



Algebraic tools for dealing with the atomic shell model. I. Wavefunctions and integrals for hydrogen-like ions [☆]

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Abstract

Today, the ‘hydrogen atom model’ is known to play its role not only in teaching the basic elements of quantum mechanics but also for building up effective theories in atomic and molecular physics, quantum optics, plasma physics, or even in the design of semiconductor devices. Therefore, the analytical as well as numerical solutions of the hydrogen-like ions are frequently required both, for analyzing experimental data and for carrying out quite advanced theoretical studies. In order to support a fast and *consistent* access to these (Coulomb-field) solutions, here we present the DIRAC program which has been developed originally for studying the properties and dynamical behavior of the (hydrogen-like) ions. In the present version, a set of MAPLE procedures is provided for the Coulomb wave and Green’s functions by applying the (wave) equations from both, the nonrelativistic and relativistic theory. Apart from the interactive access to these functions, moreover, a number of radial integrals are also implemented in the DIRAC program which may help the user to construct transition amplitudes and cross sections as they occur frequently in the theory of ion–atom and ion–photon collisions.

Program summary

Title of program: DIRAC

Catalogue number: ADUQ

Program summary URL: <http://cpc.cs.qub.ac.uk/summaries/ADUQ>

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

Licensing provisions: None

Computer for which the program is designed and has been tested: All computers with a license of the computer algebra package MAPLE [1]

Program language used: Maple 8 and 9

No. of lines in distributed program, including test data, etc.: 2186

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

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No. of bytes in distributed program, including test data, etc.: 162 591

Distribution format: tar gzip file

CPC Program Library subprograms required: None

Nature of the physical problem: Analytical solutions of the hydrogen atom are widely used in very different fields of physics [2,3]. Despite of the rather simple structure of the hydrogen-like ions, however, the underlying ‘mathematics’ is not always that easy to deal with. Apart from the well-known level structure of these ions as obtained from either the Schrödinger or Dirac equation, namely, a great deal of other properties are often needed. These properties are related to the interaction of bound electron(s) with external particles and fields and, hence, require to evaluate transition amplitudes, including wavefunctions and (transition) operators of quite different complexity. Although various special functions, such as the Laguerre polynomials, spherical harmonics, Whittaker functions, or the hypergeometric functions of various kinds can be used in most cases in order to express these amplitudes in a concise form, their derivation is time consuming and prone for making errors. In addition to their complexity, moreover, there exist a large number of mathematical relations among these functions which are difficult to remember in detail and which have often hampered quantitative studies in the past.

Method of solution: A set of MAPLE procedures is developed which provides both the nonrelativistic and relativistic (analytical) solutions of the ‘hydrogen atom model’ and which facilitates the symbolic evaluation of various transition amplitudes.

Restrictions onto the complexity of the problem: Over the past decades, a large number of representations have been worked out for the hydrogenic wave and Green’s functions, using different variables and coordinates [2]. From these, the position–space representation in spherical coordinates is certainly of most practical interest and has been used as the basis of the present implementation. No attempt has been made by us so far to provide the wave and Green’s functions also in momentum space, for which the relativistic momentum functions would have to be constructed numerically.

Although the DIRAC program supports both symbolic and numerical computations, the latter one are based on MAPLE’s standard *software* floating-point algorithms and on the (attempted) precision as defined by the global `Digits` variable. Although the default number, `Digits = 10`, appears sufficient for many computations, it often leads to a rather dramatic loss in the accuracy of the relativistic wave functions and integrals, mainly owing to MAPLE’s imprecise internal evaluation of the corresponding special functions. Therefore, in order to avoid such computational difficulties, the `Digits` variable is set to 20 whenever the DIRAC program is (re-)loaded.

Unusual features of the program: The DIRAC program has been designed for interactive work which, apart from the standard solutions and integrals of the hydrogen atom, also support the use of (approximate) *semirelativistic* wave functions for both, the bound- and continuum-states of the electron. To provide a fast and accurate access to a number of radial integrals which arise frequently in applications, the analytical expressions for these integrals have been implemented for the one-particle operators r^k , $e^{-\sigma r}$, d^m/dr^m , $j_L(kr)$ as well as for the (so-called) two-particle Slater integrals which are needed to describe the Coulomb repulsion among the electrons. Further procedures of the DIRAC program concern, for instance, the conversion of the physical results between different unit systems or for different sets of quantum numbers. A brief description of all procedures as available in the present version of the DIRAC program is given in the user manual `Dirac-commands.pdf` which is distributed together with the code.

Typical running time: Although the program replies *promptly* on most requests, the running time also depends on the particular task.

References:

[1] Maple is a registered trademark of Waterloo Maple Inc.

[2] H.A. Bethe and E.E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms, Springer, Berlin, 1957.

[3] J. Eichler and W. Meyerhof, Relativistic Atomic Collisions, Academic Press, New York, 1995.

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1. Introduction

Since the beginning of quantum mechanics, the hydrogen atom has been one of the best studied models in physics [1,2]. In a large number of textbooks and monographs, therefore, its (well-known) solutions from either

the nonrelativistic Schrödinger equation or Dirac's (relativistic) wave equation have served as standard examples in introducing atomic theory. But apart from the educational insight as obtained from the *hydrogen atom model*, the theory of the one-electron atoms and ions has found its way also into quite different fields of modern physics including molecular and plasma physics, quantum optics, or the theory of quantum information. When combined with the *atomic shell model*, i.e. the successive filling of shells as established for instance by the periodic table of elements, the (analytical) solutions of the 'hydrogen atom' help understand many atomic processes in Nature, at least qualitatively. During the last decades, moreover, Dirac's theory of the hydrogen-like ions has been applied successfully for describing energetic collisions of high-Z ions with atomic targets [3] or for testing quantum-electrodynamical (QED) effects [4], if Furry's picture and field-theoretical concepts are taken into account.

