Matrix elements of potentials in the correlation-function hyperspherical-harmonic method

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(Received 9 April 1990)

Matrix elements of two-body potentials and correlation functions between three- and four-body hyperspherical states, including their velocity-dependent parts, are calculated analytically for any value of the total orbital angular momentum. The resulting formulas contain explicitly written functions of the radial variable, and the Raynal-Revai coefficients. The latter are expressible through finite sums of 3-j and 9-j symbols. The formulas allow precise and fast evaluation of matrix elements of the effective potential in the correlation-function hyperspherical-harmonic method for atomic, molecular, and nuclear three- and four-body problems. The generalization to any number of particles is straightforward.

I. INTRODUCTION

The hyperspherical-harmonic expansion method, introduced in 1935 by Zernike and Brinkman[1] and reintroduced 25 years later in a different form by Delves[2] and Smith,[3] provides a very general and powerful approach to the N-body problem.[4] In this method the wave function, after the separation of the center-of-mass motion, is presented as a sum of products of radial functions $\phi_{\mathcal{K}}(\rho)$ and the so-called hyperspherical harmonic functions $\mathcal{Y}_{\mathcal{K}}(\Omega)$ depending on $3N-4$ angular variables Ω:

$$\Psi(\rho,\Omega)=\sum_{\mathcal{K}}\phi_{\mathcal{K}}(\rho)\mathcal{Y}_{\mathcal{K}}(\Omega) \ . \tag{1}$$

These functions are generalizations of the usual spherical functions to the N-body case and are solutions of the Laplace equation on the $(3N-3)$-dimensional sphere. They are correspondingly characterized by $3N-4$ quantum numbers $\mathcal{K}$. After the separation of $3N-4$ angular variables Ω the N-body Schrödinger equation reduces to the matrix equation for the radial functions

$$\left[\frac{1}{\rho^n}\frac{d}{d\rho}\left[\rho^n\frac{d}{d\rho}\right]-\frac{K(K+3N-5)}{\rho^2}+E\right]\phi_{\mathcal{K}}(\rho)=\sum_{\mathcal{K}'}W_{\mathcal{K},\mathcal{K}'}(\rho)\phi_{\mathcal{K}'}(\rho) \ . \tag{2}$$

Here $n=3N-4$ and

$$W_{\mathcal{K},\mathcal{K}'}(\rho)=\int[\mathcal{Y}_{\mathcal{K}}(\Omega)]^*W(\rho,\Omega)\mathcal{Y}_{\mathcal{K}'}(\Omega)d\Omega \tag{3}$$

are matrix elements of the potential W between hyperspherical functions, which are eigenfunctions of the generalized angular momentum operator $\mathcal{K}^2_{3N-3}(\Omega)$ in the $(3N-3)$-dimensional space:

$$\mathcal{K}^2_{3N-3}(\Omega)\mathcal{Y}_{\mathcal{K}}(\Omega)=K(K+3N-5)\mathcal{Y}_{\mathcal{K}}(\Omega) \ . \tag{4}$$

The set $\mathcal{K}$ contains, together with the quantum number K, also the eigenvalues of other $3N-5$ angular operators which commute with the Hamiltonian [that is, with $\mathcal{K}^2_{3N-3}(\Omega)$] and between themselves.

For systems without additional symmetry the set of conserved quantum numbers consists of the total orbital angular momentum L and its projection M. Although the other quantum numbers in principle could be chosen arbitrarily, in practice, due to the fact that most few body systems contain identical particles, it is convenient to choose them to be eigenvalues of the commuting set of operators, corresponding to the group SO$(N-1)$, which contains a group of permutations of N particles. Consequently, many further works[5-14] were devoted to finding convenient expressions for these so-called symmetrized hyperspherical harmonic functions realizing irreducible representations of the permutation group. Unfortunately the construction of the orthonormalized symmetrized hyperspherical harmonic basis turns out to be a very difficult problem even for the three particle case.[3,5-14] Simple expressions in closed form were found only for $L=0$ and $L=1$ hyperspherical functions,[5,11,12,15-17] while for $L\geq 2$ the progress was hampered by difficulties of finding the proper "fifth" operator of the complete set [containing also $\mathcal{K}^2_6(\Omega)$, $\mathbf{L}^2$, L_z, and the generator of SO(2)] which would have equally spaced, easily calculable, and nonirrational eigenvalues.[18] However the fact that the symmetrized hyperspherical function, once known, could be expressed through the Wigner $\mathcal{D}$ functions,[12,15-17] enabled analytical calculation of potential matrix elements. In the beginning analytic expressions for the matrix elements were found by Whitten[15] in the scalar case for the Coulomb, Gaussian, and harmonic oscillator potentials. This result was later generalized by Mandelzweig[19] and Barnea and Mandelzweig[16,17] who have shown that the matrix elements of an arbitrary potential for $L=0$ and $L=1$ cases could be expressed through the sum of products of the Clebsch-Gordan coefficients and explicitly written functions, defined by a power series in the radial variable ρ. The radius of convergence of the series for the matrix elements is proved to be the same as that of the power series defining the potential.[16,17,19] The power-series form of the expressions for the matrix elements is especially appealing, since an exact solution of the coupled equations is given by the power series whose coefficients are calculated by recurrence relations from the matrix coefficients in the power series for the potential matrix.[20,21]

The analytic expressions for the matrix elements as well as the power-series method of solution of coupled equations enabled an enormous saving in the computational time and extreme precision in the correlation-function hyperspherical-harmonic (CFHH) method, developed in the works,[20–27] which was used for very accurate nonvariational calculations of S states of the helium atom and of the positronium and mesonic-molecular ions. For example, for the ground state of the helium atom, this method of direct solution of the three-body Schrödinger equation yields the wave function and energy values accurate up to seven and nine significant figures,[22,23,25] respectively. The numerical computations of the potential matrix elements and the solution of the coupled equations with the precision needed for such accuracy would be extremely time consuming, if at all possible.

The idea of using the hyperspherical expansion together with the correlation functions is dating back to the works[28–30] in scattering and to works[31,32] in bound-state nuclear problems. In the CFHH method[4,20–27] the N-body bound-state wave function is presented in the product form

$$\Psi=\chi\Phi \ , \tag{5}$$

where

$$\chi=\prod_{i<j=2}^{N}\chi_{ij}(r_{ij}) \ , \tag{6}$$

r_{ij} is the distance between particles i and j, and $\chi_{ij}(r_{ij})=e^{f_{ij}(r_{ij})}$ are known Jastrow correlation factors[33] which are chosen to take into account the singularities and clustering properties of the wave function. Φ is the smooth part of the wave function to be expressed in hyperspphericals. The resulting Schrödinger equation for Φ has an effective velocity-dependent potential W, depending on the correlation factors,

$$W=V-\tfrac{1}{2}\nabla^2 f-\tfrac{1}{2}(\nabla f)^2-(\nabla f)\nabla \ , \tag{7}$$

where $f=\sum_{i<j=2}^{N} f_{ij}(r_{ij})$, V is the sum of the interparticle potentials, and

$$\nabla_k=\left[\frac{\partial}{\partial \mathbf{x}_k^1},\frac{\partial}{\partial \mathbf{x}_k^2},\frac{\partial}{\partial \mathbf{x}_k^3},\ldots,\frac{\partial}{\partial \mathbf{x}_k^{N-1}}\right] \tag{8}$$

is a $(3N-3)$-dimensional gradient and $\mathbf{x}_k^1,\mathbf{x}_k^2,\mathbf{x}_k^3,\ldots,\mathbf{x}_k^{N-1}$ are different sets of mass-weighted Jacobi coordinates.[34–36] Note that the gradients in (7) carry no set index k. This is due to the fact that the scalar product of two gradients does not change under the transformation from one set to another.

