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A wave function for three charged particles with arbitrary masses

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Abstract

In this work we present a fully correlated wave function to describe the continuum of the three-body spectra for particles with arbitrary masses interacting with Coulomb potentials. We show that this function can be related with the Φ_2 correlated model introduced few years ago for ion–atom collisions processes. The function includes important properties such as correct asymptotic conditions and Kato's cusp conditions. We discuss the properties of the wave function for one heavy and two light particles, focusing in the case of positron–electron–proton systems. A comparison between the properties of the new model and the C3 one is also performed. This analysis suggests that this function can be a successful alternative choice for the description of positron–atom collisions.

Keywords: Three-body problem; Coulomb interactions; Correlated wave function; Ion–atom; Electron–atom; Arbitrary masses

1. Introduction

Quantum mechanics started in the beginning of the 20th century with a successful description of a integrable system: the hydrogen atom. However, with the first intents of solving the helium atom, the pioneers met for first time with the mathematical difficulties related with Schrödinger equation for such a system. Many years after, Kato showed that the Schrödinger Hamiltonian operator of every atom, molecule or ion, and in general, every system composed of a finite number of particles interacting through Coulomb potentials is essentially self-adjoint. This means that there exist a complete set of eigenfunctions (discrete and/or continuous) for the n-body Coulomb problem [1]. Unfortunately, the methodology used by Kato does not give any information about how to obtain these solutions. To study the time-independent three-body Coulomb problem, we have to deal with an elliptical partial differential equation in six variables with Dirichlet–Neumann mixed-boundary conditions. In spite of the efforts, the understanding of the dynamics of three charged particles moving both in the continuum and discrete is still far from being complete. It has been shown by Poincaré that the integral of motion of the center of mass, i.e. the integrals of angular momentum, and the integral of energy are

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the only independent integrals of the three-body problem [2]. For this reason it is not possible to use the separation of variables method to solve the problem.

In general, it is possible to obtain good approximated wave functions for the case in which two particles are bound to the third one. However, the cases in which all the particles are in the continuum or one in the continuum and the other two form a bound state remains a challenging problem. The final state in processes like ion–atom ionization, electron–atom ionization, double photoionization, etc. are only some examples of the these continuum states. Much theoretical effort has been made to find approximate wave function for such a systems. One of the first approximated model has been introduced by Belkic in 1978 [3] and independently by Garibotti and Miraglia in 1980 for two protons and one electron [4]. This model is known as C3 approximation and assumes that the three-body Coulomb problem can be represented by the product of three independent two-body systems. The underlying assumption is that there exist a set of six constant of motion and then it is possible to solve the problem by separation of variables [5,7]. In terms of the Schrödinger Hamiltonian, the C3 approach results by neglecting the non-orthogonal kinetic energy [5–7]. In spite of the crude approximation, much of the relevant physical information is kept. Besides, it is a really friendly model to deal with, because it is possible to perform most of the analysis analytically. A property that makes the C3 useful is its validity for all the masses and charges of the particles and this is a consequence of the form in that it was obtained. The C3 approach has been used in the calculation of different cross sections for different processes and in this way the fails of the model have been put in evidence [8]. In the last years many works have been published with different proposal to improve the simply C3 [9–14]. Some of them introduced modifications to get a better description of the certain dynamical region [9–11], and other to improve the asymptotic behavior [12–14]. However all of them use the same form for the wave function, i.e. the product of three two-body Coulomb problem which are essentially three Kummer functions [17].

Recently the authors and co-workers have introduced an approximated wave function which overcome one of the problem that the three-body wave equation offer, its non-separability. A non-separable wave function called Φ_2 was introduced for two heavy and one light particles [15,16]. This functions, written in terms of the Kummer function [17] and degenerate hypergeometric functions of two variables [19], couple the independent two-body Coulomb problem associated with the C3 approach. The two variable hypergeometric function (which replace two of the Kummer function of the C3 one) represent the motion of, e.g., the electron in the combined field of two protons. The coupling included in the Φ_2 model can be related with part of the non-orthogonal kinetic energy neglected in the uncoupled C3 [15,16]. The application of the Φ_2 to the calculation of cross section for the ion–atom ionization has shown that the description of the dynamic of the three-body Coulomb problem is improved in some region of the configurational space in relation with the C3 [20,21].

