

Improved effective interaction for the hyperspherical formalism

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An improvement of the recently developed effective interaction method for the hyperspherical formalism is presented. The method is extended to include contributions of three-body effective forces and of the nonadiabatic kinetic energy term. The role of these two additional contributions is tested on the binding energy of ⁴He and ⁶Li using semirealistic and more realistic *NN* potential models. The rate of convergence is improved considerably, opening up the possibility to use the method with realistic two- and three-body potentials for the α -particle and for few-body nuclei with more than four nucleons.

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I. INTRODUCTION

In the last decade quite some progress was made in microscopic calculations of few-body nuclei. In fact several theoretical approaches were developed and a few of them such as the Green function Monte Carlo (GFMC) [1], the stochastic variational method (SVM) [2], the no core shell model method (NCSM) [3], and the effective interaction in the hyperspherical harmonics basis (EIHH) [4] were even applied to systems with more than four nucleons. Very recently, several of these methods were tested in a benchmark calculation for the α -particle ground state with a realistic *NN* force [5]. A very good agreement among the results of the different calculations was found. This shows the high standard of present days few-body physics calculations and opens up the possibility to tackle even more complicated microscopic *ab initio* calculations in the near future.

In particular, the effective interaction approach is a very promising new tool in few-body physics. In this field it has been first introduced by Navrátil and Barrett [6]. They have performed a NCSM calculation in an harmonic oscillator basis constructing a two-body effective interaction for a specific model space and for a given bare *NN* interaction. It is important to note that in this approach the model space is not kept fixed, but is increased up to the point that for a given observable (e.g., ground state energy, matter radius) a constant, model space independent value is reached; this value should coincide with the *true* result obtained with the bare *NN* interaction.

Recently, a similar effective interaction approach has been carried out in the hyperspherical harmonics (HH) formalism [4]. The use of the HH basis leads to various advantages, e.g., one can define a two-body effective interaction, which contains information on the residual ($A-2$)-body system; therefore the result converges faster to the asymptotic value.

The aim of this paper is to work out extensions of the EIHH method which should lead to an even faster convergence of the HH expansion. These extensions consist of (i) an inclusion of the hyper-radial kinetic energy and (ii) the incorporation of a three-body effective interaction.

The paper is organized as follows. In Sec. II the EIHH method is outlined. In Sec. III the inclusion of the hyper-

radial kinetic energy is described. The incorporation of the three-body effective interaction is discussed in Sec. IV. Results with the two improvements of the EIHH method are given in Sec. V. A detailed Appendix describes how the matrix elements of the three-body effective interaction are actually calculated for an *A*-body wave function.

II. OUTLINE OF THE EIHH METHOD

In the effective interaction approach [3,4,7] the lowest eigenvalues of an *A*-body Hamiltonian

$$H^{[A]} = H_0 + V \quad (1)$$

is treated in the following way. The Hilbert space of $H^{[A]}$ is divided into a model space and a residual space, through the use of the eigenprojectors P and Q of H_0 , which satisfy the relations

$$[H_0, P] = [H_0, Q] = 0, \quad QH_0P = PH_0Q = 0, \quad P + Q = 1. \quad (2)$$

The Hamiltonian $H^{[A]}$ is then replaced by the effective model space Hamiltonian

$$H^{[A]eff} = PH_0P + PV^{[A]eff}P \quad (3)$$

that by construction has the same energy levels as the low-lying states of $H^{[A]}$. In general, the effective interaction appearing in Eq. (3) is an *A*-body interaction. Its construction is as difficult as finding the full-space solutions. Therefore, one has to approximate $V^{[A]eff}$. However, one must build the approximate effective potential in such a way that it coincides with the bare one for $P \rightarrow 1$, so that an enlargement of the model space leads to a convergence of the eigenenergies to the *true* values. The NCSM and the EIHH methods are developed along these lines.

In the HH formalism a Hamiltonian

$$H^{[A]} = \sum_{i=1}^A \frac{\vec{p}_i^2}{2m} + \sum_{i<j}^A v_{ij} \quad (4)$$

is written as

$$H^{[A]} = T_\rho + T_K(\rho) + V^{[A]}(\rho, \Omega_A), \quad (5)$$

where

$$V^{[A]}(\rho, \Omega_A) \equiv \sum_{i < j}^A v_{ij} \quad (6)$$

denotes the bare two-body potential and

$$T_\rho = -\frac{1}{2m} \Delta_\rho \quad \text{and} \quad T_K(\rho) = \frac{1}{2m} \frac{\hat{K}_A^2}{\rho^2} \quad (7)$$

are the hyper-radial and hypercentrifugal kinetic energies, respectively. In the preceding equation, Δ_ρ is the Laplace operator with respect to the hyper-radial coordinate

$$\rho = \sqrt{\sum_{j=1}^N \eta_j^2}, \quad (8)$$

where $\vec{\eta}_j$ denote the $N=A-1$ Jacobi vectors, while \hat{K}_A is the hyperspherical grand angular momentum operator and Ω_A the $(3A-4)$ -dimensional hyperangle. The hyper-radial kinetic energy T_ρ and the residual Hamiltonian

$$\mathcal{H}^{[A]}(\rho) \equiv T_K(\rho) + V^{[A]}(\rho, \Omega_A) \quad (9)$$

are often considered separately. The Hamiltonian $\mathcal{H}^{[A]}(\rho)$, often used as a starting point in atomic and molecular calculations, is called adiabatic [8] as the hyper-radial coordinate ρ is a *slow* coordinate with respect to the hyperangles.

In Ref. [4], the effective interaction method is applied to this adiabatic Hamiltonian. The unperturbed Hamiltonian H_0 is chosen to be $T_K(\rho)$ with the hyperspherical harmonics $\mathcal{Y}_{[K_A]}$ as eigenfunctions ($[K_A]$ stands for a set of quantum numbers, see Ref. [4]). The model space P is defined as the complete set of HH basis functions with generalized angular momentum quantum number $K_A \leq K_P$, and the Q space as the complete set of HH basis functions with $K_A > K_P$. The states will be denoted by $\{|p\rangle, p=1, 2, \dots, n_P\}$ for the P space and $\{|q\rangle, q=n_{P+1}, n_{P+2}, \dots, n_Q\}$ for the Q space. Of course, in principle one has $n_Q \rightarrow \infty$, but for actual calculations one has to consider a finite Q space but with a sufficiently large n_Q .

For each value ρ of the hyper-radius, an effective adiabatic Hamiltonian is constructed as

$$\mathcal{H}^{[A]eff}(\rho, \Omega_A) = P T_K(\rho) P + P V^{[A]eff}(\rho, \Omega_A) P. \quad (10)$$

However, as already pointed out, the effective potential would be a complicated A -body interaction, therefore $V^{[A]eff}$ is approximated by a sum of *two-body* terms as

$$V^{[A]eff} \simeq \sum_{i < j}^A v_{i,j}^{[2]eff}. \quad (11)$$

In the following, it will be shown how $v_{i,j}^{[2]eff}$ is derived ensuring that the effective potential satisfies the above mentioned condition, i.e., $v_{i,j}^{[2]eff}$ tends to the bare v_{ij} for $P \rightarrow 1$. Due to the use of antisymmetric wave functions one only needs to calculate the effective interaction operator relative to one pair, since

$$\langle V^{[A]eff} \rangle \simeq \left\langle \sum_{i < j}^A v_{i,j}^{[2]eff} \right\rangle = \frac{A(A-1)}{2} \langle v_{A,(A-1)}^{[2]eff} \rangle. \quad (12)$$

Below, it will become clear why the choice to express $\langle V^{[A]eff} \rangle$ in terms of the pair potential between the last two particles A and $(A-1)$ is particularly convenient. The two-body effective potential $v_{A,(A-1)}^{[2]eff}$ is determined as follows. First, for each value ρ of the hyper-radial coordinate one defines a *quasi-two-body* adiabatic Hamiltonian containing the hypercentrifugal kinetic energy and the bare potential between the last two particles

$$\mathcal{H}^{[2]}(\rho; \theta_N, \hat{\eta}_N) = T_K(\rho) + v_{A,(A-1)}(\sqrt{2}\rho \sin \theta_N \cdot \hat{\eta}_N), \quad (13)$$

where $\hat{\eta}_N$ is the unit vector associated with the last Jacobi vector

$$\vec{\eta}_N = \sqrt{\frac{1}{2}} (\vec{r}_{A-1} - \vec{r}_A) \quad (14)$$

and θ_N is the hyperangle defined through the relation

$$\eta_N = \rho \sin \theta_N. \quad (15)$$

We emphasize here that we are using reversed order A -body Jacobi coordinates

$$\vec{\eta}_i = \sqrt{\frac{A-i}{A+1-i}} \left(\vec{r}_i - \frac{1}{A-i} \sum_{j=i+1}^A \vec{r}_j \right). \quad (16)$$

The Hamiltonian of Eq. (13) is then diagonalized on the A -body HH basis. Such a diagonalization is easily performed since ρ is only a parameter in $\mathcal{H}^{[2]}$ (there are no derivatives with respect to ρ), and for each value of ρ the Hamiltonian $\mathcal{H}^{[2]}(\rho; \theta_N, \hat{\eta}_N)$ depends only on three variables. This is just due to our choice of the $A-(A-1)$ pair. The obtained eigenstates will be denoted by $|j(\rho)\rangle$ as they are continuous functions of ρ .

