

General integral relations for the description of scattering states using the hyperspherical adiabatic basis

C. Romero-Redondo and E. Garrido

Instituto de Estructura de la Materia, CSIC, Serrano 123, E-28006 Madrid, Spain

P. Barletta

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom

A. Kievsky and M. Viviani

Istituto Nazionale di Fisica Nucleare, Largo Pontecorvo 3, 56100 Pisa, Italy

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In this work we investigate $1 + 2$ reactions within the framework of the hyperspherical adiabatic expansion method. With this aim two integral relations, derived from the Kohn variational principle, are used. A detailed derivation of these relations is shown. The expressions derived are general, not restricted to relative s partial waves, and with applicability in multichannel reactions. The convergence of the \mathcal{K} matrix in terms of the adiabatic potentials is investigated. Together with a simple model case used as a test for the method, we show results for the collision of a ^4He atom on a $^4\text{He}_2$ dimer (only the elastic channel open), and for collisions involving a ^6Li and two ^4He atoms (two channels open).

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I. INTRODUCTION

Calculation of phase shifts (or the \mathcal{K} matrix) for a given reaction is often complicated by the necessity of knowing the wave function of the full system at large distances. Extraction of the phase shifts can be in principle achieved by comparison of the large-distance part of the wave function with its known analytic asymptotic expression. For processes involving only two particles ($1 + 1$ collisions) this procedure can be easily implemented, and therefore the phase shifts can be computed. However, the more particles are involved in the reaction the more difficult is the calculation of an accurate wave function at large distances, or at least the more expensive it is from the computational point of view. Therefore, when the number of particles is increased the extraction of the phase shifts becomes progressively more and more complicated. In nuclear physics, collisions involving three and four nucleons have been extensively studied in solving the Faddeev ($A = 3$) and Faddeev-Yakubovsky ($A = 4$) equations [1,2], and the hyperspherical harmonic (HH) expansion in conjunction with the Kohn variational principle (KVP) [3,4]. These methods have been tested through different benchmarks [5,6]. When the interaction between the particles presents a hard core, as in the case of the atom-atom interaction, a direct application of these techniques could be problematic. The Faddeev equation has been modified to deal with a hard-core repulsion [7] and, in the case of the HH expansion, a correlation factor has been included [8]. In addition the hyperspherical adiabatic (HA) expansion method has proven to be a very efficient tool [9].

In the case of atom-atom interactions, the HA expansion shows a particularly fast range of convergence in the description of bound states, as has been shown, for example, in Ref. [10] for the description of rare gas trimers. In recent years there was a systematic use of the HA expansion in the description of three-atom systems in the ultracold regime

(see, for example, Refs. [11,12] and references therein). These applications raise the question about the convergence properties of the HA method for scattering states, in particular in the description of a $1 + 2$ collision. In principle the HA expansion could be applied to describe such a process since it leads to a clean distinction between all the possible incoming and outgoing channels. However, as was recently shown, the convergence of the expansion slows down significantly in applications directed to describing low-energy scattering states [13]. This problem appears at the moment of application of the proper boundary conditions to the hyperradial functions. In fact, in the HA expansion, the hyperradial functions are obtained by solving an infinite system of equations in the hyperradial variable ρ , and the convergence of the expansion is studied by increasing the number of equations considered after truncation of the system. For describing a $1 + 2$ collision, hyperradial functions are obtained requiring a hyperradial plane-wave behavior as $\rho \rightarrow \infty$. However, in such a process, this plane-wave behavior refers to the motion of the incident particle relative to the center of mass of the two-body bound system. The equivalence between the two descriptions happens at $\rho \approx \infty$ or, in other words, by inclusion of a very large number of hyperradial functions in the solutions. This is the cause of the extremely slow observed convergence.

In Ref. [14] the authors introduced a general method to compute the phase shift from two integral relations that involve only the internal part of the wave function. This method is a generalization to more than two particles of the integral relations given in [15,16] and it is derived from the KVP. In the case of the HA expansion, in Ref. [14] it was shown that for $1 + 2$ reactions, the use of the integral relations allows determination of the phase shift with a pattern of convergence similar to that in a bound state calculation. Therefore, thanks to the integral relations, the hyperspherical adiabatic expansion

method appears as a powerful tool to describe scattering processes also.

The purpose of this work is to show in detail the use of the integral relations in conjunction with the HA expansion method to describe scattering states. In Ref. [14] the particular case of a $1 + 2$ reaction with only the elastic channel open, and with only relative s waves involved, was considered. The applicability of the method is not limited to this particular case. In this work we shall consider processes involving $\ell \geq 0$ relative angular momenta, and we shall derive the integral relations for the general case in which more than one channel is open. The only limitation is that we shall restrict ourselves to energies below the breakup threshold. Above it, infinitely many adiabatic terms are in principle needed to describe the breakup channel, and although the same procedure could be used to describe it, we leave this particular case for a more careful investigation in a forthcoming work.

A different aspect is the applicability of the method to describe $1 + N$ reactions with $A = 1 + N > 3$. In this case, the main difficulty is to obtain the $N + 1$ wave function in the internal region and the N -body bound state function describing the asymptotic configuration. With this information, the integral relations apply in exactly the same way as for the $1 + 2$ case, but with the bound dimer wave function replaced by the corresponding bound N -body wave function. The extension of the adiabatic expansion to describe more than three particles is possible. The dependence of the hyperangular part consists in $(3N - 4)$ hyperangles and, in the case of systems of identical particles, the problem of constructing an A -body wave function with the proper statistic has to be faced. The first applications of the HA expansion to describe a four-body system already appeared [17]. In this work, however, we restrict the discussion to $1 + 2$ reactions.

In Sec. II we describe the details of the formalism, first describing the adiabatic expansion in a multichannel reaction, and second showing how the corresponding \mathcal{K} matrix (or equivalently the \mathcal{S} matrix) can be obtained from the asymptotic wave function. In Sec. III the integral relations for the same multichannel reaction are derived. They permit us to extract the \mathcal{K} (or \mathcal{S}) matrix, requiring only knowledge of the internal part of the wave function. The results are shown in Sec. IV. In Sec. IV A we consider a test case with only the elastic channel open. We investigate a three-body process which is fully equivalent to a two-body reaction, for which the phase shifts can be easily computed. This can then be used to test the accuracy of the integral relations method as well as the convergence pattern in the adiabatic expansion when $\ell > 0$ partial waves are involved. In Sec. IV B we investigate the elastic collision between a ^4He atom and the weakly bound $(^4\text{He})_2$ dimer. Finally, in Sec. IV C we apply the method to a collision involving a ^6Li and two ^4He atoms. In particular, we shall consider incident energies such that the two possible incoming and outgoing channels, $(^4\text{He}, (^4\text{He}-^6\text{Li}))$ and $(^6\text{Li}, (^4\text{He})_2)$, are both open. The summary and the conclusions are given in Sec. V. In Appendix A we show the derivation of the Kohn variational principle for a multichannel process and, finally, in Appendix B we have collected some technical details of the use of the integral relations when projected two-body potentials are employed.

II. FORMALISM

A. General features of the HA expansion

In this work we consider a process where a particle hits a bound two-body system. We assume the incident energy to be below the breakup threshold for the three particles. This means that the total three-body energy E , which is the sum of the incident energy $k^2/2\mu > 0$ (μ being the reduced mass between the incident particle and the dimer) and the two-body binding energy E_{2b} , is negative. In this way only elastic, inelastic, and rearrangement processes are possible.

The reaction under study is therefore a three-body process, which, as usual, can be described through the \mathbf{x} and \mathbf{y} Jacobi coordinates:

$$\begin{aligned} \mathbf{x}_i &= \sqrt{\frac{m_j m_k}{m(m_j + m_k)}} (\mathbf{r}_j - \mathbf{r}_k), \\ \mathbf{y}_i &= \sqrt{\frac{m_i(m_j + m_k)}{m(m_i + m_j + m_k)}} \left(\mathbf{r}_i - \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k} \right), \end{aligned} \quad (1)$$

where m_i and \mathbf{r}_i are the mass and coordinate of particle i and m is an arbitrary normalization mass. From the Jacobi coordinates one can construct the hyperspherical coordinates, which contain a radial one, the so-called hyperradius ρ ($\rho^2 = \sqrt{x_i^2 + y_i^2}$), and the five hyperangles Ω ($[\Omega] \equiv [\alpha_i, \Omega_x, \Omega_y]$). The hyperangle α_i is defined as $\tan \alpha_i = x_i/y_i$, and Ω_x and Ω_y give the directions of \mathbf{x}_i and \mathbf{y}_i . The five hyperangles depend on the particular ordering of the particles chosen in the definition of the Jacobi variables. Three different sets are possible by cyclic permutations of the indices i, j, k . In the following the Jacobi coordinates \mathbf{x} and \mathbf{y} and the corresponding hyperangular coordinates are given using the natural ordering of the particles $i, j, k \equiv 1, 2, 3$.

Following Ref. [9], we give a brief description of the HA method. In hyperspherical coordinates the Hamiltonian operator $\hat{\mathcal{H}}$ takes the form

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m} \hat{T}_\rho + \frac{\hbar^2}{2m\rho^2} \hat{G}^2 + V(\rho, \Omega) = -\frac{\hbar^2}{2m} \hat{T}_\rho + \hat{\mathcal{H}}_\Omega, \quad (2)$$

where $\hat{T}_\rho = \frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho}$ is the hyperradial kinetic energy operator, \hat{G}^2 is the grand angular operator, and $V(\rho, \Omega) = \sum_i V_i(x_i)$ is the potential energy (i runs over the three Jacobi systems).