In this paper we introduce a fully correlated wave function to represent the continuum of the three-body spectra. We show that this function can describe systems with arbitrary masses, keeping some important properties such as the correct asymptotic conditions. In Section 2 we introduce the notation and some important concepts related with the three-body Coulomb problem. In Section 3 we present the function Φ_M, a fully correlated wave for Coulomb systems of arbitrary masses. We also discuss two of the most important cases, the system *hhl* with two heavy ($m_{\mathrm{h}} \gg m_{\mathrm{e}}$) and a light mass, and the system *llh*, with two light and one heavy mass. We analyze the different properties and show the simplification to precedent models. Finally, we outlook some of the uses of this function in collision problems. Atomic units are used thorough the work.

2. Statement of the problem

In this section we study the way in which the Hamiltonian for three charged particles changes when the masses of the particles change. We first write the Schrödinger equation in terms of the parabolic coordinates introduced by Klar [22]. The three-body wave equation is

$$\left[\frac{1}{2\mu_{23}}\nabla^2_{\boldsymbol{r}_{23}} + \frac{1}{2v_{23}}\nabla^2_{\boldsymbol{R}_{23}} + \frac{Z_1Z_2}{r_{12}} - \frac{Z_2Z_3}{r_{23}} - \frac{Z_1Z_3}{r_{13}} - E\right]\Psi = 0, \tag{1}$$

where $\{\boldsymbol{r}_{23},\boldsymbol{R}_{23}\}$ form one of the Jacobi pairs, Z_i $(i = 1, 2, 3)$ are the charges of the particles and $\boldsymbol{r}_{ij}$ represent its the relative coordinates. We focus our attention in the continuum problem. However, simple analytical continuations can transform the next steps into bound continuum or fully bound systems. Therefore, we introduce the ansatz

$$\Psi = \mathrm{e}^{\mathrm{i}(\boldsymbol{K}_{23}\cdot\boldsymbol{R}_{23}+\boldsymbol{k}_{23}\cdot\boldsymbol{r}_{23})}\Phi \tag{2}$$

and define the energy as $E = (K^2_{23}/2v) + (k^2_{23}/2\mu)$. We end up with the following form for the Schrödinger equation:

$$[D_0 + D_1]\Phi = 0. \tag{3}$$

The operators D_0 and D_1 are given by

$$D_0 = H_1(\xi_1,\eta_1) + H_2(\xi_2,\eta_2) + H_3(\xi_3,\eta_3) \tag{4}$$

and

$$D_1 = \frac{1}{m_3}\boldsymbol{P}_1\cdot\boldsymbol{P}_2 + \frac{1}{m_2}\boldsymbol{P}_1\cdot\boldsymbol{P}_3 - \frac{1}{m_1}\boldsymbol{P}_2\cdot\boldsymbol{P}_3, \tag{5}$$

where

$$H_l(\xi_l,\eta_l) = \frac{1}{\mu_{mn}r_{mn}}\left\{\left[\xi_l\frac{\partial^2}{\partial\xi_l^2} + (1+\mathrm{i}k_{mn}\xi_l)\frac{\partial}{\partial\xi_l} - \delta_l\right] + \left[\eta_l\frac{\partial^2}{\partial\eta_l^2} + (1-\mathrm{i}k_{mn}\eta_l)\frac{\partial}{\partial\eta_l} - \gamma_l\right]\right\} \tag{6}$$

and

$$\boldsymbol{P}_i = (\nabla\xi_i)\frac{\partial}{\partial\xi_i} + (\nabla\eta_i)\frac{\partial}{\partial\eta_i}. \tag{7}$$

The constant α_i and β_i must satisfy the following condition: $\alpha_i + \beta_i = Z_jZ_k\mu_{jk}$ with i, j, $k = 1, 2, 3$ $(i \neq j \neq k)$.

Without loss of generality, we can restrict ourselves to incoming boundary conditions [5]. Then, the wave function for the continuum spectra when the particles are far ($R_{23}, r_{23} \to \infty$ and $R_{23}/r_{23} = cte$) from each other should behave as

$$\Psi \to \mathrm{e}^{\mathrm{i}(\boldsymbol{K}_{23}\cdot\boldsymbol{R}_{23}+\boldsymbol{k}_{23}\cdot\boldsymbol{r}_{23})}(k_{23}\xi_1)^{-\beta_1}(k_{13}\xi_2)^{-\beta_2}(k_{12}\xi_3)^{-\beta_3}. \tag{8}$$

This is the well-known *Redmond's* [18] asymptotic condition where $\beta_n = (\mathrm{i}Z_lZ_m\mu_{lm})/k_{lm}$ with $l \neq m \neq n$ and l, m, n = 1, 2, 3.

