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Coulomb wave functions in momentum space☆

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ABSTRACT

An algorithm to calculate non-relativistic partial-wave Coulomb functions in momentum space is presented. The arguments are the Sommerfeld parameter η, the angular momentum l, the asymptotic momentum q and the 'running' momentum p, where both momenta are real. Since the partial-wave Coulomb functions exhibit singular behavior when $p \rightarrow q$, different representations of the Legendre functions of the 2nd kind need to be implemented in computing the functions for the values of p close to the singularity and far away from it. The code for the momentum-space Coulomb wave functions is applicable for values of $|\eta|$ in the range of 10^{-1} to 10, and thus is particularly suited for momentum space calculations of nuclear reactions.

Program Summary

Program title: libcwfn
Catalogue identifier: AEUQ_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEUQ_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.: 864503
No. of bytes in distributed program, including test data, etc.: 7178021
Distribution format: tar.gz
Programming language: Fortran 90, Fortran 77, Python, make (GNU Make dialect), GNU Bash shell interpreter (available as /bin/bash).
Computer: Apple Powermac (Intel Xeon), ASUS K53U (AMD E-350 (Dual Core)), DELL Precision T3500 (Intel Xeon), NERSC Carver (Intel Nehalem Quad Core).
Operating system: Linux, Windows (using Cygwin).
RAM: less than 512 Mbytes
Classification: 17.8, 17.13, 17.16.
Nature of problem:
The calculation of partial wave Coulomb functions with integer l and all other arguments real.

☆ 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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Solution method:
Computing the value of the function using explicit formulae and algorithms.
Running time:
Less than 10^{-3} s.

1. Introduction

The problem of scattering by the long-range Coulomb force is theoretically well understood, and established computational as well as analytical techniques are available for the calculation of scattering observables for strongly interacting particles. Those procedures are defined and carried out in coordinate space (see e.g. [1]). However, if the strong interactions are nonlocal or if one is interested in problems involving three or more particles, momentum space can be preferable when carrying out calculations, since the equations can be cast in integral form and thus boundary conditions are automatically included. In this case all operators are calculated in a plane wave basis and inserted into Lippmann–Schwinger or Faddeev-type integral equations. However, due to the long-range character of the Coulomb potential, a plane-wave basis can only be used if a screening procedure of the Coulomb potential is employed [2]. Unfortunately, this screening procedure becomes unstable when charges reach values of about $Z = 20$ [3]. To remedy the situation, it would be natural to use basis functions that are better suited for the problem, which in this case are momentum-space Coulomb functions. In this basis, the Coulomb Green's function has the same form as the free Green's function in the plane wave basis. However, this is non-trivial, since the Fourier transform of the so-called coordinate-space Coulomb wave function does not exist in a functional sense, and the logarithmic singularity due to the long range of the Coulomb force is far less tractable in momentum space.

Here we present a code for computing the non-relativistic free momentum-space Coulomb wave function $\psi^C_{l,q,\eta}(p)$ in a partial-wave representation together with the analytical frame work that leads to its numerical implementation. Here q is the external, asymptotic momentum, while p is the 'running' momentum. The quantity $\eta = Z_1 Z_2 e^2 \mu/q$ represents the Sommerfeld parameter, which is positive for a repulsive Coulomb interaction, as is the case in nuclear reactions, or negative for an attractive Coulomb force, as e.g. in electron-ion reactions. The reduced mass μ of the system of two particles with masses m_1 and m_2 and charges Z_1 and Z_2 is defined as $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$. The quantity e represents the unit electric charge.

Our code is valid for arbitrary large integer values of the angular momentum l. However, it is well known (see e.g. [1]) that for a given value of η, the Coulomb wave functions for large l will eventually behave like a plane wave. In this case, a matrix element in the Coulomb basis would simply be a matrix element evaluated in a plane wave basis. In Ref. [4] momentum-space wave functions have been considered for two-particle scattering through an $l = 0$ repulsive Coulomb force. To our knowledge no code is readily available for computing momentum-space Coulomb wave functions.

