Relativistic wave and Green’s functions for hydrogen–like ions

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Abstract

The Greens library is presented which provides a set of C++ procedures for the computation of the (radial) Coulomb wave and Green’s functions. Both, the nonrelativistic as well as relativistic representations of these functions are supported by the library. However, while the wave functions are implemented for all, the bound and free–electron states, the Green’s functions are provided only for bound–state energies \( E < 0 \). Apart from the Coulomb functions, moreover, the implementation of several special functions, such as the Kummer and Whittaker functions of the first and second kind, as well as a few utility procedures may help the user with the set–up and evaluation of matrix elements.

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PROGRAM SUMMARY

Title of program: Greens

Catalogue number: To be assigned.

Program obtainable from: CPC Program Library, Queen’s University of Belfast, N. Ireland. Users may obtain the program also by downloading a tar-file from a home page at the University of Kassel

http://www.physik.uni-kassel.de/~kovalp/software/greens

Licensing provisions: None.

Computer for which the program is designed and has been tested: PC Pentium III, PC Athlon

Installation: University of Kassel (Germany).

Operating systems: Linux 6.1+, SuSe Linux 7.3, SuSe Linux 8.0, Windows 98.

Program language used: C++.

Memory required to execute with typical data: 300 kB.

No. of bits in a word: All real variables are of type double (i.e. 8 bytes long).

Distribution format: Compressed tar file.

CPC Program Library Subprograms required: None.

Keywords: confluent hypergeometric function, Coulomb–Green’s function, hydrogenic wave function, Kummer function, nonrelativistic, relativistic, two–photon ionization cross section, Whittaker function.

Nature of the physical problem:
In order to describe and understand the behaviour of hydrogen–like ions, one often needs the Coulomb wave and Green’s functions for the evaluation of matrix elements. But although these functions have been known analytically for a long time and within different representations [1,2], not so many implementations exist and allow for a simple access to these functions. In practice, moreover, the application of the Coulomb functions is sometimes hampered due to numerical instabilities.

Method of solution:
The radial components of the Coulomb wave and Green’s functions are implemented in position space, following the representation of Swainson and Drake [2]. For the computation of these functions, however, use is made of Kummer’s functions of the first and second kind [3] which were implemented for a wide range of arguments. In addition, in order to support the integration over the Coulomb functions, an adaptive Gauss–Legendre quadrature has also been implemented within one and two dimensions.
Restrictions onto the complexity of the problem:

As known for the hydrogen atom, the Coulomb wave and Green’s functions exhibit a rapid oscillation in their radial structure if either the principal quantum number or the (free–electron) energy increase. In the implementation of these wave functions, therefore, the bound–state functions have been tested properly only up to the principal quantum number \( n \approx 20 \), while the free–electron waves were tested for the angular momentum quantum numbers \( \kappa \leq 7 \) and for all energies in the range \( 0 \ldots 10|E_{1s}| \). In the computation of the two–photon ionization cross sections \( \sigma_2 \), moreover, only the long–wavelength approximation \( e^{ikr} \approx 1 \) is considered both, within the nonrelativistic and relativistic framework.

Unusual features of the program:

Access to the wave and Green’s functions is given simply by means of the GREENS library which provides a set of C++ procedures. Apart from these Coulomb functions, however, GREENS also supports the computation of several special functions from mathematical physics (see section 2.4) as well as of two–photon ionization cross sections in long–wavelength approximation, i.e. for a very first application of the atomic Green’s functions. Moreover, to facilitate the integration over the radial functions, an adaptive Gauss–Legendre quadrature has been also incorporated into the GREENS library.

Typical running time: Time requirements critically depends on the quantum numbers and energies of the functions as well as on the requested accuracy in the case of a numerical integration. One value of the relativistic two–photon ionization cross section takes less or about one minute on a Pentium III 550 MHz processor.

References:
[1] H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One–and Two–Electron Atoms, (Kluwer Academic Publishers, 1977).
[2] R. A. Swainson and G. W. F. Drake, J. Phys. A 24 (1991) 95.
[3] M. Abramowitz and I. A. Stegun, Eds., Handbook of Mathematical Functions (Dover, New York 1965).
1 Introduction

From the early days of quantum mechanics on, the 'hydrogen atom' has served not only as a well–known textbook problem but also as one of the fundamental models in the physics of atoms, molecules, and nuclei. When combined with the (atomic) shell model, namely, the —analytic— solutions for the hydrogen–like ions help understand most atomic processes in Nature, at least qualitatively. For this reason also, the 'hydrogen atom' has found its way into quite different fields of physics including, for example, astro– and plasma physics, quantum optics or even the search for more efficient x–ray lasers schemes.

Despite of the success of the hydrogen model, however, the Coulomb problem is not always that simple to deal with, in particular, if a relativistic treatment is required. Therefore, various program tools have been developed over the years to help with either the analytic or numerical manipulation of the Coulomb functions and their matrix elements. For the nonrelativistic Coulomb problem, for example, the bound–electron states can be obtained from the codes of Noble and Thompson [1], who applied a continued fraction representation of the Whittaker functions, Bell and Scott [2], or simply by using the GNU Scientific Library [3]. These functions are incorporated also into a recent library by Madsen and coworkers [4], which has been designed to support the computation of the multipole matrix elements for circular and linear polarized light. — Less attention, in contrast, has been paid to the relativistic wave functions for which a CPC program is provided only by Salvat et al. [5]. This program help integrate the radial equation for any spherical–symmetric potential for both, the (one–particle) Schrödinger and Dirac equations and also provides separate procedures to compute the Coulomb wave functions.

Apart from the bound and free–electron wave functions, however, the Coulomb Green’s functions play a similar important role, in particular, if the interaction of atoms with external fields is to be studied. In second– and higher–order perturbation theory, for instance, these functions help to carry out the summation over the complete spectrum in a rather efficient way. But although different analytic representations are known for the Green’s functions [6, 7, 8, 9, 10], until today, there are almost no reliable codes freely available.

Therefore, to facilitate the further application of the 'hydrogen atom' in different contexts, here we present the GREENS library which provides a set of C++ procedures for the computation of the Coulomb wave and Green’s functions. In GREENS, these hydrogenic functions are supported both, within a nonrelativistic as well as relativistic framework. Beside of the various routines for the computation (of the radial parts) of these functions, however, we also supply the user with a Gauss–Legendre quadrature and a set of special functions to simplify the evaluation of matrix elements. — But before we shall present details about the organization of the GREENS library, in the following section, we first compile the basic formulas from the theory of the 'hydrogen atom' with emphasize especially to those expressions, which have been implemented explicitly. In section 3, later, the program structure will be discussed and how the library is to be distributed. This section also lists all user–relevant commands, although not much is said here about the underlying algorithms. In most cases, we followed the expressions from...
sections 2 but care has been taken in order to provide a reliable code for a rather wide range of parameters which, sometimes, required quite additional effort. In section 4, we explain how (easily) the hydrogenic wave and Green’s functions can be accessed not only for a particular set of arguments but also for the computation of matrix elements. These examples may serve, therefore, also as a test bed for the installation of the code. Section 5, finally, gives a brief summary and an outlook into our future work.