In Eq. (4) each term (see Eq. (6)) can be associated with a given pair of particles, which we are going to call 1, 2 and 3, and defining a two-body Coulomb equation. If the operator D_1 is neglected then Eq. (3) can be solved by variables separation leading to a product of three two-body Coulomb wave function where the projection of the angular momentum L_z are equal to zero. The D_1 operator correlates the motion of these three pairs. We can see in Eq. (5) that the mass m_3 connect the pairs (1,2), the mass m_2 the pairs $(1, 3)$ and finally the mass m_1 correlates the pairs $(2, 3)$. That is, Eq. (5) shows us how this coupling depends upon the masses of the particles. To study this dependence more carefully we define, m_3 as m_e the mass of an electron, and we are going to see how the Schrödinger equation changes as a function of m_1 and m_2. The case of two heavy ions and one electron (*hhl*) results from setting $m_1 = m_2 \simeq \infty$. In this case, the second and third terms of Eq. (5) can be neglected and only the mixed derivatives between the pairs $\{\xi_i, \eta_i\}$ with i = 1, 2 remains. This means that only two pair of particles are correlated. This is in agreement with the common sense because in that masses configuration the motion of the pair of heavy particles, described by the coordinates ξ_3, η_3, can be modeled as independent of the movement of the electron. On the contrary, the electron should move in the field of the two heavy particles, and then the pair (1,2) should be correlated. Thus, in that masses configuration the wave function partially separates as $f(\xi_1, \eta_1, \xi_2, \eta_2)\, g(\xi_3, \eta_3)$. On the other hand, when, e.g. $m_1 = m_2 = m_e$ and $m_3 \simeq \infty$ only the first term of the D_1 can be neglected. In that situation the system does not have any separability but the coupling has a particular form. We can see that the pairs 1 and 3 are connected by the second term of Eq. (5) while the pairs 2 and 3 are correlated by the third one. The pairs 1 and 2 are not directly correlated because the first term in Eq. (5) is canceled by the mass m_3, but there is a coupling due to the correlation given by the other two terms. This means that the *l–l* interaction must be coupled with each pair forming an *l–h* interaction. Finally, in the general case where the system is completely symmetric in terms of masses, it is when $m_2 = m_1 = m_3 = m_e$ the system is completely correlated. But we can note that the coupling is still by pairs.

All the cases described above indicate that the masses connect the particles by pairs. However the connection is a little bit more complicated like that when we take a look to the coordinates. We can see that each coordinate is coupled with other four by the mix derivatives and these coupling are weighted by the masses of the particles. Additional to the coupling introduced by the cross derivatives, there exist also a coupling given by the Coulomb potentials. That is to say, even when the coordinates do not appear in a mixed derivative (for example ξ_1 and η_1) there is a coupling given by the Coulomb potential. It is well known that the two-body Coulomb problem can be understood as a superposition of two harmonic oscillators with a particular, dynamical coupling. What we see in the case of the three-body problem is that besides of this dynamical coupling there exist a *kinematic* correlation given by the cross derivatives. The D_1 operator mix each of the oscillators (there are six of them, one for each coordinate) with the other four. In the following sections we are going to use the solutions of these harmonic oscillators to construct a regular solution satisfying most of the physical properties of the three-body Coulomb problem.

3. The Φ_M approach

As we have described in the precedent section, the structure of the Schrödinger equation does not depend exclusively on the masses of the particles, but on the *relations* among these masses. This clearly suggests that any general wave function for Coulomb systems with arbitrary masses should include these relations. The simplest way to translate this particular characteristic of the differential equation to a wave function is to consider the *ratios* between the different masses. Besides, in order to treat all the interactions on equal footing, we consider a symmetric wave function of the form:

$$\Phi_M = \sum_{i,j,k=0}^{\infty} \frac{(-1)^{i+j+k}(\beta_1)_{j+k}(\beta_2)_{i+k}(\beta_3)_{i+j}}{i!j!k!(i+j+k)_{i+j+k}(1)_{2(i+j+k)}}, \tag{9}$$

$$\left(\frac{m_e}{m_1}\right)^i \left(\frac{m_e}{m_2}\right)^j \left(\frac{m_e}{m_3}\right)^k$$

$$x_3^{(i+j)} F[\beta_3 + (i+j), 1 + 2(i+j), x_3]$$

$$x_2^{(i+k)} F[\beta_2 + (i+k), 1 + 2(i+k), x_2]$$

$$x_1^{(j+k)} F[\beta_1 + (j+k), 1 + 2(j+k), x_1],$$

where the functions $F[a,b,z]$ represent the Kummer functions, m_e is the electron mass and $x_l = -\mathrm{i}(k_{mn}r_{mn} + \boldsymbol{k}_{mn} \cdot \boldsymbol{r}_{mn})$. As we shall see Φ_M can be considered an extended approximated solution of Eq. (3) based on the Φ_2 model. The function Φ_M as defined by (9) is a linear combination of harmonic oscillator solutions $x^m F[\beta + m, 1 + 2m, x]$. These functions are the analytic continuation of the set obtained by solving the bound states of the Hydrogen atom as a system of coupled harmonic oscillators.