The adiabatic expansion is based on the assumption that, in description of a particular process, the hyperangles vary much faster than the hyperradius ρ . Under this assumption it is possible to solve the Schrödinger equation $(\hat{\mathcal{H}} - E)\Psi = 0$ in two steps. In the first one the angular part is solved for a set of fixed values of ρ . This amounts to solving the eigenvalue problem

$$\hat{\mathcal{H}}_\Omega \Phi_n(\rho, \Omega) = \frac{\hbar^2}{2m} \frac{1}{\rho^2} \lambda_n(\rho) \Phi_n(\rho, \Omega) \quad (3)$$

for each ρ , which is treated as a parameter.

The angular functions $\{\Phi_n(\rho, \Omega)\}$ are used to construct the HA basis in which the basis elements form an orthonormal

basis for each value of ρ . The full three-body wave function is then expanded as

$$\Psi(\mathbf{x}, \mathbf{y}) = \frac{1}{\rho^{5/2}} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega). \quad (4)$$

Obviously the summation above has to be truncated, and only a finite number n_A of adiabatic terms are included in the calculation. For simplicity we are omitting in Ψ , f_n , and Φ_n the quantum numbers giving the total three-body angular momentum and its projection.

In a second step, the radial wave functions $f_n(\rho)$ in the expansion of Eq. (4) are obtained after solving the following coupled set of radial equations:

$$\sum_{n'=1}^{n_A} (\hat{\mathcal{H}}_{nn'} - E \delta_{nn'}) f_{n'}(\rho) = 0, \quad (5)$$

where the operator $\hat{\mathcal{H}}_{nn'}$ acts on the radial functions and takes the form

$$\hat{\mathcal{H}}_{nn}(\rho) = \frac{\hbar^2}{2m} \left[-\frac{d^2}{d\rho^2} - Q_{nn}(\rho) + \frac{1}{\rho^2} \left(\lambda_n(\rho) + \frac{15}{4} \right) \right] \quad (6)$$

for the diagonal terms, and

$$\hat{\mathcal{H}}_{nn'} = -\frac{\hbar^2}{2m} \left(2P_{nn'}(\rho) \frac{d}{d\rho} + Q_{nn'}(\rho) \right) \quad (7)$$

when $n \neq n'$.

The coupling terms $P_{nn'}$ and $Q_{nn'}$ in the expressions above follow from the dependence on ρ of the HA basis. Their explicit form is

$$P_{nn'}(\rho) = \left\langle \Phi_n(\rho, \Omega) \left| \frac{\partial}{\partial \rho} \right| \Phi_{n'}(\rho, \Omega) \right\rangle_{\Omega}, \quad (8)$$

$$Q_{nn'}(\rho) = \left\langle \Phi_n(\rho, \Omega) \left| \frac{\partial^2}{\partial \rho^2} \right| \Phi_{n'}(\rho, \Omega) \right\rangle_{\Omega},$$

where $\langle \rangle_{\Omega}$ represents integration over the five hyperangles only.

The one-dimensional set of coupled differential equations given in Eq. (5) can be written in a matrix form as

$$\begin{pmatrix} \hat{\mathcal{H}}_{11} - E & \hat{\mathcal{H}}_{12} & \cdots & \hat{\mathcal{H}}_{1n_A} \\ \hat{\mathcal{H}}_{21} & \hat{\mathcal{H}}_{22} - E & \cdots & \hat{\mathcal{H}}_{2n_A} \\ \vdots & \vdots & \vdots & \vdots \\ \hat{\mathcal{H}}_{n_A 1} & \hat{\mathcal{H}}_{n_A 2} & \cdots & \hat{\mathcal{H}}_{n_A n_A} - E \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n_A} \end{pmatrix} = 0, \quad (9)$$

and the three-body wave function is

$$\Psi(\mathbf{x}, \mathbf{y}) = \frac{1}{\rho^{5/2}} (f_1, f_2, \dots, f_{n_A}) \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{n_A} \end{pmatrix}. \quad (10)$$

It is important to note that the diagonal terms $\hat{\mathcal{H}}_{nn}$ in Eq.(6) contain the angular eigenvalues $\lambda_n(\rho)$ introduced in Eq. (3). They appear in the effective adiabatic potentials, which are

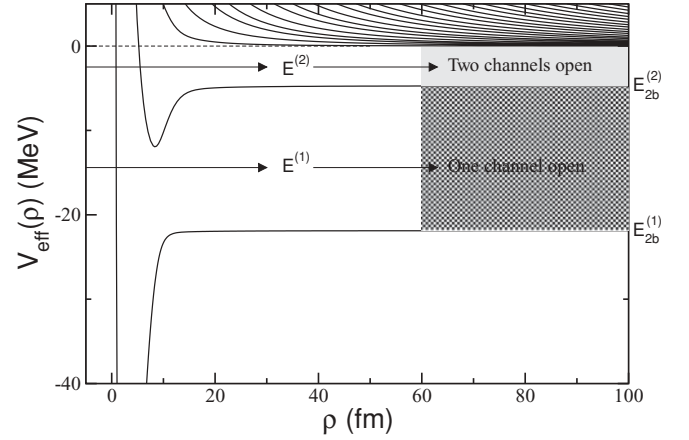


FIG. 1. Typical effective adiabatic potentials for a three-body system where two two-body bound states are present. The two lowest adiabatic potentials go asymptotically to the binding energies $E_{2b}^{(1)}$ and $E_{2b}^{(2)}$ of the two-body bound states. For a given three-body energy E , when $E_{2b}^{(1)} < E < E_{2b}^{(2)}$ only one channel is open, while when $E_{2b}^{(2)} < E < 0$ both channels are open.

given by

$$V_{\text{eff}}^{(n)}(\rho) = \frac{\hbar^2}{2m} \left(\frac{\lambda_n(\rho) + \frac{15}{4}}{\rho^2} - Q_{nn}(\rho) \right). \quad (11)$$

A typical behavior of the adiabatic potentials is shown in Fig. 1. They correspond to a three-body system where two of the two-body subsystems have a bound state. This is reflected in the fact that the two lowest effective adiabatic potentials go asymptotically to the binding energies $E_{2b}^{(1)}$ and $E_{2b}^{(2)}$ of each bound two-body system. The angular eigenfunctions associated with these two adiabatic potentials have the general asymptotic form [9]

$$\Phi_n^{JM}(\rho, \Omega) \xrightarrow{\rho \rightarrow \infty} \rho^{3/2} \left[\psi_n^{j_x}(\mathbf{x}) \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{j_y} \right]^{JM}, \quad (12)$$

where for this particular case $n = 1, 2$ and we have now made explicit the quantum numbers. The wave function $\psi_n^{j_x}(\mathbf{x})$, normalized to 1 in the \mathbf{x} Jacobi coordinate, describes the bound two-body system associated with the effective potential $V_{\text{eff}}^{(n)}$, whose angular momentum is j_x . Asymptotically it tends to the bound state wave function of the corresponding two-body subsystem. The spin function χ_{s_y} describes the spin of the third particle, which couples to the orbital angular momentum ℓ_y (associated with the Jacobi coordinate \mathbf{y}) to give total angular momentum j_y . Finally, j_x and j_y couple to the total angular momentum J with projection M of the three-body system.

The analytic form given in Eq. (12) for the asymptotic expression of the angular eigenfunction $\Phi_n^{JM}(\Omega, \rho)$ makes evident that it describes an asymptotic spatial distribution for the three particles corresponding to two of them forming a bound state, described by $\psi_n^{j_x}(\mathbf{x})$, and a free third particle moving in the continuum. In other words, the effective adiabatic potentials associated with angular eigenfunctions with the asymptotic form of Eq. (12) are the ones describing the possible incoming and outgoing channels of a process where a particle hits a bound state formed by the other two.

In Fig. 1 the different regions defined by the energy of the incident particles are depicted. All the three-body energies E such that $E_{2b}^{(1)} < E < E_{2b}^{(2)}$ (like $E^{(1)}$ in the figure) correspond to processes where only one channel is open. Only the elastic collision between the third particle and the bound two-body state with energy $E_{2b}^{(1)}$ is possible. When the three-body energy increases up to the region $E_{2b}^{(2)} < E < 0$ ($E^{(2)}$ in the figure) a second channel is open. Two different collisions are now possible, the one where a particle hits the bound state with binding energy $E_{2b}^{(1)}$, and the one where a particle hits the state with binding energy $E_{2b}^{(2)}$. In the same way, each of these reactions has two possible outgoing channels, corresponding to the two allowed bound two-body states and the third particle in the continuum. In particular, in this energy range the rearrangement process is open. When $E > 0$ the breakup channels are also open. They are described by the remaining infinitely many adiabatic potentials. Processes with breakup channels open will be investigated in a forthcoming work.