One proceeds applying the Lee-Suzuki [9,10] similarity transformation to $\mathcal{H}^{[2]}(\rho; \theta_N, \hat{\eta}_N)$ in order to get the corresponding Hermitian effective Hamiltonian

$$\mathcal{H}^{[2]eff}(\rho; \theta_N, \hat{\eta}_N) = U^\dagger(\rho) \mathcal{H}^{[2]}(\rho; \theta_N, \hat{\eta}_N) U(\rho), \quad (17)$$

where

$$U(\rho) = (P + \omega(\rho)) \frac{1}{\sqrt{P[1 + \omega(\rho)^\dagger \omega(\rho)]} P}. \quad (18)$$

The operator $\omega(\rho)$ is obtained using the following property [9]:

$$\omega(\rho) = Q \omega(\rho) P. \quad (19)$$

The matrix $\omega(\rho)$ is calculated for each value of ρ , taking the n_P states $|j(\rho)\rangle$ with the lowest eigenvalues. Each of these states leads to the following system of $(n_Q - n_P)$ equations:

$$\langle q|j(\rho)\rangle = \sum_p \langle q|\omega(\rho)|p\rangle \langle p|j(\rho)\rangle. \quad (20)$$

The $n_p(n_Q - n_p)$ matrix elements $\langle q|\omega(\rho)|p\rangle$ are obtained by solving this equation system (20). Once the effective *quasi-two-body* Hamiltonian $\mathcal{H}^{[2]eff}$ is constructed, the effective potential is obtained by a subtraction of the hypercentrifugal kinetic energy

$$v_{A,(A-1)}^{[2]eff} = \mathcal{H}^{[2]eff}(\rho) - T_K(\rho). \quad (21)$$

In the following we will denote $v_{A,(A-1)}^{[2]eff}$ simply by $v^{[2]eff}$. Using this ρ -dependent effective potential and taking into account Eqs. (10)–(12), one solves the A -body problem with the effective Hamiltonian

$$H^{[A]eff} = T_\rho + \mathcal{H}^{[A]eff} = T_\rho + T_K + \sum_{i < j} v^{[2]eff} \quad (22)$$

in the P space. One repeats the procedure enlarging the P space up to a convergence of the low-lying energies of the A -body system.

We would like to emphasize the following points.

(i) The hyper-radius is a parameter rather than a coordinate, and $v^{[2]eff}$ is determined for various fixed ρ values; therefore, while being a two-body interaction, it depends on the whole A -body system via this collective coordinate.

(ii) There is an additional dependence of $v^{[2]eff}$ on the quantum number K_{A-2} of the residual system [see Eqs. (19) and (20) of Ref. [4]].

(iii) It is evident that $U(\rho) \rightarrow 1$ for $P \rightarrow 1$ and thus $v^{[2]eff}$ converges to the bare $v_{A,(A-1)}$; therefore the energy spectrum converges to the exact one.

(iv) Via the operator $U(\rho)$ the effective potential $v^{[2]eff}$ contains information about a large part of the PQ -space interaction, hence the convergence to the exact eigenvalues of $H^{[A]}$ is accelerated with respect to the normal HH expansion.

In the present work, we would like to present two extensions of the scheme outlined above: (i) the application of the Lee-Suzuki transformation also to the hyper-radial part of the kinetic energy (Sec. III) and (ii) the incorporation of three-body effective forces (Sec. IV). The aim is to further increase the rate of convergence of the HH expansion.

III. BEYOND THE ADIABATIC APPROXIMATION

In the EHH approach outlined in the preceding section, the Lee-Suzuki unitary transformation is applied to the adiabatic *quasi-two-body* Hamiltonian of Eq. (13). The effective potential is obtained by subtraction of the hypercentrifugal term from the effective Hamiltonian of Eq. (17). One can go beyond this adiabatic approach by applying U of Eq. (18) to the nonadiabatic *quasi-two-body* Hamiltonian

$$H^{[2]}(\rho) = T_\rho + \mathcal{H}^{[2]}(\rho). \quad (23)$$

This leads to a nonadiabatic effective *quasi-two-body* Hamiltonian

$$\begin{aligned} H^{[2]eff} &= U^\dagger(\rho) T_\rho U(\rho) + \mathcal{H}^{[2]eff}(\rho) \\ &= T_\rho + \Delta T_\rho^{eff} + \mathcal{H}^{[2]eff}(\rho). \end{aligned} \quad (24)$$

A new effective interaction is then obtained by subtracting the full kinetic energy

$$\tilde{v}_{A,A-1}^{[2]eff} = H^{[2]eff} - T_K(\rho) - T_\rho = v_{A,A-1}^{[2]eff} + \Delta T_\rho^{eff}. \quad (25)$$

Here, it is worth noticing that like $T_K(\rho)$, also T_ρ satisfies the relation (2). The new effective potential $\tilde{v}_{A,A-1}^{[2]eff}$ differs from the previous $v_{A,A-1}^{[2]eff}$ by the term ΔT_ρ^{eff} , which is given by

$$\begin{aligned} \Delta T_\rho^{eff} &= -\frac{1}{2m} U^\dagger(\rho) \left[\frac{\partial^2 U(\rho)}{\partial \rho^2} + 2 \frac{\partial U(\rho)}{\partial \rho} \partial_\rho \right. \\ &\quad \left. + \frac{3A-4}{\rho} \frac{\partial U(\rho)}{\partial \rho} \right]. \end{aligned} \quad (26)$$

One can also interpret ΔT_ρ^{eff} as an *effective kinetic energy* contribution.

The matrix elements of ΔT_ρ^{eff} have to be evaluated between the HH and hyper-radial basis functions $L_m(\rho), L_n(\rho)$:

$$\begin{aligned} \langle L_n | \Delta T_\rho^{eff} | L_m \rangle &= \frac{1}{2m} \int d\rho^{3A-4} \left[\frac{\partial U^\dagger}{\partial \rho} \frac{\partial U}{\partial \rho} L_n(\rho) L_m(\rho) \right. \\ &\quad \left. + U^\dagger \frac{\partial U}{\partial \rho} \left(L_n \frac{\partial L_m}{\partial \rho} - L_m \frac{\partial L_n}{\partial \rho} \right) \right]. \end{aligned} \quad (27)$$

The first term on the right hand side is manifestly symmetric in the hyper-radial indices (as well as in the HH basis indices). As to the second term, denoting by μ, ν, λ the HH basis functions, one finds

$$\begin{aligned} \sum_\lambda U_{\mu\lambda}^\dagger \frac{\partial U_{\lambda\nu}}{\partial \rho} \left(L_n \frac{\partial L_m}{\partial \rho} - L_m \frac{\partial L_n}{\partial \rho} \right) \\ = \frac{1}{2} \sum_\lambda \left(U_{\lambda\mu}^* \frac{\partial U_{\lambda\nu}}{\partial \rho} - U_{\lambda\nu} \frac{\partial U_{\lambda\mu}^*}{\partial \rho} \right) \left(L_n \frac{\partial L_m}{\partial \rho} - L_m \frac{\partial L_n}{\partial \rho} \right). \end{aligned} \quad (28)$$

It is evident that this second term is an antisymmetric operator for interchange of both HH and hyper-radial indices. Thus, Eq. (27) gives a decomposition of ΔT_ρ^{eff} into its symmetric and antisymmetric parts, $\Delta T_\rho^{eff} = \Delta_S T_\rho^{eff} + \Delta_A T_\rho^{eff}$. Enlarging the model space, U approaches I and the contribution of ΔT_ρ^{eff} diminishes more and more. Therefore, we can estimate its contribution using first order perturbation theory. We find that the effect of $\Delta_A T_\rho^{eff}$ is much smaller in comparison to $\Delta_S T_\rho^{eff}$ (about 1% or less). So we conclude that

$$\Delta T_\rho^{eff} \approx \frac{1}{2m} \frac{\partial U^\dagger}{\partial \rho} \frac{\partial U}{\partial \rho}. \quad (29)$$

IV. THE THREE-BODY EFFECTIVE INTERACTION

The natural way to construct the three-body effective interaction is the generalization of the procedure in Sec. II.