As seen from this wide-spread use of the hydrogen atom model, therefore, a fast and interactive access to the solutions and properties of the one-electron ions is highly desirable. In the past, several programs have been developed and implemented into the CPC program library for calculating the hydrogenic wave and Green's functions, both within the nonrelativistic [5,6] and relativistic [7,8] framework. Beside of providing these functions explicitly, they have been implemented also—at least to a certain extent—in a large number of further codes including those for studying the two-photon ionization of hydrogen-like ions [8], their interaction with lasers [9] and electrons [10], the excitation and ionization of such ions by Coulomb fields [11], their bound-bound transitions in the presence of external magnetic fields [12], and at many places elsewhere. But although these programs have certainly found useful for understanding the properties and behavior of one-electron atoms and ions, they have two drawbacks in common which restrict their further application: Since these programs are designed for a very particular task, they often (i) cannot be extended so easily to other problems. Moreover, by using standard languages such as FORTRAN or C, these programs do (ii) not support any algebraic (symbolic) access to the wave functions and matrix element as required by more advanced studies. The lack of symbolic techniques, in particular, and together with the low flexibility in dealing with the input and output of the programs from above have hampered their use for a much wider range of applications.

Today, a new and promising alternative for having an algebraic access to complex (symbolic) expressions is offered by computer algebra including the general purpose systems such as MATHEMATICA or MAPLE. In the last decade, they have been increasingly utilized to provide a fast and reliable gateway to a large set of complex expressions and computations. With the development of the DIRAC program, we here provide a set of MAPLE procedures for studying the properties and the dynamical behavior of the hydrogen-like ions. In the past two years, this program has been used to support not only the interpretation of experiments but also for a detailed analysis of the polarization and correlation properties of the X-ray radiation as emitted by relativistic collisions [13,14]. Owing to its interactive design, moreover, the DIRAC program may help the user not only in his or her daily research work but also in teaching the physics of (hydrogen-like) atoms and ions.

Obviously, however, a program about the *hydrogen atom model* can neither be implemented comprehensively nor explained within a single step. Therefore, the DIRAC package will be presented in several steps, each of them dedicated to a well defined part of the theory. To provide access to the very basic elements of the theory, here we first describe a set of procedures for the symbolic (as well as numerical) computation of the wave and Green's functions. These functions are provided for both, the bound- and continuum-state solutions of the nonrelativistic as well as relativistic theory. Having once a simple access to these functions, of course, they can be rather easily applied to construct the transitions amplitudes and matrix elements for a large number of other properties. For several—frequently required—matrix elements, an algebraic evaluation of the radial integrals has been implemented also explicitly.

Although the main purpose of this work is to describe the design and the use of the DIRAC package, in the next section we first compile the basic equations and expressions from the theory of the hydrogen atom with emphasis on those which have been implemented in the code. In Section 3, we later describe the organization of the program and how it is distributed. This section also lists all the user-accessible commands together with a short description, while a detailed explanation of the parameters, optional arguments and some additional information for each procedure is given in an additional user manual and is appended to the code. This is followed in Section 4 by a

number of selected examples to illustrate the interactive use of the DIRAC program within its MAPLE environment. A short outlook onto future developments and extensions of the program is finally given in Section 5.

2. Theoretical background

Since the quantum-mechanical theory of the one-electron atoms has been worked out long time ago, both within the nonrelativistic and relativistic framework, we may refer for most details to the literature. Helpful introductions into this topic can be found, for instance, in the texts by Bethe and Salpeter [1], Messiah [15], Bransden and Joachain [2], Eichler and Meyerhof [3], and by many others. In the present work, therefore, we will restrict ourselves to rather a short compilation of the basic expressions, just enough in order to introduce the notations and formulas as implemented within the DIRAC program. In the following two Sections 2.1 and 2.2, in particular, we briefly recall the (analytically well known) radial-angular representation of the hydrogen wave and Green's functions which are later applied in Section 2.3 for evaluating a number of radial integrals. Emphasis has first been paid to those integrals which are of frequent use in the computation of the structural and dynamical properties of the hydrogen-like ions. In this paper (and also in most parts of the underlying implementation of the DIRAC code), atomic Hartree units $\hbar = m_e = e^2/4\pi\epsilon_0 = 1$, where ϵ_0 is the permittivity of free space, are used throughout unless specified otherwise.

2.1. Wavefunctions and energy levels

2.1.1. Nonrelativistic framework

In a pure Coulomb potential $V(r) = -Z/r$ of a given (nucleus with) charge Z , the motion of an electron is described by the time-independent Schrödinger equation

$$\Delta\psi(\mathbf{r}) + 2\left(E + \frac{Z}{r}\right)\psi(\mathbf{r}) = 0 \quad (1)$$

which, in polar coordinates r , ϑ , and φ , can be separated into three independent equations owing to the ansatz [1]

$$\psi(r, \vartheta, \varphi) = R(r)Y_{lm}(\vartheta, \varphi) = \frac{P(r)}{r}Y_{lm}(\vartheta, \varphi). \quad (2)$$

As seen from this ansatz (2), the electronic wavefunction $\psi(\mathbf{r}) \equiv \psi(r, \theta, \phi)$ is therefore given as a product of a *radial* function $R(r)$ or $P(r)/r$, respectively, and a spherical harmonic $Y_{lm}(\vartheta, \varphi)$ which describes the *angular* structure and which depends on the orbital angular momentum l and its projection onto the quantization axis as denoted by the magnetic quantum number m . However, not much need to be said here about the properties and treatment of the spherical harmonics as one of the standard tasks from the theory of angular momentum [16] for which meanwhile also a number of symbolic tools are available [17,18]. The (radial) function $P(r)$ from ansatz (2) obeys the *radial* Schrödinger equation