The manuscript is organized as follows: In Section 2 we review the analytical expressions of the partial-wave Coulomb functions in momentum space, and introduce the different representations of the associated Legendre functions of the 2nd kind in terms of hypergeometric functions necessary to obtain numerically stable representations of the Coulomb wave functions around the singularity point $p = q$ and far away from it. In Section 3 we give the criteria we employ to switch between the different representations. The numerical methods employed are discussed in Section 4, the computational accuracy of our code package is described in Section 5. Properties of the partial-wave Coulomb functions in momentum space such as their dependence on the parameters l and η are discussed in Section 6. The use of the code is described in Section 7, and we summarize our work in Section 8.

2. The partial-wave Coulomb scattering function in momentum space

The expression for the Coulomb scattering wave function in momentum space, $\psi^C_{\mathbf{q},\eta}(\mathbf{p})$, as function of the asymptotic momentum $\mathbf{q}$ and a 'running momentum' $\mathbf{p}$ was derived some time ago [5]. However, when considering problems which obey rotational symmetry, calculations are conventionally performed in a partial-wave basis, which takes this symmetry into account. In this work, we follow Refs. [6,7] in carrying out the angular momentum decomposition of the momentum-space Coulomb scattering wave functions to arrive at their partial-wave representation. Starting from the most general expression, we derive the two representations necessary to obtain the wave function close to the singularity point $p = q$ and far away from it.

2.1. General expression

Following Ref. [6] we start from the expression for the Coulomb scattering wave function in momentum space as Fourier transform of the coordinate-space solution of the Coulomb Schrödinger equation: $\psi^{C(+)}_{\mathbf{q},\eta}(r)$ (see e.g. Refs. [1,8]),

$$\begin{aligned}\psi^{C(+)}_{\mathbf{q},\eta}(\mathbf{p}) &= \lim_{\gamma\to+0}\int d^3\mathbf{r}\; e^{-i\mathbf{p}\cdot\mathbf{r}-\gamma r}\;\psi^{C(+)}_{\mathbf{q},\eta}(r)\\ &= -4\pi e^{-\pi\eta/2}\Gamma(1+i\eta)\\ &\quad\times\lim_{\gamma\to+0}\frac{d}{d\gamma}\left\{\frac{[p^2-(q+i\gamma)^2]^{i\eta}}{[\,|\,\mathbf{p}-\mathbf{q}\,|^2+\gamma^2]^{1+i\eta}}\right\}. \qquad (1)\end{aligned}$$

The Fourier transform given above is explicitly worked out in Ref. [9]. The wave functions are normalized in momentum space to a δ-function. It should be pointed out, that the definition of Fourier transform of Eq. (1) differs from the one in the Ref. [6] by a factor $1/(2\pi)^3$.

The partial-wave Coulomb scattering function $\psi^C_{l,q,\eta}(p)$ is then defined through

$$\psi^{C(+)}_{\mathbf{q},\eta}(\mathbf{p}) \equiv \sum_{l=0}^{\infty}(2l+1)\psi^C_{l,q,\eta}(p)P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}}), \qquad (2)$$

where $P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})$ are the Legendre polynomials. Here the decomposition of a vector $\mathbf{q}$ into its magnitude and a unit vector $\hat{\mathbf{q}}$ indicating the direction, $\mathbf{q} = q\,\hat{\mathbf{q}}$ is used. This leads to

$$\psi^C_{l,q,\eta}(p) = \frac{1}{2}\int_{-1}^{1} dz\; P_l(z)\psi^{C(+)}_{\mathbf{q},\eta}(\mathbf{p}), \qquad (3)$$

where $z = (\hat{\mathbf{p}}\cdot\hat{\mathbf{q}})$. In the following we will omit the index η to simplify the notation.