

Integral Relations for Three-Body Continuum States with the Adiabatic Expansion

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The application of the hyperspherical adiabatic expansion to describe three-body scattering states suffers from the problem of very slow convergence. Contrary to what happens for bound states, a huge number of hyper-radial equations has to be solved, and even if done, the extraction of the scattering amplitude is problematic. In this Letter we show how to obtain accurate scattering phase shifts using the hyperspherical adiabatic expansion. To this aim two integral relations, derived from the Kohn variational principle, are used. The convergence of this procedure is as fast as for bound states.

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Introduction.—Few-body collisions involving either nuclei, atoms, or molecules are frequently investigated. To this aim different methods are at present available depending on the interaction under study. In nuclear physics, collisions involving three or four nucleons have been extensively studied within the Faddeev method or the hyperspherical harmonic (HH) method [1–3]. These two methods show sufficient flexibility to treat the complexities of the nucleon-nucleon interaction. A different problem arises when the interaction presents a hard core, as in the case of the atom-atom interaction, or in systems with $A > 4$. In the first case, the Faddeev equations have been extended to deal with a hard core repulsion [4] whereas the hyperspherical adiabatic (HA) expansion method proved to be a very efficient tool [5]. In nuclear systems with $A > 4$ tentatives to describe scattering states have recently appeared [6,7].

Here we are interested in describing a $1 + 2$ collision using the HA expansion method. For bound states the convergence of the HA expansion has proved to be very fast. However, the convergence of the expansion slows down significantly in the case of low energy scattering states [8]. On the other hand, this method is extensively used to describe few-atom systems in the ultracold regime (see Refs. [9,10] and references therein) and, in particular, atom-dimer collisions. Therefore, a detailed study of its convergence properties is timely.

In this Letter we show for the first time how the HA expansion method can be used to describe elastic scattering with a pattern of convergence similar to a bound state calculation. This is achieved in a simple but very general way in which a second order estimate of the phase shift is extracted from the wave function using two integral relations derived from the Kohn variational principle (KVP) [11]. The number of HA terms needed to obtain completely stable results depends very little on the structure of the potential, exactly as for bound state calculations. The integral relations are governed by the wave function in the

interaction region. Therefore the stability of the results with a low number of HA basis elements is a clear indication that inclusion of more terms in the expansion only modifies the wave function outside the interaction range.

As derived from the KVP, the integral relations are general and their application is not limited to three particles. They can be applied to an A -body system in which the scattering wave function is known in the interaction region. Examples of applications are given below.

Continuum states in the hyperspherical adiabatic expansion method.—The details of the HA method can be found in [5,8]. For simplicity, here we restrict ourselves to three equal mass particles with total angular momentum $L = 0$ and with only s waves involved.

From the Jacobi coordinates $X_i = (\mathbf{r}_j - \mathbf{r}_k)/\sqrt{2}$ and $Y_i = (\mathbf{r}_j + \mathbf{r}_k - 2\mathbf{r}_i)/\sqrt{6}$, one defines the hyperspherical variables, $[\rho, \Omega_i] \equiv [\rho, \phi_i, \mu_i]$, with $\mu_i = \hat{X}_i \cdot \hat{Y}_i$, $X_i = \rho \cos \phi_i$, and $Y_i = \rho \sin \phi_i$, where $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$, and $\{\mathbf{r}_i\}$ are the coordinates of the three particles. In hyperspherical coordinates the Hamiltonian operator \mathcal{H} takes the form

$$\begin{aligned} \mathcal{H} &= -\frac{\hbar^2}{2m} T_\rho + \frac{\hbar^2}{2m\rho^2} G^2 + V(\rho, \Omega) \\ &= -\frac{\hbar^2}{2m} T_\rho + \mathcal{H}_\Omega, \end{aligned} \quad (1)$$

where T_ρ is the hyper-radial operator, G^2 is the grand-angular operator, $V(\rho, \Omega) = \sum_i V(X_i)$ is the potential energy, and m is set equal to the mass of the particles. The wave function Ψ for a specific bound or continuum state is expanded as

$$\Psi^{ST\Pi} = \sum_{\nu=1}^{\infty} u_\nu(\rho) \Phi_\nu^{ST\Pi}(\rho, \Omega), \quad (2)$$

where S , T , and Π are the total spin, total isospin, and parity. For simplicity, we shall suppress from now on the

corresponding labels in Ψ and $\{\Phi_\nu\}$. The HA basis elements $\{\Phi_\nu\}$ are the eigenfunctions of \mathcal{H}_Ω at fixed values of ρ . Their corresponding eigenvalues, $U_\nu(\rho)$, are the adiabatic potentials, which enter in the coupled set of differential equations (see Refs. [5,10])