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + 2E \right] \frac{P(r)}{r} = 0 \quad (3)$$

and are known to belong either to the discrete part of the spectrum with the (negative) energies

$$E_n = -\frac{Z^2}{2n^2} < 0, \quad n = 1, 2, \dots, \quad (4)$$

the so-called *bound* states, or to its continuous part for all energies $E > 0$, for which the functions $P(r)$ are said to represent the *free-electron* (or *continuum*) states. For a Coulomb potential in Eq. (3), an analytic solution of the radial functions $P(r)$ in terms of the confluent hypergeometric function $F(\alpha, \beta; x)$ are known for both, the

bound-states

$$P_{nl}(r) = r^{l+1} \frac{1}{(2l+1)!} \sqrt{\frac{(n+l)!}{(n-l-1)!2n}} \left(\frac{2Z}{n}\right)^{3/2+l} e^{(-Zr/n)} F\left(-n-l-1, 2l+2, \frac{2Zr}{n}\right), \quad (5)$$

with n and l being the principal and the orbital angular momentum quantum numbers, as well as for the *continuum* ($E > 0$)

$$P_{El}(r) = \frac{2\sqrt{Z}}{\sqrt{1 - e^{-2\pi n'}}} \prod_{s=1}^l \sqrt{s^2 + n'^2} \frac{(2kr)^l}{(2l+1)!} e^{-ikr} F(in' + l + 1, 2l + 2, 2ikr) \quad (6)$$

with $k = \sqrt{2E}$ and $n' = Z/k$. In the standard theory, moreover, the radial functions (5) and (6) are normalized due to the conditions

$$\int_0^\infty R_{nl}^2(r)r^2 dr = \int_0^\infty P_{nl}^2(r) dr = 1 \quad (7)$$

for having a single particle per bound state and due to

$$\int_0^\infty P_{El}^*(r)P_{E'l}(r) dr = \delta(E - E') \quad (8)$$

for representing one particle per unit energy as far as electrons in the continuum are concerned.

In the DIRAC package, both the full wavefunctions (2) and their radial components (5) and (6) are provided for the bound- and free-electron states by using the procedures Dirac_orbital() and Dirac_radial_orbital(), respectively.

2.1.2. Relativistic framework

Similar to Schrödinger's equation (1), the Dirac (eigenvalue) equation with a Coulomb potential

$$\left(i\boldsymbol{\alpha} \cdot \nabla + \frac{Z}{r} - (\beta - 1)c^2 + E \right) \psi(\mathbf{r}) = 0 \quad (9)$$

can be used to describe the *relativistic* motion of a spin-1/2 electron in the field of a nucleus with charge Z which, apart from the kinetic and potential energy of the electron, now also contains its rest energy as well as contributions due to the electron spin [2,3]. Analogue to the nonrelativistic case, the solution $\psi(\mathbf{r})$ of Eq. (9) can be separated again into a radial and angular part

$$\psi_{\kappa m}(r, \vartheta, \varphi) = \frac{1}{r} \begin{pmatrix} P(r)\Omega_{\kappa m}(\vartheta, \varphi) \\ iQ(r)\Omega_{-\kappa m}(\vartheta, \varphi) \end{pmatrix}, \quad (10)$$

where $\Omega_{\kappa m}(\vartheta, \varphi)$ denotes a standard Dirac spin-orbital function and where $\kappa = \pm(j + 1/2)$ for $l = j \pm 1/2$ is called the *relativistic* angular momentum quantum number. Owing to the definition of $\kappa = \pm 1, \pm 2, \dots$, this quantum number carries information about both, the total angular momentum j and the parity $(-1)^l$ of the wavefunction. As usual, the Dirac spin-orbitals can be written in terms of the spin-1/2 Pauli spinors χ_{\pm} and the spherical harmonics by

$$\Omega_{\kappa m}(\vartheta, \varphi) = \sum_{m_l} \langle l, m_l, 1/2, m - m_l | jm \rangle Y_{lm_l}(\vartheta, \varphi) \chi_{m - m_l}. \quad (11)$$

As seen from ansatz (10), moreover, the radial part of the wavefunctions is now given by the two functions $P(r)$ and $Q(r)$ which are called the *large* and *small* components, respectively. Similar to the nonrelativistic case, an analytic representation of these two components is known and is different for an electron in a bound or continuum

state where, apart from the continuum with *positive* energies $E > 0$ an additional continuous branch (of solutions) with *negative* energies $E \leq -2c^2$ exists. As known from Dirac's theory, these solutions with negative energies require special care and can be re-interpreted, for instance, in terms of positron states. For the *bound* states of hydrogen-like ions, the (discrete eigen-)energies of Eq. (9) are given by

$$E_{n\kappa} = \frac{(W_{n\kappa} - 1)}{\alpha^2} = \frac{1}{\alpha^2 [1 + (\frac{\alpha Z}{n'+s})^2]^{1/2}} - \frac{1}{\alpha^2}, \quad (12)$$

while the corresponding radial components $P_{n\kappa}$ and $Q_{n\kappa}$ can be written again in terms of the confluent hypergeometric function $F(\alpha, \beta; x)$. They read as

$$P_{n\kappa}(r) = N_{n\kappa} \sqrt{1 + W_{n\kappa} r} (2qr)^{s-1} e^{-qr} \times \left[-n' F(-n' + 1, 2s + 1; 2qr) - \left(\kappa - \frac{\alpha Z}{q\lambda_c} \right) F(-n', 2s + 1; 2qr) \right], \quad (13)$$

$$Q_{n\kappa}(r) = -N_{n\kappa} \sqrt{1 - W_{n\kappa} r} (2qr)^{s-1} e^{-qr} \times \left[n' F(-n' + 1, 2s + 1; 2qr) - \left(\kappa - \frac{\alpha Z}{q\lambda_c} \right) F(-n', 2s + 1; 2qr) \right], \quad (14)$$