The CFHH matrix elements of W in the three-body problem were obtained earlier[16,17,19] for $L=0$ and $L=1$, since only in these cases the expressions of the symmetrized orthonormal hyperspherical-harmonic functions through Wigner $\mathcal{D}$ functions, depending on kinematic variables (that is, describing particle transformations into each other and thus connecting different sets of Jacobi coordinates), are known. In the CFHH method there is no need, however, to use the symmetric basis. The reason is that even for identical particles the correlation factors $f_{ij}(r_{ij})$ could be different. For example, in the excited helium atom the correlation factor for the excited electron should be different from the one for the electron in the ground state, since the latter is influenced by the unscreened nuclear charge while the first is in a screened field; they also are in different quantum states. The symmetrization of the wave function thus should be done on the product of the correlation function χ and of the hyperspherical expansion of Φ together and not on each one of them separately. Therefore in the CFHH method there is no need to work with the symmetrized hyperspherical-harmonic functions and one can use the nonsymmetrized ones obtained by the method of trees[37,38] which form complete orthonormal sets and for which analytical expressions and properties under the kinematic rotations are very well known for arbitrary total momenta and for any number of particles.[1,37–45]

In the standard hyperspherical approach such matrix elements for the Coulomb and some other simple potentials were obtained, for example, in Refs. 46 and 47.

The purpose of this paper is to obtain explicit analytical expressions for matrix elements of the effective potential in the CFHH method using the unsymmetrized hyperspherical harmonics and thus to generalize the results of the works[16,17,19] to arbitrary L. Although the present method could be used for any number of particles we will restrict ourselves here to the cases of three- and four-body problems. The extension to the N-body case is straightforward.

The paper is organized in the following way. In Sec. II we shall obtain the matrix elements between nonsymmetrized hyperspherical harmonics for both the velocity independent and the velocity dependent parts of the effective CFHH potential W in the three-body problem. In Sec. III we shall do the same for the four-body problem. Section IV is devoted to the discussion of the results.

II. THE CFHH MATRIX ELEMENTS IN THE THREE-BODY CASE

Usually in the hyperspherical-harmonic method the pair potentials are expanded in terms of the hyperspherical-harmonic functions and one calculates overlap integrals for three hyperspherical functions. Since all pair potentials are defined by power series in interparticle distances, it is more natural and in fact leads to simpler results to take the matrix elements of an arbitrary power of any interparticle distance and to sum them with the proper coefficients in order to get the final expressions for the potential matrix elements in the form of power series in the hyperspherical radius ρ, as it was done before.[16,17,19] Such a form of the solution is necessary, as it was mentioned earlier, to obtain the exact power-series solution of coupled radial equations, since its coefficients are determined[20,21] by recurrence relations involving matrix coefficients in the power series for the potential matrix elements.

For the general case of three particles with unequal masses we introduce the usual Jacobi coordinates:

$$\mathbf{R}=\frac{1}{M}(m_i\mathbf{r}_i+m_j\mathbf{r}_j+m_k\mathbf{r}_k)\ ,$$
$$\mathbf{x}_k^1=\left[\frac{m_im_j}{m_i+m_j}\right]^{1/2}(\mathbf{r}_i-\mathbf{r}_j)\ , \tag{9}$$
$$\mathbf{x}_k^2=\left[\frac{m_k(m_i+m_j)}{M}\right]^{1/2}\left[\mathbf{r}_k-\frac{m_i\mathbf{r}_i+m_j\mathbf{r}_j}{m_i+m_j}\right]\ .$$

Here $M=m_1+m_2+m_3$, and $\{i,j,k\}$ are three numbers forming a cyclic permutation of $\{1,2,3\}$. These equations define three different equivalent sets which are connected by a linear transformation[39,40]

$$\begin{bmatrix}\mathbf{x}_i^1\\ \mathbf{x}_i^2\end{bmatrix}=\begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix}\begin{bmatrix}\mathbf{x}_k^1\\ \mathbf{x}_k^2\end{bmatrix}=\begin{bmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{bmatrix}\begin{bmatrix}\mathbf{x}_k^1\\ \mathbf{x}_k^2\end{bmatrix}\ ,$$
$$\varphi=\pi+\arctan\left[\frac{Mm_j}{m_im_k}\right]^{1/2}\ , \tag{10}$$

conserving $\rho^2=(\mathbf{x}_k^1)^2+(\mathbf{x}_k^2)^2$ which as it is easy to see, does not depend on the index k. Parametrization of the coordinates in the form

$$\mathbf{x}_k^1=\cos\alpha_k\hat{\mathbf{n}}_k^1\ ,\qquad \mathbf{x}_k^2=\sin\alpha_k\hat{\mathbf{n}}_k^2\ , \tag{11}$$

where $\hat{\mathbf{n}}_k^1$ and $\hat{\mathbf{n}}_k^2$ are unit vectors, leads to the following expression for the gradients [in the next two equations (12) and (13) we omit the index k]

$$\nabla^1=\frac{\partial}{\partial\mathbf{x}^1}=\hat{\mathbf{n}}^1\left[\cos\alpha\frac{\partial}{\partial\rho}-\frac{1}{\rho}\sin\alpha\frac{\partial}{\partial\alpha}\right]-i\frac{\hat{\mathbf{n}}^1\times\boldsymbol{l}^1}{\rho\cos\alpha}\ ,$$
$$\nabla^2=\frac{\partial}{\partial\mathbf{x}^2}=\hat{\mathbf{n}}^2\left[\sin\alpha\frac{\partial}{\partial\rho}+\frac{1}{\rho}\cos\alpha\frac{\partial}{\partial\alpha}\right]-i\frac{\hat{\mathbf{n}}^2\times\boldsymbol{l}^2}{\rho\sin\alpha}\ , \tag{12}$$

which produces a simple form for the global angular momentum operator $\mathcal{K}^2(\omega)$ in the six-dimensional space:

$$\mathcal{K}^2(\omega)=-\left[\frac{\partial^2}{\partial\alpha^2}+4\cot2\alpha\frac{\partial}{\partial\alpha}-\frac{(\boldsymbol{l}^1)^2}{\cos^2\alpha}-\frac{(\boldsymbol{l}^2)^2}{\sin^2\alpha}\right]\ . \tag{13}$$