Therefore, for processes where n_0 channels are open, the full three-body wave function has actually n_0 different components. We shall denote them by Ψ_i , corresponding to the process with incident channel i . Each of the three-body functions Ψ_i is then expanded as in Eq. (4), but the radial functions need now an additional index i ($i \leq n_0$) indicating the incident channel to which they correspond:

$$\Psi_i = \frac{1}{\rho^{5/2}} \sum_{n=1}^{n_A} f_{ni}(\rho) \Phi_n(\rho, \Omega). \quad (13)$$

For each open channel i ($i = 1, 2, \dots, n_0$) the corresponding radial wave functions $f_{ni}(\rho)$ satisfy the set of radial equations of Eq. (5), and Eq. (9) can be generalized to

$$\begin{pmatrix} \hat{\mathcal{H}}_{11} - E & \cdots & \hat{\mathcal{H}}_{1n_A} \\ \hat{\mathcal{H}}_{21} & \cdots & \hat{\mathcal{H}}_{2n_A} \\ \vdots & \vdots & \vdots \\ \hat{\mathcal{H}}_{n_A 1} & \cdots & \hat{\mathcal{H}}_{n_A n_A} - E \end{pmatrix} \begin{pmatrix} f_{11} & f_{12} & \cdots & f_{1n_0} \\ f_{21} & f_{22} & \cdots & f_{2n_0} \\ \vdots & \vdots & \vdots & \vdots \\ f_{n_A 1} & f_{n_A 2} & \cdots & f_{n_A n_0} \end{pmatrix} = 0, \quad (14)$$

which describes the full process. The full three-body wave function is now given by

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_{n_0} \end{pmatrix} = \frac{1}{\rho^{5/2}} \begin{pmatrix} f_{11} & f_{21} & \cdots & f_{n_A 1} \\ f_{12} & f_{22} & \cdots & f_{n_A 2} \\ \vdots & \vdots & \vdots & \vdots \\ f_{1n_0} & f_{2n_0} & \cdots & f_{n_A n_0} \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{n_A} \end{pmatrix}. \quad (15)$$

B. Asymptotics: \mathcal{K} matrix and \mathcal{S} matrix

For scattering states and energies below the breakup threshold ($E < 0$), Eqs. (14) decouple asymptotically, and for a given incident channel i ($i = 1, \dots, n_0$) the only equations surviving are the ones of the form

$$(\hat{\mathcal{H}}_{nn} - E) f_{ni}(\rho) = 0 \quad (n = 1, \dots, n_A), \quad (16)$$

which, by use of Eq. (6), can be written as

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{d\rho^2} + V_{\text{eff}}^{(n)}(\rho) - E \right) f_{ni}(\rho) = 0, \quad (17)$$

where $V_{\text{eff}}^{(n)}$ is given by Eq. (11).

When n corresponds to a closed channel, the radial wave functions f_{ni} vanish asymptotically. When n corresponds to an open channel, the asymptotic behavior of f_{ni} is dictated by the asymptotics of the corresponding adiabatic potential $V_{\text{eff}}^{(n)}$. A careful analysis of the large-distance behavior of the $\lambda_n(\rho)$ and $Q_{nn}(\rho)$ functions in the case of bound two-body subsystems can be found in Ref. [9]. In particular, Eqs. (91) and (93) of that reference allow the above equation to be rewritten for the case $n \leq n_0$ as

$$\left[\frac{d^2}{d\rho^2} + (k_y^{(n)})^2 - \frac{\ell_y(\ell_y + 1)}{\rho^2} \right] f_{ni}(\rho) = 0, \quad (18)$$

where

$$k_y^{(n)} = \sqrt{\frac{2m}{\hbar^2} (E - E_{2b}^{(n)})}, \quad (19)$$

$E_{2b}^{(n)}$ is the binding energy of the bound two-body system associated with the open channel n , and ℓ_y is the orbital angular momentum associated with the Jacobi coordinate \mathbf{y} , which amounts to the relative orbital angular momentum between the projectile and the two-body bound target.

From Eq. (18) it is now clear that the asymptotic behavior of the f_{ni} functions ($n, i \leq n_0$) is given by

$$f_{ni}(\rho) \rightarrow \sqrt{k_y^{(n)}} \rho [A_{in}^{(K)} j_{\ell_y}(k_y^{(n)} \rho) + B_{in}^{(K)} \eta_{\ell_y}(k_y^{(n)} \rho)], \quad (20)$$

where j_{ℓ_y} and η_{ℓ_y} are the usual regular and irregular spherical Bessel functions, respectively. The superscript (K) indicates that, with this particular choice, the coefficients $A_{in}^{(K)}$ and $B_{in}^{(K)}$ will permit extraction of the \mathcal{K} matrix. Conversely, using the spherical Hankel functions in Eq. (20) the coefficients will form the \mathcal{S} matrix and the superscript (S) will be used (see below).

Therefore, asymptotically, the matrix containing the radial wave functions in Eq. (15) reduces to the $n_0 \times n_0$ matrix $A^{(K)}J + B^{(K)}Y$, where $A^{(K)}$ and $B^{(K)}$ are $n_0 \times n_0$ matrices whose components are the $A_{ij}^{(K)}$ and $B_{ij}^{(K)}$ coefficients of Eq. (20), and J and Y are two $n_0 \times n_0$ diagonal matrices with diagonal terms $[\sqrt{k_y^{(i)}} \rho j_{\ell_y}(k_y^{(i)} \rho)]$ and $[\sqrt{k_y^{(i)}} \rho \eta_{\ell_y}(k_y^{(i)} \rho)]$, respectively. Thus, the asymptotic behavior of the full three-body wave function (15) can be finally written as

$$\Psi \rightarrow A^{(K)} F_{\rho}^{(K)} + B^{(K)} G_{\rho}^{(K)}, \quad (21)$$

where $F_{\rho}^{(K)}$ and $G_{\rho}^{(K)}$ are column vectors with n_0 terms of the forms $[\sqrt{k_y^{(n)}} j_{\ell_y}(k_y^{(n)} \rho) \Phi_n / \rho^{3/2}]$ and $[\sqrt{k_y^{(n)}} \eta_{\ell_y}(k_y^{(n)} \rho) \Phi_n / \rho^{3/2}]$, respectively.

From Eq. (21) we then have that for a given incident channel i the asymptotic form of the corresponding three-body wave function (13) takes the form

$$\Psi_i \rightarrow \sum_{n=1}^{n_0} (A_{in}^{(K)} F_{\rho,n}^{(K)} + B_{in}^{(K)} G_{\rho,n}^{(K)}), \quad (22)$$

where

$$\begin{aligned} F_{\rho,n}^{(K)} &= \sqrt{k_y^{(n)}} j_{\ell_y}(k_y^{(n)} \rho) [\psi_n^{j_x} \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{j_y}]^{JM}, \\ G_{\rho,n}^{(K)} &= \sqrt{k_y^{(n)}} \eta_{\ell_y}(k_y^{(n)} \rho) [\psi_n^{j_x} \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{j_y}]^{JM}, \end{aligned} \quad (23)$$

and where we have made use of Eq. (12), which relates the angular eigenfunction Φ_n^{JM} and the two-body wave function $\psi_n^{j_x}$. When two or three identical particles are present in the system, these functions should be correctly symmetrized or antisymmetrized depending on whether they are bosons or fermions.

From Eq. (21) we can now easily write

$$\Psi \rightarrow A^{(K)}(F_{\rho}^{(K)} - \mathcal{K}G_{\rho}^{(K)}), \quad (24)$$

where

$$\mathcal{K} = -A^{(K)-1}B^{(K)} \quad (25)$$

is the \mathcal{K} matrix of the reaction, whose dimension is $n_0 \times n_0$ (with n_0 being the number of open channels).

The discussion in this subsection could also have been made by replacing j_{ℓ_y} and η_{ℓ_y} in Eq. (20) with the spherical Hankel functions $h_{\ell_y}^{(2)}$ and $h_{\ell_y}^{(1)}$, respectively. This would then lead to

$$\Psi \rightarrow A^{(S)}F_{\rho}^{(S)} + B^{(S)}G_{\rho}^{(S)}, \quad (26)$$

where now $F_{\rho}^{(S)}$ and $G_{\rho}^{(S)}$ are column vectors with n_0 terms of the forms $[\sqrt{k_y^{(n)}}h_{\ell_y}^{(2)}(k_y^{(n)}\rho)\Phi_n/\rho^{3/2}]$ and $[\sqrt{k_y^{(n)}}h_{\ell_y}^{(1)}(k_y^{(n)}\rho)\Phi_n/\rho^{3/2}]$, respectively. We can then write

$$\Psi \rightarrow A^{(S)}(F_{\rho}^{(S)} + \mathcal{S}G_{\rho}^{(S)}), \quad (27)$$

where

$$\mathcal{S} = A^{(S)-1}B^{(S)} \quad (28)$$

is the so called \mathcal{S} matrix of the reaction. The \mathcal{S} and \mathcal{K} matrices are related through the well-known simple expression

$$\mathcal{S} = (1 + i\mathcal{K})(1 - i\mathcal{K})^{-1}. \quad (29)$$

It is important to keep in mind that while $A^{(K)}$, $B^{(K)}$, and \mathcal{K} are real, the matrices $A^{(S)}$, $B^{(S)}$, and \mathcal{S} are in general complex.

III. SECOND-ORDER INTEGRAL RELATIONS

In Ref. [14] the applicability of the HA expansion for extraction of phase shifts for $1+2$ reactions when only the elastic channel is open has been discussed. In that reference it was found that, when the number of adiabatic channels n_A included in the calculation is increased as much as possible, the difference between the computed phase shift and the exact value remains significant. As mentioned in the Introduction, this is related to the fact that the asymptotic structure of the system has to be describe in terms of spherical Bessel functions depending on $k_y y$, where y is the modulus of the Jacobi coordinate between the center of mass of the outgoing bound two-body system and the third particle. Instead, the asymptotic behavior using the HA basis is given in terms of spherical Bessel functions depending on $k_y \rho$. Since the equivalence between $k_y y$ and $k_y \rho$ is not achieved for any finite value of ρ , the correct boundary condition is achieved only at $\rho \approx \infty$ and $n_A \rightarrow \infty$.