where $n' = n - |\kappa| = 0, 1, 2, \dots$ denotes the number of nodes of the radial components, $\lambda_c = \hbar/m_e c$ the Compton length of the electron, and

$$s = \sqrt{\kappa^2 - (\alpha Z)^2}, \quad (15)$$

$$q = \frac{Z}{\sqrt{(\alpha Z)^2 + (n' + s)^2}}. \quad (16)$$

Moreover, the normalization factor

$$N_{n\kappa} = \frac{\sqrt{2} q^{5/2} \lambda_c}{\Gamma(2s + 1)} \left[\frac{\Gamma(2s + n' + 1)}{n'! (\alpha Z) (\alpha Z - \kappa q \lambda_c)} \right]^{1/2} \quad (17)$$

is chosen in such a way that the two radial components satisfy the condition

$$\int_0^\infty (P_{n\kappa}^2(r) + Q_{n\kappa}^2(r)) dr = 1, \quad (18)$$

i.e. that the wavefunction (10) represents one electron per bound state.

For the free-electron states with energies $E \leq -2c^2$ or $E > 0$, the explicit expressions of the radial components $P_{E\kappa}(r)$ and $Q_{E\kappa}(r)$ are quite elaborate when compared with the bound solutions in Eqs. (13) and (14) and are not displayed here. They are shown and discussed, for example, in the text by Eichler and Meyerhof [3]. However, these continuum states are also implemented in the DIRAC package and can be accessed as well by means of the procedures `Dirac_spinor()` and `Dirac_radial_component()`.

2.1.3. Semirelativistic framework

The two radial functions (13) and (14) represent, together with Eq. (10), an *exact* solution of the Dirac equation for a pure Coulomb potential. In practice, however, the use of these radial components often leads to rather lengthy and complicated computations. Instead of the exact form, therefore, the *approximate* Darwin wavefunctions [19] have been widely used in applications such as the theoretical description of the Coulomb ionization [20] or the electron–positron pair creation [21]. For a Coulomb potential, $-Z/r$, the Darwin wavefunctions

$$\phi_{nlm}^{(\pm)}(\mathbf{r}) = \left(1 - \frac{i}{2c} \boldsymbol{\alpha} \cdot \nabla \right) u^{(\pm)} \psi_{nlm}(\mathbf{r}) \quad (19)$$

are expressed in terms of the nonrelativistic solutions (2)–(5) of the Schrödinger equation from Section 2.1.1, where $u^{(+)} = (1, 0, 0, 0)^+$ and $u^{(-)} = (0, 1, 0, 0)^+$ are the two four-component spinors for a particle at rest with either spin-up or spin-down, respectively. Obviously, the Darwin functions (19) have a much simpler structure when compared with the exact bound-state solutions (13) and (14) from above; they are accurate to first-order in αZ in the expansion of the Dirac equation and are normalized to the same order.

Apart from the bound states (19), approximate continuum wavefunctions can be derived which are accurate to αZ in the relativistic motion of the electron and which are known as Sommerfeld–Maue wavefunctions [22] from the literature. Again, these functions can be expressed in terms of the nonrelativistic functions and have been widely used in applications [21,23]. Although the explicit form of these functions is slightly more complicated than in the bound case, their derivation follows very similar lines. Here, we will not display these functions in detail but simply refer to the procedures `Dirac_Darwin()` and `Dirac_Sommerfeld_Maue` of the `DIRAC` code which facilitates the access to both, the Darwin and the Sommerfeld–Maue semirelativistic approximations.

2.2. Green’s function

Apart from the wavefunctions, which describe the electron in some particular quantum state, one often needs the summation over all the (unoccupied) states, especially if parts of the atomic interaction are treated as a perturbation. Such a summation over the *complete* spectrum is required, for example, for describing the two- (and multi-)photon processes in hydrogen-like ions [24] or for the computation of hyperpolarizabilities. Although, in principle, it appears straightforward to carry out such a summation explicitly by using the function from above, the large number of terms and the need for integrating over the electron continuum may hamper such an approach. Instead, the use of the Green’s function

$$G(\mathbf{r}, \mathbf{r}'; E) = \sum_v \frac{|\psi_v(\mathbf{r})\rangle\langle\psi_v(\mathbf{r}')|}{E_v - E} \tag{20}$$

is usually much more favorable since it provides a simple access to the perturbative treatment of various types of interactions in the computation of atomic properties.

As easily shown, the Green’s function (20) can be obtained generally as solution of the inhomogeneous differential equation

$$[\hat{H} - E]G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}'), \tag{21}$$

where \hat{H} denotes the Hamiltonian operator of the system. Similar to the case of the wavefunctions, the form of the Hamiltonian \hat{H} and, hence, the explicit expressions for the Green’s function depends of course on the *framework* in which the system is described. For the Schrödinger operator $\hat{H} = -\nabla^2/2 - V(r)$ (the nonrelativistic case), for example, the solutions of Eq. (21) can be separated—again—into radial and angular functions by means of the ansatz

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{rr'} \sum_{l=0}^{\infty} \sum_m g_l(r, r'; E) Y_{lm}^*(\vartheta', \varphi') Y_{lm}(\vartheta, \varphi). \tag{22}$$

For a Coulomb-potential $V(r) = -Z/r$ in the Hamiltonian above, the radial functions are known analytically in terms of (special) Whittaker functions of the first and second kind

$$g_l(r, r'; E) = \frac{v}{Z} \frac{\Gamma(l+1-v)}{\Gamma(2l+2)} M_{v,l+1/2} \left(\frac{2r_{<}}{v} \right) W_{v,l+1/2} \left(\frac{2r_{>}}{v} \right), \tag{23}$$

where $v = Z/\sqrt{-2E}$ and $r_{>} = \max(r, r')$ and where $r_{<} = \min(r, r')$ refer to the larger and smaller values of the two radial coordinates, respectively.