(i) Approximate the matrix element of the A -body effective interaction by

$$V^{[A]eff} \simeq \frac{1}{A-2} \sum_{i < j < k}^A v^{[3]eff}(i, j, k). \quad (30)$$

(ii) Calculate its matrix element via

$$\begin{aligned} \langle V^{[A]eff} \rangle &\simeq \left\langle \frac{1}{A-2} \sum_{i < j < k}^A v^{[3]eff}(i, j, k) \right\rangle \\ &= \frac{A(A-1)}{6} \langle v^{[3]eff}(A, A-1, A-2) \rangle. \end{aligned} \quad (31)$$

(iii) Replace the adiabatic *quasi-two-body* Hamiltonian of Eq. (13) with the adiabatic *quasi-three-body* Hamiltonian

$$\begin{aligned} \mathcal{H}^{[3]}(\rho) &= \frac{1}{2m} \frac{\hat{K}_A^2}{\rho^2} + v_{A,(A-1)} + v_{(A-1),(A-2)} + v_{(A-2),A} \\ &\equiv \frac{1}{2m} \frac{\hat{K}_A^2}{\rho^2} + v^{[3]}(A, A-1, A-2). \end{aligned} \quad (32)$$

(iv) Diagonalize it in the $P+Q$ space of the A -body system.

(v) Calculate the new $\omega(\rho)$ [Eq. (19)] and apply the Lee-Suzuki similarity transformation to obtain $v^{[3]eff}$; add the nonadiabatic effective kinetic energy contribution as outlined in Sec. III, to obtain $\tilde{v}^{[3]eff}$.

(vi) Solve the A -body problem with

$$H^{[A]eff} = T_\rho + \mathcal{H}^{[A]eff} = T_\rho + T_K + \frac{1}{A-2} \sum_{i < j < k} \tilde{v}^{[3]eff}(i, j, k) \quad (33)$$

considering point (ii).

A closer look, however, reveals that solving $\mathcal{H}^{[3]}$ is more complicated than solving the three-body problem. This point will become clearer in the following. While for the two-body effective interaction one needs to consider only the hyperspherical coordinates connected to the A - $(A-1)$ pair explicitly, for the three-body effective interaction one has to take into account additional coordinates. In order to clarify this point, we present the general transformation from the reversed order A -body Jacobi coordinates [Eq. (16)] to hyperspherical coordinates. Each Jacobi vector $\vec{\eta}_j$ consists of a radial coordinate η_j and a pair of angular coordinates $\hat{\eta}_j$. The radial coordinates are transformed into the hyperspherical coordinates $\rho, \theta_2, \dots, \theta_{A-1}$ through the relations

$$\sin \theta_n = \frac{\eta_n}{\rho_n} \quad \text{and} \quad \rho_n^2 = \rho_{n-1}^2 + \eta_n^2 = \sum_{j=1}^n \eta_j^2. \quad (34)$$

Note that the hyper-radial coordinates ρ_n are symmetric with respect to the permutation of particles $1, 2, \dots, n$. The A -body hyper-radial coordinate $\rho \equiv \rho_{A-1}$ is symmetric with respect to any particle permutation. In order to focus on the *interacting* three-body subsystem, we transform the (3A-4) hyperangular coordinates

$$\Omega_A = (\theta_2, \dots, \theta_{A-1}, \hat{\eta}_1, \dots, \hat{\eta}_{A-1}) \quad (35)$$

into a new set of hyperangles

$$\Omega_{3,A-3} = (\theta_2, \dots, \theta_{A-3}, \Theta^{[3,A-3]}, \theta_{int}^{[3]}, \hat{\eta}_1, \dots, \hat{\eta}_{A-1}). \quad (36)$$

The new hyperangles reflect the splitting of the A -body system into a three- and an $(A-3)$ -body subsystems. The hyperangle $\Omega_{3,A-3}$ can be written as

$$\Omega_{3,A-3} = (\Theta^{[3,A-3]}, \Omega_{int}^{[3]}, \Omega_{res}^{[A-3]}), \quad (37)$$

where

$$\Omega_{int}^{[3]} = (\theta_{int}^{[3]}, \hat{\eta}_{A-2}, \hat{\eta}_{A-1}) \quad (38)$$

are the hyperangles of the *interacting* three-body subsystem, and

$$\Omega_{res}^{[A-3]} = (\theta_2, \dots, \theta_{A-3}, \hat{\eta}_1, \dots, \hat{\eta}_{A-3}) \quad (39)$$

are the hyperangles of the *residual* $(A-3)$ -body subsystem. The two new angles $\Theta^{[3,A-3]}, \theta_{int}^{[3]}$, replacing θ_{A-2} and θ_{A-1} , are given through the relations

$$\rho_{int}^{[3]} \equiv \sqrt{\eta_{A-1}^2 + \eta_{A-2}^2} = \rho \sin \Theta^{[3,A-3]}, \quad (40)$$

$$\rho_{A-3} = \rho \cos \Theta^{[3,A-3]} \quad (41)$$

and

$$\eta_{A-1} = \rho_{int}^{[3]} \sin \theta_{int}^{[3]}, \quad (42)$$

$$\eta_{A-2} = \rho_{int}^{[3]} \cos \theta_{int}^{[3]}. \quad (43)$$

The new coordinates $(\rho_{int}^{[3]}, \Omega_{int}^{[3]})$ form a complete set for the three-body problem and $\mathcal{H}^{[3]}$ can be written as

$$\mathcal{H}^{[3]}(\rho) = \frac{1}{2m} \frac{\hat{K}_A^2}{\rho^2} + v^{[3]}(\rho, \Theta^{[3,A-3]}, \Omega_{int}^{[3]}). \quad (44)$$

Now we can proceed to point (iv) of the list above. In order to do so we follow Ref. [11] and construct $v^{[3]eff}$ through a sequence of steps as follows.

Step 1. We solve the Schrödinger equation with the Hamiltonian of Eq. (13) for the A -body system and construct the “nonadiabatic” *two-body* effective interaction $\tilde{v}^{[2]eff}(\rho)$. We label with $K_P^{[2]}$ the top of the P_2 space and with $K_Q^{[2]}$ the top of the Q_2 space.

Step 2. We solve the Schrödinger equation with the Hamiltonian of Eq. (44), replacing the bare interaction $v^{[3]}$ with the sum of the effective two-body interactions $(\tilde{v}_{A,A-1}^{[2]eff} + \tilde{v}_{A-1,A-2}^{[2]eff} + \tilde{v}_{A-2,A}^{[2]eff})$ and construct the effective interaction $\tilde{v}^{[3]eff}(\rho)$. We label with $K_P^{[3]}$ and K_P ($K_P^{[3]} = K_P$) the top of the P_3 and P_A spaces, respectively, and we take $K_Q^{[3]} \equiv K_P^{[2]}$ as top of the Q_3 space.