For a general multichannel process the adiabatic expansion obviously shows the same deficiency. The correct asymptotic wave function is given by Eq. (21), but where $F_{\rho}^{(K)}$ and $G_{\rho}^{(K)}$ in Eq. (23) have to be replaced by $F^{(K)}$ and $G^{(K)}$, which are column vectors whose n th element is

$$\begin{aligned} F_n^{(K)} &= \sqrt{k_y^{(n)}} j_{\ell_y}(k_y^{(n)} y_n) [\psi_n^{j_x} \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{j_y}]^{JM}, \\ G_n^{(K)} &= \sqrt{k_y^{(n)}} \eta_{\ell_y}(k_y^{(n)} y_n) [\psi_n^{j_x} \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]^{j_y}]^{JM}. \end{aligned} \quad (30)$$

In these expressions y_n refers to the modulus of the Jacobi coordinate describing the center of mass of the bound two-body system $\psi_n^{j_x}$ and the third particle.

It is important to recall that the Bessel functions η_{ℓ} are irregular at the origin, which creates difficulties from the numerical point of view. It is then convenient to regularize such functions, in such a way that $G_n^{(K)}$ given in Eq. (30) has to be replaced by

$$\tilde{G}_n^{(K)} = (1 - e^{-\gamma y_n})^{\ell_y+1} G_n^{(K)}, \quad (31)$$

where γ is a nonlinear parameter. The results are stable for values of γ within a small range around $\gamma \sim 1/r_0$, with r_0 the range of the potential.

For simplicity in the notation, from now on, we shall refer to the matrices $\{F^{(K)}, \tilde{G}^{(K)}\}$ as $\{F, G\}$, in such a way that we can write the asymptotic behavior of the wave function as

$$\Psi \rightarrow AF + BG, \quad (32)$$

and $\mathcal{K} = -A^{-1}B$.

The vectors F and G satisfy the following normalization condition:

$$-\frac{2m}{\hbar^2} [\langle F | \hat{\mathcal{H}} - E | G \rangle - \langle G | \hat{\mathcal{H}} - E | F \rangle^T] = \mathbb{I}, \quad (33)$$

where \mathbb{I} is the identity matrix. In Eq. (33) we have introduced a notation to be used from now on in which the overlap of two vectors is a matrix whose elements are, for example, $\langle F | \hat{\mathcal{H}} - E | G \rangle_{ij} = \langle F_i | \hat{\mathcal{H}} - E | G_j \rangle$. The normalization condition allows us to extract a first-order estimate of the matrices A and B from the scattering wave function Ψ as

$$B^{1st} = -\frac{2m}{\hbar^2} [\langle F | \hat{\mathcal{H}} - E | \Psi \rangle^T - \langle \Psi | \hat{\mathcal{H}} - E | F \rangle], \quad (34)$$

$$A^{1st} = -\frac{2m}{\hbar^2} [\langle \Psi | \hat{\mathcal{H}} - E | G \rangle - \langle G | \hat{\mathcal{H}} - E | \Psi \rangle^T]. \quad (35)$$

Clearly, when Ψ is an exact solution of $(\hat{\mathcal{H}} - E)\Psi = 0$, the above expressions reduce to the following integral relations:

$$B = \frac{2m}{\hbar^2} \langle \Psi | \hat{\mathcal{H}} - E | F \rangle, \quad (36)$$

$$A = -\frac{2m}{\hbar^2} \langle \Psi | \hat{\mathcal{H}} - E | G \rangle.$$

Explicitly, each matrix element B_{ij} and A_{ij} is given by

$$B_{ij} = \frac{2m}{\hbar^2} \langle \Psi_i | \hat{\mathcal{H}} - E | F_j \rangle, \quad (37)$$

$$A_{ij} = -\frac{2m}{\hbar^2} \langle \Psi_i | \hat{\mathcal{H}} - E | G_j \rangle, \quad (38)$$

which can be seen as the extension to multichannel scattering of the expressions valid for the single-channel case. Now the same formula applies for each possible incoming channel described by Ψ_i and each possible outgoing channel whose asymptotic analytic form is given by a linear combination of F_j and G_j .

As demonstrated in Refs. [14,18] for a single-channel process, the relation $\mathcal{K} = -A^{-1}B$ computed using Eqs. (37) and (38) can be considered accurate up to second order when a trial wave function Ψ_t is used. Moreover the two integral relations of Eqs. (37) and (38) can be directly derived from the Kohn variational principle. As shown in Appendix A, the matrix form of the KVP, necessary to describe a multichannel process, establishes that each matrix element of $A^{-1}B^{2\text{nd}}$ is a functional given by

$$A^{-1}B^{2\text{nd}} = A^{-1}B + \frac{2m}{\hbar^2} A^{-1} \langle \Psi_t | \hat{\mathcal{H}} - E | \Psi_t \rangle (A^{-1})^T, \quad (39)$$

which is stationary with respect to variations of the wave function. Taking into account the general asymptotic behavior in Eq. (32), we can write the full trial wave function schematically as

$$\Psi_t = \Psi_c + AF + BG, \quad (40)$$

with $\Psi_c \rightarrow 0$ as $\rho \rightarrow \infty$. Furthermore Ψ_c can be expanded in terms of a (square integrable) complete basis $\{b_i, i = 1, \dots, m\}$:

$$\Psi_c = \begin{pmatrix} \Psi_{c,1} \\ \Psi_{c,2} \\ \vdots \\ \Psi_{c,n_0} \end{pmatrix} = \frac{1}{\rho^{5/2}} \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1m} \\ c_{21} & c_{22} & \cdots & c_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ c_{n_0 1} & c_{n_0 2} & \cdots & c_{n_0 m} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}. \quad (41)$$

The variation of the functional with respect to the linear parameters c_{ij} and with respect to the matrix elements of $A^{-1}B$ leads to

$$\begin{aligned} \langle \Psi_c | \hat{\mathcal{H}} - E | \Psi_t \rangle &= 0, \\ \langle G | \hat{\mathcal{H}} - E | \Psi_t \rangle &= 0. \end{aligned} \quad (42)$$

When Ψ is replaced by Ψ_t , the second expression above and Eq. (35) result in

$$A = -\frac{2m}{\hbar^2} \langle \Psi_t | \hat{\mathcal{H}} - E | G \rangle. \quad (43)$$

Replacing now Eq. (40) into (39), and making use of Eqs. (42), we also get

$$B^{2\text{nd}} = B^{1\text{st}} + \frac{2m}{\hbar^2} \langle F | \hat{\mathcal{H}} - E | \Psi_t \rangle^T, \quad (44)$$

and, taking into account that $B^{1\text{st}}$ is given by Eq. (34) we can then obtain the final result:

$$\begin{aligned} B^{2\text{nd}} &= \frac{2m}{\hbar^2} \langle \Psi_t | \hat{\mathcal{H}} - E | F \rangle, \\ A &= -\frac{2m}{\hbar^2} \langle \Psi_t | \hat{\mathcal{H}} - E | G \rangle, \end{aligned} \quad (45)$$

which according to Eqs. (25) and (29) permit one to obtain the second-order estimate of the \mathcal{K} matrix or the \mathcal{S} matrix, $\mathcal{K}^{2\text{nd}}$ or $\mathcal{S}^{2\text{nd}}$, respectively.

In practical cases, application of the integral relations given in Eq. (45) requires the calculation of each individual matrix element A_{ij} and B_{ij} , which relate each possible incoming channel i , described by Ψ_i , with each possible outgoing asymptotic given by F_j and G_j . Details about the calculation of these matrix elements are given in Appendix B, in particular for the case of two-body potentials projecting on the partial waves.

The integral relations of Eq. (45) depend on the short-range structure of the scattering wave function Ψ_t as F and G are asymptotically solutions of $(\mathcal{H} - E)F, G = 0$. This property allows for different applications of the integral relations, as discussed in Ref. [18]. In the present work interest is in the study of the pattern of convergence of $\mathcal{K}^{2\text{nd}}$ in terms of the number of equations n_A considered in the description of Ψ_t using the HA expansion. As we will see, with increase in n_A , both matrices A and $B^{2\text{nd}}$ slightly change, showing individually a very slow rate of convergence. Conversely, the rate $\mathcal{K}^{2\text{nd}} = -A^{-1}B^{2\text{nd}}$ shows a pattern of convergence similar to that observed in a bound state calculation.

IV. RESULTS

A. Test of the method: A model 1 + 2 collision

To test the method we have chosen a 1 + 2 reaction where the target dimer is made up of an infinitely heavy particle and a light one, and where we consider a projectile interacting only with the heavy particle (see Fig. 2). In the collision particle 2 does not play any role, and the process is equivalent to a two-body reaction between particles 3 and 1. Therefore the results obtained through the three-body calculation and the integral relations can be easily tested by means of a simple two-body calculation.