A similar *radial-angular* representation can be found for the (relativistic) Dirac Hamiltonian in Eq. (21) but leads to a quite complicated form for the radial part which is given then by a 2×2 matrix. In the `DIRAC` program,

we provide the procedure `Dirac_Greens_radial()` which supports the computation of the radial functions (23) or of the corresponding relativistic Green's functions.

2.3. Integrals with hydrogenic wavefunctions

The Coulomb wave and Green's functions from the previous subsections can be applied for studying the properties and dynamics of hydrogen-like ions. Usually, they are the basic ingredients in defining the transition amplitudes and cross sections and, by using their *radial-integral* decompositions in Eqs. (2), (10), and (22) immediately lead to a number of *radial-integrals* including various types of (transition) operators. While, of course, these integrals can always be determined *numerically*, an *analytic* (pre-)evaluation of these integrals is in many cases possible and results in a considerable gain in the computation of the transition amplitudes. Often, moreover, the analytic evaluation of the radial integrals is faster and more accurate when compared with a (straightforward) numerical integration. For several integrals, which frequently arise in applications, therefore, the analytic formulas have been implemented explicitly into the DIRAC code. Below, we first discuss the matrix elements containing the operators r^k , $e^{-\sigma r}$, d^m/dr^m , the integrals for studying the light-matter interaction or for collisions with external particles, but turn later also to the (well-known) Slater integrals for treating the interaction among the electrons.

2.3.1. Radial integrals of r -dependent operators

Nonrelativistic framework: For calculating the structure of the hydrogen-like ions and their cross sections in collisions with atoms and electrons, one often needs the matrix elements for the operators r^k , d^m/dr^m , $e^{-\sigma r}$, or various combinations of these operators. Within the nonrelativistic Schrödinger theory, the analytic calculation of such r -dependent matrix elements have been analyzed and discussed especially by Sánchez and López Piñeiro [25] who applied the hypervirial theorem along with a second quantization formalism. They showed that these matrix elements can be typically reduced to radial integrals of the form

$$\begin{aligned} \langle nl|r^k e^{-\sigma r}|n'l'\rangle &= \int_0^\infty P_{nl}(r)r^k e^{-\sigma r} P_{n'l'}(r)dr \\ &= N_{n'l'}N_{nl} \sum_{m=0}^{n-l-1} \sum_{m'=0}^{n'-l'-1} \frac{(-1)^{m+m'}}{m!m'!} \binom{n'+l'}{n'-l'-1-m'} \binom{n+l}{n-l-1-m} \\ &\quad \times \left(\frac{2Z}{n'}\right)^{l'+m'} \left(\frac{2Z}{n}\right)^{l+m} \left(\frac{Z}{n'} + \frac{Z}{n} + \sigma\right)^{-(k+l+l'+m+m'+3)} \\ &\quad \times \Gamma(k+l+l'+m+m'+3), \end{aligned} \tag{24}$$

which can then be utilized also (if necessary) in order to compute the matrix elements including some derivatives $d^m/dr^m P_{nl}(r)$ of the wave functions. For the sake of brevity, however, we will not display these recursion formulas but only mention that, for all the operators from above, the corresponding radial integrals can be evaluated by means of the procedure `Dirac_r_matrix_element()` of the DIRAC program. In this procedure, an analytic evaluation of the integrals is carried out whenever possible.

Relativistic framework: Of course, an analytical expression of the matrix elements with operators $r^k e^{-\sigma r}$ can be found also for the relativistic Dirac wavefunctions. However, in order to derive such expressions it is more convenient not to start from the standard representation of the hydrogenic functions (13)–(14) but first to re-write them in terms of a series expansion in r as it was suggested originally by Rose [26]. By using such r -series

representation, the $r^k e^{-\sigma r}$ matrix elements can be written, similar to (24), in term of Γ -functions as

$$\begin{aligned} \langle n\kappa | r^k e^{-\sigma r} | n'\kappa' \rangle &= \int_0^\infty (P_{n\ell}(r)P_{n'\ell'}(r) + Q_{n\ell}(r)Q_{n'\ell'}(r))r^k e^{-\sigma r} dr \\ &= N_{n\kappa}N_{n'\kappa'} \sum_{v=0}^{n-|\kappa|} \sum_{v'=0}^{n'-|\kappa'|} (c_{n\kappa,v}^+ c_{n'\kappa',v'}^+ + c_{n\kappa,v}^- c_{n'\kappa',v'}^-) \\ &\quad \times \frac{q^{s+v-1} q'^{s'+v'-1}}{(q+q'+\sigma)^{1+v+v'+s+s'+k}} \Gamma(v+v'+k+s+s'+1), \end{aligned} \tag{25}$$

where the parameters q, s and the normalization factor $N_{n\kappa}$ were defined by Rose [26], and where the coefficients $c_{n\kappa,v}^\pm$ are given by

$$c_{n\kappa,v}^\pm = (1 \pm \sqrt{1-q^2})^{1/2} \frac{((-n+|\kappa|)_v 2^v)}{v!(2s+1)_v} [(v-n+|\kappa|) \pm (\alpha Z/q - \kappa)] \tag{26}$$

with $(a)_v$ being the Pochhammer symbol.

In contrast to the radial integral (25), no analytic expressions for the matrix elements containing the derivative d^m/d^m within the relativistic framework are implemented explicitly in DIRAC program. For all such matrix elements, however, the (straightforward) numerical integration is applied by making use of the standard MAPLE command `int()`.