To show the connection between the Φ_2 model and the Φ_M function we consider the case *hhl*. For example, $m_1 = m_2 = m_p \to \infty$ (m_p being the proton mass) and $m_3 = m_e$. In that limit, the function Φ_M reduces to

$$\Phi_M^{ppe} = F[\beta_3, 1, x_3] \sum_{k=0}^{\infty} \frac{(-1)^k (\beta_1)_k (\beta_2)_k}{k!(k)_k (\gamma)_{2k}}, \tag{10}$$

$$x_2^k F[\beta_2 + k, \gamma + 2k, x_2] x_1^k F[\beta_1 + k, \gamma + 2k, x_1].$$

The series appearing in this equation is the harmonic oscillator expansion of the Φ_2 hypergeometric function, and in that limit Φ_M reduces to the Φ_2 wave function [15]. As we can verify this limit is fulfilled by each of the possible combination of two heavy and one light particles, due to the symmetry of the wave function. The approximated wave function Φ_M connect the different limits of masses. In each of the limits the Φ_M function satisfy the approximated Schrödinger equation satisfied by the Φ_2 model. According with the discussion of the previous section there must be a unique solution (within the model) connecting the different masses regions. The Φ_M is the one which connect the different Φ_2 models.

The *llh* system result form Eq. (9) by introducing the limit $m_1 = m_2 = m_e$ and $m_3 \simeq m_p \to \infty$, obtaining

$$\Phi_M^{llh} = \sum_{i,j=0}^{\infty} \frac{(-1)^{i+j}(\beta_1)_j(\beta_2)_i(\beta_3)_{i+j}}{i!j!(i+j)_{i+j}(1)_{2(i+j)}} x_1^j \times F[\beta_1 + j, 1+2j, x_1] x_2^i F[\beta_2 + i, 1+2i, x_2] x_3^{(i+j)} \times F[\beta_3 + (i+j), 1+2(i+j), x_3]. \quad (11)$$

The Kummer functions depending on x_1 and x_2 represent the dynamics of each of the electrons in relation with the nucleus represented by the particles 3. The third Kummer function represents the interaction between the electrons. As we can see the whole wave function is non-separable and the correlation presented is in agreement with the discussion of Section 2. We should emphasize that the first order of Eq. (11) is the C3 wave function, but due to the presence of the other terms of the series the normalization of the function is different. Asymptotically the Φ_M^{eep} model satisfy the Redmond's condition

$$\Psi_M^{llh} = \frac{1}{N^{eep}} e^{i(\mathbf{K}_{23}\cdot\mathbf{R}_{23} + \mathbf{k}_{23}\cdot\mathbf{r}_{23})} (ix_1)^{-\beta_1} (ix_2)^{-\beta_2} (ix_3)^{-\beta_3},$$

where the normalization constant is given by

$$N^{eep} = \frac{N_{C3}}{\sum_{i,j=0}^{\infty} \frac{(-1)^{i+j}(\beta_1)_j(\beta_2)_i(\beta_3)_{i+j}(1)_{2j}(1)_{2i}}{i!j!(i+j)_{i+j}(1-\beta_1)_j(1-\beta_2)_i(1-\beta_3)_{i+j}}}. \quad (12)$$

Clearly this constant can be also obtained by using the general definition of Φ_M. N_{C3} is the normalization of the C3 wave function $N_{C3} = \prod_{j=1}^{3} e^{-\pi\beta_j/2}\Gamma(1 - i\beta_j)$.

The normalization constant of the C3 model is mostly responsible for the cusp-like structures appearing in positron–atom ionization (as well as ion–atom ionization). Also it takes a major role in the energy behavior in the Wannier region. However, the normalization in the correlated models like the Φ_2 is different. Within the Φ_2 model the normalization constant is more symmetric than the C3 one, but the differential cross-sections around the cusp is more asymmetric, giving a better agreement with the experimental data. This means that the energy behavior around the cusp also depend on the transition matrices in the correlated models. The C3 wave function describes the electron capture to the continuum in e^+ atom but fails to describes correctly the Wannier law when the excess energy tends to zero [10]. This is similar to the wrong description observed in antiproton–atom ionization [4]. This effect is a consequence of the fact that the C3 wave function describes the three-body Coulomb problem as the product of three non-interacting two-body ones. In this sense we can see clearly that the Φ_M^{eep} changes completely the representation since it is a non-separable wave function. The normalization N^{eep} shows the same kind of behavior than the Φ_2 one in ion–atom collision. In Fig. 1 we plot the normalization for the case of two electrons and one proton while in Fig. 2 we represent the normalization for one positron, one electron and one proton. The asymmetry is decreased in the eep and the $e^+e^-p^+$. The calculation of the T matrices within the Φ_M model would show the behavior as a function of the energy.