In particular, we consider a two-body target made by two spin-zero bosons with masses $0.5m$ and $10^{12}m$ (with $m = 938.69461$ MeV) interacting via a simple central potential given by

$$V_{12}(r) = -80 e^{-r^2/1.6^3}, \quad (46)$$

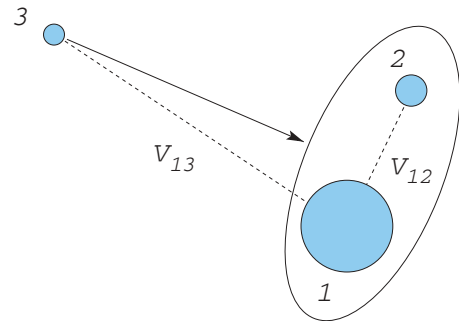


FIG. 2. (Color online) Scheme of the model reaction used to test the integral relations. The light projectile 3 hits the dimer made by particles 1 and 2. Particle 1 is infinitely heavy and particles 2 and 3 do not interact.

TABLE I. Partial wave phase shifts δ_ℓ for different values of n_A [number of adiabatic terms used in the expansion (4)]. In the last row, the result using a two-body calculation is shown.

n_A	δ_s	δ_p	δ_d
1	40.554	0.6658	0.0136
2	38.988	0.6892	0.0113
3	38.642	0.6921	0.0121
5	38.693	0.6911	0.0119
8	38.702	0.6918	0.0118
10	38.701	0.6918	0.0118
Two body	38.699	0.6917	0.0117

where r is given in fermi (fm) and the strength in MeV. This system has only one s -wave bound state with binding energy -6.2757 MeV.

The projectile, which is chosen to have a mass of $0.51m$, does not interact with particle 2, while it does it with particle 1 through the Gaussian potential

$$V_{13}(r) = -30 e^{-r^2/1.6^2}, \quad (47)$$

where again r is in fm and the strength in MeV. This potential is not able to bind particles 1 and 3. Finally, as described above, $V_{23} = 0$.

We have chosen an incident energy of 3 MeV, which implies a total three-body energy of -3.2757 MeV. We are then below the threshold for breakup of the two-body target, and only the elastic channel is open. Therefore, B and A in Eq. (45) are just numbers, and they are such that $\tan \delta_\ell = -B/A$ (note that the definitions of B here and in [14,18] have opposite signs).

We have computed the phase shift for this reaction for relative s , p , and d waves between the projectile and the target. The convergence of the expansion (4) is shown in Table I, where we show the phase shift for the different partial waves and for different values of n_A , which is the number of adiabatic terms included in the calculation. As we can see, inclusion of eight to ten adiabatic potentials is enough to reach convergence for the three partial waves. Furthermore, the converged result agrees with the phase shift obtained from the two-body calculation describing the collision between particles 3 and 1.

The efficiency of using the integral relations in Eq. (45) is made evident in Fig. 3, where we show the partial wave phase shifts δ_ℓ as functions of n_A . The solid line gives the results obtained from the integral relations (given in Table I), and the thick dashed line shows the results extracted by direct comparison of the computed asymptotic radial wave functions and the analytic expression in Eq. (20). The thin dashed line indicates the phase shifts obtained from a two-body calculation. As we can immediately see in the figure, the pattern of convergence of the phase shifts obtained from Eq. (20) (thick dashed curves) is very slow. A simple extrapolation of these curves up to the correct value permits one to foresee that the number of adiabatic terms needed to obtain accurate values of δ_ℓ is far larger than that needed when the integral relations are used. In fact, at the scale of the figure, the calculations with the integral relations are already indistinguishable from the correct result for $n_A = 4$ (see also Table I).

As seen in Table I, the d -wave phase shift is already rather small and therefore, at the considered energy, the cross

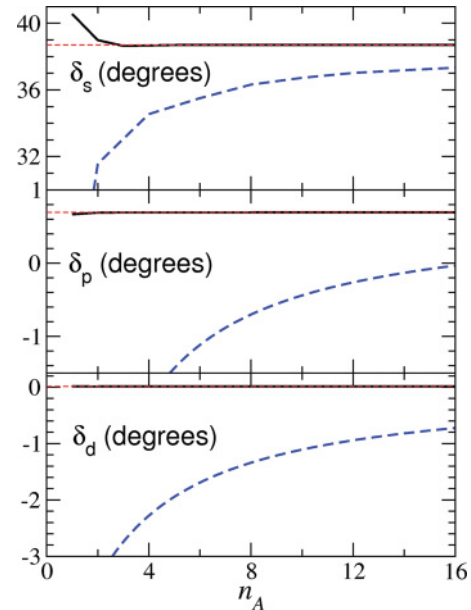


FIG. 3. (Color online) Phase shift for s , p , and d partial waves for the model reaction in Sec. IV A as a function of the number of adiabatic terms included in the calculation. The solid line is the result obtained through the integral relations, and the thick dashed curve has been obtained from the asymptotic expression (20). The thin dashed line is the result obtained from a two-body calculation.

section contributions from higher angular partial waves are negligible. In Fig. 4 the differential cross section of the process with cumulative inclusion of one (solid), two (dashed), and three (dot-dashed) partial waves is shown. As can be seen, s , p , and d partial waves are enough to obtain a converged cross section of the process. In fact, the partial waves beyond the s wave have a modest contribution, and the total cross section approaches quite closely the characteristic $\sin \theta$ function of the s waves.

B. A realistic case: The ${}^4\text{He}$ - ${}^4\text{He}_2$ collision

In this section we discuss an interesting simple physical case, but one that is technically similar to the model case described in the previous section. This is the collision of a ${}^4\text{He}$ atom with the weakly bound ${}^4\text{He}_2$ dimer. The helium dimer

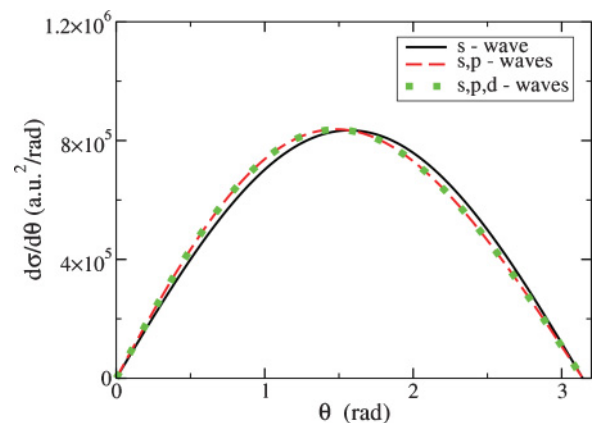


FIG. 4. (Color online) Cumulative contributions to the differential cross section as a function of the scattering angle θ for the model collision in Sec. IV A.

has a single s -wave bound state, and as soon as the incident energy is below the dimer breakup threshold, again only the elastic channel is open.

The two-body helium-helium interaction is chosen to be the simple effective Gaussian potential given in [19]. This is enough for our purpose of illustrating how this kind of processes can be easily described by use of the integral relations. This potential is built to reproduce the s -wave scattering length (189.054 a.u.) and effective range (13.843 a.u.) of the LM2M2 interaction [20], which is the second mimic of the second Liu and McLean potential introduced in [21], and it is given by

$$V_{2B}(r) = -1.227e^{-r^2/10.03^2}, \quad (48)$$

where r is given in a.u. and the strength is in kelvin (K). This potential leads to a bound $0^+ \text{ } ^4\text{He}_2$ dimer with a binding energy $E_d = -1.2959$ mK, a scattering length $a = 189.947$ a.u., and an effective range of 13.846 a.u. Simple representations of the atom-atom potentials are often used to describe reactions in the ultracold regime (see for example Refs. [22,23]). In this regime the process is largely independent of the shape of the potential and can be characterized only by the scattering length.

With this interaction the helium trimer has two bound states at -150.0 and -2.467 mK. These states have been obtained using the Gaussian potential active only in s waves. Increase in the number of partial waves up to $\ell_x = \ell_y = 8$ results in a very small change for the ground and excited state binding energies, which become now 150.4 and -2.472 mK, respectively. In fact, more than 99% of the norm of the bound state wave functions is provided by the lowest adiabatic term, whose corresponding adiabatic potential is close to identical in both calculations. Accordingly, in the following we restrict the calculations to include only the $\ell_x = 0$ channel.

When the LM2M2 potential is used, these two states are found to have binding energies -126.4 and -2.265 mK, respectively [8]. As we can see, the ground state is not very well reproduced when the Gaussian version of the potential is used. In this very deep state, the three atoms are close to each other and the correct structure cannot be described with the simplified potential. Conversely, the excited state, which has the characteristics of an Efimov state, has a structure in which the third atom orbits very far from the bound state of the other two. This particular structure is well described by the attractive Gaussian potential.

In order to study the convergence properties of the HA expansion for a $1 + 2$ collision, we have chosen an incident energy of 0.5 mK (or a three-body energy $E = -0.7959$ mK). The phase shifts for the different partial waves have been computed as in the previous subsection. The results are shown in Table II for s , p , d , and f waves. A good convergence is obtained already after inclusion of about 10 adiabatic terms, except for s waves, where about 18 are needed. The last row in the table shows the phase shift obtained for an s -wave collision when the hyperspherical harmonic method is used. The two methods are in close agreement.

At this particular energy we have calculated the differential cross section. Figure 5 shows the cumulative contributions of

TABLE II. Partial wave phase shifts δ_ℓ showing convergence of these values with the number n_A of adiabatic potentials used in the calculation. The last row shows the result when the hyperspherical harmonic method [4] is used.

n_A	δ_s	δ_p	δ_d	δ_f
1	-39.72	-13.19	2.01	-0.27
2	-40.30	-13.13	2.11	-0.28
4	-40.43	-13.11	2.13	-0.28
8	-40.50	-13.11	2.14	-0.28
18	-40.54	-13.11	2.14	-0.28
22	-40.54	-13.11	2.14	-0.28
HH calculation	-40.55			

the s , p , d , and f partial waves. We observe that the p -wave contribution is rather important and produces a deviation from the $\sin\theta$ shape. Moreover, four partial waves are needed to reach a good convergence.

