Multichannel reactions using the adiabatic expansion method

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Abstract. In this work we describe a method to study scattering processes. The method, which is based on the Kohn Variational Principle, has been generalized to be applicable for calculating any partial wave phase shift and studying multichannel processes. It shows fast convergence when applied to three-body reactions described with the hyperspherical adiabatic method. The pattern of convergence is similar to the one found when the method is applied to obtain bound states.

1. Introduction
The most immediate way of studying scattering processes is to compare the long distance wave functions with the known asymptotic behavior. However, for reactions involving more than two particles the calculation of an accurate enough wave function at long distances requires soon an increasingly large basis, which implies a big numerical effort that can become at some point unaffordable.

In particular, when using the Hyperspherical Adiabatic Expansion Method [1] the calculation of the wave functions at long distances implies to calculate a large amount of accurate adiabatic potentials in the same asymptotic region. This makes the calculation very delicate and computationally very expensive. However, using the Adiabatic Expansion Method to study a given reaction has the great advantage of giving a clear distinction between all the possible outgoing channels.

In Ref.[2] we have described a general method derived from the Kohn Variational principle that permits to obtain the phase shifts from two integral relations that involve only the internal part of the scattering wave function. As a consequence, a detailed knowledge of the wave function at large distances is not needed. The method was carefully described for studying processes with only one open channel and it was restricted to s-wave processes.

In this work we study the general form of the integral relations in multichannel processes making possible the application of the method in different low energy reactions, including elastic, inelastic and rearrangement processes. We study the convergence of the scattering K-matrix in terms of adiabatic potentials as well as the convergence of the cross section in terms of partial waves.

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2. Generalization of the Integral Relations

Let us consider a process in which a particle hits a bound two-body target with an incident energy below the breakup energy threshold. Different processes could occur below this breakup energy. We will study systems in which one or more of these processes are allowed. Therefore the method will permit to investigate reactions with multiple open channels that can include elastic scattering, inelastic scattering or rearrangement processes.

When studying multichannel reactions it is very useful to introduce a vectorial notation for the wave function. Each of the components \( \{\Psi_i\} \) of this vector represents a different open channel in the process.

When \( \Psi \) is the exact wave function, its asymptotic form is given by:

\[
\Psi_i \to \sum_{n=1}^{n_0} (A_{in} F_n + B_{in} G_n),
\]

where

\[
F_n = \sqrt{k_y^n j_{\ell_y}(k_y^n y_n)} \left[ \psi^{i\ell_y}(x_n) \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]_{J^M} \right],
\]
\[
G_n = \sqrt{k_y^n \eta_{\ell_y}(k_y^n y_n)} \left[ \psi^{i\ell_y}(x_n) \otimes [Y_{\ell_y}(\Omega_y) \otimes \chi_{s_y}]_{J^M} \right].
\]

The functions \( F_n \) and \( G_n \) are two linearly independent asymptotic solutions of the Hamiltonian, \( n_0 \) is the number of open channels and \( x_n \) and \( y_n \) are the Jacobi coordinates. The matrices \( A \) and \( B \) are given by:

\[
B_{ij} = \frac{2m}{\hbar^2} \langle \Psi_i | \hat{H} - E | F_j \rangle
\]
\[
A_{ij} = -\frac{2m}{\hbar^2} \langle \Psi_i | \hat{H} - E | G_j \rangle,
\]

When \( \Psi \) is a trial wave function the same integral relations in Eqs.(3) will give \( A \) and a second order approximation \( B^{2nd} \). This result is derived from the Kohn Variational Principle similarly to how it is done for a single channel process in [2].

Due to the fact that functions \( F_n \) and \( G_n \) are two linearly independent asymptotic solutions of the Hamiltonian, these integral relations have integrands which tend rapidly to zero when increasing the distance. Therefore, to accurately calculate the matrices \( A \) and \( B \) it is not necessary to use a test wave function \( \Psi \) with an exact asymptotic form. It is enough that its inner part is correctly calculated. The \( n_0 \times n_0 \) K-matrix can be finally obtained as:

\[
K^{2nd} = -A^{-1}B^{2nd}
\]