The main advantage of the proposed scheme lays in the first step, where excitations of the two-body subsystem into the Q_3 -space part of the Q_A space are taken care of, thus accelerating the convergence of Eq. (44). For a better understanding of the effective interaction, we show in Figs. 1 and 2 the various Hilbert spaces of the two-, three-, and A -body

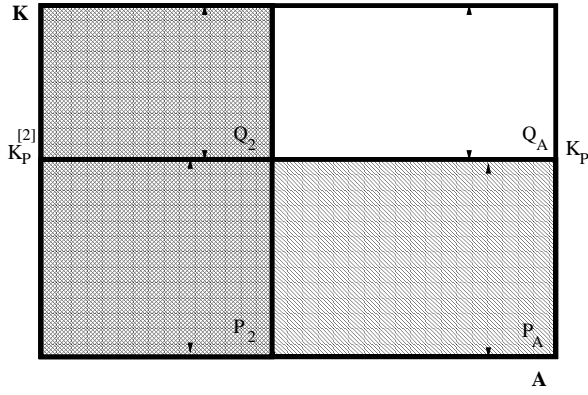


FIG. 1. The various P and Q spaces relevant for the construction of the two-body effective interaction (see text).

systems. In Fig. 1, we illustrate the construction of two-body effective interaction. The hyperangular part of the A -body Hilbert space is divided into a two-body and a residual Hilbert space. The Lee-Suzuki procedure guarantees that $\tilde{v}^{[2]eff}$ takes into account besides P_A also the shaded area Q_2 of the Q_A space. In Fig. 2, the construction of the three-body effective interaction is illustrated. It depicts the spaces P_2 , Q_2 , P_3 , and Q_3 of the three-body HH space. The information about Q_2 is contained via $\tilde{v}^{[2]eff}$ (step 1), while the information about the horizontally shaded area of Q_3 is taken into account via $\tilde{v}^{[3]eff}$ (step 2). The so constructed $\tilde{v}^{[3]eff}$ is used in the A -body system as a bare three-body interaction. One should note that, in the limit in which the A -body P space includes all the horizontally shaded area of Q_3 space, one remains with the two-body effective interaction.

It should be noticed that there are three *energy scales* in the scheme. The first scale is that determined by $K_Q^{[2]}$. This should be fixed so that the lower eigenenergies of $\mathcal{H}^{[2]}$ for the “three-body” problem are in convergence. In accordance, the three-body scale determined by $K_Q^{[3]} \equiv K_P^{[2]} < K_Q^{[2]}$ has to be high enough, so that the lower eigenenergies of $\mathcal{H}^{[3]}$ for the “three-body” problem are also in convergence. The third scale $K_P \equiv K_P^{[3]} < K_Q^{[3]}$ should be varied until the spectra of the A -body system is established. It should be

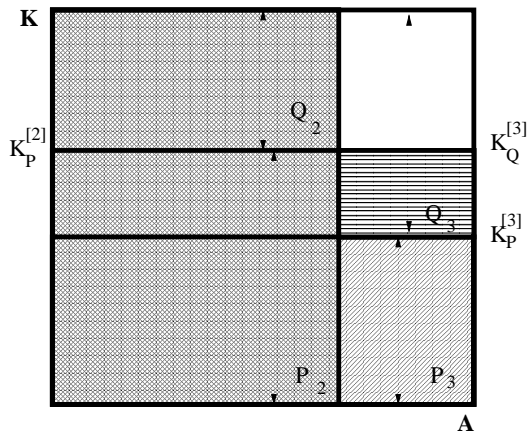


FIG. 2. The various P and Q spaces relevant for the construction of the three-body effective interaction (see text).

TABLE I. Convergence of the HH expansion for the ${}^4\text{He}$ ground state energy (in MeV) with the AV8' potential. Here H_{eff} stands for the effective Hamiltonian in the adiabatic approximation, and $H_{eff} + \Delta_S T_\rho^{eff}$ is the effective Hamiltonian including the nonadiabatic correction $\Delta_S T_\rho^{eff}$. The reference energy is taken to be $E_\infty = -25.934$ (MeV) (see text).

K_{max}	$\langle H_{eff} \rangle$	$ E - E_\infty $	$\langle H_{eff} + \Delta_S T_\rho^{eff} \rangle$	$ E - E_\infty $	$\langle \Delta_S T_\rho^{eff} \rangle$
2	-27.522	1.588	-25.464	0.470	2.058
4	-28.135	2.201	-27.052	1.118	1.083
6	-27.004	1.070	-26.498	0.564	0.506
8	-26.672	0.738	-26.421	0.487	0.250
10	-26.081	0.147	-25.949	0.015	0.131
12	-26.135	0.201	-26.064	0.130	0.070
14	-26.004	0.070	-25.963	0.029	0.040
16	-25.977	0.043	-25.953	0.019	0.024
18	-25.944	0.010	-25.929	0.005	0.015
20	-25.944				

evident from the above discussion that using two-, three-, and if possible more-body effective interactions, the convergence of the spectrum of the A -body system should become faster and faster since the information on large parts of the Q space are already taken into account via those effective operators.

The actual calculation of the three-body effective interaction is quite complicated and technically rather challenging. The difficulty has its origin in the separation of the A -body system into two subsystems [the interacting three- and the residual ($A-3$)-body systems]. Expressing the A -body matrix elements of the interaction in terms of the matrix elements for the three-body subsystems, one has to pay the price of evaluating the overlap between the antisymmetric A -body basis functions and basis functions constructed in the ($3, A-3$) scheme. In the Appendix, it is described in detail how such matrix elements are calculated.

V. RESULTS AND DISCUSSION

Results for the nonadiabatic kinetic energy contribution and the three-body effective interaction are studied for the binding energies of ${}^4\text{He}$ and ${}^6\text{Li}$ using semirealistic and more realistic NN interactions. First, we discuss the importance of the effective kinetic energy $\Delta_S T_{eff}$. We choose a case that has been considered in a recent benchmark paper [5] presenting in Table I results for the ${}^4\text{He}$ ground state energy with the Argonne AV8' NN force [12]. The result for the calculation with the effective Hamiltonian in the adiabatic approximation at $K_{max}=20$ is our EHH result published in Ref. [5]. It was obtained in a rather time consuming calculation which we were not able to repeat this time and thus other results are only shown up to $K_{max}=18$. From the table it is evident that $\Delta_S T_{eff}$ has a rather regular convergence pattern. This enables us to estimate $\Delta_S T_{eff}$ also for $K_{max}=20$ leading to the value of about 10 keV. With this result we estimate a binding energy of 25.934 MeV for the nonadiabatic calculation at $K_{max}=20$. This value is used as a reference energy in Table I. One sees that the rates of con-

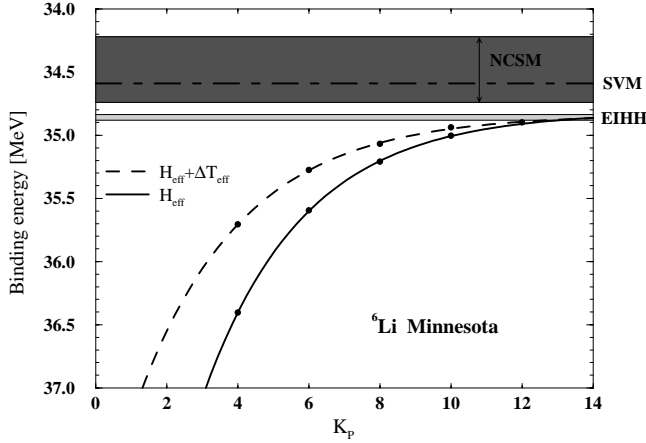


FIG. 3. Convergence of the HH expansion for the ${}^6\text{Li}$ ground state energy with the Minnesota NN potential. The solid (dashed) line connects the results of the adiabatic (nonadiabatic) effective two-body interaction calculation. The dashed area corresponds to the energy range $E_\infty = -34.86 \pm 0.02$ (MeV) (see text). Also given the SVM [2] (dot-dashed line) and NCSM [14] (shaded area) results.

vergence for adiabatic and nonadiabatic calculations are quite similar, but it is also evident that the inclusion of $\Delta_S T_{eff}$ improves the results considerably. It reduces the difference to the reference energy for any value of K_{max} by about a factor of 2.