2 Theoretical Background

Since the theory of the ‘hydrogen atom’ has been presented at quite many places before (see, for instance, the texts of Messiah [11] and Drake [12]), we shall restrict ourselves to rather a short compilation of formulas, just enough in order to provide the basic notations and those expressions which are implemented in the code. In the next two subsections, therefore, we first recall the (analytic) form of the Coulomb wave and Green’s functions while, in subsection 2.3, these functions are applied to calculate the two–photon ionizations cross sections for linear and circular polarized light. In all these subsections, the nonrelativistic and relativistic formulas are always presented in turn of each other in order to display the similarities but also the differences in the numerical treatment of these functions. Subsection 2.4, moreover, provides reference to a few special functions from mathematical physics, which frequently occur in the computations of the Coulomb wave or Green’s functions and, hence, need to be part of the Greens library.

2.1 Coulomb wave functions

2.1.1 Nonrelativistic wave function

In a time–independent external field, the motion of a particle is described by the stationary Schrödinger equation

$$\left( \hat{H} (r) - E \right) \psi (r) = 0 \quad (1)$$

which, obviously, is an eigenvalue equation for the total energy $E$ of the particle. As known from the nonrelativistic Schrödinger theory, the Hamiltonian $\hat{H}$ just includes the kinetic and potential energy of the particle and, thus, takes the form

$$\hat{H} (r) = -\frac{\nabla^2}{2} - \frac{Z}{r} \quad (2)$$

in the case of a (pure) Coulomb field of a nucleus with charge $Z$. For such a spherical–symmetric potential, of course, Eq. (1) and the wave functions $\psi (r)$ can be separated

$$\psi_{n l m} (r, \theta, \varphi) = \frac{P_{n l} (r)}{r} Y_{l m} (\theta, \varphi) \quad (3)$$

into a radial and an angular part where, in most practical computations, the angular structure of the wave functions is often treated by means of the techniques from Racah’s algebra [14]. In expression (3), $n$ and $l$ denote the principal and orbital angular momentum quantum numbers, respectively, while $m$ describes the projection of the $z$–component of the orbital

\[^1\text{Here and in the following, we use atomic units} \ (m_e = \hbar = e^2/4\pi\varepsilon_0 = 1) \text{if not stated otherwise.}\]
angular momentum onto the quantization axis and is called the magnetic quantum number. The radial part of the wave function, \( P_{nl}(r)/r \), is a solution of the *radial* Schrödinger equation

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + 2E \frac{P_{nl}(r)}{r} = 0
\]

which has (normalizable) physical solutions for a discrete set of negative energies

\[
E_n = -\frac{Z^2}{2n^2} < 0, \quad n = 1, 2, \ldots,
\]

the so-called bound states, as well as for all positive energies \( E > 0 \), i.e. the continuum or free-electron states. Both, the bound and continuum solutions of (4) can be represented in terms of a single Whittaker function of the first kind \( M_{a,b}(z) \)

\[
P_{nl}(r) = C(n,l,Z) M_{n,l+\frac{1}{2}}(2Zr/n)
\]

\[
P_{E,l}(r) = C(E,l,Z) M_{i\sqrt{2EZ},l+\frac{1}{2}}(-2i\sqrt{2EZ}r)
\]

with real or complex arguments, and where \( C(n,l,Z) \) and \( C(E,l,Z) \), respectively, denote the corresponding normalization factors. The Whittaker functions are closely related to the Kummer functions of first and second kind as we will discuss in subsection 2.2.1. In the standard theory, moreover, the radial wave functions (6) and (7) are often normalized due to

\[
\int_0^\infty P_{nl}^2(r) \, dr = 1,
\]

\[
\int_0^\infty P_{E,l}^*(r)P_{E,l}'(r) \, dr = \delta(E - E'),
\]

in order to represent a single particle per bound state or per energy unit, respectively, if particles in the continuum are concerned.

### 2.1.2 Relativistic wave functions

An eigenvalue equation analogue to (4) also applies, if the motion of the particle is described within the relativistic theory. For an electron with spin \( s = 1/2 \), however, then the Hamiltonian \( \hat{H} \) needs to be replaced by the Dirac–Hamiltonian

\[
\hat{H}_D(r) = -ic\boldsymbol{\alpha} \cdot \nabla + \beta c^2 - \frac{Z}{r}
\]

which, apart from the kinetic and potential energy of the electron in the field of the nucleus, now also incorporates the rest energy of the electron as well as energy contributions owing to its spin. As in the nonrelativistic case, a separation of the wave function

\[
\psi_{n\kappa m}(r) = \frac{1}{r} \begin{pmatrix} P_{\kappa}(r) \Omega_{nm}(\theta,\varphi) \\ iQ_{\kappa}(r) \Omega_{-nm}(\theta,\varphi) \end{pmatrix}
\]

into a radial and angular part is possible for any spherical–symmetric potential, where the two radial functions \( P_{\kappa}(r) \) and \( Q_{\kappa}(r) \) are often called the large and small components. These
two functions also form a radial spinor \( \left( \frac{P_{\nu \kappa}(r)}{Q_{\nu \kappa}(r)} \right) \) and have to be obtained as solutions of the first–order, coupled equations \[13\]

\[
\left[ -\frac{Z}{r} - E \right] \frac{P_{\nu \kappa}(r)}{r} + \left[ \frac{\kappa}{\alpha r} - \frac{1}{\alpha} \frac{\partial}{\partial r} \right] \frac{Q_{\nu \kappa}(r)}{r} = 0 \quad (12)
\]

\[
\left[ \frac{1}{\alpha^2} \frac{\partial}{\partial r} + \frac{\kappa}{\alpha r} \right] \frac{P_{\nu \kappa}(r)}{r} - \left[ \frac{2}{\alpha^2} + \frac{Z}{r} + E \right] \frac{Q_{\nu \kappa}(r)}{r} = 0 \quad (13)
\]

where, however, the (total) energy \( E \) is taken here to represent the energy of the electron without its rest energy \( c^2 \), similar to Eq. \[14\] in the Schrödinger theory. In Eqs. \[11\]–\[13\], moreover, \( \kappa = \pm (j + 1/2) \) for \( l = j \pm 1/2 \) is called the relativistic angular momentum quantum number and carries information about both, the total angular momentum \( j \) as well as the parity \((-1)^l\) of the wave function. Again, (normalizable) physical solutions to the Dirac operator \[10\] can be found for a discrete set of negative energies

\[
E_{\nu \kappa} = \alpha^{-2} \left[ 1 + \left( \frac{\alpha Z}{n - \kappa + \sqrt{\kappa^2 - \alpha^2 Z^2}} \right)^2 \right]^{-\frac{1}{2}} - \alpha^{-2} < 0,
\]

\[
n = 1, 2, \ldots; \, \kappa = -n, \ldots, n-1, \, \kappa \neq 0 \quad (14)
\]

and for all positive energies \( E \geq 0 \) as well as for the (negative) energies \( E \leq -2c^2 \). The two latter —continuous— parts of the spectrum are also called the positive and negative continuum whereby the negative branch, in particular, requires some re–interpretation of the theory (in terms of positron states, for example) and often introduces additional complications in the treatment of many–electron systems. When compared with the nonrelativistic energies \[5\], however, the degeneracy of the (relativistic) energies \[14\] is partially resolved and now depends on both, the principal quantum number \( n \) and the relativistic quantum number \( \kappa \).