2.3.2. Grant's integrals

Relativistic framework: As known from relativistic collision theory [3,27], the interaction of (atomic) electrons with the radiation field or with other atoms and ions can usually be traced back to the computation of the following three radial integrals

$$I_L^\pm(q; a, b) = \int_0^\infty dr j_L(qr) (P_a(r)Q_b(r) \pm Q_a(r)P_b(r)), \tag{27}$$

$$I_L^0(q; a, b) = \int_0^\infty dr j_L(qr) P_a(r)Q_b(r), \tag{28}$$

$$J_L(q; a, b) = \int_0^\infty dr j_L(qr) (P_a(r)P_b(r) + Q_a(r)Q_b(r)), \tag{29}$$

where $j_L(qr)$ denotes a spherical Bessel function of order L and, as before, $P(r)$ and $Q(r)$ are the radial components of the one-electron wavefunctions (10). Because of the oscillations in the Bessel as well as the radial wavefunctions, however, an accurate value of these integrals is not always easy to obtain numerically. In the DIRAC program, we therefore implemented the analytic formulas for these integrals in terms of a finite series over the confluent hypergeometric functions as known for the *bound-bound* and *bound-free* transitions [28,29]. While this typically results in a much faster (and more accurate) computation of the integrals, it requires however that at least one set of radial components—either $P_a(r), Q_a(r)$ or $P_b(r), Q_b(r)$ —has to represent some bound-state electron.

Nonrelativistic framework: Since, in the limit $c \rightarrow \infty$, the small component $Q(r)$ becomes negligible, only contributions from the last integral (29) survives in the nonrelativistic description of interaction processes with the

radiation field and gives rise to the integral

$$J_L(q; a, b) = \int_0^{\infty} dr j_L(qr) P_a(r) P_b(r). \quad (30)$$

An analytic evaluation of this integral with nonrelativistic radial orbital functions is supported by the procedure `Dirac_IJ_radial()` of the DIRAC program for both, *bound–bound* and *bound–free* electronic transitions.

2.3.3. Slater integrals

Although the main emphasis in developing the DIRAC program has been placed on studying the properties and behaviors of the hydrogen-like ions, the wave functions from above can be used also to estimate the effects of the electron–electron interaction for *few-electron* atoms and ions. For such systems, one often needs to compute the (two-electron) matrix elements for the Coulomb repulsion operator $1/r_{12}$ which, after some algebra, leads to the so-called Slater integrals

$$R^k(a, b, c, d) = \int_0^{\infty} dr_1 \int_0^{\infty} dr_2 P_{n_a l_a}(r_1) P_{n_b l_b}(r_2) \frac{r_{<}^k}{r_{>}^{k+1}} P_{n_c l_c}(r_1) P_{n_d l_d}(r_2), \quad (31)$$

where $r_{>} = \max(r_1, r_2)$ and $r_{<} = \min(r_1, r_2)$ refer to the larger and smaller values of the two radial coordinates, respectively. The analytic evaluation of this integral in terms of confluent hypergeometric functions has been implemented in the DIRAC package for the nonrelativistic framework. For reasons of efficiency, however, no attempt has been made to incorporate also the ‘relativistic version’ of the Slater integrals which would raise much larger demands regarding the accurate computation of these values.

3. Program organization

3.1. Overview about the DIRAC package

The DIRAC package has been developed as an interactive tool within the framework of MAPLE (version 8). It is designed in order to provide a simple and consistent access to the wave functions, the excitation and decay properties as well as the dynamical behavior of the hydrogen-like ions. To allow for a rather large flexibility in the use of the program, most of the functions and quantities from the *hydrogen atom model* are supported both, within the nonrelativistic as well as the relativistic theory. With the present version of DIRAC, we start with compiling different (analytical) representations of the Coulomb wave and Green’s functions using polar coordinates. In addition, both the analytical and numerical evaluation of the—most frequently—required integrals are supported and now facilitate their accurate computation for a large number of properties.

Following MAPLE’s philosophy, the DIRAC program is organized in a *hierarchical* order. In the current version, there are about 50 procedures at quite different level of complexity from which most however are kept hidden to the user. As in MAPLE’s own design, these procedures mainly serve as language elements in order to build up commands at some higher level of the hierarchy. Therefore, only about 15 procedures at top level need to be known by the user and are briefly summarized in [Table 1](#). More detailed information about the use of these procedures, their optional arguments, or the output can be obtained from the user manual `Dirac-commands.pdf` which is distributed together with code. In this manual, we mainly follow the style of the help pages of MAPLE and *The Maple Handbook* by Redfern [30] from earlier years. To illustrate some of the basic features of the program, moreover, a few selected examples are displayed below.

As known from MAPLE’s recent up-grades, most of its internal commands make use of rather short names and often of some abbreviations for the various quantities and methods. Although such a name convention might be

Table 1

Main commands of the DIRAC package. A more detailed description of these and a few less important procedures is given in the user manual `Dirac-commands.pdf` and is distributed together with the code

Procedure	Description
<code>Dirac_convert()</code>	Converts the physical results between different unit systems.
<code>Dirac_energy()</code>	Returns the nonrelativistic energy E_n from Eq. (4) or the relativistic energy $E_{n\kappa}$ from Eq. (12) for bound-electron states.
<code>Dirac_evalf()</code>	Attempts to simplify an algebraic expression for either the energies, wavefunctions, or matrix elements by substituting the numerical values for some fundamental constants.
<code>Dirac_Greens_radial()</code>	Calculates the radial part of either the nonrelativistic Coulomb Green's functions (23) or of the corresponding relativistic Green's functions.
<code>Dirac_IJ_radial()</code>	Evaluates the radial integrals (27)–(30) for both, the bound-bound and bound-free electron transitions.
<code>Dirac_orbital()</code>	Returns the nonrelativistic hydrogenic orbitals $\psi_{n(E)lm}(r, \vartheta, \varphi)$ from Eq. (2) as function of the given arguments.
<code>Dirac_r_matrix_element()</code>	Evaluates the radial matrix elements for various r -dependent operators between hydrogenic wavefunctions, both within the nonrelativistic and the relativistic framework.
<code>Dirac_radial_component()</code>	Returns the large and small radial components, $P_{n(E)\kappa}(r)$ and $Q_{n(E)\kappa}(r)$, of the relativistic orbital functions (13)–(14). These components are supported for both, the bound and free-electron states.
<code>Dirac_radial_orbital()</code>	Returns a nonrelativistic radial orbital $P_{n(E)lm}(r)$ for both, the bound and free-electron states.
<code>Dirac_settings()</code>	Specifies the framework, nuclear charge and the units which are to be used by the DIRAC program.
<code>Dirac_Slater_radial()</code>	Evaluates the Slater integral (31) with nonrelativistic orbital functions.
<code>Dirac_spin_orbital()</code>	Returns the Dirac spherical spinor $\Omega_{\kappa m}$ from Eq. (11).
<code>Dirac_spinor()</code>	Returns the relativistic hydrogenic spinor $\psi_{n(E)\kappa m}(r, \vartheta, \varphi)$ from Eq. (10).
<code>Dirac_Ylm()</code>	Return the spherical harmonic $Y_{lm}(\vartheta, \varphi)$.