Here $\boldsymbol{l}^1=-i\mathbf{x}^1\times\nabla^1$ and $\boldsymbol{l}^2=-i\mathbf{x}^2\times\nabla^2$ are operators of the angular momenta corresponding to the two Jacobi coordinates of the given set. The orthonormalized eigenfunctions which have the eigenvalues $K(K+4), K=0,1,2,\ldots$, are given by the expression

$$\mathcal{Y}_K^{l_k^1l_k^2LM}(\omega_k)=\langle\omega_k|Kl_k^1l_k^2LM\rangle=N_K^{l_k^1l_k^2}\sum_{m_1,m_2}\langle LM|l_k^1m_1l_k^2m_2\rangle(\cos\alpha_k)^{l_k^1}(\sin\alpha_k)^{l_k^2}P_n^{(l_k^2+1/2,l_k^1+1/2)}(\cos2\alpha_k)\times Y_{l_k^1m_1}(\hat{\mathbf{n}}_k^1)Y_{l_k^2m_2}(\hat{\mathbf{n}}_k^2)\ . \tag{14}$$

Here $\langle LM|l_k^1m_1l_k^2m_2\rangle$ is the Clebsch-Gordan coefficient, $P_n^{(\alpha,\beta)}$ is a Jacobi polynomial, Y_{lm} are the ordinary spherical harmonic functions, $n=(K-l_k^1-l_k^2)/2$, and $N_K^{l_k^1l_k^2}$ is the normalization constant

$$N_c^{a,b}=\left[\frac{2(c+2)n!\Gamma(n+a+b+2)}{\Gamma(n+a+\frac{3}{2})\Gamma(n+b+\frac{3}{2})}\right]^{1/2},\quad n=\frac{c-a-b}{2}\ . \tag{15}$$

$\omega_k=(\alpha_k,\omega_k^1,\omega_k^2)$ denote the five angular coordinates on the six-dimensional hypersphere; $0\le\alpha_k\le\pi/2$ and ω_k^1,ω_k^2 are solid angles connected with the vectors $\hat{\mathbf{n}}_k^1$, $\hat{\mathbf{n}}_k^2$, respectively; and the angular volume element is given by

$$d\omega_k=\tfrac{1}{4}\sin^22\alpha_k\,d\omega_k^1d\omega_k^2\ .$$

The eigenfunctions are characterized, together with K, by the eigenvalues of the three-body angular momentum L, its projection M and by the "partial" angular momenta l_k^1, l_k^2.

The transformation properties of the basis set (14) under the kinematic rotation (10),

$$\mathcal{Y}_K^{l_i^1l_i^2LM}(\omega_i)=\sum_{l_k^1,l_k^2}\langle l_k^1l_k^2|l_i^1l_i^2\rangle_{KL}\mathcal{Y}_K^{l_k^1l_k^2LM}(\omega_k)\ , \tag{16}$$

are defined with the help of the Raynal-Revai coefficients:[39,40]

$$\langle l_k^1l_k^2|l_i^1l_i^2\rangle_{KL}=\tfrac{1}{4}\pi[C_{l_i^1l_i^2}^{n_i}C_{l_k^1l_k^2}^{n_k}]^{-1/2}\times\sum_{\lambda_1,\lambda_2,\lambda_3,\lambda_4}i^{\lambda_3+\lambda_4+l_i^2-l_k^2}(-1)^{\lambda_1+\lambda_2+K}f(\lambda_1,\lambda_3;l_k^1)f(\lambda_4,\lambda_2;l_k^2)f(\lambda_1,\lambda_4;l_i^1)$$
$$\times f(\lambda_3,\lambda_2;l_i^2)\begin{Bmatrix}\lambda_1 & \lambda_3 & l_k^1\\ \lambda_4 & \lambda_2 & l_k^2\\ l_i^1 & l_i^2 & L\end{Bmatrix}\sum_{\mu,\nu}(-1)^{\mu}C_{\lambda_3\lambda_4}^{\mu}C_{\lambda_1\lambda_2}^{\nu}a_{11}^{\nu+\lambda_1}a_{22}^{\nu+\lambda_2}a_{12}^{\mu+\lambda_3}a_{21}^{\mu+\lambda_4}\ , \tag{17}$$

where

$$C_{rs}^{n}=\frac{\Gamma(2n+r+s+2)}{\Gamma(n+1)\Gamma(n+r+\frac{3}{2})\Gamma(n+s+\frac{3}{2})\Gamma(n+r+s+2)}, \quad n=\frac{K-r-s}{2}, \quad f(a,b;c)=\sqrt{(2a+1)(2b+1)}\langle a0b0|c0\rangle , \tag{18}$$

and the summation is restricted by the following condition:

$$K=2n_i+l_i^1+l_i^2=2n_k+l_k^1+l_k^2 =2\mu+2\nu+\lambda_1+\lambda_2+\lambda_3+\lambda_4 . \tag{19}$$

Another expression for the Raynal-Revai coefficient is given in the work[41] and the equivalence of both forms is proven in Ref. 13.

In the case of the total orbital angular momentum L the hyperspherical expansion of Φ is given by

$$\Phi^{LM}=\sum_{K,l_k^1l_k^2}\phi_{l_k^1l_k^2}^{K}(\rho)\mathcal{Y}_K^{l_k^1l_k^2LM}(\omega_k) , \tag{20}$$

where ω_k are the angular coordinates corresponding to the chosen Jacobi set. For example, for the case of i and j being identical particles, the set k is usually the most convenient one since the transformation properties of $\mathcal{Y}_K^{l_k^1l_k^2LM}(\omega_k)$ under the exchange of particles i and j, that is, under $\mathbf{x}_k^1\to-\mathbf{x}_k^1$ or $\alpha_k\to\pi-\alpha_k$, are then simplest:

$$\mathcal{Y}_K^{l_k^1l_k^2LM}(\omega_k)\to(-1)^{l_k^1}\mathcal{Y}_K^{l_k^1l_k^2LM}(\omega_k) . \tag{21}$$

