $\Delta K_{max} = 12$ for 4 He, $\Delta K_{max} = 10$ for ${}^{4.5}$ H, $\Delta K_{max} = 8$ for ${}^{5.6}$ He, $\Delta K_{max} = 6$ for ${}^{6.7}$ H, and 8 He and $\Delta K_{max} = 4$ for ${}^{7.9.10}$ He, where $\Delta K_{max} = K_{max} - K_{min}$. The number N(K) of the hyperspherical basis states with chosen [f]LST for ${}^{3-7}$ H and ${}^{4-10}$ He as a function of $\Delta K = K - K_{min}$ is shown in Fig. 1. As expected, the number N(K) increases strongly with the increasing number of nucleons.

For the nuclei from Fig. 1 the hyperradial potentials $V_{K\gamma,K'\gamma'}(\rho)$ were calculated up to some ρ_{max} in about 25 to 50 points with the step $\Delta\rho$ varying from 0.1 to 0.5 fm depending on the number of nucleons. Beyond ρ_{max} the inverse power expansion (29) was used to calculate $V_{K\gamma,K'\gamma'}(\rho)$, which significantly reduced the size of the arrays where the hyperradial potentials were stored. The expansion coefficients $v_{K\gamma,K'\gamma'}^{(\nu)}$ were calculated up to some ν_{max} that depended on ΔK_{max} and A. In the majority of cases, the choice $\nu_{max}=9$ has provided at least six correct digits for large and 1% for small $V_{K\gamma,K'\gamma'}(\rho)_{max}$. However, in some cases, to get the same accuracy, ν_{max} has been increased up to 15.

An example of the inverse power expansion for the case of ¹⁰He is shown in Fig. 2 where the hyperradial potential $V(\rho)$ of the K_{min} approximation is compared with its asymptotics $V^{as}(\rho)$ calculated for ν_{max} from 0 to 7. One can see



FIG. 1. The number N(K) of the hyperspherical basis states with chosen [f]LST for ³⁻⁷H (a) and ⁴⁻¹⁰He (b) as a function of $\Delta K = K - K_{min}$.

that, because of the slow decrease, the hyperradial potential still significantly differs from zero even for very large values of ρ . In the particular case of ¹⁰He, the nuclear hyperradial potential at $\rho \approx 200$ fm is still about 10% of the centrifugal potential. Using only a few points in the inverse power expansion helps to avoid the calculation of the nuclear hyperradial potentials at such large distances. Generally, the quality of the inverse power approximation deteriorates with increasing *A* and *K*.

After the hyperradial potentials are calculated, the system of hyperradial differential equations (5) has been solved with the computer code STURMXX that is based on the algorithm described in Ref. [31]. This code uses an expansion on a Sturmian basis and explicitly treats the long-range asymptotic tails of the hyperradial potentials represented by the inverse power expansion (29). For the present calculations, the total number of the hyperradial channels is less than 400.

The present method has been tested for the ³H and ⁴He nuclei for which the results obtained with the same *NN* potential by different authors exist [4,7,8]. The binding energies of ³H, calculated in the present paper up to $K_{max} = 16$, are in excellent agreement with those in Refs. [4,8]. The binding energy of ⁴He has been calculated up to $K_{max} = 12$. The Coulomb interaction has been switched off for this test case. A very good agreement has been obtained for lower harmonics with the results of Ref. [7]. For $K_{max} \ge 10$ the binding energies obtained in the present work, are about 0.05% lower than the corresponding values from Ref. [7]. Such a difference may arise because only the optimal set of



FIG. 2. Hyperradial potential $V(\rho)$ for ¹⁰He calculated for K_{min} and its inverse power approximations $V^{as}(\rho)$. The centrifugal and Coulomb potentials are included in all the curves and the centrifugal potential is also shown separately.

hyperspherical basis states has been used in Ref. [7] while all the basis states have been taken into account in the present work. Another source of this difference can be a lack of accuracy while solving the coupled set of differential equations (5) either in the present work or in Ref. [7].