Explicit representation of the bound and free–electron solutions of Eqs. \[12\]–\[13\] are known from the literature (cf. \[13\]–\[15\]) but typically result in rather lengthy expressions. For the bound states, for example, the two radial components are given by

\[
P_{\nu \kappa}(r) = C_P(n, \kappa, Z) \ r^s e^{-qr} \left[ (-n + |\kappa|) M(-n + |\kappa| + 1, 2s + 1, 2qr) \right.
\]

\[
- (\kappa - Z q^{-1}) \ M(-n + |\kappa|, 2s + 1, 2qr) \] \quad (15)
\]

\[
Q_{\nu \kappa}(r) = C_Q(n, \kappa, Z) \ r^s e^{-qr} \left[ (-n + |\kappa|) M(-n + |\kappa| + 1, 2s + 1, 2qr) \right.
\]

\[
- (\kappa - Z q^{-1}) \ M(-n + |\kappa|, 2s + 1, 2qr) \] \quad (16)
\]

where \( M(a, b; z) \) is the Kummer function of the first kind, \( s = \sqrt{\kappa^2 - (\alpha Z)^2} \), and \( q = Z [\sqrt{(\alpha Z)^2 + (n - |\kappa| + s^2)^{-1}}] \), while even more elaborate expressions arise for the free–electron states \[15\]. Similiar to \[8\] and \[9\],the bound and free–electron radial wave functions can be normalized also due to

\[
\int_0^\infty \left( P_{\nu \kappa}^2(r) + Q_{\nu \kappa}^2(r) \right) \, dr = 1 \quad (17)
\]

\[
\int_0^\infty \left( P_{E \kappa}(r)P_{E' \kappa}(r) + Q_{E \kappa}(r)Q_{E' \kappa}(r) \right) \, dr = \delta(E - E') \quad (18)
\]

\[2\]In atomic units, the speed of light \( c = 1/\alpha \) is the inverse of the fine–structure constant.
to represent one electron per bound state or per energy unit, respectively.

In the Greens library, the radial functions of the bound and free–electron states can be accessed by means of the two library procedures `greens_radial_orbital()` and `greens_radial_spinor()` in the nonrelativistic and relativistic case, respectively; for further details, see section 3.

### 2.2 Coulomb Green’s functions

Apart from the wave functions, which describe the electron in particular quantum states, one often needs a summation over all (unoccupied) states, especially, if parts of the atomic interaction are treated as a perturbation. A full summation is required in second– and higher–order perturbation theory, for instance, if the behaviour of the atom is studied in a — not too weak — radiation field or in the presence of external electric or magnetic fields. Although, in principle, it appears straightforward to carry out such a summation explicitly, the large number of terms and the need of free–free matrix elements may hamper such an approach. Instead, the use of Green’s functions often provides a much simpler access to the spectrum of the atom and, hence, to a perturbative treatment of atomic processes. In the following, therefore, we first recall a representation of the radial Coulomb Green’s functions as appropriate for numerical computations. The application of these functions in the computation of two–photon ionization cross sections $\sigma_2$ for hydrogen–like is discussed later in subsection 2.3.

#### 2.2.1 Nonrelativistic Green’s function

Analogue to the wave functions, the Coulomb Green’s functions $G_E(r, r')$ are obtained as solutions of a linear equation

$$ (\hat{H}(r) - E) G_E(r, r') = \delta(r - r') $$

with the same Schrödinger operator as in but for an additional $\delta$–like inhomogenity on the right–hand side, which allows for solutions for any arbitrary $E$. For a spherical–symmetric potential, again, this equation can be separated into a radial and angular part by using the ansatz

$$ G_E(r, r') = \sum_{lm} g_{El} \frac{Y_{lm}(\theta, \varphi)}{r_{r'}} Y^*_{lm}(\theta', \varphi') $$

for the Green’s function in spherical coordinates. By substituting ansatz into Eq. 20, one easily shows that the radial Green’s function $g_{El}(r, r')$, which just depends on the energy $E$ and the orbital angular momentum $l$, must satisfy the equation

$$ \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + 2E \right] g_{El}(r, r') = -2 \frac{\delta(r - r')}{r_{r'}}. $$

Solutions to this single equation can be determined by taking a proper superposition of the regular and irregular solutions (near the origin) of Schrödinger’s equation. An explicit representation for the radial Green’s function reads as

$$ g_{El}(r, r') = \frac{\Gamma(l + \frac{1}{2})}{\pi \Gamma(2l + 2)} M_{\tau, l+\frac{1}{2}}(2x r_<) W_{\tau, l+\frac{1}{2}}(2x r_>), $$
where \( x = (-2E)^{1/2} \), \( \tau = \frac{Z}{r} \), and where \( r_\geq = \max(r, r') \) and \( r_\leq = \min(r, r') \) refer to the larger and smaller value of the two radial coordinates, respectively. In this representation, moreover, \( M_{a,b}(z) \) and \( W_{a,b}(z) \) denote the two Whittaker functions of the first and second kind which can be expressed also in terms of the Kummer functions \( M(a, b; z) \) and \( U(a, b; z) \) of the corresponding kinds [17]

\[
M_{a,b}(z) = z^{b+\frac{1}{2}} e^{-z/2} M(b-a+1/2, 2b+1; z), \quad (23)
\]

\[
W_{a,b}(z) = z^{b+\frac{1}{2}} e^{-z/2} U(b-a+1/2, 2b+1; z). \quad (24)
\]

In practise, the two Kummer functions are used more frequently (than the Whittaker functions) in the mathematical literature and in various program libraries since \( M(a, b; z) \) is closely related to the hypergeometric series and since the Kummer function \( U(a, b; z) \) of the second kind can be expressed in terms of \( M(a, b; z) \). In addition, several improved algorithms have been worked out recently in order to calculate the regular Kummer function \( M(a, b; z) \) more efficiently, see section 2.4 for further details.