In Fig. 3, we present the effect of the nonadiabatic term on the convergence of the binding energy of ${}^6\text{Li}$ with the Minnesota NN force [13]. The effect of $\Delta_S T_{eff}$ is very similar to the just discussed ${}^4\text{He}$ case again leading to a considerable improvement of the convergence of the ground state energy. In order to estimate the converged binding energy ($K_p \rightarrow \infty$), we fit the results of the nonadiabatic calculation with the formula $E(K) = E_\infty + C e^{-\alpha K}$. Using all the points from $K=4$ to $K=12$ we obtain $E_\infty = -34.836$ MeV, while using only the three higher values ($K=8, 10, 12$) we find $E_\infty = -34.881$ MeV. With these results we estimate a converged value of $E_{gs} = -34.86 \pm 0.02$ [MeV]. A comparison with available results of other methods (SVM [2], NCSM [14]) is shown in Table II. There is a difference of about 200–400 keV between the different methods. In order to improve the comparison further convergence checks should be made in the various calculations.

Next we discuss the effect of the three-body effective interaction. The convergence of the calculation with $\tilde{v}^{[3]eff}$ depends, of course, on the size of the model space $P_A(K_p)$, but also on the size of the Q_3 space ($K_Q^{[3]}$). As described in

TABLE II. Results for the ${}^6\text{Li}$ ground state energy (in MeV) with the Minnesota potential.

Method	E_{gs} (MeV)
EIHH	-34.86 ± 0.02
NCSM [14]	-34.48 ± 0.26
SVM [2]	-34.59

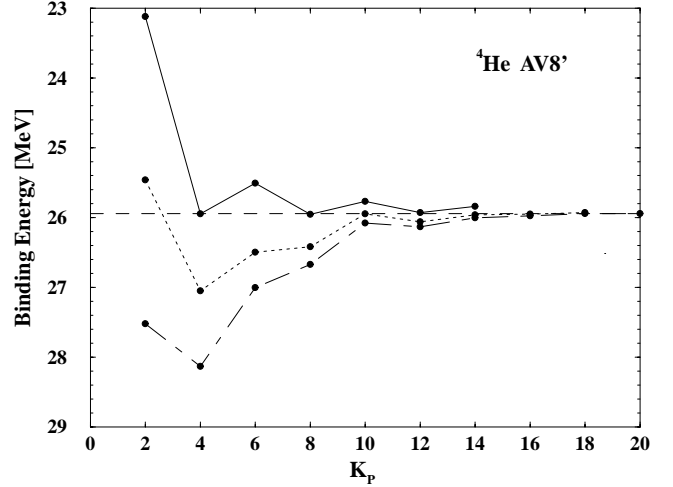


FIG. 4. Convergence of the HH expansion for the ${}^4\text{He}$ ground state energy with the AV8' NN potential. The dot-dashed (dotted) line connects the results of the adiabatic (nonadiabatic) two-body effective calculation and the solid line the results of the nonadiabatic three-body effective interaction.

Sec. IV, both spaces enter in the construction of $\tilde{v}^{[3]eff}$. In the calculation, one encounters computational difficulties due to the fact that one has to solve many different “three-body” systems. Taking into account each hyper-radial grid point, each value of K_{A-3} and the possible values of J_3, T_3, T_3^z the number of “three-body” systems one has to consider amounts to a few thousand. For a $K_Q^{[3]}$ of about 20 the average number of basis states is about 1500. Thus one faces the problem of diagonalizing a matrix of 1500×1500 a few thousand times. The computational effort can be reduced if one restricts the range of J_3 values for which $\tilde{v}^{[3]eff}$ is constructed.

In Fig. 4, the convergence of the ${}^4\text{He}$ ground state energy is shown for the AV8' NN potential as function of K_p with $K_Q^{[3]} = 24$ and limiting value of $J_3 = 3/2$. With respect to the last two quantum numbers one finds an excellent convergence of the three-body effective interaction. In fact with $K_Q^{[3]} = 20$ and $J_3 = 1/2$ one has essentially the same results as those shown in Fig. 4. We would like to emphasize once again that for $K_p^{[3]} = K_Q^{[3]}$ one gets the identical results with two- and three-body effective interactions. Therefore the advantage of the three-body effective interaction can only be a faster convergence for the lower $K_p^{[3]}$ values. In fact the results of Fig. 4 show that this is the case. This is particularly important for systems with more than four particles, where one cannot easily work with larger P_A spaces. In order to study this point better, we have considered with ${}^6\text{Li}$ also a six-body system. Different from the ${}^6\text{Li}$ case above (see discussion of Fig. 3), where we use the semirealistic central Minnesota potential, we take the more realistic AV8' potential. Such a more realistic potential model leads to a P space, which grows very fast with K_p . At present we can consider only $K_p \leq 6$. The results of our calculation are shown in Fig. 5. One sees that in contrast to the discussed four-body cases, the six-body binding energy depends very much on the limiting value of J_3 . Though we are restricted to relatively small

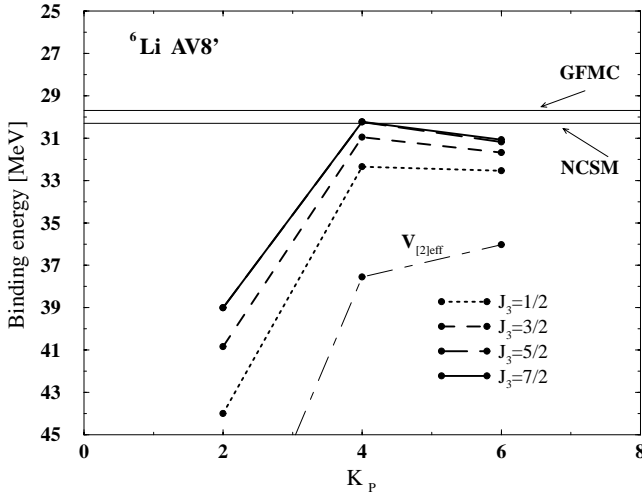


FIG. 5. Convergence of the HH expansion for the ${}^6\text{Li}$ ground state energy with the AV8' NN potential. The dotted, dashed, and the thick solid line connect the results for the nonadiabatic three-body effective interaction with different limiting values of J_3 as illustrated in the figure. The dash-dotted line connects the results for the nonadiabatic two-body effective interaction. The thin solid lines stand for GFMC [20] and NCSM [14] results as marked in the figure.

values of K_p , it can be seen that the obtained energy is in reasonable agreement with those of other methods.

We summarize our results as follows. We have extended the HH effective interaction method in two different directions. On one hand we include a nonadiabatic correction for the hyper-radial kinetic energy and on the other hand we introduce a three-body HH effective interaction. Both extensions accelerate the convergence of the HH expansion for the binding energy as explicitly shown for the cases of ${}^4\text{He}$ and ${}^6\text{Li}$, where for both nuclei we used semirealistic, but also more realistic NN interactions. The nonadiabatic correction leads to better converged energies for all grandangular momentum values K , while for the three-body HH effective interaction one obtains particularly strong improvements for lower K values. Our results show that the improved HH effective interaction facilitates more realistic calculations for p -shell nuclei. With an increase of computational efforts (parallelization of the codes, more powerful computers) it will be possible to bring our calculations to a better convergence in the near future. We would also like to point out that the three-body effective interaction opens up the way for incorporating genuine three-body forces in the EHH method.

ACKNOWLEDGMENT

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APPENDIX: MATRIX ELEMENTS FOR THREE-BODY INTERACTION

A meaningful effective interaction can be derived from $\mathcal{H}^{[3]}$, only if we employ a physical basis set consisting of

functions antisymmetric with respect to three-body permutations and with good three-body and A -body quantum numbers $(J_3, J_3^z, T_3, T_3^z, J_A, J_A^z, T_A, T_A^z)$. The construction of such basis functions and the evaluation of the Hamiltonian matrix elements are given below.