The C3 model satisfies the Kato cusp conditions, due to the fact that each of the two-body Coulomb wave function which form the whole wave function does. The Φ_M wave function does

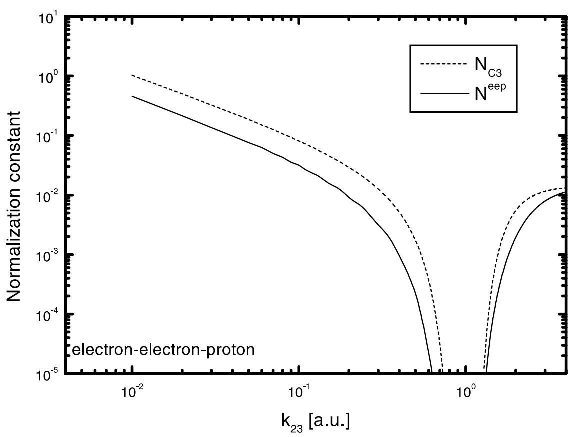

Fig. 1. Normalization factors as a function of the electron–proton relative momentum for a $e^-e^-p^+$ system. The velocity of the incoming electron is set to 1 a.u.

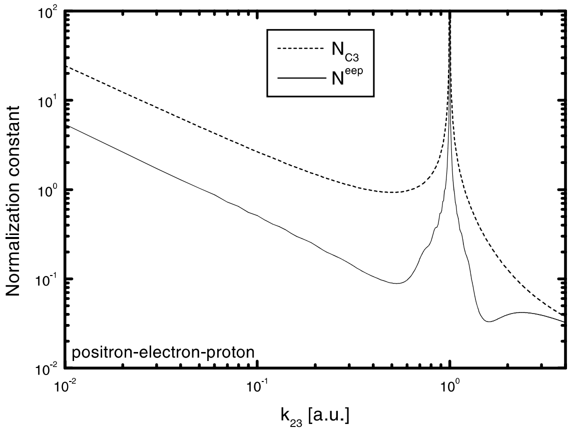

Fig. 2. Same as Fig. 1 for a $e^+e^-p^+$ system.

satisfy a first order in the Kato conditions in the sense explained by Miraglia et al. [24]. Actually, to fully satisfy the Kato conditions within a harmonic oscillator representation it is necessary to include the η_i coordinates [23]. The approximated wave function Φ_M can be considered as an alternative model to the introduced by Miraglia et al. in 1999 [24]. We should note that their wave functions are not valid for system with arbitrary masses.

4. Outlook

In this paper we introduced a new model to deal with three-charged particles with arbitrary masses. The Φ_M wave function can be viewed as the generalization of the approximated solution for a ppe system Φ_2. Even when this is an approximate model, it is based in two physically sound assumptions. First, the wave function reproduces the dependence of the differential equation not in the masses of the particles, but in the *ratios* of them. Second, it correlates all the variables in the problem, only restricted by asymptotic conditions. In this way, different approximations for *hhl* or *llh* systems can be derived naturally from the wave function. The structure showed by the wave function in this two limiting cases arises with proper limits in the ratios of masses and reproduce the correlation observed at the wave equation level. We showed that the Φ_M function correctly behaves in the asymptotic regime, and also fulfills approximately the Kato's cusp conditions. This two properties are necessary for any useful calculation in three-body Coulomb collisions.

Further extensions of this function can be glimpsed. The introduction of all the six coordinates of the problem is straightforward, giving rise to a six-index summation of products of six two-body Coulomb functions. Although this function can have some interesting properties, it is unlikely to be useful for calculation processes due to the calculation time that could be required. On the other hand, generalized bound continuum and fully bound functions can be obtained. The last ones can be a good test for the accuracy of the approximation.

In this paper two particular system of particles were considered, but other system can be also studied. Three electron-like paritcles (including positrons) and other exotic system can be described with the Φ_M wave function. Its application to different processes involving different kind of particles would be the ideal test to the approximation. Finally, the Φ_M function accepts the modifications in the parameters (such as dynamic charges or position-dependent momenta) proposed by some authors [9–14] but the final expressions are cumbersome. Currently our efforts are devoted to test this function in ion–atom and $e^{\pm}$–atom collisions.

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