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Two–body Coulomb problems with sources for the J-matrix method

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Abstract. The two-body Coulomb problem with sources is studied. Closed form solutions are provided for particular non-homogeneities used within the J-matrix method. The results are employed to build analytical solutions having incoming, outgoing and standing wave asymptotic conditions.

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1 Introduction

Scattering theory is of fundamental importance in atomic physics. It allows for a description and an interpretation of many atomic collision processes such as, e.g., excitation and ionization by particle or radiation impact, among many others. In many cases, the wave function satisfying the full (time-independent) Schrödinger equation may be written as the sum of a known initial state of a simplified hamiltonian and an unknown scattering solution which describes the dynamics of the collision [1, 2]. This separation leads straightforwardly to a non–homogeneous (driven) equation where the source is the product of the neglected interactions and the asymptotic solution. For example, this is the line followed by the Exterior Complex Scaling approach [3–5], which has been widely and successfully used in treating a large variety of scattering problems.

In a previous paper [6], we studied a two-body driven Schrödinger equation which includes a Coulomb interaction, a case of fundamental importance for the atomic physics community. Here, we shall apply some of the closed form results to the construction of an asymptotical cosine-like stationary function used by the J-matrix approach [7–9].

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The J-matrix has proven to be a very successful method to treat a large variety of scattering problems, as reviewed by Alhaidari *et al.* [7]. It has been formulated for two-body problems without [10] and with [8,11] Coulomb interaction, but also for multichannel processes [10–12]. The method can be considered as a variant of the variational approach for continuum states [13]. It bears some analogy with the R-matrix theory which divides the coordinate space into two regions, an inner region and an asymptotic region. The main idea of the J-matrix method is to separate the wave function into two parts: (i) an internal term which contains the information about the dynamics of the problem associated to a given potential V, and (ii) a term containing the asymptotic solution of the problem. The first part depends upon a large number of parameters which are used to solve the Schrödinger equation in the reaction zone where the interaction potential V is not negligible. This term is usually expanded in a complete and orthogonal basis set. The second – asymptotic – part, on the other hand, ignores V and is written as a linear combination $\varphi_s(r)+\tan\delta\,\varphi_c(r)$ of two stationary functions which at large distances r from the origin behave as free particle – or Coulomb – waves with sine-like (φ_s) and cosine–like (φ_c) behaviors. This linear combination involves the coefficient $\tan\delta$ usually associated to the transition matrix of the scattering problem. The transition matrix and the expansion coefficients are determined by enforcing the proposal to satisfy the Schröginger equation.

The two functions φ_s and φ_c used to represent the asymptotic part must be linearly independent functions satisfying a Schrödinger equation which does not contain the interaction potential V. However, a problem arises: for a given radial Schrödinger equation, two solutions with the asymptotic behavior of φ_s and φ_c, and being both regular at the origin, are not available. Thus the J-Matrix method makes use of a function φ_c which, having cosine–like behavior, satisfies a non–homogeneous Schrödinger equation; its expansion on L^2 Laguerre basis functions was proposed, e.g., in Refs. [8,11,12]. The primary purpose of this paper is to give a closed form solution for φ_c.

The paper is arranged as follows. In Sec. II, we provide in closed form the particular solution for the two-body Coulomb Schrödinger equation with a particular non–homogeneity. This involves a two-variable hypergeometric function which can be considered as a generalization of the Kummer function associated to the pure Coulomb problem. In Sec. III, we give the asymptotic behavior of this solution, as well as that of the regular and irregular homogeneous solutions. We then use these results to construct, through an appropriate linear combination, pure incoming, outgoing or cosine-like waves which can be used within the J-matrix method. Atomic units are used throughout.

2 The two-body Coulomb problem with a particular source

The J-matrix method makes use of a function φ_c which is solution of the following radial non–homogeneous equation [8,12]

$$\left[-\frac{1}{2\mu}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)+\frac{z_1z_2}{r}-E\right]h_{l,\sigma}(r)=a_{l,\sigma}e^{-\lambda r}r^{l+\sigma}, \tag{1}$$