$$\left[-\frac{\hbar^2}{2m} T_\rho + U_\nu(\rho) - \frac{\hbar^2}{2m} Q_{\nu\nu}(\rho) - E \right] u_\nu(\rho) - \frac{\hbar^2}{2m} \sum_{\nu' \neq \nu}^{N_A} \left[Q_{\nu\nu'}(\rho) + P_{\nu\nu'}(\rho) \left(\frac{5}{\rho} + 2 \frac{d}{d\rho} \right) \right] u_{\nu'}(\rho) = 0 \quad (3)$$

with N_A the number of adiabatic channels included in the calculation, E the three-body energy, and from which the hyper-radial functions $u_\nu(\rho)$ are obtained. At energies below the two-body breakup E^{2B} and $\rho \rightarrow \infty$, the total scattering wave function behaves asymptotically as [8]

$$\Psi \rightarrow \phi_d(r) \left[\frac{\sin(k_\rho \rho)}{\sqrt{k_\rho \rho}} + \tan \delta_\rho \frac{\cos(k_\rho \rho)}{\sqrt{k_\rho \rho}} \right] |ST\rangle. \quad (4)$$

However, as we will show below, even increasing N_A as much as possible, the computed value of δ_ρ does not converge to the expected one. This can be understood from the fact that the asymptotic structure of the system can be constructed in terms of the functions

$$F_{ST} = \sum_{i=1}^3 F_{ST}(i) = \sum_{i=1}^3 \phi_d(X_i) \frac{\sin[k_y y_i]}{\sqrt{k_y y_i}} |ST\rangle \quad (5)$$

$$G_{ST} = \sum_{i=1}^3 G_{ST}(i) = \sum_{i=1}^3 \phi_d(X_i) \frac{\cos[k_y y_i]}{\sqrt{k_y y_i}} |ST\rangle,$$

where particle i is assumed to hit the bound state made by j and k , and where $y_i = \frac{\sqrt{6}}{2} Y_i$ is the distance between i and the j - k center of mass, and $k_y^2 = \frac{2}{3} k_\rho^2$. The asymptotic configuration in the limit $y_i \rightarrow \infty$ is then

$$\Psi \rightarrow F_{ST} + \tan \delta G_{ST}. \quad (6)$$

When $\rho \rightarrow \infty$, the distance X_i is limited by ϕ_d and the approximate relation $k_y y_i \approx k_\rho \rho$ holds. However, the exact equivalence between $k_y y_i$ and $k_\rho \rho$ is not matched for any finite value of ρ and, accordingly, the boundary condition of Eq. (4) is equivalent to the one in (6) only at $\rho \approx \infty$ and $N_A \rightarrow \infty$. As a consequence, δ_ρ converges extremely slowly to δ by increasing the number of adiabatic states. This situation has reduced the applicability of the method.

Second order integral relations.—From the above discussion and observing that in the expansion of the functions F_{ST} and G_{ST} in terms of HA basis elements [8], the two terms of Eq. (4) represent the first term of that expansion, respectively, the wave function Ψ can be expressed asymptotically as

$$\Psi = \sum_\nu^{N_A} u_\nu(\rho) \Phi_\nu(\rho, \Omega) \rightarrow AF_{ST} + BG_{ST}. \quad (7)$$

In order to extract the coefficients A and B ($\tan \delta = B/A$), we derive from the KVP two integral relations accurate up to second order. The KVP states that the following functional is stationary:

$$[\tan \delta]^{2^{\text{nd}}} = \tan \delta - \langle (1/A)\Psi | \mathcal{L} | (1/A)\Psi \rangle \quad (8)$$

with respect to variations of the wave function, where $\mathcal{L} = \frac{2}{\sqrt{3}} \frac{m}{\hbar^2} (\mathcal{H} - E)$. The scattering wave function can be schematically written as $(1/A)\Psi = \Psi_c + F_{ST} + \tan \delta \tilde{G}_{ST}$. The function \tilde{G}_{ST} , representing a regularization of the function G_{ST} , introduces a nonlinear parameter γ to eliminate a term proportional to $\delta(y_i)$ originated by $(\mathcal{H} - E)G_{ST}$, and Ψ_c is the part of the wave function inside the interaction region constructed in terms of some parameters (e.g., a linear combination of basis elements). It verifies $\Psi_c \rightarrow 0$ asymptotically. The other parameter in Ψ is $\tan \delta$. In the present work we have used

$$\tilde{G}_{ST} = \sum_i \phi_d(X_i) \frac{\cos[k_y y_i]}{\sqrt{k_y y_i}} (1 - e^{-\gamma y_i}) |ST\rangle. \quad (9)$$