favorable for the frequent use of the commands, these names are usually not easy to remember and to recognize in their output if implemented in a code. In the DIRAC program, therefore, we follow a slightly different concept by making use of rather long names to better explain the purpose of the procedures. In the long run, hopefully, this will simplify the readability and the maintenance of the program. Moreover, all the commands of the DIRAC package begin with the additional prefix `Dirac_` in order to distinguish them from MAPLE's internal functionality.

3.2. Getting started with DIRAC

The DIRAC package is distributed as a compressed tar-file `dirac.tar` from which the `dirac` root directory is obtained by the command `tar -xvf dirac.tar`. This root contains the source code library (for MAPLE 8), a `Read.me` for the installation of the package as well as the program manual `dirac-commands.pdf`. This latter document explains all the user relevant commands along with the output format, their optional arguments and some additional information which might be of interest for the application of the procedures. The `dirac` root directory also contains an example of a `.mapleinit` file which can be easily modified and incorporated into the user's home. Making use of such a `.mapleinit` file, the module `dirac` should then be available like any other module of MAPLE simply by typing

```
> with(dirac);
Welcome to Dirac

Dirac_save_nuclear_charge := Z
Dirac_save_framework := nonrelativistic
Dirac_save_units := atomic
```

As seen from the printout above, the settings of the DIRAC program are specified by the three *global* variables which must not be overwritten interactively. The (global) variable `Dirac_save_ framework`, for instance, specifies the theoretical *framework* in which the various commands will respond to the user; it may take the two

values `relativistic` and `nonrelativistic` and determines of how the input and output of the procedures is to be treated internally. In practice, of course, the input/output data of the procedures depend not only on the framework but often also on the present choice of the *units* as specified by the variable `Dirac_save_units`. In the DIRAC program, we presently support atomic Hartree ($\hbar = m_e = e^2/4\pi\epsilon_0 = 1$), natural ($m_e = c = e = 1$), SI, and Gaussian units which are recognized by setting `Dirac_save_units` to one of its allowed values: `atomic`, `natural`, `SI`, or `cgs`, respectively. Moreover, most of the solutions and output of interest will depend on the *nuclear charge* Z as internally specified by the global variable `Dirac_save_nuclear_charge`. To change these particular specifications of the DIRAC program, the command `Dirac_settings()` can be used; if instead of ‘atomic’ units, the user wishes to employ ‘natural’ units for the input and output of the procedures, the initial specification can be modified by entering

```
> Dirac_settings(units, natural);
    Units are changed to natural
```

Therefore, by specifying the global variables properly due to the demands of the user, the procedures of the DIRAC program can be adapted to the particular task. A proper choice of these global definitions makes the program appropriate for a wide range of applications.

4. Interactive work with the DIRAC program

To illustrate the use of the DIRAC program and to provide some test cases, below we will display and explain a few examples concerning the fine-structure of the hydrogen-like ions as well as the (algebraic) access to their wave functions. A more advanced example later shows the computation of matrix elements within the relativistic framework as they arise frequently in the study of light–matter interactions. For all these examples, we assume the DIRAC program to be loaded into the current MAPLE session as explained in the previous Section 3.2.

4.1. Fine structure of hydrogen-like ions

In the nonrelativistic Schrödinger theory, the level energies (4) only depend on the principal quantum number n and, hence, are *degenerate* with respect to the orbital quantum number l and the magnetic quantum number m . This $2n^2$ degeneracy (the factor 2 arises from the spin of the electrons), however, is partially removed if Dirac’s theory is applied. In the relativistic case (12), namely, the nonrelativistic levels with energy E_n split into n different sublevels according to the total angular momentum $j = 1/2, 3/2, \dots, n - 1/2$ of the state. This splitting, which is known as the fine-structure of the hydrogen-like ions, can be easily illustrated below by means of the DIRAC program.

To obtain insight into this splitting as a function of the nuclear charge Z , let us first compare the relativistic and nonrelativistic level energies for $n = 2$. Since the *nonrelativistic* framework is predefined whenever the DIRAC program is (re-)loaded, we start with the Schrödinger energy (4) which is returned for an arbitrary nuclear charge $Z = Z_0$ by entering

```
> Dirac_settings(charge, Z0);

    Nuclear charge is changed to Z0

> E_2(Z0) := Dirac_energy(2);

                2
                Z0
E_2(Z0) := - ----
                8
```

Of course, the well-known nonrelativistic energy expression $E_{n=2} = -Z_0^2/8$ is returned, given in *atomic* units as the default setting. Analogue, we may obtain the $n = 2$ energy levels as predicted by the Dirac theory. To this end, we first need to change to the *relativistic* framework for all subsequent calls of the DIRAC procedures

```
> Dirac_settings( framework, relativistic );
```

