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Three-body wave functions in the continuum.

Application to the Coulomb case

Received: date / Accepted: date

Abstract In this work we describe a method that permits to obtain full three-body continuum wave functions regardless the short- or long-range character of the two-body potentials involved. Within this method all the possible incoming channels are automatically taken into account. When applied to systems where only the Coulomb interaction enters the method provides the corresponding regular three-body Coulomb functions, from which their irregular partners can be obtained.

1 Introduction

The three-body problem in the continuum is equivalent to a multichannel problem. Therefore, knowledge of the full three-body continuum wave function requires knowledge of the wave function for all the possible incoming channels. In Ref.[1] we have shown that the discretization of the continuum by imposing a simple box boundary condition automatically provides the full continuum wave function, meaning that all the possible incoming channels are automatically taken into account. Therefore, no information is lost when this discretization procedure is employed. The main problem of the method is that the components corresponding to the different possible incoming channels are actually computed at slightly different energies. Only for an eventually infinitely big box the energies for each of the components would be exactly the same. This problem can be to a large extent solved by means of very small modifications of the size of the discretization box for each of the components, in such a way that they all provide a discrete state at exactly the same energy. As shown [1], the price to pay is a very small different normalization for each of the components, but whose effect in the final results is clearly negligible.

Obviously, this method can be applied for the particular case in which only the Coulomb interaction between the pairs of particles is considered. In this way, one can immediately obtain the regular three-body continuum wave functions just as solutions of the corresponding hamiltonian [2]. From the regular solutions the irregular partners are obtained after diagonalization of the regular radial function, and replacing the regular Coulomb functions in the diagonal by their corresponding irregular counterparts.

As shown in [2], four different tests were found to be successfully fulfilled by the regular and irregular Coulomb functions: i) The irregular functions are solution of the coupled set of radial equations, ii) the sum of the squares of the regular and irregular functions goes asymptotically to the identity matrix, iii)

This work was partially supported by funds provided by DGI of MINECO (Spain) under contract No. FIS2014-51971-P

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Fig. 1 (a): Discrete energies obtained after discretizing the spectrum of the three-alpha system with a box boundary condition at 300 fm. The ellipses are put to identify the different groups of states obtained. (b): Radial wave functions $f_{ii}(\rho)$ for $i = 1, \dots, 4$ for the three-alpha system after tuning the energy at 3.5 MeV by means of a small change in the box size.

the Wronskian relation is satisfactorily fulfilled, and iv) the computed $\mathcal{S}$ -matrix satisfies the unitarity condition.

2 Sketch of the method

The continuum three-body wave function for a given total energy E can be written in a matrix form as :

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

where the index i in Ψ_i runs over all the possible n_0 incoming channels and the functions $\{\Phi_i\}$ ($i = 1, \dots, n_A$) constitute the complete basis used to expand the three-body wave functions (in general n_A is a truncation of an infinitely big basis set). A very common basis is the one formed by the hyperspherical harmonics, but in this work we shall use the eigenfunctions of the angular part of the hamiltonian, which form the basis set used in the adiabatic expansion method [3]. This choice has the advantage that the required truncation n_A in the basis expansion is by far smaller than when the expansion in terms of the hyperspherical harmonics is used. As a consequence, the size of the matrices involved in Eq.(1) is rather modest, and therefore the number of radial functions to be computed is drastically reduced. Note that when the three-body system contains bound dimer subsystems, we then, together with the genuine three-body continuum states, also have continuum dimer-particle states. In this way, if $E < 0$ only some (or all, depending on the value of E) of these continuum dimer-particle states are open, and therefore $n_0 \neq n_A$ in Eq.(1). Also, in this case n_0 is finite in typically a very small number. For $E > 0$ we always have that $n_0 = n_A$.

As described in [1; 3] the radial functions in the radial matrix R in Eq.(1) are obtained as solutions of a coupled set of differential equations. The difficult part when working in the continuum is to obtain

the different Ψ_i solutions, all of them corresponding to the same three-body energy, but to a different incoming channel. This problem can be solved as shown in Ref.[2] by simply solving the coupled set of radial equations by imposing a box boundary condition. When done, the different discrete states appear in groups of states with a very similar energy, and in such a way that each group of states contains n_0 terms, which is the number of open channels. It is important to note that the bigger the box used for the discretization the closer to degeneracy the states in the same group. Eventually, for an infinitely big box, all the states in each group are degenerate. It is then clear that the n_0 states belonging to a certain group provide the n_0 Ψ_i functions in Eq.(1), or, in other words, they provide the full three-body continuum wave function Ψ . This is illustrated in Fig.1a, where we show the discrete spectrum obtained for a three-alpha system with $n_0 = 8$ and using a box of size equal to 300 fm. The groups containing 8 states are indicated by the ellipses.