For Gaussian *NN* potentials, the HSFM binding energies converge exponentially [3]. Since the V1 potential has Gaussian shape, exponential extrapolation can be used to estimate the converged binding energies. For ³H, the extrapolated energy is -8.448 MeV and -8.476 MeV for the *K* $=4, \ldots, 16$ and $K=6, \ldots, 16$ model spaces, respectively, which means that the accuracy of the exponential extrapolation in this case is 0.3%. For ⁴He, the exponential extrapolation gave the binding energy of -30.46 MeV for *K* $=4, \ldots, 12$ and -30.40 MeV for $K=6, \ldots, 12$. With this accuracy, the value obtained agrees well with the binding energies of -30.40 MeV and -30.42 MeV obtained with the optimal set of the hyperspherical functions in Ref. [8] and by the stochastic variational method in Ref. [32], respectively.

The calculated ground state binding energies of ${}^{3-7}$ H and ${}^{4-10}$ He, together with experimental data, taken from Refs. [33,34], are shown in Figs. 3 and 4 and Table I. For the *NN* potential chosen the binding energies of 3 H and 4 He have almost converged for ΔK_{max} =12. The converged energy of 3 H, shown in Table II, is very close to the experi-



FIG. 3. The ground state binding energies of the hydrogen isotopes calculated with different ΔK_{max} .

mental one. For ⁴He, the converged energy is about 1 MeV lower than the experimental one. In fact, the binding energies of ³H and ⁴He are not very sensitive to increases in the model space. These energies, calculated in the minimal approximation, are already close to the converged ones and the contribution of the lowest order hyperharmonics to the total norm of the wave functions of ³H and ⁴He are 99.3% and 99.1% (see Tables I and II).

The situation is different for all the other isotopes considered, as, for them, the contribution of higher order hyperharmonics is very important. To illustrate this, the calculated probabilities $P_{\Delta K} = \sum_{\gamma} P_{K\gamma}$ of the hypermoment $K = K_{min}$



FIG. 4. The ground state binding energies of the helium isotopes calculated with different ΔK_{max} .

TABLE I. The binding energies E (in MeV) and the probabilities $P_{\Delta K}$ (in %) of the hypermoment $K = K_{min} + \Delta K$ for the ground states of the ³⁻⁷H and ⁴⁻¹⁰He nuclei in the model space determined by ΔK_{max} .

Nucleus	ΔK_{max}	Ε	P_0	P_2	P_4	P_{6}	P_8
³ H	4	-8.078	99.571	0	0.429		
³ H	6	- 8.329	99.385	0	0.464	0.151	
$^{3}\mathrm{H}$	8	-8.376	99.359	0	0.470	0.152	0.019
³ H	10	-8.416	99.337	0	0.477	0.154	0.019
³ H	12	-8.443	99.318	0	0.486	0.155	0.019
³ H	14	-8.451	99.311	0	0.490	0.156	0.019
³ H	16	-8.457	99.303	0	0.495	0.158	0.019
⁴ H	2	-1.450	91.407	8.593			
$^{4}\mathrm{H}$	4	-3.318	80.990	12.547	6.463		
$^{4}\mathrm{H}$	6	-4.284	73.165	14.776	9.503	2.556	
$^{4}\mathrm{H}$	8	-4.918	65.249	16.648	12.556	4.081	1.466
$^{4}\mathrm{H}$	10	-5.387	57.994	17.742	15.064	5.748	2.494
⁵ H	2	-1.745	89.806	10.194			
⁵ H	4	-3.925	81.917	11.739	6.344		
⁵ H	6	-5.316	75.116	13.131	8.459	3.294	
⁵ H	8	-6.070	69.435	13.976	10.539	4.526	1.524
⁵ H	10	- 6.589	64.536	14.326	12.106	5.880	2.233
⁶ H	6	-1.55	70.26	14.15	10.88	4.71	
⁷ H	6	-1.878	71.077	13.429	10.498	4.997	
⁴ He	4	-28.450	99.506	0	0.494		
⁴ He	6	-28.978	99.308	0	0.495	0.197	
⁴ He	8	-29.328	99.209	0	0.493	0.193	0.105
⁴ He	10	-29.444	99.182	0	0.494	0.190	0.104
⁴ He	12	-29.532	99.150	0	0.508	0.189	0.102
⁵ He	2	-21.821	91.420	8.580			
⁵ He	4	-23.957	82.818	12.763	4.419		
⁵ He	6	-25.017	76.217	15.121	7.097	1.565	
⁵ He	8	-25.780	70.578	16.330	9.384	2.829	0.088
⁶ He	2	-24.726	88.893	11.107			
⁶ He	4	-27.205	82.134	13.427	4.439		
⁶ He	6	-28.418	76.998	14.980	6.358	1.662	
⁶ He	8	-29.140	73.576	15.512	7.742	2.446	0.723
⁷ He	2	- 19.655	88.295	11.705			
⁷ He	4	-23.204	78.632	14.754	6.614		
⁸ He	2	- 22.255	89.051	10.949			
⁸ He	4	-26.036	80.245	13.184	6.571		
⁸ He	6	-27.866	73.429	15.079	8.922	2.570	
⁹ He	2	-18.024	88.608	11.392			
⁹ He	4	-22.461	78.318	13.564	8.119		
¹⁰ He	2	-20.560	90.287	9.713			
¹⁰ He	4	-25.165	80.354	11.438	8.208		