When using the hyperspherical adiabatic expansion, the wave function can be written in a matrix way as follows:

\[
\Psi = \left( \begin{array}{c} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_{n_0} \end{array} \right) = \frac{1}{\rho^{5/2}} \left( \begin{array}{cccc} f_{11} & f_{21} & \cdots & f_{n_A1} \\ f_{12} & f_{22} & \cdots & f_{n_A2} \\ \vdots & \vdots & \ddots & \vdots \\ f_{1n_0} & f_{2n_0} & \cdots & f_{n_An_0} \end{array} \right) \left( \begin{array}{c} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_{n_A} \end{array} \right),
\]

where \( n_A \) is the number of adiabatic potentials included in the calculation.
The asymptotic form of each component will be:

\[
\psi_i \rightarrow \sum_{n=1}^{n_0} \sqrt{k_y} \left( A_{in} \hat{r}_y(k_y) \rho \right) + B_{in}^{1st} \eta_{yp}(k_y) \rho \right) \left[ \psi_{jn}^{s} \otimes \left[ Y_{\ell y}(\Omega_y) \otimes \chi_{s p} \right] \right]^{JM}
\]

where \( \rho \) is the hyperradius and \( \psi_{jn}^{s} \) is the dimer wave function. We can finally use this \( \Psi \) as a trial wave function in order to obtain a second order approximation of the \( K \)-matrix using Eqs.(3) and (4).

3. Results

3.1. Collision \( ^4He-{^4He}_2 \)

As a first case, we study the collision of a \( ^4He \) atom into the weakly bound \( ^4He_2 \) dimer. The helium dimer has a single bound state, which implies that for incident energies below the dimer breakup threshold, only the elastic channel is open.

The two-body helium-helium interaction is chosen to be the simple effective gaussian potential given in [3]. This potential leads to a bound \( 0^+ \) dimer with a binding energy of \( -1.2959 \) mK.

To investigate the behavior of the method for different angular momenta, we have calculated for this system the partial wave phase shifts up to \( f \)-wave for an incident energy of \( 0.5 \) mK. The convergence of these partial wave phase shifts has been reached with about 18 adiabatic potentials for \( s \)-wave and about 5 for higher partial waves. We have obtained a phase shift of \( -40.54, -13.11, 2.14 \) and \( -0.28 \) degrees for \( \delta_s, \delta_p, \delta_d \) and \( \delta_f \), respectively. For the case of \( \delta_s \) the hyperspherical harmonic expansion method gives a value of \( -40.55 \) degrees. The differential cross section is found to be converged when partial waves up to \( \ell = 3 \) are included.

3.2. Multichannel Collision \( ^4He-{^4He}-^6Li \)

As a next step we have applied the method to the \( ^4He-{^4He}-^6Li \) system. In this case, we can have two different open channels. In channel 1 there is a dimer formed by one helium atom and one lithium atom with the second helium atom in the continuum. In channel 2 the dimer is formed by the two helium atoms and the lithium atom in the continuum. Therefore, for each incoming channel there will be two possible outgoing channels, one corresponding to the elastic scattering and the other one to a rearrangement process.

The existence of two possible outgoing channels implies that now the matrices \( S \) and \( K \) are two by two matrices. Therefore, four different elements have to be calculated for each of them. This will allow us to calculate the population rate of each channel.

For the \( ^4He-{^4He} \) interaction we used the same gaussian as in the previous case. For the \( ^4He-{^6Li} \) interaction potential we have taken a gaussian whose parameters have been adjusted to reproduce the scattering length and effective range obtained in [4] with the more sophisticated KTTY potential. This gaussian potential gives rise to a two-body binding energy of \( -1.42246 \) mK.

We have found, for a three-body energy of \(-0.7959\) mK, a good convergence of the four \( K \)-matrix elements with about 18 adiabatic potentials. The matrix terms \( K_{11}, K_{12}, K_{21} \) and \( K_{22} \), have been found to be \(-2.712, -0.791, -0.790 \) and \(-1.474 \) respectively. Once the \( K \)-matrix has been obtained, it is then possible to calculate the \( S \)-matrix with the simple expression:

\[
S = (1 + iK)(1 - iK)^{-1}.
\]

The elastic scattering or rearrangement probability is then easily calculated by taking the modulus square of the corresponding element of the \( S \)-matrix. In this particular case we have found an elastic scattering probability of 0.892 and a rearrangement probability of 0.108.
4. Conclusions
In Refs. [2] and [5] two integral relations for studying continuum states with the adiabatic expansion method were presented. These relations were derived from the Kohn Variational Principle and it was shown that they solved the convergence problems appearing when the adiabatic expansion is used to study scattering problems. This happens because when using the integral relations the long distance behavior of the wave function is no longer needed to extract the phase shifts. In this work, we have introduced the generalization of the integral relations to include any partial wave and allow multichannel processes. To this aim we proposed a vectorial notation for the wave functions in order to represent each of the possible open channels.

We have applied the method to two physical cases, first to the $^4$He-$^4$He$_2$ collision in which we had just one open channel and calculated different partial waves phase shifts and second, the $^4$He-$^4$He-$^6$Li system in which we had two open channels. In both cases we could see a good convergence of the method, making this a promising method for studying scattering processes.

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