We have to calculate

$$\langle Kl_k^1l_k^2LM|V|K'l_k^{1'}l_k^{2'}L'M'\rangle .$$

The potential V is a sum of pair potentials:

$$V=V^i(y_i)+V^j(y_j)+V^k(y_k) , \tag{22}$$

where

$$y_k=|\mathbf{r}_i-\mathbf{r}_j|=\left[\frac{m_i+m_j}{m_im_j}\right]^{1/2}x_k^1$$

is the distance between particles i and j. The matrix element

$$\langle Kl_k^1l_k^2LM|V|K'l_k^{1'}l_k^{2'}L'M'\rangle$$

could easily be evaluated by using the power expansion for the potential,

$$V^k(y_k)=\sum_{p=-2}^{\infty}V_p^k(y_k)^p =\sum_{p=-2}^{\infty}\tilde{V}_p^k(x_k^1)^p, \quad \tilde{V}_p^k=\left[\frac{m_i+m_j}{m_im_j}\right]^{p/2}V_p^k , \tag{23}$$

and tabulated integrals involving the Jacobi polynomials. We obtain

$$\langle Kl_k^1l_k^2LM|V^k|K'l_k^{1'}l_k^{2'}L'M'\rangle =\delta_{LL'}\delta_{MM'}\delta_{l_k^1l_k^{1'}}\delta_{l_k^2l_k^{2'}}\langle K|V^k|K'\rangle_{l_k^1l_k^2} , \tag{24}$$

where

$$\langle K|V^k|K'\rangle_{l_k^1l_k^2}=\sum_{p=-2}^{\infty}\tilde{V}_p^k\langle K|(\cos\alpha_k)^p|K'\rangle_{l_k^1l_k^2}\rho^p . \tag{25}$$

We shall express all integrals through the following integral:[48]

$$\begin{aligned}\mathcal{C}(t;n,a,b;m,r,s)&=\int_{-1}^{1}dx\,(1-x)^t(1+x)^bP_n^{(a,b)}(x)P_m^{(r,s)}(x)\\&=\frac{2^{b+t+1}\Gamma(a-t+n)\Gamma(b+n+1)\Gamma(r+m+1)\Gamma(t+1)}{m!n!\Gamma(r+1)\Gamma(a-t)\Gamma(b+t+n+2)}\\&\quad\times{}_4F_3(-m,r+s+m+1,t+1,t-a+1;r+1,b+t+n+2,t-a-n+1;1) ,\end{aligned}$$

$$\mathrm{Re}\,b>-1, \quad \mathrm{Re}\,t>-1 , \tag{26}$$

where ${}_4F_3$ is the generalized hypergeometric function defined by the equation[49]

$${}_pF_q(\alpha_1,\alpha_2,\ldots,\alpha_p;\beta_1,\beta_2,\ldots,\beta_q;x)=\sum_{k=0}^{\infty}\frac{(\alpha_1)_k(\alpha_2)_k\cdots(\alpha_p)_k}{(\beta_1)_k(\beta_2)_k\cdots(\beta_q)_k}\frac{x^k}{k!} . \tag{27}$$

After a change of variable to $x=-\cos2\alpha$ we obtain

$$\langle K|(\cos\alpha)^p|K'\rangle_{l^1l^2}=N_K^{l^1l^2}N_{K'}^{l^1l^2}(-1)^{n+n'}2^{-(l^1+l^2+p/2+3)}\mathcal{C}(l^1+p/2+\tfrac{1}{2};n,l^1+\tfrac{1}{2},l^2+\tfrac{1}{2};n',l^1+\tfrac{1}{2},l^2+\tfrac{1}{2}) , \tag{28}$$

where

$$n=\frac{(K-l^1-l^2)}{2}, \quad n'=\frac{(K'-l^{1'}-l^{2'})}{2} .$$

For the case $\alpha_1=-n'$ the function (27) reduces to a polynomial of the order n'. For large z,

$$\Gamma(z)\approx\sqrt{2\pi}e^{-z}z^{z-1/2}\ ,$$

and the expressions of the type $\Gamma(a+pc)/\Gamma(b+pc)$ in which power p enters Eq. (28) are of the order of $(ecp)^{b-a}$ for large p. The ratio of coefficients $\langle K|(\cos\alpha)^p|K'\rangle_{l^1l^2}$ and $\langle K|(\cos\alpha)^{p+1}|K'\rangle_{l^1l^2}$ for large p therefore tends to 1, which means that the radius of convergence of the series (25) is the same as that of the series (23) for the potential itself.

Finally we have, using the Raynal-Revai coefficients to calculate the matrix elements of potentials $V^i(y_i)$ and $V^j(y_j)$ in their respective hyperspherical bases $\mathcal{Y}_K^{l_i^1l_i^2LM}(\omega_i)$ and $\mathcal{Y}_K^{l_j^1l_j^2LM}(\omega_j)$,

$$\langle Kl_k^1l_k^2LM|V|K'l_k^{1'}l_k^{2'}L'M'\rangle=\delta_{LL'}\delta_{MM'}\sum_{m=i,j,k}\sum_{l_m^1,l_m^2}\langle l_k^1l_k^2|l_m^1l_m^2\rangle_{KL}\langle K|V^m|K'\rangle_{l_m^1l_m^2}\langle l_m^1l_m^2|l_k^{1'}l_k^{2'}\rangle_{K'L}\ . \tag{29}$$

The evaluation of the term

$$-\tfrac{1}{2}\nabla^2f=-\frac{1}{2}\left[\frac{1}{\rho^5}\frac{d}{d\rho}\left[\rho^5\frac{d}{d\rho}\right]-\frac{\mathcal{K}^2}{\rho^2}\right]f$$

in the effective potential is rather easy since this term, like the potential V itself, in view of (6) also separates into the sum of terms which depend on one interparticle distance only:

$$f=\sum_{m=i,j,k}f^m(y_m)\ . \tag{30}$$

Acting with the operator $\mathcal{K}^2$ on the bra, we obtain

$$\langle Kl_k^1l_k^2LM|\nabla^2f|K'l_k^{1'}l_k^{2'}L'M'\rangle$$
$$=\delta_{LL'}\delta_{MM'}\sum_{m=i,j,k}\sum_{l_m^1l_m^2}\langle l_k^1l_k^2|l_m^1l_m^2\rangle_{KL}\left\{\left[\frac{1}{\rho^5}\frac{d}{d\rho}\left[\rho^5\frac{d}{d\rho}\right]-\frac{K(K+4)}{\rho^2}\right]\langle K|f^m|K'\rangle_{l_m^1l_m^2}\right\}\langle l_m^1l_m^2|l_k^{1'}l_k^{2'}\rangle_{K'L}\ , \tag{31}$$

where the expression for $\langle K|f^m|K'\rangle_{l_m^1l_m^2}$ is given by Eq. (25) in which the expansion coefficients $\tilde{V}_p^m$ in the power series for the potential are substituted by the corresponding coefficients $\tilde{f}_p^m=[(m_i+m_j)/(m_im_j)]^{p/2}f_p^m$ in the expansion of the correlation function.