TABLE II. Experimental binding energies E_{exp} (in MeV) and the exponentially extrapolated binding energies E_{extr} (in MeV) and weights of the lowest order hyperharmonics P_0^{extr} (in %).

	E_{exp}	E _{extr}	P_0^{extr}
³ H	-8.48	- 8.45	99.3
$^{4}\mathrm{H}$	-5.57	-5.90	
⁵ H	-6.78	-7.34	41.2
^{7}H		-7.61	
⁴ He	-28.30	-29.63	99.1
⁵ He	-27.40	-26.80	34.2
⁶ He	-29.27	-29.67	66.8
⁸ He	-31.41	-31.60	47.3

 $+\Delta K$ in the model space determined by ΔK_{max} are shown in Table I. For the model space used, convergence of $P_{\Delta K}$ has only been achieved for ³H and ⁴He. The results of the calculations clearly indicate that for the neutron-rich isotopes of hydrogen and helium the weights of the lowest hyperharmonics can be significantly smaller than one. One can see from Table I a general trend that the decreased contribution of the minimal hypermoment with enlargement of the model space is somehow correlated to the cluster structure of the nuclei under consideration.

For ⁴H, which is a two-body resonance in the ³H + n continuum, the contribution of the lowest order hyperharmonic P_0 decreases almost linearly for the model space used in the calculations, which makes it impossible to estimate its convergent value by exponential extrapolation. One can only say that the contribution of lowest order hyperharmonic is less than 57%. The ⁴H binding energy starts to converge and an exponential extrapolation gives for the converged energy -5.90 MeV, which is slightly lower than the experimental one -5.57 MeV.

For ⁵H and ^{5,6}He, the decreasing contributions of the lowest order hyperharmonics with increasing model space follows an exponential law. The possible converged weights P_0^{extr} of the lowest hyperharmonic for these nuclei are given in Table II. One can see that the weight of the minimal hyperharmonic for the particle-stable nucleus ⁶He, is larger than for the particle unstable isotopes ^{4,5}H and ⁵He. The binding energies of these isotopes tend to converge. The exponential extrapolation gives $E({}^{5}\text{H}) = -7.34 \text{ MeV},$ $E({}^{5}\text{He}) = -26.80 \text{ MeV}$, and $E({}^{6}\text{He}) = -29.67 \text{ MeV}$ (see Table II), which are reasonably close to the experimental values -6.7 ± 0.3 , -27.40, and -29.27 MeV, respectively. However, in these cases the estimates of the converged values are less accurate than in case of ³H and ⁴He because of smaller model space used.

For all the other isotopes considered, the model space is not large enough to make any definite conclusions about convergence. The only case where the binding energies $E_{\Delta K_{max}}$ follow approximately an exponential decrease is ⁸He. An exponential extrapolation made with E_0 , E_2 , E_4 , and E_6 gives an estimate for $E(^{8}\text{He}) = -31.60$ MeV, which is unexpectedly close to the experimental value of -31.41 MeV. The extrapolated converged contribution of the lowest order hyperharmonics for ⁸He is 47.3%.

The ⁶H and ⁷H isotopes become particle stable with respect to the six- and seven-body decays only for $\Delta K_{max} = 6$. In the case of ⁷H a possible value of the converged energy has been estimated by calculating the positions of the sevenbody resonances for $\Delta K_{max} = 2$ and $\Delta K_{max} = 4$. With $E_2 = 2.85$ MeV, $E_4 = 0.133$ MeV, and $E_6 = -1.878$ MeV the estimated possible value for converged energy is -7.61 MeV, which is about 300 keV below the estimated binding energy of ⁵H obtained in this work. It should be mentioned, however, that such an extrapolation is not very reliable. It should only be used to give a rough idea of where the converged energy may be.