2.2.2 Relativistic Green’s function

Of course, the relativistic Coulomb Green’s function must refer to the Dirac Hamiltonian [10] and, hence, is given by a \( 4 \times 4 \)–matrix which satisfies the equation

\[
\left( \hat{H}_D(r) - E - c^2 \right) G_E(r, r') = \delta(r - r') I_4,
\]

where \( I_4 \) denotes the \( 4 \times 4 \) unit–matrix and where, as for the wave functions from Eqs. [12, 13], the rest energy \( c^2 \) has not been incorporated into the (total) energy \( E \). Solutions to this equation are known again from the literature for a radial–angular representation of the Coulomb Green’s function [9]

\[
G_E(r, r') = \sum_{\kappa m} \frac{1}{rt} \begin{pmatrix}
  g_{LL}^{\kappa m}(r, r') \Omega_{\kappa m}(r) \Omega_{\kappa m}^\dagger(r') & -i g_{LS}^{\kappa m}(r, r') \Omega_{\kappa m}(r) \Omega_{\kappa m}^\dagger(r') \\
  i g_{SL}^{\kappa m}(r, r') \Omega_{\kappa m}(r) \Omega_{\kappa m}^\dagger(r') & g_{SS}^{\kappa m}(r, r') \Omega_{\kappa m}(r) \Omega_{\kappa m}^\dagger(r')
\end{pmatrix},
\]

where the radial part

\[
\begin{pmatrix}
g_{LL}^{\kappa m}(r, r') & g_{LS}^{\kappa m}(r, r') \\
g_{SL}^{\kappa m}(r, r') & g_{SS}^{\kappa m}(r, r')
\end{pmatrix}/rr' \text{ of this function is now a } 2 \times 2 \text{ matrix which must satisfy the matrix equation}
\]

\[
\begin{pmatrix}
  \left[ \frac{1}{rt} - \frac{Z}{r} - E \right] & \left[ \frac{\kappa}{ar} - \frac{1}{ar} \frac{\partial}{\partial r} \right] \\
  \left[ \frac{1}{ar} \frac{\partial}{\partial r} + \frac{\kappa}{ar} \right] & \left[ -2 + \frac{Z}{a^2} - \frac{Z}{r} - E \right]
\end{pmatrix} \frac{1}{rr'} \begin{pmatrix}
g_{LL}^{\kappa m}(r, r') & g_{LS}^{\kappa m}(r, r') \\
g_{SL}^{\kappa m}(r, r') & g_{SS}^{\kappa m}(r, r')
\end{pmatrix} = \frac{\delta(r - r')}{rr'} I_2.
\]

In this representation of the Green’s function, we make use of the two superscripts \( T \) and \( T' \) to denote the individual components in the \( 2 \times 2 \) radial Green’s matrix. They may take both the values \( T = [L, S] \) to refer to either the large or small components, when multiplied with a wave function spinor [11]. An explicit representation of the (four) components \( g_{E\kappa}^{TT'}(r, r') \) of the radial Green’s function is found by Swainson and Drake [9]

\[
\begin{pmatrix}
g_{LL}^{E\kappa} & g_{LS}^{E\kappa} \\
g_{SL}^{E\kappa} & g_{SS}^{E\kappa}
\end{pmatrix} = \frac{1}{(1 - X)^2} \begin{pmatrix}
h_{11} - X(h_{12} + h_{22}) + X^2 h_{22} - X(h_{11} + h_{22}) + h_{12} + X^2 h_{21} \\
-X(h_{11} + h_{22}) + X^2 h_{12} + h_{21} X^2 h_{11} - X(h_{12} + h_{21}) + h_{22}
\end{pmatrix}, \quad (26)
\]
with

\[ h^{11}(r', r) = \frac{(1 - X^2)((E\alpha^2 + 1)\kappa\gamma^{-1} + 1)}{2\omega} \frac{\Gamma(\gamma + 1 - \nu)}{\Gamma(2\gamma + 2)} M_{\nu, \gamma+\frac{1}{2}}(2\omega r) W_{\nu, \gamma+\frac{1}{2}}(2\omega r) \]  

(27)

\[ h^{22}(r', r) = \frac{(1 - X^2)((E\alpha^2 + 1)\kappa\gamma^{-1} - 1)}{2\omega} \frac{\Gamma(\gamma - \nu)}{\Gamma(2\gamma)} M_{\nu, \gamma-\frac{1}{2}}(2\omega r) W_{\nu, \gamma-\frac{1}{2}}(2\omega r) \]  

(28)

\[ h^{21}(r', r) = h^{12}(r', r) \]  

= \frac{(1 - X^2)\Gamma(\gamma + 1 - \nu)\alpha\gamma^{-1}}{2\Gamma(2\gamma + 2)} \left[ 2\gamma(2\gamma + 1)\theta(r' - r) M_{\nu, \gamma-\frac{1}{2}}(2\omega r) W_{\nu, \gamma+\frac{1}{2}}(2\omega r') 
- (\nu + \gamma)\theta(r - r') W_{\nu, \gamma-\frac{1}{2}}(2\omega r) M_{\nu, \gamma+\frac{1}{2}}(2\omega r') \right] \]  

(29)

and

\[ X = (-\kappa + \gamma)(\alpha Z)^{-1}, \quad \gamma = (\kappa^2 - \alpha^2 Z^2)^{1/2}, \quad \omega = \alpha^{-1}(1 - (E\alpha^2 + 1)^2)^{1/2}, \quad \nu = Z(E\alpha^2 + 1)\omega^{-1}, \]  

and where \( \theta(x) \) denotes the Heaviside function.

In the GREENS library, we provide the two procedures \texttt{greens_radial_function()} and \texttt{greens_radial_matrix()} which support the computation of the radial functions (27) and (28) for any proper set of parameters.

### 2.3 Two–photon transition amplitudes and ionization cross sections

The Green’s function (21) and (25) can be utilized directly to evaluate, for instance, the two–photon cross sections \( \sigma_2 \) for a non–resonant excitation, ionization, or decay process. They also occur rather naturally in the theory of the photon scattering on hydrogen–like ions. In the following, we briefly outline the perturbative calculation of the two–photon ionization cross section for hydrogen–like ions which, for an unpolarized target and in atomic units, is given by

\[ \sigma_2 = \frac{8\pi^3\alpha^2}{E_\gamma^2} \sum_{\nu} \frac{1}{2j_i + 1} \sum_{m_i} |M_{fi}|^2, \]  

(30)

where \( E_\gamma \) is the photon energy and \( M_{fi} \) the two–photon transition amplitude

\[ M_{fi} = \sum_{\nu} \frac{\langle \psi_f | \mathbf{u}_{\lambda 2} e^{ik_2 r} \cdot \mathbf{p} | \psi_i \rangle \langle \psi_{\nu} | \mathbf{u}_{\lambda 1} e^{ik_1 r} \cdot \mathbf{p} | \psi_i \rangle}{E_{\nu} - E_\gamma - E_i}. \]  

(31)

In this amplitude, moreover, \( (\psi_i, E_i), (\psi_\nu, E_\nu), \) and \( (\psi_f, E_f) \) denote the wave functions and energies of the initial, intermediate and final atomic states, respectively. Here, the energy of the final state, \( E_f \), does not appear explicitly in (31) but follows from

\[ E_f = E_i + 2E_\gamma \]

due to the conservation of energy. Furthermore, the two vector quantities \( \mathbf{u}_\lambda \) and \( \mathbf{p} \) in the transition amplitude (31) refer to the polarization of the two photons as well as to the electron momentum operator.