The fact that in an actual calculation the n_0 states in a group have slightly different energies can be solved by computing each of the Ψ_i functions with a slightly different box size, which can be used to fine tune the energy. As an example we show in Fig.1b the tail of the radial functions f_{ii} with $i = 1, \dots, 4$ obtained for a three-alpha system at an energy of 3.5 MeV and with $n_0 = 8$. Note that the most important contribution in each Ψ_i component in Eq.(1) is given by the diagonal f_{ii} function [2]. As seen in the figure, a variation in the box size not bigger than 2 fm is enough to fine tune the energy to the desired value. Since each Ψ_i function is normalized to 1 inside the box, we have that a change in the box size implies a change in the normalization. However, a size variation from 300 fm to 298 fm amounts to a global factor in the wave function of 1.003, which has no visible effects in the results.

The procedure described above can be applied as well in order to compute the regular solutions of the free hamiltonian. If no long-range interactions are involved, the free radial matrix R is diagonal, and the corresponding diagonal terms are given by regular Bessel functions, which, in fact, are known analytically.

When the Coulomb interaction (or any other long-range potential) is involved, the radial matrix of the free Coulomb solutions is not diagonal anymore. All the adiabatic channels are coupled. The free solutions computed in this way are the regular three-body Coulomb functions for that particular system. The numerical calculation of these functions is of great importance, since their analytical form is so far not known.

From the regular solutions it is possible to extract the corresponding irregular partners simply taking into account that the radial matrix R can always be decomposed as (singular value decomposition):

$$R = UWV^T, \quad (2)$$

where $U^T U = \mathbb{1}$, $V^T V = \mathbb{1}$, and W is diagonal. The diagonal terms are regular Coulomb functions whose order and Sommerfeld parameter can be extracted numerically. From these regular Coulomb functions it is simple to construct their irregular counterparts, and from them, by means of Eq.(2) the irregular Coulomb function G can be obtained.

3 $\mathcal{S}$ -matrix and recombination rate

The importance of the regular and irregular Coulomb functions F and G relies on the fact that they are necessary ingredients in order to compute the $\mathcal{S}$ -matrix, which contains all the information about the system. As shown for instance in [4], the $\mathcal{S}$ -matrix is given in terms of the $\mathcal{K}$ -matrix by $\mathcal{S} = (1 + i\mathcal{K})(1 - \mathcal{K})^{-1}$, and $\mathcal{K} = -A \cdot B$. The matrices A and B can be obtained by means of the integral relations:

$$A = -\frac{2m}{\hbar^2} \langle \Psi | \hat{\mathcal{H}} - E | G \rangle \quad (3)$$

$$B = \frac{2m}{\hbar^2} \langle \Psi | \hat{\mathcal{H}} - E | F \rangle, \quad (4)$$

where $\hat{\mathcal{H}}$ is the total three-body hamiltonian and E is the three-body energy.

In the particular case that the three-body system contains bound two-body dimers, it is then possible to compute the three-body recombination rate at a given energy E , which is given in terms

of the $\mathcal{S}$ -matrix by the expression:

$$K_3 = \nu! \sum_{J\Pi} \sum_{i=1}^{N_d} \frac{32\hbar\pi^2(2J+1)}{\mu k^4} \sum_{\lambda=N_d+1}^N \left| \mathcal{S}_{i\lambda}^{J\Pi}(E) \right|^2, \quad (5)$$

where ν is the number of identical particles, J and Π are the total spin and parity of the three-body system, the channels $i = 1, \dots, N_d$ correspond to those containing a bound dimer, and the channels $\lambda = N_d + 1, \dots, N$ are the genuine three-body continuum channels included in the calculation. The mass μ is defined as $\mu^2 = M_1 M_2 M_3 / (M_1 + M_2 + M_3)$, where M_i is the mass of particle i , and, finally, $k^2 = 2\mu E / \hbar^2$.

In the expression above the term $\left| \mathcal{S}_{i\lambda}^{J\Pi}(E) \right|^2$ gives the probability for an incoming three-body continuum channel λ going out in through the dimer+particle channel i . Making now use of the unitarity condition of the $\mathcal{S}$ -matrix we can also write $\sum_{\lambda=N_d+1}^N \left| \mathcal{S}_{i\lambda}^{J\Pi}(E) \right|^2 = 1 - \sum_{j=1}^{N_d} \left| \mathcal{S}_{ij}^{J\Pi}(E) \right|^2$. For the particular case of three identical particles the recombination rate finally reads:

$$K_3 = \frac{\hbar^5}{M^3} \frac{144\sqrt{3}\pi^2}{E^2} \sum_{J\Pi} (2J+1) \sum_{i=1}^{N_d} \left(1 - \sum_{j=1}^{N_d} \left| \mathcal{S}_{ij}^{J\Pi}(E) \right|^2 \right), \quad (6)$$

where M is the mass of the particle.

4 Summary

Three-body Coulomb functions are a necessary ingredient in order to describe three-body continuum states for charged particles. Since they are not known analytically a numerical calculation is therefore in order. In this work we have described how the discretization of the continuum with a simple box boundary condition permits to obtain full continuum wave functions, meaning that all the possible incoming channels are automatically accounted for. Furthermore, the method can be used no matter the short- or long-range character of the interactions involved in the system. In particular, when employed with three-body systems where only the Coulomb interaction enters, the method provides the full regular solutions of the hamiltonian, i.e., the regular three-body Coulomb wave functions. After diagonalization of the regular Coulomb function, their corresponding irregular partners can be easily obtained.

References

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