The antisymmetric A -body hyperspherical-spin-isospin basis functions with total angular momentum J_A , J_A^z and isospin $T_A T_A^z$ can be written as

$$\begin{aligned} & |K_A J_A J_A^z T_A T_A^z \Gamma_A \alpha_A \beta_A \rangle \\ &= \sum_{Y_{A-1}} \frac{\Lambda_{\Gamma_A, Y_{A-1}}}{\sqrt{|\Gamma_A|}} [|K_A L_A M_A \Gamma_A Y_{A-1} \alpha_A \rangle \\ & \times |S_A S_A^z T_A T_A^z \tilde{\Gamma}_A, \tilde{Y}_{A-1} \beta_A \rangle]^{J_A J_A^z}, \end{aligned} \quad (\text{A1})$$

where

$$\langle \Omega_A | K_A L_A M_A \Gamma_A Y_{A-1} \alpha_A \rangle \equiv \mathcal{Y}_{K_A L_A M_A \Gamma_A Y_{A-1} \alpha_A}^{[A]}(\Omega_A) \quad (\text{A2})$$

are HH functions with hyperspherical angular momentum $K=K_A$, and orbital angular momentum quantum numbers L_A, M_A that belong to well defined irreducible representations (irreps) $\Gamma_1 \in \Gamma_2 \in \dots \in \Gamma_A$ of the permutation group-subgroup chain $\mathcal{S}_1 \subset \mathcal{S}_2 \subset \dots \subset \mathcal{S}_A$, denoted by the Yamanouchi symbol $[\Gamma_A, Y_{A-1}] \equiv [\Gamma_A, \Gamma_{A-1}, \dots, \Gamma_1]$. The dimension of the irrep Γ_m is denoted by $|\Gamma_m|$ and $\Lambda_{\Gamma_A, Y_{A-1}}$ is a phase factor [15]. Similarly, the functions

$$\begin{aligned} & \langle s_1^z \dots s_A^z, t_1^z \dots t_A^z | S_A S_A^z T_A T_A^z \tilde{\Gamma}_A, \tilde{Y}_{A-1} \beta_A \rangle \\ & \equiv \chi_{S_A S_A^z T_A T_A^z \tilde{\Gamma}_A, \tilde{Y}_{A-1} \beta_A}^{[A]}(s_1^z \dots s_A^z, t_1^z \dots t_A^z) \end{aligned} \quad (\text{A3})$$

are the symmetrized spin-isospin basis functions. The quantum numbers α_A, β_A are used to remove the degeneracy of the HH and spin-isospin states, respectively.

In analogy to Eq. (A1), we can construct antisymmetric three-body basis functions that correspond to the particles $A, A-1, A-2$ and to the Jacobi vectors $\vec{\eta}_{A-1}, \vec{\eta}_{A-2}$ as

$$\begin{aligned} & |K_3 J_3 J_3^z T_3 T_3^z \Gamma_3 \alpha_3 \beta_3 \rangle = \sum_{Y_2} \frac{\Lambda_{\Gamma_3, Y_2}}{\sqrt{|\Gamma_3|}} [|K_3 L_3 M_3 \Gamma_3 Y_2 \alpha_3 \rangle \\ & \times |S_3 S_3^z T_3 T_3^z \tilde{\Gamma}_3, \tilde{Y}_2 \beta_3 \rangle]^{J_3 J_3^z} \end{aligned} \quad (\text{A4})$$

and the antisymmetric $(A-3)$ -body basis functions that correspond to the particles $1, 2, \dots, A-3$ and to the Jacobi vectors $\vec{\eta}_1, \dots, \vec{\eta}_{A-3}$ [note that these $(A-3)$ Jacobi vectors contain also the relative orientation of the three- and the $(A-3)$ -body subsystems] as

$$\begin{aligned}
& |K_{A-3}J_{A-3}J_{A-3}^z T_{A-3}T_{A-3}^z \Gamma_{A-3} \alpha_{A-3} \beta_{A-3} \rangle \\
&= \sum_{Y_{A-4}} \frac{\Lambda_{\Gamma_{A-3}, Y_{A-4}}}{\sqrt{|\Gamma_{A-3}|}} [|K_{A-3}L_{A-3}M_{A-3} \Gamma_{A-3} Y_{A-4} \alpha_{A-3} \rangle \\
&\quad \times |S_{A-3}S_{A-3}^z T_{A-3}T_{A-3}^z \tilde{\Gamma}_{A-3}, \tilde{Y}_{A-4} \beta_{A-3} \rangle]^{J_{A-3}J_{A-3}^z}. \quad (A5)
\end{aligned}$$

The corresponding HH functions are given by

$$\begin{aligned}
& | (K_3 J_3 T_3 \Gamma_3 \alpha_3 \beta_3; K_{A-3} J_{A-3} T_{A-3} \Gamma_{A-3} \alpha_{A-3} \beta_{A-3}) K_A J_A J_A^z T_A T_A^z \rangle \\
&= \mathcal{N}_n^{a,b} (\sin \Theta^{[3,A-3]})^{K_3} (\cos \Theta^{[3,A-3]})^{K_{A-3}} P_n^{(a,b)} (\cos 2\Theta^{[3,A-3]}) \\
&\quad \times [|K_3 J_3 J_3^z T_3 T_3^z \Gamma_3 \alpha_3 \beta_3 \rangle |K_{A-3} J_{A-3} J_{A-3}^z T_{A-3} T_{A-3}^z \Gamma_{A-3} \alpha_{A-3} \beta_{A-3} \rangle]^{J_A J_A^z T_A T_A^z}. \quad (A8)
\end{aligned}$$

Here $P_n^{(a,b)}$ are the Jacobi polynomials, with the arguments

$$a = K_3 + 2, \quad (A9)$$

$$b = K_{A-3} + \frac{3A-11}{2}, \quad (A10)$$

$$n = \frac{K_A - K_{A-3} - K_3}{2}. \quad (A11)$$

The numerical factor

$$\mathcal{N}_n^{a,b} = \sqrt{\frac{2(2n+a+b)n! \Gamma(n+a+b+1)}{\Gamma(n+a+1) \Gamma(n+b+1)}} \quad (A12)$$

is a normalization constant.

For the sake of brevity we use the following notations:

$$[K_3] \equiv K_3 J_3 J_3^z T_3 T_3^z \Gamma_3 \alpha_3 \beta_3,$$

$$[K_{A-3}] \equiv K_{A-3} J_{A-3} J_{A-3}^z T_{A-3} T_{A-3}^z \Gamma_{A-3} \alpha_{A-3} \beta_{A-3},$$

$$\langle \Omega_{int}^{[3]} | K_3 L_3 M_3 \Gamma_3 Y_2 \alpha_3 \rangle \equiv \mathcal{Y}_{K_3 L_3 M_3 \Gamma_3 Y_2 \alpha_3}^{[3]} (\Omega_{int}^{[3]}), \quad (A6)$$

$$\begin{aligned}
& \langle \Omega_{res}^{[A-3]} | K_{A-3} L_{A-3} M_{A-3} \Gamma_{A-3} Y_{A-4} \alpha_{A-3} \rangle \\
& \equiv \mathcal{Y}_{K_{A-3} L_{A-3} M_{A-3} \Gamma_{A-3} Y_{A-4} \alpha_{A-3}}^{[A-3]} (\Omega_{res}^{[A-3]}), \quad (A7)
\end{aligned}$$

and equivalent expressions for the spin-isospin part. These two sets of basis functions, Eqs. (A4) and (A5), can be combined into an A -body HH basis function with quantum numbers $K_A J_A J_A^z T_A T_A^z$ through the relation

and

$$[K_A] \equiv K_A J_A J_A^z T_A T_A^z \Gamma_A \alpha_A \beta_A.$$

With the help of these notations Eq. (A8) can be rewritten as

$$\begin{aligned}
& | ([K_3]; [K_{A-3}]) K_A J_A J_A^z T_A T_A^z \rangle \\
&= \mathcal{N}_n^{a,b} (\sin \Theta^{[3,A-3]})^{K_3} \\
&\quad \times (\cos \Theta^{[3,A-3]})^{K_{A-3}} P_n^{(a,b)} (\cos 2\Theta^{[3,A-3]}) \\
&\quad \times [| [K_3] \rangle | [K_{A-3}] \rangle]^{J_A J_A^z T_A T_A^z}. \quad (A13)
\end{aligned}$$

The basis of Eq. (A13) is the desired one for the calculation of the three-body effective interaction, as the residual $(A-3)$ -body subsystem is factorized out.