\(^3\)The cross section \( \sigma_2 \) has the dimension length\(^4 \times \) time and, thus, can be converted into cgs–units \( \text{cm}^4 \cdot \text{s} \) by using the multiplication factor \( 1.896792 \cdot 10^{-50} \).
As mentioned before, the summation over $\nu$ in (31) runs over the complete spectrum of the atom including the continuum. This summation can be replaced, therefore, by a single Green’s function (19), so that the transition amplitude (31) finally takes the form

$$M_{fi} = \int \psi^+_f(r) \ u_{\lambda_2} \ e^{ik_2 \cdot r} \cdot p \ G_{E_i+E_\gamma} (r,r') \ u_{\lambda_1} \ e^{i k_1 \cdot r'} \cdot p' \ \psi_i (r') \ dr \ dr'.$$

(32)

It is this form of the transition amplitude which has often been used in the literature to study non–resonant, two–photon processes [10, 18].

2.3.1 Nonrelativistic ionization cross sections

For the sake of brevity, let us restrict ourselves to the two–photon ionization cross sections within the long–wavelength approximation, i.e. we assume $e^{ikr} \equiv 1$ for the coupling of the radiation field in (32). Apart from the electric–dipole field, of course, this approximation neglects the contribution from all higher multipoles, but is known to describe well the ionization of light atoms with a nuclear charge of, say, $Z \lesssim 30$ and for photon energies below the ionization threshold $E_\gamma < E_T$. By substituting $p \rightarrow r$ and $E_\gamma \rightarrow 1/E_\gamma$ into Eqs. (30) and (31), moreover, we may obtain the ionization cross section in length gauge

$$\sigma_{2}^{\text{length}} = 8 \pi^3 \alpha^2 E_\gamma^2 \sum_{l,m_f} \frac{1}{2l_i + 1} \sum_{m_i} |M_{fi}^{\text{length}}|^2,$$

(33)

with

$$M_{fi}^{\text{length}} = \int \psi^+_f (r) \ u_{\lambda_2} \cdot r \ G_{E_i+E_\gamma} (r,r') \ u_{\lambda_1} \cdot r' \ \psi_i (r') \ dr \ dr'.$$

(34)

Using the radial–angular representations (3) and (21) of the wave and Green’s functions, respectively, and by making use of some angular momentum algebra, the 6–dimensional integral in the transition amplitude (34) can be reduced further to just a two–dimensional integration over the radial coordinates $r$ and $r'$. In addition, if we assume the ion initially in its 1s ground–state and circular polarized light, i.e. two photons with the same helicity $\lambda_1 = \lambda_2 = \pm 1$, the two–photon ionization cross section (in length gauge) simply takes the form

$$\sigma_{2}^{\text{length, circular}} = 8\pi^3 \alpha^2 E_\gamma^2 \left| \int P_{E_f 2} (r) \ g_{E_i+E_\gamma,1} (r,r') \ P_{10} (r') \ dr \ dr' \right|^2.$$  

(35)

2.3.2 Relativistic two–photon ionization cross sections

The long–wavelength approximation for the coupling of the radiation field can be considered also within the framework of the relativistic theory. In this framework, however, an useful estimate of the total cross section $\sigma_2$ are obtained only if the photon energy is well below the threshold energy $E_\gamma < E_T$ of the two–photon ionization. In the relativistic theory, the (long–wavelength) transition amplitude (32) takes the form

$$M_{fi} = c^2 \int \psi^+_f (r) \ u_{\lambda_2} \cdot \alpha \ G_{E_i+E_\gamma} (r,r') \ u_{\lambda_1} \cdot \alpha' \ \psi_i (r') \ dr \ dr',$$

(36)

where $\alpha$ denotes Dirac’s velocity operator. Using the radial–angular representation (25) of the Green’s functions, then the total two–photon ionization cross section $\sigma_2$ for circular–polarized
light can be written as
\[
\sigma_2^{(\text{velocity, circular})} = \frac{8\pi^3}{\alpha^2 E^2} \left\{ \frac{32}{25} U^{SL} \left( d_{\frac{1}{2}}, p_{\frac{1}{2}}, s_{\frac{1}{2}} \right)^2 + \frac{12}{2025} \left[ 5 U^{LL} \left( d_{\frac{1}{2}}, p_{\frac{1}{2}}, s_{\frac{1}{2}} \right) + 
\right. \right.
\]
\[
+ 3 U^{SL} \left( d_{\frac{1}{2}}, p_{\frac{1}{2}}, s_{\frac{1}{2}} \right) - 5 U^{LL} \left( d_{\frac{1}{2}}, p_{\frac{1}{2}}, s_{\frac{1}{2}} \right) - 15 U^{LS} \left( d_{\frac{1}{2}}, p_{\frac{1}{2}}, s_{\frac{1}{2}} \right) \right\}^2, \tag{37}
\]
where we introduced the radial integral
\[
U^{TT'}(\kappa_f, \kappa_{\nu}, \kappa_i) = \int g^{T}_{E_f, \kappa_f}(r) g^{TT'}_{E_i+E_{\nu}, \kappa_{\nu}}(r, r') g^{T'}_{n_i, \kappa_i}(r') dr dr'. \tag{38}
\]
In this integral, a superscript $\overline{T}$ refers to the conjugate of $T$, i.e. $\overline{T} = S$ for $T = L$ and vice versa, and $g^{T}_{E, \kappa}(r)$ and $g^{T}_{n, \kappa}(r)$ are used to denote the large and small components of the radial spinor $\langle 11 \rangle$. This notation allows for a very compact representation of the multiphoton transition amplitudes which can be applied also well beyond the long-wavelength approximation.

In the GREENS library, the procedure `greens_two_photon_cs()` is presented to compute two-photon ionization cross sections in various approximations.

### 2.4 Special functions

Of course, the main emphasize in developing the GREENS library has been paid to the computation of the Coulomb wave and Green’s functions as appropriate for a theoretical description of hydrogen-like ions. As seen from sections 2.1 and 2.2, however, for an explicit representation of these functions we usually need to refer to a few special functions such as the $\Gamma(z)$ and $\Psi(z)$ functions, or the Kummer and Whittaker functions of the first and second kind which are known from the mathematical literature [17]. Therefore, in order to facilitate the implementation of the Coulomb functions, we have to provide also a simple interface to these special functions; in the following, we briefly summarize the definition of these functions and for which type of arguments they are needed for the GREENS library.