The variation of the functional (8) with respect to the parameters in Ψ_c and with respect to $\tan \delta$ leads to

$$\langle \Psi_c | \mathcal{L} | \Psi \rangle = 0; \quad \langle \tilde{G}_{ST} | \mathcal{L} | \Psi \rangle = 0. \quad (10)$$

These two equations can be interpreted in two different ways. In the case in which Ψ is explicitly separated in the three terms Ψ_c , F_{ST} , \tilde{G}_{ST} , the above equations are used to determine Ψ_c and the first order estimate of $\tan \delta$ ($\tan \delta^{1^{\text{st}}}$). Accordingly, Ψ is constructed after solving these equations. A different case arises when Ψ is known (for example using the HA expansion) but the separation in the three terms is not explicitly known. For this case the two equations can be used to define of Ψ_c and $\tan \delta^{1^{\text{st}}}$.

Introducing Eq. (10) into the functional, the second order estimate of $\tan \delta$ is obtained

$$[\tan \delta]^{2^{\text{nd}}} = (\tan \delta)^{1^{\text{st}}} - \langle F_{ST} | \mathcal{L} | (1/A)\Psi \rangle, \quad (11)$$

with $A = \langle \Psi | \mathcal{L} | \tilde{G}_{ST} \rangle$. This is a consequence of the general relation $A = \langle \Psi | \mathcal{L} | \tilde{G}_{ST} \rangle - \langle \tilde{G}_{ST} | \mathcal{L} | \Psi \rangle$ (obtained by transforming the Laplacian term in a surface integral), the normalization relation $\langle F_{ST} | \mathcal{L} | \tilde{G}_{ST} \rangle - \langle \tilde{G}_{ST} | \mathcal{L} | F_{ST} \rangle = 1$ and the last equation derived from the KVP in Eq. (10). The same relation can be used to obtain a first order estimate for the coefficient B as

$$B^{1^{\text{st}}} = \langle F_{ST} | \mathcal{L} | \Psi \rangle - \langle \Psi | \mathcal{L} | F_{ST} \rangle. \quad (12)$$

After multiplying Eq. (11) by A one gets that $B^{2^{\text{nd}}} = B^{1^{\text{st}}} - \langle F_{ST} | \mathcal{L} | \Psi \rangle$, which by use of Eq. (12) leads to a second order integral relation for B and, accordingly, a second order estimate for $\tan \delta$. These results are the main con-

clusions of this Letter and can be summarized as

$$\begin{aligned} B^{2\text{nd}} &= -\langle \Psi | \mathcal{L} | F_{ST} \rangle \\ A &= \langle \Psi | \mathcal{L} | \tilde{G}_{ST} \rangle \end{aligned} \quad \tan \delta^{2\text{nd}} = B^{2\text{nd}}/A. \quad (13)$$

The relations of Eq. (13) are equivalent to the KVP and are useful in the cases in which Ψ is known but its explicit asymptotic form in terms of the functions F_{ST} and G_{ST} is not. This is the case, for example, when Ψ is obtained from the solution of the HA equations. The integrands in the integral relations of Eq. (13) go rapidly to zero as $\rho \rightarrow \infty$ since F_{ST} and \tilde{G}_{ST} are solutions of \mathcal{L} in that limit. Therefore, an accurate knowledge of Ψ outside the range of interaction is not needed. In the present case, the explicit form of the integrals in Eq. (13) are

$$\begin{aligned} B^{2\text{nd}} &= -C \int d\rho \rho^5 d\Omega \Psi(\rho, \Omega) V(X_i) [F_{ST}(j) + F_{ST}(k)] \\ A &= C \int d\rho \rho^5 d\Omega \Psi(\rho, \Omega) V(X_i) [G_{ST}(j) + G_{ST}(k)] + I_\gamma, \end{aligned} \quad (15)$$

where $C = 2\sqrt{3}m/\hbar^2$ and I_γ is a (short-range) integral including all terms depending on γ . Let us note that the last integral is largely independent of γ provided that the regularization is performed inside the interaction region and Ψ tends to the exact wave function. The dependence of $\tan \delta$ on γ is studied below. We have found that values of $\gamma \approx \sqrt{m|E^{2B}|/\hbar^2}$ are a convenient choice.