Using these basis functions one can easily reduce the A -body matrix elements of a scalar-isoscalar three-body operator into the matrix elements of the three-body subsystem,

$$\begin{aligned}
\langle [K_A] | v^{[3]}(A, A-1, A-2) | [K'_A] \rangle &= \sum_{[K_3], [K'_3], [K_{A-3}], [K'_{A-3}]} \langle [K_A] | ([K_3]; [K_{A-3}]) K_A J_A J_A^z T_A T_A^z \rangle \\
&\quad \times \langle [K'_A] | ([K'_3]; [K'_{A-3}]) K'_A J'_A J'^z_A T'_A T'^z_A \rangle * \langle ([K_3]; [K_{A-3}]) \\
&\quad \times K_A J_A J_A^z T_A T_A^z | v^{[3]}(\rho^{[3]}, \Omega^{[3]}) | ([K'_3]; [K'_{A-3}]) K'_A J'_A J'^z_A T'_A T'^z_A \rangle. \quad (A14)
\end{aligned}$$

The matrix elements $\langle [K_A] | ([K_3]; [K_{A-3}]) K_A J_A J_A^z T_A T_A^z \rangle$ are the overlaps between the A -body functions, Eq. (A1), and the $(3, A-3)$ -body functions, Eq. (A13). The potential matrix element can be conveniently written as

$$\begin{aligned}
& \langle ([K_3]; [K_{A-3}]) K_A J_A J_A^z T_A T_A^z | v^{[3]}(\rho^{[3]}, \Omega^{[3]}) | ([K'_3]; [K'_{A-3}]) K'_A J'_A J'^z_A T'_A T'^z_A \rangle \\
&= \delta_{J_A, J'_A} \delta_{T_A, T'_A} \delta_{[K_{A-3}], [K'_{A-3}]} \delta_{J_3, J'_3} \delta_{T_3, T'_3} \delta_{J_A^z, J'^z_A} \delta_{T_A^z, T'^z_A} V_{[K_3] K_A, [K'_3] K'_A}^{[3, K_{A-3}]}(\rho), \quad (A15)
\end{aligned}$$

with

$$\begin{aligned}
V_{[K_3]K_A, [K'_3]K'_A}^{[3 K_{A-3}]}(\rho) &= \sum_{\Gamma_2 \Gamma'_2} \Lambda_{\Gamma_3 \Gamma_2} \Lambda_{\Gamma_2 \Gamma_1} \Lambda_{\Gamma'_3 \Gamma'_2} \Lambda_{\Gamma'_2 \Gamma_1} \frac{1}{\sqrt{|\Gamma_3| |\Gamma'_3|}} \\
&\times \sum_{\ell_2 \ell'_2 \ell_1 \ell'_1} \sum_{\alpha_2 \alpha'_2} \Pi H S C F P_3 \quad \Pi H S C F P'_3 \sum_{T_2 T'_2} \sum_{S_2 S'_2} \Pi T S C F P_3 \quad \Pi T S C F P'_3 V_{[K_3]_u K_A, [K'_3]_u K'_A}^{[3 K_{A-3}]}(\rho),
\end{aligned} \tag{A16}$$

where the products of the three-body coefficients of fractional parentage (CFPs [17,18]) are given by

$$\begin{aligned}
\Pi H S C F P_3 &= \langle K_3 L_3 \Gamma_2 \alpha_2 | K_3 L_3 \Gamma_3 \alpha_3 \rangle \\
&\times \langle (\ell_1 \Gamma_1; \ell_2) K_3 L_3 | K_3 L_3 \Gamma_2 \alpha_2 \rangle,
\end{aligned} \tag{A17}$$

$$\begin{aligned}
\Pi T S C F P_3 &= \langle S_3 S_2 T_3 T_2, \tilde{\Gamma}_2 \beta_2 | S_3 T_3 \tilde{\Gamma}_3 \beta_3 \rangle \\
&\times \langle S_2, S_1 T_2, T_1 \tilde{\Gamma}_1 \beta_1 | S_2, T_2, \tilde{\Gamma}_2 \beta_2 \rangle,
\end{aligned} \tag{A18}$$

and the notation $[K_3]_u$ stands for the unsymmetrized three-body HH-spin-isospin state,

$$|[K_3]_u\rangle \equiv |[(\ell_1; \ell_2) K_3 L_3; S_1 S_2 S_3] J_3 T_1 T_2 T_3\rangle.$$

Here S_1 (T_1) stands for the spin (isospin) of particle $A-2$, while S_3 (T_3) stands for the total spin (isospin) of the three-body subsystem. It should be noted however that in $[K_3]_u$, ℓ_2 stands for the relative angular momentum of particles A and $A-1$ but S_2 , (T_2) is the coupled spin (isospin) quantum number of particles $A-1$ and $A-2$ (and therefore the notation $2'$).

Using standard angular momentum technique it is easy to evaluate the matrix elements

$$\begin{aligned}
&\langle [(\ell_1; \ell_2) L_3; S_1 S_2 S_3] J_3 T_1 T_2 T_3 \\
&\times |[(\ell_1; S_1) J_1 (\ell_2; S_2) J_2] J_3 T_1 T_2 T_3\rangle,
\end{aligned}$$

where S_2 (T_2) is the spin (isospin) quantum number of particles A and $A-1$. The basis

$$|[K_3]_n\rangle \equiv |[(\ell_1; S_1) J_1 (\ell_2; S_2) J_2] K_3 J_3 T_1 T_2 T_3\rangle$$

is the most convenient one for evaluating matrix elements of two-body and three-body forces. Let us start by considering the case of three-body forces. We can use Eqs. (40) and (A13) to get

$$\begin{aligned}
V_{[K_3]_n K_A, [K'_3]_n K'_A}^{[3 K_{A-3}]}(\rho) &= \mathcal{N}_n^{a,b} \mathcal{N}_{n'}^{a',b} \int_0^{\pi/2} d\Theta^{[3,A-3]} (\sin \Theta^{[3,A-3]})^{K_3 + K'_3 + 5} \\
&\times (\cos \Theta^{[3,A-3]})^{2K_{A-3} + 3A - 10} P_n^{(a,b)} \\
&\times (\cos 2\Theta^{[3,A-3]}) P_{n'}^{(a',b)} (\cos 2\Theta^{[3,A-3]}) \\
&\times W_{[K_3], [K'_3]}(\rho_{int}^{[3]}),
\end{aligned} \tag{A19}$$

where $W_{[K_3], [K'_3]}$ stands for the three-body matrix elements

$$W_{[K_3], [K'_3]}(\rho_{int}^{[3]}) = \langle [K_3] | v^{[3]}(\rho_{int}^{[3]}, \Omega^{[3]}) | [K'_3] \rangle \tag{A20}$$

of either a genuine or a pseudo-three-body force

$$v^{[3]}(\rho_{int}^{[3]}, \Omega^{[3]}) = v_{A, (A-1)} + v_{(A-1), (A-2)} + v_{(A-2), A}.$$

An alternative way for calculating matrix elements of the latter case can be realized by

$$\begin{aligned}
V_{[K_3]_n K_A, [K'_3]_n K'_A}^{[3 K_{A-3}]}(\rho) &= 3 \sum_{K_{A-2}} T_{K_3, K_{A-2}}^{K_A; \ell_2 \ell_1 K_{A-3}} T_{K'_3, K_{A-2}}^{K'_A; \ell'_2 \ell'_1 K_{A-3}} \\
&\times V_{(\ell_2 S_2) J_2 T_2 K_A, (\ell'_2 S'_2) J_2 T_2 K'_A}^{[2 K_{A-2}]}(\rho),
\end{aligned} \tag{A21}$$

where the HH transformation coefficients $T_{K_{ab}, K_{bc}}^{K_a K_b K_c}$ first derived by Kil'dyushov [19] are the HH analogs of the $6j$ symbol. The two-body matrix elements can now be reduced to an one-dimensional integral as

$$\begin{aligned}
V_{(\ell_2 S_2) J_2 T_2 K_A, (\ell'_2 S'_2) J_2 T_2 K'_A}^{[2 K_{A-2}]}(\rho) &= \mathcal{N}_n^{a,b} \mathcal{N}_{n'}^{a',b} \int_0^{\pi/2} d\theta_{A-1} (\sin \theta_{A-1})^{\ell_2 + \ell'_2 + 2} \\
&\times (\cos \theta_{A-1})^{2K_{A-2} + 3A - 7} P_n^{(a,b)} \\
&\times (\cos 2\theta_{A-1}) P_{n'}^{(a',b)} (\cos 2\theta_{A-1}) \\
&\times \langle (\ell_2 S_2) J_2 T_2 | v^{[2]}(\sqrt{2}\rho \sin \theta_{A-1}) | (\ell'_2 S'_2) J_2 T_2 \rangle
\end{aligned} \tag{A22}$$

with

$$a = \ell_2 + \frac{1}{2}, \tag{A23}$$

$$b = K_{A-2} + \frac{3A-8}{2}, \tag{A24}$$

$$n = \frac{K_A - K_{A-2} - \ell_2}{2}. \tag{A25}$$

It should be noted that $V_{[K_3]K_A, [K'_3]K'_A}^{[3 K_{A-3}]}(\rho)$ are the matrix elements that appear when evaluating the adiabatic *quasi-three-*

body Hamiltonian of Eq. (32). Recalling that $[K_3]$ is a complete set of quantum numbers for the three-body system one understands why Eq. (32) is more complicated than a three-body bound state problem, where quantum numbers for total angular momentum and isospin are fixed. As pointed out above, for a genuine three-body force one has to consider the matrix elements $W_{[K_3],[K'_3]}$, they are exactly those that are needed in the three-body problem. Therefore, our formulation is very convenient for such a case. If one considers only genuine two-body forces, one can use Eq. (A21) replacing

the potential matrix elements by the matrix elements of the two-body effective interaction. This simplifies the construction of the three-body effective potential.