Let us now evaluate the velocity-dependent part of the effective potential,

$$\Theta=(\nabla f)\nabla=[(\nabla_m^1f)\nabla_m^1+(\nabla_m^2f)\nabla_m^2]\ . \tag{32}$$

Here m can be equal to any of the indicies i,j,k. The use of Eq. (12) yields, after a simple calculation,

$$\Theta=\frac{\partial f}{\partial\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial f}{\partial\alpha_m}\frac{\partial}{\partial\alpha_m}-\frac{(\mathbf{l}_m^1f)\cdot\mathbf{l}_m^1}{\rho^2\cos^2\alpha_m}-\frac{(\mathbf{l}_m^2f)\cdot\mathbf{l}_m^2}{\rho^2\sin^2\alpha_m}\ . \tag{33}$$

In view of (32) and arbitrariness of m there, one can write

$$\Theta=\sum_m\Theta^m\ ,$$
$$\Theta^m=\frac{\partial f^m}{\partial\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial f^m}{\partial\alpha_m}\frac{\partial}{\partial\alpha_m}-\frac{(\mathbf{l}_m^1f^m)\cdot\mathbf{l}_m^1}{\rho^2\cos^2\alpha_m}-\frac{(\mathbf{l}_m^2f^m)\cdot\mathbf{l}_m^2}{\rho^2\sin^2\alpha_m}\ . \tag{34}$$

As f^m is a scalar function depending only on the interparticle distance x_m^1, the last two terms in expression (34) are zero and we finally have

$$\Theta^m=\frac{\partial f^m}{\partial\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial f^m}{\partial\alpha_m}\frac{\partial}{\partial\alpha_m}\ . \tag{35}$$

A straightforward calculation gives

$$\langle K|\Theta^m|K'\rangle_{l_m^1l_m^2}=\sum_{p=-2}^{\infty}\tilde{f}_p^m\left[\langle K|(\cos\alpha_m)^p|K'\rangle_{l_m^1l_m^2}p\rho^{p-1}\frac{\partial}{\partial\rho}+\left\langle K\left|\frac{\partial(\cos\alpha_m)^p}{\partial\alpha_m}\frac{\partial}{\partial\alpha_m}\right|K'\right\rangle_{l_m^1l_m^2}\rho^{p-2}\right]\ , \tag{36}$$

where

$$\left\langle K\left|\frac{\partial(\cos\alpha)^p}{\partial\alpha}\frac{\partial}{\partial\alpha}\right|K'\right\rangle_{l^1l^2}=N_K^{l^1l^2}N_{K'}^{l^1l^2}(-1)^{n+n'}2^{-(l^1+l^2+p/2+3)}$$
$$\times\{pl^1[2\mathcal{C}(l^1+p/2-\tfrac{1}{2};n,l^1+\tfrac{1}{2},l^2+\tfrac{1}{2};n',l^1+\tfrac{1}{2},l^2+\tfrac{1}{2})$$
$$-\mathcal{C}(l^1+p/2+\tfrac{1}{2};n,l^1+\tfrac{1}{2},l^2+\tfrac{1}{2};n',l^1+\tfrac{1}{2},l^2+\tfrac{1}{2})]$$
$$-pl^2\mathcal{C}(l^1+p/2+\tfrac{1}{2};n,l^1+\tfrac{1}{2},l^2+\tfrac{1}{2};n',l^1+\tfrac{1}{2},l^2+\tfrac{1}{2})$$
$$-p(l^1+l^2+n'+2)\mathcal{C}(l^1+p/2+\tfrac{1}{2};n,l^1+\tfrac{1}{2},l^2+\tfrac{1}{2};n'-1,l^1+\tfrac{3}{2},l^2+\tfrac{3}{2})\} \tag{37}$$

The expression for the matrix elements of the operator Θ is therefore given by

$$\langle K l_k^1 l_k^2 LM|\Theta|K' l_k^{1'} l_k^{2'} L'M'\rangle = \delta_{LL'}\delta_{MM'} \sum_{m=i,j,k} \sum_{l_m^1, l_m^2} \langle l_k^1 l_k^2 | l_m^1 l_m^2 \rangle_{KL} \langle K|\Theta^m|K'\rangle_{l_m^1 l_m^2} \langle l_m^1 l_m^2 | l_k^{1'} l_k^{2'} \rangle_{K'L} . \quad (38)$$

The matrix elements of the remaining part of the effective potential $(\nabla f)^2 = \Theta f$ could be calculated analytically by inserting the completeness condition $\sum_{\mathcal{K}} |\mathcal{K}\rangle\langle\mathcal{K}| = 1$ after the operator Θ and thus presenting the matrix elements of Θf as a sum of products of the matrix elements of Θ and f. This sum, however, is infinite, and has a power-law-type convergence in K. The precise evaluation of the matrix elements of Θf could therefore involve many terms. We have verified, for example, that in the case $L=0$ the evaluation of the Θf matrix elements for the linear correlation function $f = \sum_{i<j} a_{ij} r_{ij}$ in the helium atom ground state calculation with the precision of seven digits demands a sum on K up to $K=400$, which due to additional quantum numbers (restricted by K) leads to a summation over about 10 000 intermediate states. Therefore in the case of the operator Θf, as well as in the cases when a three-body potential is present, the numerical evaluation of matrix elements of this part of the effective potential should be considered.

III. THE CFHH MATRIX ELEMENTS IN THE FOUR-BODY CASE

The generalization to the four-body case is straightforward, albeit tedious. One can introduce, for example, the following set of Jacobi coordinates:

$$\begin{aligned} \mathbf{R} &= \frac{1}{M}(m_i\mathbf{r}_i + m_j\mathbf{r}_j + m_k\mathbf{r}_k + m_l\mathbf{r}_l) , \\ \mathbf{x}_{kl}^1 &= \left[\frac{m_i m_j}{m_i+m_j}\right]^{1/2} (\mathbf{r}_i - \mathbf{r}_j) , \\ \mathbf{x}_{kl}^2 &= \left[\frac{(m_i+m_j)(m_k+m_l)}{M}\right]^{1/2} \\ &\quad \times \left[\frac{m_k\mathbf{r}_k + m_l\mathbf{r}_l}{m_k+m_l} - \frac{m_i\mathbf{r}_i + m_j\mathbf{r}_j}{m_i+m_j}\right] , \\ \mathbf{x}_{kl}^3 &= \left[\frac{m_k m_l}{m_k+m_l}\right]^{1/2} (\mathbf{r}_k - \mathbf{r}_l) , \end{aligned} \quad (39)$$

where $M = m_1+m_2+m_3+m_4$ and $\{i,j,k,l\}$ are four numbers forming a permutation of $\{1,2,3,4\}$.

All other possible sets of Jacobi coordinates could be obtained with the help of orthogonal kinematic rotations[36]

$$\begin{bmatrix} \mathbf{x}^{1'} \\ \mathbf{x}^{2'} \\ \mathbf{x}^{3'} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \\ \mathbf{x}^3 \end{bmatrix} \quad (40)$$

conserving the length of the radius vector $\rho, \rho^2 = (\mathbf{x}^1)^2 + (\mathbf{x}^2)^2 + (\mathbf{x}^3)^2$ in the nine-dimensional space. The explicit form of the transformation (40) for the set (39) in the case of permutations of the four particles is given in Ref. 45.