Euler’s Gamma function $\Gamma(z)$ and the Psi–function $\Psi(z)$ occur very frequently and in quite different fields of physics. While the $\Gamma$–function is defined by the integral
\[
\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt
\]
the $\Psi$–function refers to the derivative
\[
\Psi(z) = \frac{d \ln \Gamma(z)}{dz}. \tag{40}
\]
These functions are defined for all complex arguments $z$ except of the real negative integers $z \neq -1, -2, ...$ where they have their poles. In GREENS, the $\Gamma(z)$ function with real arguments $z$ is needed for the computation of the bound–state wave and Green’s functions, respectively, while complex arguments arise in the representation of the free–electron waves [17]. The $\Psi$–function, in addition, arises in the calculation of the Kummer function $U(a, b; z)$ of the second type if the argument $b$ refers to an integer in the computation of nonrelativistic Green’s functions.
Although the Coulomb wave and Green’s functions are often expressed in terms of the Whittaker functions $M_{a,b}(z)$ and $W_{a,b}(z)$ of the first and second kind, in practical computations one makes better use of the Kummer functions of the corresponding kind, as discussed in subsection 2.2.1 above. The Kummer functions $M(a,b;z)$ and $U(a,b;z)$ of the first and second kind refer to the regular and irregular solutions of Kummer’s equation

$$z \frac{d^2 M}{dz^2} + (b - z) \frac{dM}{dz} - a M = 0; \quad (41)$$

in the literature, however, also several other notations are used for these functions such as $M(a,b;z) = {}_1F_1(a;b;z)$ or $U(a,b;z) = \Psi(a,b,z)$, respectively. Usually, the function $M(a,b;z)$ of the first kind is solved for the initial value $M(a,b;0) = 1$ and, hence, is given by the confluent hypergeometric series

$$M(a,b;z) = 1 + \frac{a}{b} z + \frac{1}{2} \frac{a(a+1)}{b(b+1)} z^2 + \cdots. \quad (42)$$

The Kummer function of the first kind $M(a,b;z)$ is needed for both, real $a, b, z$ and complex arguments $a, z$ to represent the radial wave and Green’s function components. In contrast, the Kummer function $U(a,b;z)$ of the second kind is required only for real argument $b$, for which it can be expressed as a linear combination

$$U(a,b;z) = \frac{\pi}{\sin \pi b} \left[ \frac{M(a,b;z)}{\Gamma(1 + a - b) \Gamma(b)} - z^{1-b} \frac{M(a+1-b,2-b;z)}{\Gamma(a) \Gamma(2-b)} \right] \quad (43)$$

of two Kummer functions of the first kind; the function $U(a,b;z)$ arises in the computation of the radial Green’s function.

The following section explains how these special functions from the Greens library can be used also in applications other than the computation of Coulomb wave and Green’s functions.

3 Program organisation

3.1 Overview about the Greens library

The Greens library has been designed mainly in order to facilitate numerical applications of the Coulomb wave and Green’s functions from section 2. It provides the user with a set of C++ procedures to compute the radial components of these functions within both, a nonrelativistic as well as relativistic framework. Apart from the radial components, however, we also support the numerical integration of the Coulomb functions as well as the computation of a few selected matrix elements which, below, will help us demonstrate the application of the Greens library. To provide the user with a simple access to the various functions, the concepts of object–oriented programming such as structures, classes and members as well as the overloading of procedures and operators have been utilized carefully.

Table 1 lists the main procedures of the Greens library for calculating the energies and radial components of the Coulomb functions. To simplify the use of the library, the classes `spinor2.col`, `spinor2.raw`, and `matrix2x2` have been implemented to describe the radial spinor (11), its adjunct raw spinor, and the radial Green’s matrix (26), respectively. The classes `spinor2.col` and `spinor2.raw`, for instance, contain each the two members .L and
.S to represent the large and small components of a relativistic wave function, while the class \texttt{matrix}\_2\_x\_2\_x\_2\_x\_2\_x\_2 has the four members \texttt{.LL}, \texttt{.LS}, \texttt{.SL}, and \texttt{.SS} with an obvious meaning. The class \texttt{matrix}\_2\_x\_2\_x\_2\_x\_2\_x\_2, moreover, also contains the member \texttt{.e} which just returns all the four matrix elements together within a $2 \times 2$ array.

In order to treat the bound– and free–electron states in a similar way, the two wave function procedures \texttt{green}\_\_radial\_\_orbital()} and \texttt{green}\_\_radial\_\_spinor() have been overloaded. For these two procedures, a first \emph{integer} argument $n \geq 1$ is used to represent the principal quantum number and to return the corresponding bound–state solution, while a (first) argument $E > 0$ of type \texttt{double} refers to the kinetic energy of a free–electron state (in Hartree units). As mentioned above, however, this energy $E$ does not include the electron rest energy, neither in the nonrelativistic nor relativistic framework. The two additional procedures \texttt{greens}\_\_set\_\_nuclear\_\_charge()} and \texttt{greens}\_\_get\_\_nuclear\_\_charge()} from table 1 can be called to re–define or to return the current value of the nuclear charge which is utilized for the computation of all radial functions. The default value of the nuclear charge is $Z = 1$.

In most applications, the (radial) Coulomb wave and Green’s function components usually occur as part of some matrix element and, hence, first require an additional integration (over $r$ and/or $r’$) before any \textit{observable} quantity is obtained. Therefore, to facilitate such applications, we also provide the utility procedure \texttt{greens}\_\_integral\_\_GL()} which evaluates a 1– or 2–dimensional integral over a finite or infinite area with a \textit{user–defined} accuracy, see table 2. In this procedure, a Gauss–Legendre quadrature [17] of appropriate order is applied, independently for each dimension of the integrand. Moreover, to ensure a result which is accurate up to a given number of $d$ valid digits, the domain of integration is divided by steps into subdomains until the required accuracy is obtained. A \textbf{Warning} arises during the execution, if the requested precision cannot be guaranteed by the procedure. As seen from table 2, the procedure name \texttt{greens}\_\_integral\_\_GL()} is \textit{overloaded} and, thus, can be invoked with rather different lists of parameters, from which the dimension of the integral, the integration domain as well as the type of the function is deduced. Apart from a real–valued integrand $f(x)$ or $f(x,y)$, respectively, \texttt{greens}\_\_integral\_\_GL()} also supports a \texttt{matrix}\_\_2\_\_x\_\_2\_x\_2–valued integrand as appropriate for the computation of matrix elements such as (38) from the relativistic theory. In the latter case, for instance, all the four integrals $U_{LL}$, $U_{LS}$, $U_{SL}$ and $U_{SS}$ in (37) could be treated simultaneously.

A second utility procedure \texttt{greens}\_\_two\_\_photon\_\_cs()} from table 2 enables the user to calculate two–photon ionization cross sections in various approximations. Obviously, this procedure makes use of \texttt{greens}\_\_integral\_\_GL()} and is mainly provided for test purposes below. It helps compute the total two–photon ionization cross sections $\sigma_2$ for linear or circular polarized light and within either the nonrelativistic or relativistic framework, respectively. In all of these cases, however, the computation of the cross sections is restricted to the long–wavelength approximation $e^{ikr} = 1$ for the coupling of the radiation field and to the ionization of an electron from the unpolarized $1s$ ground state. In addition, the photon energy $E_{\gamma}$, i.e. the third argument of the procedure \texttt{greens}\_\_two\_\_photon\_\_cs()} must be in the range $-E_{1s}/2 < E_{\gamma} < -E_{1s}$ where $E_{1s}$ is the (negative) $1s$–binding energy from Eqs. (5) or (14). Again, the last argument $d$ refers to the requested accuracy of the cross section of (at least) $d$ valid digits and is transfered directly to the underlying integration procedure \texttt{greens}\_\_integral\_\_GL()}. Of course, the wave and Green’s functions from section 2 can hardly be implemented without
Table 1  Main procedures of the GREENS library to calculate the energies and radial wave and Green’s functions for hydrogen–like ions. The (expected) type of parameters is shown by using the syntax of C++; all quantities below must be given in atomic units.