As for ^{7,9,10}He, the numerical calculations have been performed only up to ΔK_{max} =4 and these calculations clearly show the importance of the higher order hyperharmonics. For the model space used in these cases the contribution of these harmonics is more than 20%.

It is very important to note here that the parts of the many-body wave function described by the lowest order hyperharmonics correspond to the $0\hbar\omega$ no-core shell model with all possible oscillator frequencies [2]. Therefore, the probabilities P_0 of these hyperharmonics show how good the standard shell model description is for the nucleus of interest. For nuclei with $P_0 \approx 1$, the shell model description is well justified. However, the case of P_0 being significantly less than one indicates a strong presence of particle-hole excitations. For some of the hydrogen and helium isotopes considered above, the probabilities P_0^{extr} , obtained by exponential extrapolation, are shown in Table II. Only ³H and ⁴He have displayed a well defined shell model structure with nucleons occupying the 0s shell. In the particle unstable nuclei ⁵H and ⁵He the probabilities for their nucleons to occupy only 0s and 0p shell model states are 41.2% and 34.2%, respectively. For the particle stable nucleus 6 He, the shell model picture of a closed 0s shell plus two valent nucleons in the 0p shell is justified only by 66.8%. The rest are the particle-hole excitations that are responsible for the three-cluster nature of this nucleus displayed in fragmentation reactions. Surprisingly, the present calculations have revealed only 47.3% probability for the particle-stable isotope ⁸He to be described as a closed 0s core plus four 0p valence particles. ⁸He is more bound than ⁶He and has a smaller radius, which was considered as a consequence of the $p_{3/2}$ subshell closure. The HSFM calculations suggest one half probability for the nucleons in ⁸He to spend in other energy shells. At the same time, the HSFM calculations reproduce the enhanced binding energy of ⁸He as compared to ⁶He.

VI. DISCUSSION AND CONCLUSIONS

In this paper a new method to calculate the matrix elements in the hyperspherical basis beyond the minimal approximation has been presented, and applied to the calculation of binding energies of the hydrogen and helium isotopes. The method is based on the link between the translationinvariant shell model and the hyperspherical functions method and uses the Slater determinant representation of the hyperspherical functions. It has been shown that the HSFM matrix elements are just the inverse Laplace transforms of the matrix elements of the large scale no-core oscillator shell model, on the condition that the center-of-mass motion and the hyperradial excitations are removed from the shell model states. Such a condition is the crucial point that makes the shell model formalism applicable in the calculations of the HSFM matrix elements. Unlike the HCFP technique, the shell model based method is not recursive and can be directly applied to any nucleus including nonclosed shell nuclei and nuclei far from stability. For these purposes, existing shell model computer codes can be adapted to perform the HSFM calculations.

The method proposed in this paper is a further development of the ideas of Refs. [18–20,25]. However, the expressions for the HSFM matrix elements derived here are simpler and better suited to the numerical calculations than those suggested in these works. Such an improvement has been achieved by the independent choice of the individual nucleon coordinates from the center-of-mass of the many-nucleon system. However, the price that has to be paid is the requirement to remove the center-of-mass excitations from the shell model functions. This removal is simply done by the well-defined procedure of diagonalizing the matrix R_A^2 . Other improvements relate to a different choice of methods for the elimination of hyperradial excitations and the orthogonalization procedure used to construct the orthonormal set of hyperspherical functions.

The Slater determinant representation of hyperspherical functions, as proposed in this work, does not have any relation to the "realistic" shell model with the experimentally determined single particle wave functions and energies. This representation only helps to express one mathematical function, namely, a hyperspherical function, which is a fully antisymmetric function of 3A-4 angular variables and 3A spin and isospin variables, by some linear combination of other mathematical functions, namely, by exponentials, polynomials, and spherical functions, of 3A spatial and 3A spin and isospin variables. It is this apparent increase of the number of variables that makes it possible to replace the difficult problem of calculating the HSFM matrix elements by the well-known easier problem of calculating the matrix elements in the oscillator shell model.