In order to complete our discussion, we evaluate the product

$$\langle [K_A] | ([K_3]; [K_{A-3}]) K_A J_A J_A^z T_A T_A^z \rangle.$$

This matrix element is evaluated with the help of $6j$ and $9j$ symbols, the hyperspherical CFPs and the spin-isospin CFPs [16],

$$\begin{aligned} \langle [K_A] | ([K_3]; [K_{A-3}]) K_A J_A J_A^z T_A T_A^z \rangle &= \sqrt{(2J_{A-3}+1)(2J_3+1)(2S_A+1)(2L_A+1)} \begin{Bmatrix} S_3 & S_{A-3} & S_A \\ L_3 & L_{A-3} & L_A \\ J_3 & J_{A-3} & J_A \end{Bmatrix} \\ &\times \sum_{\Gamma_{A-1}\Gamma_{A-2}\Gamma_2} \Lambda_{\Gamma_A, \Gamma_{A-1}} \Lambda_{\Gamma_{A-1}, \Gamma_{A-2}} \Lambda_{\Gamma_{A-2}, \Gamma_{A-3}} \Lambda_{\Gamma_3, \Gamma_2} \Lambda_{\Gamma_2, \Gamma_1} \sqrt{\frac{|\Gamma_{A-3}|}{|\Gamma_A||\Gamma_3|}} \\ &\times \langle K_A L_A Y_A \alpha_A | (K_3 L_3 Y_3 \alpha_3; K_{A-3} L_{A-3} Y_{A-3} \alpha_{A-3}) K_A L_A \rangle \\ &\times \langle S_A T_A \tilde{Y}_A \beta_A | (S_3 T_3 \tilde{Y}_3 \beta_3; S_{A-3} T_{A-3} \tilde{Y}_{A-3} \beta_{A-3}) S_A T_A \rangle. \end{aligned} \quad (\text{A26})$$

The hyperspherical matrix elements are then written as

$$\begin{aligned} \langle K_A L_A Y_A \alpha_A | (K_3 L_3 Y_3 \alpha_3; K_{A-3} L_{A-3} Y_{A-3} \alpha_{A-3}) K_A L_A \rangle &= \sum_{\alpha_{A-1}} \sum_{K_{A-2} L_{A-2} \alpha_{A-2}} \sum_{\ell_2 \ell_1} \sum_{\alpha_3 \alpha_2} \Pi H S C F P_A \Pi H S C F P_3 \langle (K_{A-3} L_{A-3}; \ell_1) \\ &\times K_{A-2} L_{A-2}; \ell_2 \rangle K_A L_A | (K_{A-3} L_{A-3}; (\ell_1; \ell_2) K_3 L_3) K_A L_A \rangle, \end{aligned} \quad (\text{A27})$$

where the CFPs products are given by Eq. (A17), and

$$\begin{aligned} \Pi H S C F P_A &= \langle K_A L_A \Gamma_{A-1} \alpha_{A-1} | K_A L_A \Gamma_A \alpha_A \rangle \langle (K_{A-2} L_{A-2} \Gamma_{A-2} \alpha_{A-2}; \ell_2) K_A L_A | K_A L_A \Gamma_{A-1} \alpha_{A-1} \rangle \\ &\times \langle (K_{A-3} L_{A-3} \Gamma_{A-3} \alpha_{A-3}; \ell_1) K_{A-2} L_{A-2} | K_{A-2} L_{A-2} \Gamma_{A-2} \alpha_{A-2} \rangle. \end{aligned} \quad (\text{A28})$$

The spin-isospin term is evaluated in a similar way as follows:

$$\begin{aligned} \langle S_A T_A \tilde{Y}_A \beta_A | (S_3 T_3 \tilde{Y}_3 \beta_3; S_{A-3} T_{A-3} \tilde{Y}_{A-3} \beta_{A-3}) S_A T_A \rangle &= \sum_{S_{A-1} T_{A-1} \beta_{A-1}} \sum_{S_{A-2} T_{A-2} \beta_{A-2}} \Pi T S C F P_A \\ &\times \sum_{S_2' T_2' \beta_2} \Pi T S C F P_3 \langle S_{A-3} S_{A-2} S_{A-1} S_A | (S_{A-3}; S_2' S_3) S_A \rangle \langle T_{A-3} T_{A-2} T_{A-1} T_A | (T_{A-3}; T_2' T_3) T_A \rangle \end{aligned} \quad (\text{A29})$$

with CFPs products

$$\begin{aligned} \Pi T S C F P_A &= \langle S_A S_{A-1} T_A T_{A-1} \tilde{\Gamma}_{A-1} \beta_{A-1} | S_A T_A \tilde{\Gamma}_A \beta_A \rangle \langle S_{A-1} S_{A-2} T_{A-1} T_{A-2} \tilde{\Gamma}_{A-2} \beta_{A-2} | S_{A-1} T_{A-1} \tilde{\Gamma}_{A-1} \beta_{A-1} \rangle \\ &\times \langle S_{A-2} S_{A-3} T_{A-2} T_{A-3} \tilde{\Gamma}_{A-3} \beta_{A-3} | S_{A-2} T_{A-2} \tilde{\Gamma}_{A-2} \beta_{A-2} \rangle \end{aligned} \quad (\text{A30})$$

and Eq. (A17). The remaining HH and spin-isospin matrix elements can then be easily evaluated using standard hyperspherical and angular momentum techniques,

$$\begin{aligned} &\langle [(K_{A-3} L_{A-3}; \ell_1) K_{A-2} L_{A-2}; \ell_2] K_A L_A | [K_{A-3} L_{A-3}; (\ell_1; \ell_2) K_3 L_3] K_A L_A \rangle \\ &= \sqrt{(2L_{A-2}+1)(2L_3+1)} (-)^{L_A+L_{A-3}+\ell_1+\ell_2} \begin{Bmatrix} \ell_2 & \ell_1 & L_3 \\ L_{A-3} & L_A & L_{A-2} \end{Bmatrix} T_{K_3, K_{A-2}}^{K_A; \ell_2 \ell_1 K_{A-3}} \end{aligned} \quad (\text{A31})$$

and

$$\begin{aligned}
\langle T_{A-3}T_{A-2}T_{A-1}T_A | (T_{A-3}; T_2, T_3) T_A \rangle &= \sum_{T_2} (-)^{T_{A-2}+T_{A-3}+T_2+T_3+2T_A+3} (2T_2+1) \\
&\times \sqrt{(2T_{A-1}+1)(2T_{A-2}+1)(2T_3+1)(2T_2'+1)} \begin{Bmatrix} T_{A-2} & t & T_{A-1} \\ t & T_A & T_2 \end{Bmatrix} \\
&\times \begin{Bmatrix} T_{A-3} & t & T_{A-2} \\ T_2 & T_A & T_3 \end{Bmatrix} \begin{Bmatrix} t & t & T_2 \\ t & T_3 & T_2' \end{Bmatrix}. \tag{A32}
\end{aligned}$$

Here $t = \frac{1}{2}$ stands for the isospin of a single nucleon. The spin matrix element can be obtained by simply replacing in Eq. (A32) the isospin quantum numbers by corresponding spin quantum numbers.

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