| Procedure                      | Arguments                  | Description and comments                                                                 |
|--------------------------------|----------------------------|------------------------------------------------------------------------------------------|
| double greens_energy          | (int n)                    | Returns the nonrelativistic energy $E_n$ (in a. u.) of a bound–state solution with principal quantum number $n$; see Eq. (5). |
|                               | (int n, int kappa)         | Returns the relativistic energy $E_{n\kappa}$ (in a. u.) of a bound–state solution quantum numbers $n$ and $\kappa$; see Eq. (14). |
| double greens_radial_orbital  | (int n, int l, double r)   | Computes the value of the radial function $P_{nl}(r)$ at $r$ of a bound state with principal quantum number $n$ and orbital angular momentum $l$. |
|                               | (double E, int l, double r)| Computes the value of the radial function $P_{El}(r)$ at $r$ of a free–electron state with energy $E > 0$ and orbital angular momentum $l$. |
| spinor2_col                   | (int n, int kappa, double r) | Computes the value of the radial spinor function $\begin{pmatrix} P_{n\kappa}(r) \\ Q_{n\kappa}(r) \end{pmatrix}$ at $r$ of a bound state with principal quantum number $n$ and relativistic angular momentum quantum number $\kappa$. |
| greens_radial_spinor          | (double E, int kappa, double r) | Computes the value of the radial spinor function $\begin{pmatrix} P_{E\kappa}(r) \\ Q_{E\kappa}(r) \end{pmatrix}$ at $r$ of a free–electron state with energy $E$ and relativistic angular momentum quantum number $\kappa$. |
| double greens_radial_function | (double E, int l, double r, double r') | Computes the radial Coulomb Green’s function $g_{El}(r, r')$ at $r$ and $r'$ for the energy $E < 0$ and orbital angular momentum $l$. |
| matrix_2x2                    | (double E, int kappa, double r, double r') | Computes the radial Coulomb Green’s matrix $\begin{pmatrix} g_{L}^{LL} & g_{L}^{LS} \\ g_{L}^{LS} & g_{L}^{SS} \end{pmatrix}$ from $g_{EL}$ at $r$ and $r'$ for the energy $E < 0$ and the relativistic angular momentum quantum number $\kappa$. |
Table 2  Utility procedures of the GREENS library for the numerical integration of 1– and 2–dimensional functions and the computation of two–photon ionization cross sections $\sigma_2$ in various approximations. The same notation as in table 1 is used.

| Procedure                 | Arguments                                      | Description and comments                                                                 |
|----------------------------|-----------------------------------------------|------------------------------------------------------------------------------------------|
| double                    | (double(*funct)(double x), double a, double b, int d) | Calculates the definite (1–dimensional) integral $\int_a^b f(x)\,dx$ with an accuracy of (at least) d valid digits. This procedure applies an adaptive Gauss–Legendre integration formula, independently in each dimension. |
| double                    | (double(*funct)(double x), int d)             | Calculates the definite (1–dimensional) integral $\int_0^\infty f(x)\,dx$ with an accuracy of (at least) d valid digits if $f(x)$ does not oscillate rapidly and vanishes sufficiently fast for large values of x. |
| double                    | (double(*funct)(double x, double y), double ax, double bx, double ay, double by, int d) | Calculates the definite (2–dimensional) integral $\int_{a_x}^{b_x} \int_{a_y}^{b_y} f(x,y)\,dxdy$ with an accuracy of (at least) d valid digits. |
| double                    | (double(*funct)(double x, double y), int d)   | Calculates the definite (2–dimensional) integral $\int_0^\infty \int_0^\infty f(x,y)\,dxdy$ with an accuracy of (at least) d valid digits if $f(x,y)$ does not oscillate rapidly and vanishes sufficiently fast for large values of x and y. |
| double                    | ("nonrelativistic", "circular", double E_ph, int d) | Computes the nonrelativistic two–photon ionization cross section $\sigma_2$ for circular polarized light, in long–wavelength approximation, and for a photon energy $E_{ph} > E_{1s}/2$. A cross section value in atomic units and with an accuracy of (at least) d valid digits is returned. |
| double                    | ("nonrelativistic", "linear", double E_ph, int d) | Computes the nonrelativistic two–photon ionization cross section for linear polarized light and in long–wavelength approximation. |
| double                    | ("relativistic", "circular", double E_ph, int d) | Computes the relativistic two–photon ionization cross section for circular polarized light, in long–wavelength approximation, and for a photon energy $E_{ph} > E_{1s}/2$. |
| double                    | ("relativistic", "linear", double E_ph, int d) | Computes the relativistic two–photon ionization cross section for linear polarized light and in long–wavelength approximation. |
Table 3  Special function procedures of the GREENS library. The same notation as in table 1 is used. The type of all procedures is double if all arguments are double, and is of type complex otherwise.

| Procedure   | Arguments                                                                 | Description and comments                                                                 |
|-------------|---------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| GAMMA       | (double z) or (complex z)                                                 | Returns the Γ(z) function $^{39}$ for either a real or complex argument z.                |
| Psi         | (double z) or (complex z)                                                 | Returns the Ψ(z) function $^{40}$ for either a real or complex argument z.                |
| KummerM     | (double a, double b, double z) or (complex a, double b, complex z)        | Calculates the Kummer function $M(a,b;z)$ of the first kind $^{12}$ for real and/or complex arguments a, b, and z. |
| KummerU     | (double a, double b, double z)                                            | Calculates the Kummer function $U(a,b;z)$ of the second kind $^{43}$ for real arguments a, b, and z. |
| WhittakerM  | (double a, double b, double z) or (complex a, double b, complex z)        | Calculates the Whittaker function $M_{a,b}(z)$ of the first kind $^{23}$ for either real or complex arguments a, b, and z; b must be real. |
| WhittakerW  | (double a, double b, double z)                                            | Calculates the Whittaker function $W_{a,b}(z)$ of the second kind $^{24}$ for real arguments a, b, and z. |

a proper set of special function procedures. Therefore, table 3 displays those procedures which are provided by the GREENS library and which we briefly discussed in section 2.4. The allowed types of the parameters are also displayed in this table.

3.2 Distribution and compilation of the GREENS library

The GREENS library will be distributed as the gzipped tar–file greens.tar.gz from which the greens root directory is obtained by gunzip greens.tar.gz and tar -xvf greens.tar. This root contains a Read.me file, the src subdirectory for the source code as well as six subdirectories for various examples. In src, we provide the header file greens.h and a makefile to facilitate the compilation of the (static) library libgreens.a in the greens root directory. It also incorporates about 50 source files for all of the individual procedures.

In the following section, two examples from the subdirectories example-coulomb-funct and example-twophoton-cs are discussed in more detail and are taken as the test for the installation of the library. Each of these example subdirectories, again, contain a makefile from which an executable (a.out) is generated simply by typing make within the corresponding subdirectory. Since these makefiles also compile and link the library libgreens.a, the user may start directly from a copy of one of these subdirectories for his own application of the GREENS library.