The integral relations, as given above, are a generalization of the relation used in the two-body case [12]. However, an attempt to identify the single term $B^{2\text{nd}} = \tan \delta_B$ as a corrected phase shift fails as we show below. The validity of Eq. (13) is not limited to the three-body case and to wave functions obtained using the HA method. It can be applied to any wave function Ψ which verifies $(\mathcal{H} - E)\Psi = 0$ in the interaction region without any explicit indication of its asymptotic behavior. An example is represented by the solution of $(\mathcal{H} - E)\Psi = 0$ in a box in which Ψ is set to zero at some distance. Using Eq. (13) a second order estimate of a phase shift can be obtained studying its convergence in terms of the dimension of the box.

Results.—As a first application we consider a three-body system of identical spinless bosons interacting through a central, s wave, Gaussian potential $V(r) = V_0 \exp[-(r/r_0)^2]$, with $V_0 = -51.5$ MeV and $r_0 = 1.6$ fm. Though this potential is unrealistic, it will serve to the purpose of testing the method due to the very extended dimer wave function ($E^{2B} = 0.397743$ MeV and $\hbar^2/m = 41.4696$ MeV fm²). Such three-body system has two $L = 0$ bound states with separation energies $E_{3B}^{(0)} = -9.7574$ MeV and $E_{3B}^{(1)} = -0.4816$ MeV, respectively. In Table I we show the convergence of these two states in terms of the HH and HA expansions. From the table we observe the fast convergence of the HA even in the

TABLE I. Convergence of the bound state energies (in MeV) as a function of the number N of HH and HA basis functions.

N	$E_{3B}^{(0)}$		N	$E_{3B}^{(1)}$	
	HH	HA		HH	HA
1	-9.2062	-9.7347	1	...	-0.4781
2	-9.5810	-9.7552	4	...	-0.4815
3	-9.7247	-9.7573	10	-0.2323	-0.4816
4	-9.7424	-9.7574	30	-0.4635	-0.4816
6	-9.7558	-9.7574	50	-0.4790	-0.4816
8	-9.7571	-9.7574	70	-0.4811	-0.4816
10	-9.7574	-9.7574	100	-0.4815	-0.4816

case of the shallow state $E_{3B}^{(1)}$. We can conclude that 10 HA basis states are sufficient to describe simultaneously both bound states.

We now show results for the $L = 0$ phase shift at $E = -0.1$ MeV. Equation (3) has been solved up to $\rho = 500$ fm with the boundary condition of Eq. (4) for increasing values of N_A . Because of the large extension of the $P_{\nu\nu'}$ and $Q_{\nu\nu'}$ coupling terms, the higher N_A the larger the value of ρ at which the asymptotic form of u_1 is verified. For example, using only one HA basis state (only one hyper-radial equation has to be solved), u_1 reaches its asymptotic form at $\rho \approx 100$ fm. When 40 HA terms are used, this happens beyond 500 fm. The results for δ_ρ , $\delta_B = \arctan(B^{2\text{nd}})$, $\delta^{2\text{nd}} = \arctan(B^{2\text{nd}}/A)$ (for different values of γ), and A , are given in Table II up to 40 HA basis functions.

We observe that δ_ρ and δ_B converge very slowly to a value that, by extrapolation, can be estimated in the interval $72.8^\circ - 72.9^\circ$ as $N_A \rightarrow \infty$. This is at variance with the value $\delta^{2\text{nd}} = 73.18^\circ$, which shows a rate of convergence extremely fast and a large stability with γ , as N_A increases. The calculation of $\delta^{2\text{nd}}$ requires the knowledge of the radial functions up to values of ρ not larger than 70–80 fm, for

TABLE II. Patterns of convergence for δ_ρ , $\delta_B = \arctan B$, $\delta^{2\text{nd}}$ (in degrees) and A , in terms of N_A for $E = -0.1$ MeV. The values of A have been calculated using $\gamma = 0.25$.

N_A	δ_ρ	δ_B	A	$\delta^{2\text{nd}} = \arctan(B^{2\text{nd}}/A)$			
				$\gamma = 0.1$	$\gamma = 0.25$	$\gamma = 0.5$	$\gamma = 1.0$
1	65.23	67.85	0.607	75.895	76.212	75.479	74.727
4	71.65	71.89	0.909	73.385	73.446	73.450	73.429
8	72.32	72.42	0.951	73.222	73.237	73.245	73.259
12	72.56	72.62	0.965	73.190	73.194	73.196	73.203
16	72.67	72.71	0.971	73.182	73.183	73.185	73.189
20	72.72	72.76	0.974	73.180	73.180	73.182	73.186
24	72.75	72.79	0.976	73.179	73.179	73.180	73.184
28	72.77	72.81	0.977	73.179	73.179	73.180	73.184
32	72.78	72.82	0.978	73.179	73.179	73.180	73.184
36	72.79	72.82	0.978	73.179	73.179	73.180	73.183
40	72.79	72.83	0.978	73.179	73.179	73.180	73.183