In Fig. 6 we show the computed s -wave phase shift as a function of the incident energy ($E - E_d$). Our results are given by the stars. For comparison we also show the results reported in [24], [25], and [26] (solid curve, squares, and dashed curve, respectively). As we can see, the phase shifts obtained in this work are a few degrees above the ones obtained in the previous calculations, where the $^4\text{He}-^4\text{He}$ interaction is treated in more detail. In fact the reason for this discrepancy is the hard core repulsion present in the $^4\text{He}-^4\text{He}$ interactions used in [24–26]. For the same reason the atom-dimer scattering length a_{a-d} obtained with the Gaussian potential used in this work, $a_{a-d} = 166$ a.u., differs from the typical values of around $a_{a-d} = 220$ a.u. (≈ 116 Å) obtained when hard core potentials are used [25,27].

C. A multichannel collision: The $^4\text{He}-^4\text{He}-^6\text{Li}$ system

In this section a reaction where more than one channel is open is discussed. To this end, we have chosen a process involving two helium and one lithium atoms. The cross section for this kind of reaction is the necessary ingredient to obtain the recombination rate for such three-body systems. As quoted in [28], where the three-body recombination for cold-helium–helium–alkali-metal systems is investigated, such collision

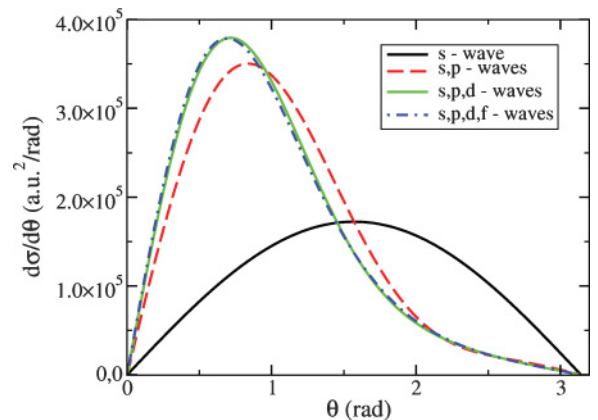


FIG. 5. (Color online) The same as Fig. 4 for the $^4\text{He}-^4\text{He}_2$ collision. With four partial waves the convergence is fairly good.

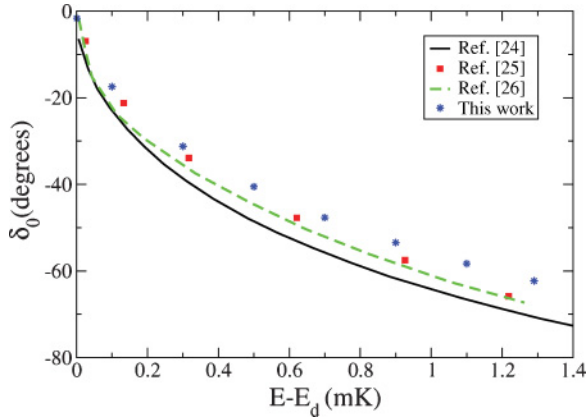


FIG. 6. (Color online) s -wave phase shift δ_s as a function of the incident energy for the ${}^4\text{He}$ - ${}^4\text{He}_2$ collision. The stars are the results obtained in the present work. The solid curve, the squares, and the dashed curve correspond to the results given in [24], [25], and [26], respectively.

processes are important in ultracold gas experiments using buffer-gas cooling, since it might limit the lifetimes of the trapped atoms.

To describe this three-body system we take the same helium-helium interaction as in the previous section, which leads to a 0^+ ${}^4\text{He}_2$ dimer with a binding energy of -1.2959 mK. The lithium-helium interaction is also chosen to have a Gaussian shape, and it is taken to be

$$V_{({}^6\text{Li}-{}^4\text{He})}(r) = -0.273\,68e^{-r^2/20.14^2}, \quad (49)$$

where r is in a.u. and the strength is in K. The parameters have been adjusted to give a scattering length of -173.5 a.u. and an effective range of 26.475 a.u. in agreement with the values obtained in [29] ($a = -173.8$ a.u. and $r_e = 26.483$ a.u.), where the more sophisticated Kleinekaöhfer-Tang-Toennies-Yiu potential is used. This potential leads to a 0^+ bound ${}^6\text{Li}$ - ${}^4\text{He}$ system with a binding energy of -1.4225 mK.

The adiabatic potentials obtained for the ${}^4\text{He}$ - ${}^4\text{He}$ - ${}^6\text{Li}$ three-body system follow the same pattern as the potentials in Fig. 1, where $E_{2b}^{(1)}$ corresponds now to the binding energy of the ${}^6\text{Li}$ - ${}^4\text{He}$ dimer (-1.4225 mK) and $E_{2b}^{(2)}$ corresponds to the binding energy of the ${}^4\text{He}_2$ dimer (-1.2959 mK). The three-body system presents one bound state at $E = -58.12$ mK.

Thus, as soon as the three-body energy lies in the same region as $E^{(2)}$ in the figure, two different channels are open. One of them corresponds to a bound ${}^6\text{Li}$ - ${}^4\text{He}$ dimer and the second ${}^4\text{He}$ atom in the continuum (we shall refer to it as channel 1), and the other one corresponds to the bound ${}^4\text{He}_2$ dimer and the ${}^6\text{Li}$ atom in the continuum (we shall refer to it as channel 2). In other words, when taking channel 1 as the incoming channel we are considering a process where the ${}^4\text{He}$ atom hits a bound ${}^6\text{Li}$ - ${}^4\text{He}$ dimer, while when choosing channel 2 as the incoming channel we are then considering the process of a ${}^6\text{Li}$ atom hitting a ${}^4\text{He}_2$ dimer. For each of the two possible incoming channels we have two different outgoing channels, the elastic one, and a rearrangement process where the projectile is captured by one of the

TABLE III. \mathcal{K} -matrix elements are given as a function of the number of adiabatic potentials used in the calculation (n_A).

n_A	\mathcal{K}_{11}	\mathcal{K}_{12}	\mathcal{K}_{21}	\mathcal{K}_{22}
2	-2.460	-0.650	-0.648	-1.411
3	-2.765	-0.821	-0.801	-1.496
4	-2.691	-0.775	-0.776	-1.468
6	-2.699	-0.781	-0.781	-1.471
8	-2.702	-0.783	-0.783	-1.471
10	-2.710	-0.787	-0.787	-1.473
14	-2.714	-0.790	-0.789	-1.474
18	-2.712	-0.791	-0.790	-1.474

constituents of the dimer, while the second dimer constituent is released.

The existence of two open channels implies that the \mathcal{K} matrix (or the \mathcal{S} matrix) is a 2×2 matrix, that can be obtained through the 2×2 matrices A and $B^{2\text{nd}}$ in Eq. (45). Each of the four terms in A and $B^{2\text{nd}}$ can be obtained as in Eqs. (38) and (37), where Ψ_i is the trial three-body wave function for the incoming channel i . F_j and G_j are the asymptotic functions given in Eqs. (30) for the outgoing channel j . These functions have to be symmetrized when the outgoing channel is 1, since the helium atom in the dimer is identical to the one moving in the continuum. For outgoing channel 2 this is not necessary, since the dimer wave function in (30) is already properly symmetrized. In practice, the symmetrization introduces a factor of $\sqrt{2}$ in Eqs. (37) and (38) when $j = 1$. The calculation of each of these terms is formally identical to the case with only the elastic channel open.

In the calculation here we have chosen a three-body energy of -0.7959 mK, which represents an incident energy of 0.6266 mK when channel 1 is the incoming channel and 0.5 mK when channel 2 is the incoming channel. For simplicity we restrict our attention in this section to relative s waves between the projectile and the dimer target. The computed results for the four terms of the \mathcal{K} matrix are shown in Table III for different values of n_A . As seen in the table, again a reduced number of adiabatic terms permits us to reach a reasonable convergence in the \mathcal{K} matrix.

From the computed \mathcal{K} matrix we can now easily obtain the \mathcal{S} matrix by means of Eq. (29). This leads to $\mathcal{S}_{11} = -0.673 - 0.663i$, $\mathcal{S}_{12} = \mathcal{S}_{21} = -0.285 + 0.162i$, and $\mathcal{S}_{22} = -0.224 - 0.918i$. The square of these elements, $|\mathcal{S}_{ij}|^2$, indicates the probability for the process with incoming channel i to end up in channel j . In this particular case we get $|\mathcal{S}_{11}|^2 = |\mathcal{S}_{22}|^2 = 0.892$ and $|\mathcal{S}_{12}|^2 = |\mathcal{S}_{21}|^2 = 0.108$.

It is important to note that the matrices A and $B^{2\text{nd}}$ are not unique. A different definition of the normalization of the asymptotic states would result in new A and $B^{2\text{nd}}$ matrices which would obviously lead to the same \mathcal{K} matrix. In particular, A and $B^{2\text{nd}}$ do not fulfill the property of being symmetric, but they lead to a \mathcal{K} matrix with the correct Hermitian condition. Moreover, using Eq. (29), the computed \mathcal{S} matrix automatically satisfies the unitarity condition $\mathcal{S}^\dagger \mathcal{S} = \mathbb{I}$.