4 Examples

To illustrate the use of the GREENS library, we first show how the (radial) Coulomb wave and Green’s functions can be calculated for any point $r$ or $(r,r')$, respectively. Hereby,
```c
#include "greens.h"

int main(void) {
    int n, l, kappa; // quantum numbers
    double r, rp, E, wf_nr, gf_nr; // coordinates, energies, etc.
    spinor2_col wf_r; // relativistic spinor
    matrix_2x2 gf_r; // relativistic Green's matrix

    print("#Test of the Coulomb radial functions");

    for(double Z=1.0; Z<93.0; Z=Z+91.0) {
        print();
        greens_set_nuclear_charge(Z); // set nuclear charge
        E = -greens_energy(1) * 0.8;

        rp = 2.5/Z; n = 4; l = 2; kappa = -3;
        write("# coord wf_nr wf_r.L ");
        print("gf_nr gf_r.e[0][0] gf_r.LL");
        for (r=0.0; r<25.0/Z; r=r+0.1/Z){
            wf_nr = greens_radial_orbital(n, l, r);
            wf_r = greens_radial_spinor (n, l, r);
            gf_nr = greens_radial_function(-E, l, r, rp);
            gf_r = greens_radial_matrix (-E, l, r, rp);

            printf("%E %E %E %E %E %E\n", r, wf_nr, wf_r.L, 
                    gf_nr, gf_r.e[0][0], gf_r.LL); }}

    return 0;}
```

Figure 1: Calculation of the Coulomb wave and Green's functions for nuclear charge $Z = 1$ and $Z = 92$. The printout of this procedure is shown in the Test Run Output and in the file printout.txt in the subdirectory example-coulomb-funct.

A simple comparison between the nonrelativistic and relativistic theory — in the limits of a low and high nuclear charge $Z$ — is achieved by setting $Z = 1$ (hydrogen) and $Z = 92$ (hydrogen–like uranium), respectively. Figure 1 displays the source code which evaluates the two radial functions $P_{4d}(r)$ and $P_{4d/2}(r)$, respectively, for $r$–values in the range $r = 0., . . . . , 25./Z$ with a stepsize of $\Delta r = 0.1/Z$. Beside of these wave function components, this code also calculates the Coulomb Green's functions at the same values of $r$ and for a fixed $r' = 2.5/Z$. For a call of this procedure, the printout is (partially) shown in the Test Run Output below. The source of this example and the complete printout can be found in the subdirectory example-coulomb-funct. In order to obtain the —full— radial part of the Coulomb wave and Green's functions, of course, the results of `greens_radial_orbital()` and `greens_radial_spinor()` must be multiplied with $1/r$, while the values from `greens_radial_function()` and `greens_radial_matrix()` have to be multiplied with $1/rr'$, respectively.

A second example concerns the computation of the two–photon ionization cross sections for the two ions from above. For these ions, the $1s$ binding energies are $-1/2$ and $-4232$ Hartrees within the nonrelativistic theory. In the Test Run Output below, the two–photon ionization cross sections for circular and linear polarized light and within both, the nonrelativistic and relativistic approximation. For each of these ions, the cross sections are calculated with an accuracy of about six digits for the ten energies $E_0, E_o + 0.01 * Z^2, . . . . , E_o + 0.09 * Z^2$ where $E_o = 0.3 * Z^2$ corresponds to 60 % of the nonrelativistic $1s$ binding energy. Again, the full source of this example is provided with the Greens library in the subdirectory example-coulomb-funct.
example-twophoton-cs and, thus, can easily be modified for any other photon energy.

5 Summary and outlook

To facilitate applications of the 'hydrogen ion model' in quite different fields of physics, the GREENS library is presented and provides a set of C++ procedures for the computation of the Coulomb wave and Green's functions within both, a nonrelativistic as well as relativistic framework. Since C++ is today freely available for most architectures, an object-oriented approach to the Coulomb problem could be realized without the need for special compilers or other mathematical libraries. Apart from the radial Coulomb functions, however, GREENS also provides a set of special functions as well as a few utility procedures to evaluate, for instance, the two-photon ionization cross sections in long-wavelength approximation.

In the future, various extensions of the GREENS library might be of great interest for the physics community. Owing to the current design of several free-electron laser (FEL) facilities worldwide, for example, systematic investigations on multiphoton processes become more and more likely also in the EUV and x-ray region, where the inner-shell electron get involved. For such investigations, which will consider also many-electron atoms and ions, the generation of effective one-particle Green's functions are certainly desirable. First steps into this direction, including the combination with the well-known RATIP package [19], are currently under work in our group.

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A. Computation of the radial Coulomb wave and Green’s functions

#Test of the Coulomb radial functions

#Nuclear charge is changed to 1.000000
#coord  wf_nr  wf_r.L  gf_nr  gf_r.e[0][0]  gf_r.LL
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
1.000000E-01 6.758392E-06 6.761076E-06 9.861696E-05 9.861644E-05
2.000000E-01 5.228909E-05 5.230066E-05 7.642130E-04 7.643481E-04
...
2.480000E+01 -2.307241E-01 -2.307229E-01 8.979656E-09 8.980284E-09
2.490000E+01 -2.295400E-01 -2.295388E-01 8.243999E-09 8.244579E-09

#Nuclear charge is changed to 92.000000
#coord  wf_nr  wf_r.L  gf_nr  gf_r.e[0][0]  gf_r.LL
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
1.086957E-03 6.482422E-05 4.346958E-04 1.071923E-06 5.170738E-06
2.173913E-03 5.015393E-04 1.952599E-03 8.306663E-06 2.311893E-05
...
2.706522E-01 -2.01670E+00 -2.088423E+00 8.960868E-11 1.641947E-10
2.717391E-01 -2.190133E+00 -2.074839E+00 8.226371E-11 1.512671E-10

B. Computation of two-photon ionization cross sections

#Test of the two-photon ionisation cross sections
#Digits is changed to 6

#Nuclear charge is changed to 1.000000
#E  cs_nr_c  cs_r_c  cs_nr_l  cs_r_l
3.000000E-01 8.728681E-01 8.727765E-01 5.849625E-01 5.849002E-01
3.100000E-01 8.819793E-01 8.818399E-01 5.889291E-01 5.888364E-01
3.200000E-01 9.143732E-01 9.143980E-01 6.095973E-01 6.096138E-01
...
3.800000E-01 5.778480E+00 5.794808E+00 4.829547E+00 4.843563E+00
3.900000E-01 1.792990E+01 1.796899E+01 2.330477E+01 2.333333E+01

#Nuclear charge is changed to 92.000000
#E  cs_nr_c  cs_r_c  cs_nr_l  cs_r_l
2.539200E+03 1.439533E-12 6.927729E+13 9.647196E-13 4.629667E-13
2.623840E+03 1.454559E-12 6.763950E+13 9.712612E-13 4.510878E-13
2.708480E+03 1.507983E-12 6.588038E+13 1.005347E-12 4.392479E-13
...
3.216320E+03 9.529863E-12 6.744809E-13 7.968848E-12 4.646710E-13
3.309600E+03 2.956996E-13 7.498654E-13 3.843421E-13 5.232579E-13