Following the work,[44] we introduce the notations

$$\begin{aligned} \mathbf{x}^1 &= \rho(\cos\alpha)(\sin\beta)\hat{\mathbf{n}}^1 , \\ \mathbf{x}^2 &= \rho(\sin\alpha)(\sin\beta)\hat{\mathbf{n}}^2 , \\ \mathbf{x}^3 &= \rho(\cos\beta)\hat{\mathbf{n}}^3, \quad 0 \le \alpha,\beta \le \frac{\pi}{2} . \end{aligned} \quad (41)$$

From here on we omit the indices k,l in most equations and retain them only if necessary for definiteness. The eight angular coordinates on the nine-dimensional hypersphere are α,β and the solid angles $\omega^1,\omega^2,\omega^3$ corresponding to the unit vectors $\hat{\mathbf{n}}^1,\hat{\mathbf{n}}^2,\hat{\mathbf{n}}^3$. The angular part of the volume element is $d\Omega = \sin^5\beta\cos^2\beta\, d\beta\, d\omega^3 d\omega$, where $d\omega$ was defined in Sec. II.

The square of the generalized angular momentum operator on the nine-dimensional sphere $\mathcal{Q}^2(\Omega) = \mathcal{K}_9^2(\Omega)$ is now given by

$$\mathcal{Q}^2(\Omega) = \frac{1}{\sin^2\beta}\mathcal{K}^2(\omega) - \frac{\partial^2}{\partial\beta^2} - \frac{7\cos^2\beta - 2}{\sin\beta\cos\beta}\frac{\partial}{\partial\beta} + \frac{(\mathbf{l}^3)^2}{\cos^2\beta} , \quad (42)$$

where $\mathcal{K}^2(\omega) = \mathcal{K}_6^2(\omega)$ is, as before, the square of the generalized six-dimensional angular momentum operator, given by Eq. (13), and $\mathbf{l}^1, \mathbf{l}^2, \mathbf{l}^3$ are the usual three-dimensional orbital angular momentum operators, related to the Jacobi coordinates $\mathbf{x}^1,\mathbf{x}^2,\mathbf{x}^3$. The orthonormalized set of the hyperspherical-harmonic functions, corresponding to the eigenvalues $Q(Q+7)$ of $\mathcal{Q}^2(\Omega)$ and $K(K+4)$ of $\mathcal{K}^2(\omega)$, is given by

$$\begin{aligned} Z_{QK}^{l^1 l^2 l l^3 LM}(\Omega) &= \langle \Omega | QK l^1 l^2 l l^3 LM \rangle \\ &= \sum_{m,m^3} \langle LM | l^3 m^3 l m \rangle N_{Q+3/2}^{l^3, K+3/2} (\cos\beta)^{l^3} \\ &\quad \times (\sin\beta)^K P_q^{(K+2, l^3+1/2)}(\cos 2\beta) \\ &\quad \times Y_{l^3 m^3}(\hat{\mathbf{n}}^3) \mathcal{Y}_K^{l^1 l^2 l m}(\omega) . \end{aligned} \quad (43)$$

Here $q = (Q - K - l^3)/2$ and $N_{Q+3/2}^{l^3, K+3/2}$ is given by Eq. (15).

The Raynal-Revai coefficients, connecting the different basis sets through the formula

$$Z_{QK}^{l^1 l^2 l l^3 LM}(\Omega) = \sum_{l^{1'}, l^{2'}, l^{3'}, l', K'} \langle l^{1'} l^{2'} l' l^{3'} K' | l^1 l^2 l l^3 K \rangle_{QL} \times Z_{QK'}^{l^{1'} l^{2'} l' l^{3'} LM}(\Omega') , \quad (44)$$

were calculated for the four-particle case by Jibuti, Krupennikova, and Shubitidze:[45]

$$
\begin{aligned}
\langle l^{1'} l^{2'} l' l^{3'} K' | l^1 l^2 l l^3 K \rangle_{QL} = {} & \tfrac{1}{128} \pi^3 G^{q'K'}_{l^{1'} l^{2'} l^{3'}} G^{qK}_{l^1 l^2 l^3} \\
& \times \sum_{\substack{\lambda_1,\lambda_2,\lambda_3,\lambda_4,\lambda_5,\lambda_6,\lambda_7,\lambda_8,\lambda_9, \\ \lambda_{12},\lambda_{45},\lambda_{78},\lambda_{14},\lambda_{25},\lambda_{36}}} (-1)^{\lambda_3+\lambda_6} i^{\lambda_3+\lambda_6+\lambda_7+\lambda_8+K-K'} \\
& \times f(\lambda_1\lambda_2;\lambda_{12}) f(\lambda_{12}\lambda_3;l^1) f(\lambda_4\lambda_5;\lambda_{45}) f(\lambda_{45}\lambda_6;l^2) f(\lambda_7\lambda_8;\lambda_{78}) f(\lambda_{78}\lambda_9;l^3) \\
& \times f(\lambda_1\lambda_4;\lambda_{14}) f(\lambda_{14}\lambda_7;l^{1'}) f(\lambda_2\lambda_5;\lambda_{25}) f(\lambda_{25}\lambda_8;l^{2'}) f(\lambda_3\lambda_6;\lambda_{36}) f(\lambda_{36}\lambda_9;l^{3'}) \sqrt{(2l'+1)(2l+1)} \\
& \times \left\{ \begin{array}{cccccccc}
\lambda_1 & \lambda_2 & \lambda_{12} & & & & & \\
\lambda_4 & \lambda_5 & & \lambda_{45} & & & & \\
\lambda_{14} & & & & \lambda_7 & l^{1'} & & \\
& \lambda_{25} & & & \lambda_8 & l^{2'} & & \\
& & \lambda_3 & \lambda_6 & & & \lambda_{36} & \\
& & l^1 & l^2 & & & & l \\
& & & & \lambda_{78} & & \lambda_9 & l^3 \\
& & & & & l' & l^{3'} & L
\end{array} \right\} \\
& \times \sum_{\tau_1,\tau_2,\tau_3,\tau_4,\tau_5,\tau_6,\tau_7,\tau_8,\tau_9} (-1)^{\tau_3+\tau_6+\tau_7+\tau_8} \left[\prod_{k=1}^{9} \tau_k! \Gamma(\lambda_k+\tau_k+\tfrac{3}{2}) \right]^{-1} \\
& \times (a_{11})^{\lambda_1+2\tau_1} (a_{21})^{\lambda_2+2\tau_2} (a_{31})^{\lambda_3+2\tau_3} (a_{12})^{\lambda_4+2\tau_4} (a_{22})^{\lambda_5+2\tau_5} (a_{32})^{\lambda_6+2\tau_6} (a_{13})^{\lambda_7+2\tau_7} (a_{23})^{\lambda_8+2\tau_8} \\
& \times (a_{33})^{\lambda_9+2\tau_9} B(\rho/2+\tfrac{3}{2},\sigma/2+\tfrac{3}{2}) B(\rho'/2+\tfrac{3}{2},\sigma'/2+\tfrac{3}{2}) \\
& \times {}_3F_2(-n, l^1+l^2+n+2, \rho/2+\tfrac{3}{2}; l^2+\tfrac{3}{2}, (\rho+\sigma)/2+3; 1) \\
& \times {}_3F_2(-n', l^{1'}+l^{2'}+n'+2, \rho'/2+\tfrac{3}{2}, l^{2'}+\tfrac{3}{2}, (\rho'+\sigma')/2+3; 1) ,
\end{aligned}
\tag{45}
$$

where $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the β function, ${}_3F_2$ is given by Eq. (27), and

$$
G^{qK}_{l^1 l^2 l^3} = \left[\frac{\Gamma(q+l^3+\frac{3}{2})\Gamma(q+K+3)}{\begin{bmatrix} Q+\frac{5}{2} \\ q \end{bmatrix}} \right]^{1/2} N_K^{l^1 l^2} \frac{\Gamma(n+l^2+\frac{3}{2})}{\Gamma(n+1)\Gamma(l^2+\frac{3}{2})} . \tag{46}
$$