V. SUMMARY AND CONCLUSIONS

In this work we have discussed the general form of the integral relations that were introduced in [14,18]. These relations are derived from the Kohn variational principle and they permit the particularities of the adiabatic expansion method to be exploited to describe scattering states. In particular, in [14,18] it was shown that the convergence of the computed scattering phase shifts in terms of the adiabatic terms included in the calculation is rather fast. The resulting convergence pattern is similar to that of a bound state calculation. The reason for this success is that when the integral relations are used only the internal part of the wave function is needed, and an accurate calculation of it requires a smaller number of adiabatic terms than when the wave function is computed in the asymptotic region.

The applications given in [14,18] were limited to processes involving only relative s waves and with only one channel open. In this work we have explicitly derived the integral relations from the KVP in the case of multichannel reactions and we have computed phase shifts up to f waves. Furthermore, we have used a vectorial notation for the wave function such that all the possible channels are simultaneously represented. With this notation the coefficients weighting the regular and irregular parts of the asymptotic wave function are $n_0 \times n_0$ matrices (with n_0 being the number of open channels) and each term of these two matrices is obtained from an integral relation. Finally, the \mathcal{K} matrix for a given process is obtained as the product of two $n_0 \times n_0$ matrices.

Although the method derived is completely general, in this work we have restricted ourselves to describing $1 + 2$ reactions with projectile energy below the breakup threshold in three outgoing particles. Therefore, only elastic, inelastic, and rearrangement processes are possible.

To test the method when relative partial waves higher than zero are included, we first used a toy model such that the three-body reaction is fully equivalent to a two-body process. In this way the correct phase shift can be easily computed through a simple two-body calculation. We found a slow convergence of the phase shifts when they were extracted from the asymptotic parts of the radial wave functions. Conversely, the rate $A^{-1}B$ converges much more quickly and the result stabilizes with a rather small number of adiabatic channels. The convergence is equally fast for all the partial waves, and around ten adiabatic terms are enough to reach a good convergence. Furthermore, the phase shifts obtained with the two-body calculations are well reproduced.

As the next step, we analyzed a more physical case, in particular the ${}^4\text{He}-{}^4\text{He}_2$ collision. Since we considered energies below the ${}^4\text{He}_2$ breakup threshold, in this reaction only the elastic channel is open. This is a process technically analogous to the previous schematic case for which the method has been proved to work. In fact, a similar pattern of convergence is found for the different partial waves included in the calculation. Inclusion of partial waves with ℓ up to 3 is needed to obtain a converged cross section for the process. For s waves the computed phase shift reproduces the one obtained with the hyperspherical harmonic expansion method.

Finally, we considered a process with two open channels. We chose a three-body system made by two ${}^4\text{He}$ and one

${}^6\text{Li}$ atoms, where two different dimers, ${}^4\text{He}_2$ and ${}^4\text{He}-{}^6\text{Li}$, are possible. We therefore simultaneously investigated the collision between a ${}^4\text{He}$ atom and a ${}^4\text{He}-{}^6\text{Li}$ dimer and the one between a ${}^6\text{Li}$ atom and a ${}^4\text{He}_2$ dimer. For both reactions two possible outgoing channels (elastic and rearrangement) are permitted. We then used the method to obtain the 2×2 \mathcal{K} matrix. Again, we found a fast convergence of the four terms in \mathcal{K} . Furthermore, the computed \mathcal{K} matrix satisfies the required Hermitian condition, as well as the fact of leading to a unitary \mathcal{S} matrix.

Summarizing, we have shown that the integral relations can be easily applied to reactions involving nonzero partial waves and with more than one channel open. Also in this case, the hyperspherical adiabatic expansion method is a highly efficient tool that permits scattering wave functions to be obtained. The \mathcal{K} matrix, and therefore also the \mathcal{S} matrix, converges rather fast. Also, since the hyperspherical adiabatic expansion method permits identification of every single incoming and outgoing open channel with a single adiabatic term, the dimension of the matrices to be computed is rather modest, typically of the same size as the number of open channels in the reaction.

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APPENDIX A: MATRIX FORM OF THE KOHN VARIATIONAL PRINCIPLE

This derivation is completely analogous to the derivation presented in Ref. [30]. The only difference is that, in order to represent each possible incoming channel, we use the vectorial notation for the wave functions as introduced in the present work, where the total wave function Ψ has the form given in Eq. (15).

We start by taking the matrix given by

$$I \equiv \langle \Psi | \hat{\mathcal{H}} - E | \Psi \rangle, \quad (\text{A1})$$

which vanishes when Ψ is the exact wave function. We then introduce a test wave function $\Psi_t = \Psi + \delta\Psi$ so that its radial wave functions verify

$$\begin{aligned} f_{ni}^t(0) &= 0, \\ f_{ni}^t(\rho \rightarrow \infty) &\rightarrow \sqrt{k_y^{(n)}} \rho [A_{in}^t j_{\ell_y}(k_y^{(n)} \rho) + B_{in}^t \eta_{\ell_y}(k_y^{(n)} \rho)]. \end{aligned} \quad (\text{A2})$$

We can then write $f_{ni}^t = f_{ni} + \delta f_{ni}$, where δf_{ni} satisfies

$$\delta f_{ni}(\rho) \rightarrow \sqrt{k_y^{(n)}} \rho \eta_{\ell_y}(k_y^{(n)} \rho) \delta B_{in}. \quad (\text{A3})$$

The matrix in Eq. (A1), evaluated at the test wave function, is

$$I_t = \delta I = \langle \Psi_t | \hat{\mathcal{H}} - E | \Psi_t \rangle. \quad (\text{A4})$$

Using now that the exact wave function verifies that $(\hat{\mathcal{H}} - E)|\Psi\rangle = 0$, and keeping only the first order terms, the matrix above can be written as

$$\delta I = \langle \Psi | \hat{\mathcal{H}} - E | \delta \Psi \rangle - \langle \delta \Psi | \hat{\mathcal{H}} - E | \Psi \rangle^T \quad (\text{A5})$$

Using the expansion of Ψ given in Eq. (13) and the analytical expression of the operator $\hat{\mathcal{H}}$ from Eq. (2), it can be seen that each matrix element of δI takes the form

$$\begin{aligned} \delta I_{ij} = & \frac{\hbar^2}{2m} \sum_n \int_0^\infty d\rho \frac{d}{d\rho} \left(\frac{df_{ni}}{d\rho} \delta f_{nj} - \frac{d(\delta f_{nj})}{d\rho} f_{ni} \right) \\ & - \frac{\hbar^2}{m} \sum_n \int_0^\infty d\rho \frac{d}{d\rho} (P_{ij}(\rho) f_{ni} \delta f_{nj}), \end{aligned} \quad (\text{A6})$$

where $P_{ij}(\rho)$ are the coupling terms appearing in Eq. (7) and given in Eq. (8), which vanish when ρ tends to zero or to infinity. Therefore the last term in the previous expression vanishes, and, since $f_{ni}(0) = 0$, we get

$$\delta I_{ij} = \frac{\hbar^2}{2m} \sum_n \left[\frac{df_{ni}}{d\rho} \delta f_{nj} - \frac{d(\delta f_{nj})}{d\rho} f_{ni} \right]_{\rho=\infty}, \quad (\text{A7})$$

which, using Eqs. (20) and (A3), leads to

$$\delta I_{ij} = -\frac{\hbar^2}{2m} \sum_n A_{in} \delta B_{jn} = -\frac{\hbar^2}{2m} \{A \delta B^T\}_{ij}, \quad (\text{A8})$$

or, in a more compact way,

$$\delta \left(I + \frac{\hbar^2}{2m} A B^T \right) = 0. \quad (\text{A9})$$

Since for the exact wave function Ψ we have that $I = 0$, we finally get

$$\frac{\hbar^2}{2m} A B^T = I_t + \frac{\hbar^2}{2m} A B_t^T, \quad (\text{A10})$$

which becomes a variational principle for $A B^T$. Therefore, given a test wave function Ψ_t , we obtain a second order correction for $A B^T$ as

$$A(B^{2\text{nd}})^T = A B^T + \frac{2m}{\hbar^2} \langle \Psi_t | \hat{\mathcal{H}} - E | \Psi_t \rangle. \quad (\text{A11})$$

If we now multiply from the left by A^{-1} and from the right by $(A^{-1})^T$, and make use of the fact that the \mathcal{K} matrix is symmetric, i.e., $A^{-1} B = B^T (A^{-1})^T$, we then finally get the expression given in Eq. (39).

APPENDIX B: CALCULATION OF THE INTEGRALS IN A AND B

In this appendix we give details of the calculation of the integrals A and B , in particular when using two-body potentials projecting on partial waves. With this aim let us start from the general expression for A and B in Eq. (45), and write the \mathcal{L} operator in its explicit form,

$$\begin{aligned} \mathcal{L} = & \frac{2m}{\hbar^2} (\hat{\mathcal{H}} - E) = \frac{2m}{\hbar^2} \left(-\frac{\hbar^2}{2m} \nabla_{y_1}^2 - \frac{\hbar^2}{2m} \nabla_{x_1}^2 + \hat{V}_1(x_1) \right. \\ & \left. + \hat{V}_2(x_2) + \hat{V}_3(x_3) - E_d - E_0 \right), \end{aligned} \quad (\text{B1})$$

where E_d is the binding energy of the dimer and E_0 is the incident energy of the projectile. The Jacobi coordinates $(\mathbf{x}_1, \mathbf{y}_1)$ are defined such that \mathbf{x}_1 connects the two particles in the dimer (particles 2 and 3). The coordinates x_2 and x_3 are related to the distances between particles 1 and 3, and between particles 1 and 2, respectively.