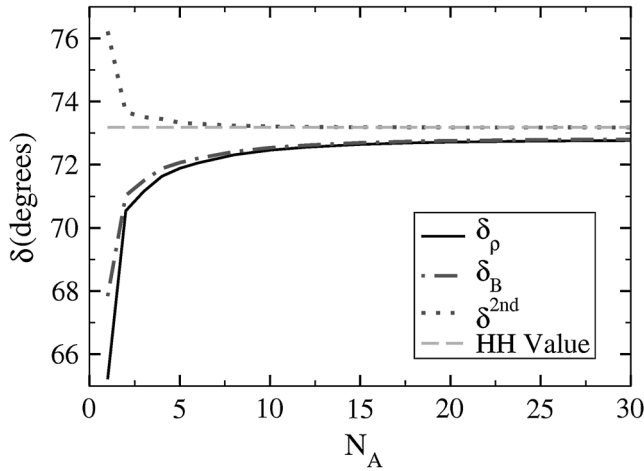


FIG. 1. Convergence of δ_ρ , δ_B , and δ^{2nd} as a function of the number N_A of HA basis functions. The converged value obtained from the HH expansion is shown for comparison.

which a relatively small number of HA terms is enough. Conversely, δ_ρ and δ_B would converge to the correct phase shift only after imposing the boundary condition to the wave function at $\rho = \infty$, for which in principle infinitely many HA basis terms are needed. For comparison, a converged value of 73.180° is obtained for the phase shift using the HH expansion method with 120 basis elements. This result is in complete agreement with the one obtained with Eq. (13). The different patterns of convergence can be clearly seen on Fig. 1.

Reference [8] reports calculations at three different energies using the MT-III potential [13], which has a yukawian repulsion at short distances, in the $S = 3/2$, $T = 0$ state. When the HH expansion is used, more than 120 basis states have to be included to reach convergence in the phase shifts. In Table III we show the corresponding results when using Eq. (13). In the last row the results from Ref. [8] using the HH expansion are given for comparison. The results obtained with the integral relations are in complete agreement with those obtained using the HH expansion and show a very fast pattern of convergence.

Conclusions.—We have derived two integral relations from the KVP which are accurate up to second order. Their ratio, the phase shift, converges in terms of the HA basis elements as fast as the binding energy in a bound state calculation. The fast convergence has been shown for different types of interactions. We would like to stress the general validity of Eq. (13). Its application will be very useful in the case in which Ψ is known in the interaction region but the exact construction of its asymptotic form is difficult. The HA expansion has been applied in Refs. [10,14] to compute phase shifts in a $1 + 2$ and a $2 + 2$ helium atom collisions. Accordingly, Eq. (13) can be used directly to obtain a second order estimate of the phase shifts. In Ref. [6], $n - \alpha$ scattering has been studied using Quantum Monte Carlo techniques. The wave function of

TABLE III. Convergence of $\delta^{2nd} = \arctan(B^{2nd}/A)$ (in degrees) at three incident energies with the MT-III potential.

N_A	0.2 MeV	1.0 MeV	2.0 MeV
4	-28.277	-55.875	-71.507
8	-28.290	-55.865	-71.475
12	-28.293	-55.864	-71.473
16	-28.294	-55.863	-71.473
20	-28.294	-55.863	-71.473
HH	-28.294	-55.863	-71.474

the system was obtained solving $(\mathcal{H} - E)\Psi = 0$ in a box. The knowledge of Ψ in the interaction region allows for a direct application of Eq. (13) also in this case. To be noticed that in the case in which more than one elastic channel is open, the coefficients A and B of Eq. (13) correspond to matrices

$$\left. \begin{aligned} B_{ij}^{2nd} &= -\langle \Psi_i | \mathcal{L} | F_j \rangle \\ A_{ij} &= \langle \Psi_i | \mathcal{L} | \tilde{G}_j \rangle \end{aligned} \right\} R^{2nd} = A^{-1} B^{2nd}. \quad (14)$$

with R^{2nd} the second order estimate of the scattering matrix whose eigenvalues are the phase shifts and the indices (i, j) indicate the different asymptotic configurations accessible at the specific energy under consideration. Finally, we would like to mention the possibility of using Eq. (13) to describe a $1 + 2$ elastic collision with charged particles using a screened Coulomb potential and free asymptotic conditions.

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