From the fact that the hyperspherical functions with the hypermoment $K = K_{min}^0 + \Delta K$ can be constructed using the $\Delta K \hbar \omega$ oscillator shell model space it follows that the upper limit on K_{max} , achievable with the technique of the present work, is determined by the dimension of the $\Delta K_{max} \hbar \omega$ nocore shell model space that modern computers are able to deal with. It should be noticed, however, that the hyperradial function $R_{K\nu}(\rho)$ can be represented by the sum over all possible monopole excitations of the oscillator hyperradial wave functions $R_{\kappa K}^{(\omega)}(\rho)$ with an arbitrarily chosen oscillator frequency ω : $R_{K\gamma}(\rho) = \sum_{\kappa=0}^{\infty} c_{\kappa K\gamma} R_{\kappa K}^{(b)}(\rho)$. Therefore, with the same value of ΔK_{max} , the HSFM takes more basis states into account than the no-core shell model where the number of radial monopole excitations is restricted by the condition $2\kappa + K = K_{max}$. Besides, in the shell model, the oscillator frequency ω , chosen to minimize the total binding energy, is the same for all the single particle wave functions and, therefore, for all the hyperradial functions. By contrast, in the HSFM, the hyperradial functions are the superpositions of the oscillator wave functions with the oscillator frequencies determined by the spatial separations of nucleons [1], or they can be represented by an integral of oscillator wave functions over all possible frequencies [2]. In both cases the weights of such configurations are generated by a self-consistent hyperradial field, which, in turn, is generated by the *NN* interaction potential. Therefore, the HSFM hyperradial functions, corresponding to different values of *K*, have their own unique shapes.

Until now, for light nuclei the no-core shell model calculations have been performed up to $6\hbar\omega$ and $4\hbar\omega$ for $A \leq 7$ and $8 \le A \le 11$, respectively [35]. Recently, calculations of ⁸Be up to $10\hbar\omega$ have been reported [36]. Therefore, one can expect that, using the proposed shell model technique, the hyperspherical basis for these nuclei can be constructed at least up to $K_{max} = K_{min} + 4$ or $K_{min} + 6$. With the current version of the computer code written for the purposes of the present paper, it was possible to go up to $\Delta K_{max} = 10$ for ^{4,5}H, $\Delta K_{max} = 8$ for ^{5,6}He, $\Delta K_{max} = 6$ for ^{6,7}H, and ⁸He and $\Delta K_{max} = 4$ for ^{7,9,10}He. On the other hand, for A = 6, the calculations have been performed up to the same value of K_{max} that was achieved in Ref. [11] with the HCFP technique. It should be mentioned, however, that for the same K_{max} the model space of the present work is larger than that in Ref. [11] because the states with well-defined orthogonal symmetry have not been selected here.

In this work the Volkov V1 effective *NN* interaction has been used only for simplicity. With this potential, the ³H and ⁴He ground states binding energies are found to converge rapidly. The binding energies of ^{4,5}H and ^{5,6,8}He decrease exponentially with *K* and, for K_{max} used, these nuclei are underbound by maximum of 12% with respect to the values obtained by the exponential extrapolation. Exponential extrapolation estimates of the converged energies for the ³H, ^{4,6,8}He isotopes agree surprisingly well with experiment while the estimated converged energies of ⁴H and ⁵H are only 0.33 MeV and 0.6 MeV lower than the experimental ones. It is also important to note that the binding energy of ⁷H estimated by exponential extrapolation is about 300 keV lower that that for ⁵H. If this result is confirmed by more detailed calculations, this would agree with the hypothesis of Ref. [34] that ⁷H may exist as a low lying resonance with the only decay channel being ⁷H \rightarrow ³H+*n*+*n*+*n*+*n*.

In general, to solve the many-body problem, modern realistic NN potentials should be used instead of V1. With realistic potentials, the convergence of the simple HSFM will deteriorate. However, the hyperspherical basis can still be used in many-body calculations if, for example, either shortrange correlation factors or effective interactions are introduced. The increase in binding with K, obtained in this paper for V1, gives a rough idea of what one can expect when such convergence accelerating methods are used.

Summarizing, in this paper a new method to construct the hyperspherical basis for *A* identical particles using the Slater determinant representation of the hyperspherical functions has been proposed. This method made it possible to apply the hyperspherical functions technique to real systems up to A = 10 fermions using a simple model for the *NN* interaction. The presented calculations suffer in some cases, seriously, convergence problems, but this drawback can be overcome by different convergence accelerating methods. Future improvements of the proposed method, and in computer power, could allow realistic microscopic calculations for A > 4 nuclei, a problem that is still very difficult to tackle. Such calculations will help to understand nuclear structure from first principles, and will test models for the *NN* interactions.

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