



An algorithm for the calculation of the partial wave expansion of the Coulomb-distorted plane wave[☆]



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ABSTRACT

The partial wave expansion of the Coulomb-distorted plane wave is determined by the help of the complex generalized hypergeometric function ${}_2F_2(a, a; a + l + 1, a - l; z)$. An algorithm for the calculation of ${}_2F_2(a, a; a + l + 1, a - l; z)$ is created and it is implemented as a FORTRAN-90 code. The code is fast and its accuracy is 14 significant decimal digits.

Program summary

Program title: Hyp2F2spec_v1

Catalogue identifier: AEXR_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEXR_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, <http://cpc.cs.qub.ac.uk/licence/licence.html>

No. of lines in distributed program, including test data, etc.: 1067

No. of bytes in distributed program, including test data, etc.: 8394

Distribution format: tar.gz

Programming language: FORTRAN-90.

Computer: x86-64.

Operating system: LINUX, MAC OS X, Windows.

RAM: < 1 MB

Classification: 4.7.

Nature of problem: The partial wave expansion of the Coulomb distorted plane wave is given by a generalized hypergeometric function with special indexes. An algorithm is developed for the calculation of this function.

Solution method: Taylor-series and asymptotic expansion in both cases estimates for the remainder terms are determined. Explicit expression is also used.

Running time: Less than 0.01 s

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1. Introduction

Scattering of charged particles is an important field in quantum mechanics. Even the two-body case is peculiar since it does not fit into the conventional time-dependent scattering theory formalism. Several methods are invented to overcome the difficulties caused by the long range behavior of the Coulomb interaction. In the time-dependent framework the formalism of

[☆] This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

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Dollard [1] modifies the Møller wave operator. In stationary approach the method of van Haeringen [2] introduced Coulomb asymptotic states and Mulherin and Zinnes [3] promoted distorted asymptotic states. The connection of the latter two formalism was also investigated [4]. Following the works [5,6] we will call the asymptotic state of Mulherin and Zinnes as Coulomb-distorted plane wave (CDPW).

The recently introduced surface integral formalism of quantum scattering theory [5–7] is valid not only for two-body scattering but it can be extended to scattering of three charged particles. Another advantage of this formalism is that it handles the short and long range interactions on an equal footing. It is said in [6] “All the results... rely on the asymptotic forms of the plane wave and the Coulomb-distorted plane waves”. The CDPW indeed plays an important role in the surface integral formalism. In this framework the full scattering wave function is composed of as a sum of the CDPW and a so called scattered part. Furthermore the surface integral expression of the scattering amplitude also refers to the CDPW.

The explicit three-dimensional form of the CDPW is given by

$$e^{i\mathbf{k}\mathbf{r}}(k\mathbf{r} - \mathbf{k}\mathbf{r})^{i\gamma}. \quad (1)$$

Here γ is the Sommerfeld parameter and \mathbf{k} is the momentum vector. The bold face letters \mathbf{k} and \mathbf{r} denote elements of the three-dimensional Euclidean space \mathbb{R}^3 , while k and r denote the corresponding magnitudes.

Interestingly the partial wave expansion of the CDPW has been given only recently [8,9] and there is no computer program to evaluate the partial wave components. Here we present an algorithm and FORTRAN-90 code for numerical calculations.

The basic notations are introduced in Sections 2 and 3. Since the CDPW can be expressed by the help of hypergeometric function ${}_2F_2(a, a; a + l + 1, a - l; z)$ we derive an algorithm for the calculation of it in Section 4. The numerical results, test runs are presented in Section 5. Instead of using the direct expression for the CDPW, for two regions, we developed special methods for the calculation. Around the origin we use the Taylor expansion and we determined an upper bound for the error term. Similarly in the asymptotic regions we derived an asymptotic expansion with an estimate for the error term. The detailed mathematical descriptions of the algorithms used for different regions of the complex plane are contained in the [Appendices A and B](#).

2. The partial wave expansion of the Coulomb-distorted plane wave

As we have shown in [9] the partial wave expansion of the Coulomb-distorted plane wave is

$$e^{i\mathbf{k}\mathbf{r}}(k\mathbf{r} \mp \mathbf{k}\mathbf{r})^{\pm i\gamma} = \sum_{l=0}^{\infty} (2l+1) \tau_l^{(\pm)}(\gamma, kr) P_l(\cos(\vartheta)), \quad (2)$$

where the upper and lower signs correspond to the post and prior form of the CDPW. The angle between the vectors \mathbf{k} and \mathbf{r} is signed by ϑ and the Legendre polynomial is denoted by $P_l(x)$. The radial function $\tau_l^{(\pm)}(\gamma, kr)$ can be calculated by the integral

$$\tau_l^{(\pm)}(\gamma, kr) = \frac{1}{2}(kr)^{\pm i\gamma} \int_{-1}^1 e^{\pm ikrx} (1 \mp x)^{\pm i\gamma} P_l(x) dx. \quad (3)$$