Using F and G as defined in (30) we can rewrite Eq. (45) as

$$B^{2\text{nd}} = \frac{2m}{\hbar^2} \langle \Psi | \hat{V}_2(x_2) + \hat{V}_3(x_3) | F(\mathbf{x}_1, \mathbf{y}_1) \rangle, \quad (\text{B2})$$

$$A = -\frac{2m}{\hbar^2} \langle \Psi | \hat{V}_2(x_2) + \hat{V}_3(x_3) | \tilde{G}(\mathbf{x}_1, \mathbf{y}_1) \rangle + I_\nabla,$$

where

$$I_\nabla = -\langle \Psi | \nabla_{y_1}^2 - k_{y_1}^2 | \tilde{G}(x_1, y_1) \rangle, \quad (\text{B3})$$

and where \tilde{G} refers to the regularized function (31).

If we set $B^{2\text{nd}} = I_B$ and $A = I_A + I_\nabla$, we have that, after substitution of Eq. (30), the integrals in (B2) can also be written as

$$\begin{aligned} I_{A,B} = & \frac{2m}{\hbar^2} \sum_{i=2,3} \int d\rho \rho^5 d\Omega_i \Psi(\rho, \Omega_i) \hat{V}_i(x_i), \\ & g_{A,B}^{\ell_{y_1}}(y_1, k_{y_1}) [\psi_{\ell_{x_1}}(\mathbf{x}_1) \otimes Y_{\ell_{y_1}}(\Omega_{y_1})]^{LM_L}, \end{aligned} \quad (\text{B4})$$

where

$$\begin{aligned} g_B^{\ell_y}(y, k_y) &= j_{\ell_y}(k_y y), \\ g_A^{\ell_y}(y, k_y) &= -\eta_{\ell_y}(k_y y) (1 - e^{\gamma y})^{\ell_y + 1}, \end{aligned} \quad (\text{B5})$$

and where for simplicity in the notation we have assumed that the particles have zero spin. The corresponding expressions in this appendix for particles with spin will follow immediately by coupling the orbital part in the expressions above to the corresponding spin part.

If the potential operator is given as a sum of projectors on partial waves, we have that

$$\hat{V}_i(x_i) = \sum_{\ell_{x_i} m_{\ell_{x_i}}} V_{\ell_{x_i}}(x_i) |\ell_{x_i} m_{\ell_{x_i}}\rangle \langle \ell_{x_i} m_{\ell_{x_i}}|, \quad (\text{B6})$$

where $V_{\ell_{x_i}}$ represents the interaction between particles j and k when they are in a relative partial wave with angular momentum ℓ_{x_i} .

If we also consider Eq. (4) and expand the angular functions $\Phi_n(\rho, \Omega)$ in terms of the hyperspherical harmonics $[\Phi_n(\rho, \Omega)^{LM} = \sum_{K \ell_x \ell_y} C_{K \ell_x \ell_y}^{(n)}(\rho) \mathcal{Y}_{\ell_x \ell_y}^{KLM}(\Omega)]$, we can then obtain the following expression for the potential operator acting over the three-body wave function:

$$\begin{aligned} \langle \Psi | \hat{V}(x) = & \frac{1}{\rho^{5/2}} \sum_n f_n(\rho) \sum_{K \ell_x \ell_y} \sum_{\tilde{K} \tilde{\ell}_x \tilde{\ell}_y} C_{\tilde{K} \tilde{\ell}_x \tilde{\ell}_y}^{(n)} \\ & \times \langle \mathcal{Y}_{\tilde{\ell}_x \tilde{\ell}_y}^{\tilde{K}LM} | V_{\ell_x}(x) | \mathcal{Y}_{\ell_x \ell_y}^{KLM} \rangle \langle \mathcal{Y}_{\ell_x \ell_y}^{KLM} |. \end{aligned} \quad (\text{B7})$$

Expanding now the hyperspherical harmonics in terms of the Jacobi polynomials $P_\nu^{\ell_x+1/2, \ell_y+1/2}$ ($K = 2\nu + \ell_x + \ell_y$) with normalization coefficients $N_K^{\ell_x \ell_y}$ (see [9] for details), we have that the the integrals I_A and I_B can then be explicitly

written as

$$\begin{aligned}
I_{A,B} = & \sum_{i=2,3} \int d\rho \rho^5 (\sin \alpha_i)^2 (\cos \alpha_i)^2 d\alpha_i \frac{1}{\rho^{5/2}} \\
& \times \sum_n f_n(\rho) \sum_{K \ell_x \ell_y} \sum_{\bar{K} \bar{\ell}_x \bar{\ell}_y} C_{K \ell_x \ell_y L}^{(n)} N_{\bar{K}}^{\bar{\ell}_x \bar{\ell}_y} (\sin \alpha_i)^{\bar{\ell}_x} (\cos \alpha_i)^{\bar{\ell}_y} \\
& \times P_v^{\bar{\ell}_x+1/2, \bar{\ell}_y+1/2} (2 \cos \alpha_i) \langle \mathcal{Y}_{\bar{\ell}_x \bar{\ell}_y}^{\bar{K} LM} | V_{\ell_x}(x_i) | \mathcal{Y}_{\ell_x \ell_y}^{K LM} \rangle \\
& \times R_{i1}^{\bar{\ell}_x \bar{\ell}_y, \ell_{x1} \ell_{y1}} \left[\phi_d^{\ell_{x1}}(x_1) g_{A,B}^{\ell_{y1}}(k_{y1}, y_1) \right], \quad (\text{B8})
\end{aligned}$$

where $\phi_d^{\ell_{x1}}$ is the radial part of the dimer wave function $\psi_{\ell_{x1}}(\mathbf{x}_1)$.

It is important to note that in Eqs. (B2) and (B4) the potential operators and the functions F and \tilde{G} are written in different Jacobi sets. Therefore, when computing the integrals one has to rotate the whole integrand into the same Jacobi set. This is done in the expression above by the function R_{ij} , which is a rotation function defined as

$$\begin{aligned}
R_{ij}^{\ell_{x1} \ell_{y1}, \ell_{xj} \ell_{yj}} & \left[W_{\ell_{xj} \ell_{yj}}(x_j, y_j) \right] \\
= & \int d\Omega_{x_i} d\Omega_{y_i} \left[Y_{\ell_{x_i}}^*(\Omega_{x_i}) \otimes Y_{\ell_{y_i}}^*(\Omega_{y_i}) \right]^{LM_L} \\
& \times W_{\ell_{x_j} \ell_{y_j}}(x_j, y_j) \left[Y_{\ell_{x_j}}(\Omega_{x_j}) \otimes Y_{\ell_{y_j}}(\Omega_{y_j}) \right]^{LM_L}. \quad (\text{B9})
\end{aligned}$$

It rotates any function $W_{\ell_{xj} \ell_{yj}}(x_j, y_j)$ written in terms of the coordinates and angular momenta defined in the Jacobi set j

into the coordinates and angular momenta corresponding to the Jacobi set i .

As already mentioned, $V_{\ell}(x)$ is the total two-body interaction when the two particles are in a relative partial wave with angular momentum ℓ_x . In general, for particles with spin, the partial waves are identified by the quantum numbers $\{\ell_x, s_x, j_x\}$, where s_x is the coupling of the spins of the two particles, which in turn couples to ℓ_x to give the total two-body angular momentum j_x . In this case the matrix element $\langle \mathcal{Y}_{\bar{\ell}_x \bar{\ell}_y}^{\bar{K} LM} | V_{\ell_x}(x) | \mathcal{Y}_{\ell_x \ell_y}^{K LM} \rangle$ in Eq. (B7) or (B8) has to be replaced by

$$\left(\left[\mathcal{Y}_{\bar{\ell}_x \bar{\ell}_y}^{\bar{K} L} \otimes \chi_{s_x, s_y}^S \right]^{JM} \left| V_{\ell_x s_x j_x}(x) \right| \left[\mathcal{Y}_{\ell_x \ell_y}^{K L} \otimes \chi_{s_x, s_y}^S \right]^{JM} \right), \quad (\text{B10})$$

where s_y is the spin of the third particle, χ_{s_x, s_y}^S is the three-body spin wave function, and J, M are the total three-body angular momentum and its projection. In general, the partial wave two-body potential $V_{\ell_x s_x j_x}(x)$ could consist of a sum of central, spin-orbit, spin-spin, and tensor potentials. Therefore, in this case, calculation of the matrix element in (B10) implies calculation of the matrix element of the corresponding spin-spin, spin-orbit, and tensor operators. In the simplest case with only a central potential and particles with zero spin the matrix elements of the potential operator reduce to:

$$\langle \mathcal{Y}_{\bar{\ell}_x \bar{\ell}_y}^{\bar{K} LM} | V_{\ell_x}(x) | \mathcal{Y}_{\ell_x \ell_y}^{K LM} \rangle = V_{\ell_x}(x) \delta_{\ell_x, \bar{\ell}_x} \delta_{\ell_y, \bar{\ell}_y} \delta_{K, \bar{K}}, \quad (\text{B11})$$

simplifying the expression (B8).

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