The summation is restricted by

$$
Q = \sum_{k=1}^{9} (\lambda_k + 2\tau_k) , \tag{47}
$$

$N_K^{l^1 l^2}$ is given by Eq. (15), $q=(Q-K-l^3)/2$ as defined after Eq. (43), $n=(K-l^1-l^2)/2$, and

$$
\begin{aligned}
& \sigma = l^1+\lambda_1+2\tau_1+\lambda_2+2\tau_2+\lambda_3+2\tau_3, \quad \sigma' = l^{1'}+\lambda_1+2\tau_1+\lambda_4+2\tau_4+\lambda_7+2\tau_7 , \\
& \rho = l^2+\lambda_4+2\tau_4+\lambda_5+2\tau_5+\lambda_6+2\tau_6, \quad \rho' = l^{2'}+\lambda_2+2\tau_2+\lambda_5+2\tau_5+\lambda_8+2\tau_8 .
\end{aligned}
\tag{48}
$$

The 24-j symbols can be expressed through a sum of products of four 9-j symbols as follows:[45]

$$\left\{\begin{array}{cccccccc} \lambda_1 & \lambda_2 & \lambda_{12} & & & & & \\ \lambda_4 & \lambda_5 & & \lambda_{45} & & & & \\ \lambda_{14} & & & & \lambda_7 & l^{1'} & & \\ & \lambda_{25} & & & \lambda_8 & l^{2'} & & \\ & & \lambda_3 & \lambda_6 & & & \lambda_{36} & \\ & & l^1 & l^2 & & & & l \\ & & & & \lambda_{78} & & \lambda_9 & l^3 \\ & & & & & l' & l^{3'} & L \end{array}\right\} = \sum_{\lambda} (2\lambda+1) \begin{Bmatrix} \lambda_{12} & \lambda_3 & l^1 \\ \lambda_{45} & \lambda_6 & l^2 \\ \lambda & \lambda_{36} & l \end{Bmatrix} \begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_{12} \\ \lambda_4 & \lambda_5 & \lambda_{45} \\ \lambda_{14} & \lambda_{25} & \lambda \end{Bmatrix} \begin{Bmatrix} \lambda & \lambda_{36} & l \\ \lambda_{78} & \lambda_9 & l^3 \\ l' & l^{3'} & L \end{Bmatrix} \begin{Bmatrix} \lambda_{14} & \lambda_{25} & \lambda \\ \lambda_7 & \lambda_8 & \lambda_{78} \\ l^{1'} & l^{2'} & l' \end{Bmatrix} . \tag{49}$$

Let us choose now the set Ω_{kl} of the hyperspherical angles and the set of hyperspherical states

$$|QK_{kl}l^1_{kl}l^2_{kl}l_{kl}l^3_{kl}LM\rangle$$

as the expansion basis for the wave function

$$\Phi^{LM} = \sum_{Q,K,l^1,l^2,l,l^3} \phi^{QK}_{l^1l^2ll^3}(\rho) \mathcal{Z}^{l^1l^2ll^3LM}_{QK}(\Omega) . \tag{50}$$

The indices k,l, marking the quantum numbers K,l^1,l^2,l,l^3 and the hyperspherical angles, are omitted.

The calculation of the matrix element of the potential

$$V = \sum_{m<n=i,j,k,l} V^{mn}(y_{mn}), \quad y_{mn} = \left[\frac{m_m+m_n}{m_m m_n}\right]^{1/2} \mathbf{x}^3_{mn} , \tag{51}$$

proceeds as in the three-body case. The matrix element of V^{mn} first reduces to

$$\langle QKl^1l^2ll^3LM|V^{mn}|Q'K'l^{1'}l^{2'}l'l^{3'}L'M'\rangle = \delta_{LL'}\delta_{MM'}\delta_{KK'}\delta_{ll'}\delta_{l^1l^{1'}}\delta_{l^2l^{2'}}\delta_{l^3l^{3'}}\langle Q|V^{mn}|Q'\rangle_{Kl^3} , \tag{52}$$

where, as before, the indices m,n marking K,l^1,l^2,l,l^3 and $K',l^{1'},l^{2'},l',l^{3'}$ are not displayed. The reduced matrix element on the right-hand side of Eq. (52) is

$$\langle Q|V^{mn}|Q'\rangle_{Kl^3} = \sum_{p=-2}^{\infty} \tilde{V}^{mn}_p \langle Q|(\cos\beta)^p|Q'\rangle_{Kl^3}\rho^p ,$$
$$\tilde{V}^{mn}_p = \left[\frac{m_m+m_n}{m_m m_n}\right]^{p/2} V^{mn}_p , \tag{53}$$

where as in Eq. (28),

$$\langle Q|(\cos\beta)^p|Q'\rangle_{Kl^3} = N^{l^3,K+3/2}_{Q+3/2} N^{l^3,K+3/2}_{Q'+3/2}(-1)^{q+q'}2^{-(K+l^3+p/2+9/2)}\mathcal{C}(l^3+p/2+\tfrac{1}{2};q,l^3+\tfrac{1}{2},K+2;q',l^3+\tfrac{1}{2},K+2) . \tag{54}$$

Finally,

$$\langle QK_{kl}l^1_{kl}l^2_{kl}l_{kl}l^3_{kl}LM|V|Q'K'_{kl}l^{1'}_{kl}l^{2'}_{kl}l'_{kl}l^{3'}_{kl}L'M'\rangle$$
$$= \delta_{LL'}\delta_{MM'} \sum_{m<n=i,j,k,l} \sum_{l^1_{mn},l^2_{mn},l^3_{mn},l_{mn},K_{mn}} \langle l^1_{kl}l^2_{kl}l_{kl}l^3_{kl}K_{kl}|l^1_{mn}l^2_{mn}l_{mn}l^3_{mn}K_{mn}\rangle_{QL}\langle Q|V^{mn}|Q'\rangle_{K_{mn}l^3_{mn}}$$
$$\times\langle l^1_{mn}l^2_{mn}l_{mn}l^3_{mn}K_{mn}|l^{1'}_{kl}l^{2'}_{kl}l'_{kl}l^{3'}_{kl}K'_{kl}\rangle_{Q'L} . \tag{55}$$