A compact expression for the partial wave component $\tau_l^{(\pm)}(\gamma, kr)$ can be given for arbitrary l . Using (3) and the formula 2.17.5.6 in [10] we get

$$\tau_l^{(+)}(\gamma, kr) = \frac{(-i\gamma)_l}{(1+i\gamma)_{l+1}} (2kr)^{i\gamma} e^{i\mathbf{k}\mathbf{r}} {}_2F_2(1+i\gamma, 1+i\gamma; l+2+i\gamma, 1+i\gamma-l; -2ikr) \quad (4)$$

and

$$\tau_l^{(-)}(\gamma, kr) = (-1)^l \frac{(i\gamma)_l}{(1-i\gamma)_{l+1}} (2kr)^{-i\gamma} e^{-i\mathbf{k}\mathbf{r}} {}_2F_2(1-i\gamma, 1-i\gamma; l+2-i\gamma, 1-i\gamma-l; 2ikr), \quad (5)$$

where $(a)_n$ is the Pochhammer symbol and ${}_2F_2$ is the generalized hypergeometric function [11].

3. General description of the program

The expressions (4) and (5) show that the CDPW can be expressed by the help of the function ${}_2F_2(a, a; a + l + 1, a - l; z)$, where $a = 1 + i\gamma$ and $a = 1 - i\gamma$ for the post and prior form of the function. We developed an algorithm for the determination of the hypergeometric function ${}_2F_2(a, a; a + l + 1, a - l; z)$ for almost arbitrary complex a and z , some restrictions will be given in the next sections. The calculation of the CDPW can be carried out using the expressions (4) and (5).

The present code uses two freely available FORTRAN-90 codes for the calculation of the Gamma function and for the incomplete Gamma function. The Gamma function is calculated by the CGAMMA code developed by A.H. Morris which can be found in the Naval Surface Warfare Center (NSWC) Library of Mathematics Subroutines. The references [12–14] contain the description of the algorithms used by the code CGAMMA. The accuracy of this code is 14 significant decimal digits. The FORTRAN-90 version of this code is due to Alan Miller [15]. The complementer of the incomplete Gamma function is calculated by the code CINCGAM developed by Eric Kostlan and Dmitry Gokhman [16]. Actually we use the FORTRAN 90 version of Alan Miller [15]. Arbitrary accuracy can be achieved with the code CINCGAM. Although the $\Gamma(z)$ function can be calculated with the code CINCGAM but in order to increase the speed of the calculation we used the code CGAMMA.

For physical applications there are no large parameters the typical values are $l < 20$ and $|a| < 100$. We have to deal with however with the cases when the variable z is small or large. In the case of $|z| < 1$ we used the Taylor series of the function ${}_2F_2(a, a; a + l + 1, a - l; z)$ and gave an estimate for the remainder if we use only the first N terms of the Taylor series (see [Appendix A](#)). In this way we can do arbitrary accuracy calculation in the $|z| < 1$ region of the variable z . If $|z|$ is large we derived an asymptotic expression for ${}_2F_2(a, a; a + l + 1, a - l; z)$ (see (B.1) and (B.15) in [Appendix B](#)) and developed an estimate for the error term.

The code HYP2F2SPEC_V1 in the general case ($|z| \geq 1$ and z is not in the asymptotic region (see [Appendix B](#))) applies the expression

$$\begin{aligned} & {}_2F_2(a, a; a + l + 1, a - l; z) \\ &= (-z)^{-a} \frac{(a)_{l+1}}{(1-a)_l} \sum_{k=0}^l \binom{l}{k} \frac{(l+1)_k}{k!} \gamma(a+k, -z) z^{-k} \end{aligned} \quad (6)$$

(see: [9]).

4. Algorithm of HYP2F2SPEC_V1

The code HYP2F2SPEC_V1 in the case of $|z| \geq 1$ can be used for $l \geq 0$, l is integer, $a \in \mathbb{C} \setminus \mathbb{Z}$ and $\text{Re}[a] > 0$, in the case of $|z| < 1$ it is supposed that $l \geq 0$, l is integer and $a \in \mathbb{C} \setminus \mathbb{Z}$. The input parameters of the code are a, l, z, M, E . The first three correspond to the parameters of the hypergeometric function ${}_2F_2(a, a; a + l + 1, a - l; z)$. The error term of the asymptotic expansion is determined by the integer parameter M such that $M \geq 1$ (see Eq. (B.15)). The absolute error ϵ is determined by the integer E ($E \geq 0$) such that $\epsilon = 10^{-E}$.

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