The matrix elements of $\nabla^2 f$ evaluated similarly as in the three-body case have the form of Eq. (55) with $\langle Q|V^{mn}|Q'\rangle_{K_{mn}l^3_{mn}}$ changed to

$$\left[\left[\frac{1}{\rho^8}\frac{d}{d\rho}\left[\rho^8\frac{d}{d\rho}\right] - \frac{Q(Q+7)}{\rho^2}\right]\langle Q|f^{mn}|Q'\rangle_{K_{mn}l^3_{mn}}\right] , \tag{56}$$

where the matrix elements of the correlation function between particles m and n are given by Eq. (53) in which the expansion coefficients $\tilde{V}^{mn}_p$ in the power series of the potential are exchanged for the expansion coefficient $\tilde{f}^{mn}_p$ of the correlation function.

We now turn to the matrix elements of the velocity-dependent part of the effective potential, which according to the same arguments as were used in the three-body case, could be written in the form

$$\Theta = \sum_{m<n=i,j,k,l} \Theta^{mn} . \tag{57}$$

Θ^{mn} for a scalar two-particle correlation function f^{mn} has the following expression:

$$\Theta^{mn} = \frac{\partial f^{mn}}{\partial \rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\left[\frac{\partial f^{mn}}{\partial \beta_{mn}}\frac{\partial}{\partial \beta_{mn}} + \frac{1}{\sin^2\beta_{mn}}\frac{\partial f^{mn}}{\partial \alpha_{mn}}\frac{\partial}{\partial \alpha_{mn}}\right] . \tag{58}$$

The evaluation of the matrix elements in the Jacobi coordinate set m,n gives

$$\langle Q|\Theta^{mn}|Q'\rangle_{K_{mn}l^3_{mn}} = \sum_{p=-2}^{\infty} \tilde{V}_p^{mn}\left[\langle Q|(\cos\beta_{mn})^p|Q'\rangle_{K_{mn}l^3_{mn}} p\rho^{p-1}\frac{\partial}{\partial\rho} + \left\langle Q\left|\frac{\partial(\cos\beta_{mn})^p}{\partial\beta_{mn}}\frac{\partial}{\partial\beta_{mn}}\right|Q'\right\rangle_{K_{mn}l^3_{mn}}\rho^{p-2}\right] , \tag{59}$$

where

$$\begin{aligned}\left\langle Q\left|\frac{\partial(\cos\beta)^p}{\partial\beta}\frac{\partial}{\partial\beta}\right|Q'\right\rangle_{Kl_3} = {} & N_{Q+3/2}^{l^3,K+3/2}N_{Q'+3/2}^{l^3,K+3/2}(-1)^{q+q'}2^{-(K+l^3+p/2+9/2)} \\ & \times\{pl^3[2\mathcal{C}(l^3+p/2-\tfrac{1}{2};q,l^3+\tfrac{1}{2},K+2;q',l^3+\tfrac{1}{2},K+2) \\ & -\mathcal{C}(l^3+p/2+\tfrac{1}{2};q,l^3+\tfrac{1}{2},K+2;q',l^3+\tfrac{1}{2},K+2)] \\ & -pK\mathcal{C}(l^3+p/2+\tfrac{1}{2};q,l^3+\tfrac{1}{2},K+2;q',l^3+\tfrac{1}{2},K+2) \\ & -p(K+l^3+\tfrac{3}{2}+q'+2)\mathcal{C}(l^3+p/2+\tfrac{1}{2};q,l^3+\tfrac{1}{2},K+2;q'-1,l^3+\tfrac{3}{2},K+3)\} .\end{aligned} \tag{60}$$

The matrix element of Θ is thus given by

$$\begin{aligned}\langle QK_{kl}l^1_{kl}l^2_{kl}l_{kl}l^3_{kl}LM|\Theta|Q'K'_{kl}l^{1'}_{kl}l^{2'}_{kl}l'_{kl}l^{3'}_{kl}L'M'\rangle \\ = \delta_{LL'}\delta_{MM'}\sum_{m<n=i,j,k,l}\ \sum_{l^1_{mn},l^2_{mn},l^3_{mn},l_{mn},K_{mn}} & \langle l^1_{kl}l^2_{kl}l_{kl}l^3_{kl}K_{kl}|l^1_{mn}l^2_{mn}l_{mn}l^3_{mn}K_{mn}\rangle_{QL}\langle Q|\Theta^{mn}|Q'\rangle_{K_{mn}l^3_{mn}} \\ & \times\langle l^1_{mn}l^2_{mn}l_{mn}l^3_{mn}K_{mn}|l^{1'}_{kl}l^{2'}_{kl}l'_{kl}l^{3'}_{kl}K'_{kl}\rangle_{Q'L} .\end{aligned} \tag{61}$$

IV. CONCLUSION

We have derived explicit analytic formulas for the evaluation of the matrix elements of the effective potential in the correlation-function hyperspherical-harmonic (CFHH) method for the three- and four-body problem. These formulas express the coefficients in the power-series expansions of the matrix elements in the variable ρ through the known coefficients of the power series in the interparticle distances, defining the two-body potentials and correlation functions. They allow very fast and precise evaluation of these coefficients, which in turn serve as input to the matrix recursion relations, determining the coefficients of the power series solution[20,21] of the matrix equation (2) and thus the bound-state energy and wave function. Indeed, although the final expressions for the matrix elements look rather cumbersome, they contain only finite sums of 3-j and 9-j symbols and of the hypergeometric functions (which in our case are reduced to polynomials), and are easily implemented on the computer. The precision of the evaluation of the potential matrix coefficients with the help of similar formulas obtained in the $L=0$ case in the symmetrized hyperspherical basis, and the precision of the power-series coefficients of the solution of the coupled equations (2) obtained with the recurrence relations, depends only on the length of the computer word. It is by many orders of magnitude higher than the error introduced by the truncation of the system (2) to a finite dimension. The time spent on their calculation was a small part of the total computational time in the calculations.[22–27] The accuracy of these calculations was up to nine significant digits for the energy and seven digits for the wave function. The use of the current formulas will allow the extension of the CFHH method to any value of the total angular momentum and to the four-particle atomic, molecular and nuclear bound-state problems. The extension of the given expressions to more particles can be performed in an analogous manner.

ACKNOWLEDGMENTS

The authors would like to thank Professor Jibuti for useful comments and verification of expressions for the four-body Raynal-Revai coefficients. The stay of the authors at the Max-Planck-Institut für Kernphysik in Heidelberg was made possible for R. K. by a grant from the Research Council of Slovenia and for V. M. by the support of the Minerva Foundation for cooperation between German and Israeli research institutions.

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