Framework is changed to relativistic

and, again, make use of the same command `Dirac_energy()`. In the relativistic framework, this procedure now expects the two arguments n and κ to return the level energy $E_{n\kappa}$ from Eq. (12). To get the energy of a $2s_{1/2}$ electron with quantum numbers $n = 2$ and $\kappa = -1$, we type

```
> E_2s(Z0) := Dirac_energy(2, -1);
```

$$E_{2s}(Z_0) := \frac{1}{2} \frac{1}{\text{Dirac_Constant_alpha}} \frac{1}{\sqrt{1 + \frac{Z_0^2 \text{Dirac_Constant_alpha}^2}{(1 + (1 - \text{Dirac_Constant_alpha}^2 Z_0^2)^{1/2})^2}}}$$

which returns this energy in the most general form, including the nuclear charge Z_0 and the (unevaluated) fine structure constant α as yet given by the global variable `Dirac_Constant_alpha`. At the first glance, such a general form may look quite complicated but it helps of course in treating the expressions algebraically. For our discussion of the fine-structure behavior as a function of Z , we may first assume the αZ parameter small when compared with unity and apply the standard MAPLE command `series()` to expand this expression for the $2s_{1/2}$ energy in powers of Z

```
> series(E_2s(Z0), Z0);
> E_2s_exp(Z0) := convert(% , polynom);
```

$$E_{2s_exp}(Z_0) = -1/8 Z_0^2 - 5/128 \text{Dirac_Constant_alpha}^2 Z_0^4$$

Subtracting from this expression the Schrödinger energy $E_{n=2}$ from above

```
> E_2s_exp(Z0) - E_2(Z0);
5 Dirac_Constant_alpha^2 Z0^4
-----
128
```

we find the so-called relativistic Pauli correction $\Delta E_{n\kappa}$ to the (nonrelativistic) level energy [1,2] which, as seen from the printout, scales like $\alpha^2 Z_0^4$ and, thus, will strongly increase for high- Z ions.

The result above for the Pauli correction $\Delta E_{n\kappa}$ displays the analytic behavior of the fine-structure splitting; to get a better impression on the size of this splitting, we may evaluate this expression for $n = 2$ also *numerically*. To substitute the value $\alpha = 1/137.036$ of the fine-structure constant for `Dirac_Constant_alpha`, we may use the command `Dirac_evalf()` in the DIRAC program and obtain

```
> E_2s(Z0) := Dirac_evalf(E_2s(Z0));
```

$$E_{2s}(Z_0) := \frac{18778.865231694104538}{\left(1 + \frac{0.000053251353990881516089 Z_0^2}{(1 + (1 - 0.000053251353990881516089 Z_0^2)^{1/2})^2}\right)^{1/2}} - 18778.865231694104538$$

By evaluating in a similar way also the level energy for the $2p_{3/2}$ shell ($n = 2$, $\kappa = -2$)

```
> E_2p(Z0) := Dirac_energy(2, -2);
> E_2p(Z0) := Dirac_evalf(E\2p(Z0)):
```

we can finally calculate the level shifts of the $j = 1/2$ and $j = 3/2$ fine-structure levels with respect to the value from the nonrelativistic theory. For atomic hydrogen ($Z_0 = 1$), this gives rise to

```
> subs(Z0 = 1, E_2s(Z0) - E_2(Z0));
> subs(Z0 = 1, E_2p(Z0) - E_2(Z0));
```

```
-5
-0.208018917100000 10
```

```
-5
-0.41602897100000 10
```

in atomic units and can be compared immediately to the values of 0.46 cm^{-1} (0.208×10^{-5} a.u.) and 0.09 cm^{-1} (0.416×10^{-6} a.u.), respectively, as known from the literature [1,2].

4.2. Relativistic contraction of the s-orbitals

In Section 2, we have displayed the radial components for a bound-state electron for both, the nonrelativistic (5) and relativistic theory (13)–(14). The spatial behavior of these one-electron solutions for different nuclear charges Z has been discussed in detail at a number of places [1,3] to illustrate the ‘relativistic effects’ for high- Z ions. While, for small charges Z , the radial Schrödinger function (5) and the large component (13) from the Dirac theory are practically the same, a comparison of these functions for high- Z ions shows a clear contraction of the large component towards the nucleus. This effects, which is known as the *relativistic contraction of the wavefunctions*, influences not only the structure of heavy (hydrogen-like) ions but, for instance, also their ionization behavior [31] or the chemical binding in materials containing heavy elements.

To illustrate the contraction of the 3s wavefunction for a hydrogen-like uranium ion U^{91+} by means of the DIRAC program, we shall extract and compare the radial function (5) with the large component (13) from Dirac’s theory. The algebraic expression for the $P_{n=3,l=0}(r)$ nonrelativistic function can be obtained by

```
> Dirac_settings(framework, nonrelativistic);
```

```
Framework is changed to nonrelativistic
```

```
> Dirac_settings(charge, 92);
```

```
Nuclear charge is changed to 92
```

```
> P_3s(r) := Dirac_radial_orbital(3, 0, r);
```

$$P_{3s}(r) := \frac{368}{243} r^{1/2} \exp\left(-\frac{92}{3} r\right) \left(27 - 1656 r + 16928 r^2\right) r$$

where, in the first two lines of printout, we set the nonrelativistic framework and define the nuclear charge to be $Z = 92$.

Returning to the relativistic framework as before, the large component of a $3s_{1/2}$ electron is generated in the DIRAC program by calling

```
> P_3s_r(r) := Dirac_radial_component(large, 3, -1, r):
```

for which, we suppress here the printout to screen (using the colon at the end of the line) as this would result in quite a lengthy expression in terms of the hypergeometric function and various physical constants (cf. Eq. (13)). For the present purpose, instead, we first better ‘evaluate’ all the physical constants to their numerical values by calling

```
> P_3s_r(r) := Dirac_evalf(P_rel(r));
```

```
0.74113463002424792093
```

```
P_3s_r(r) := 69.235282776899202095 r
```

```
exp(-32.599243267231110742 r) (3.8221513992160292467
```

```
hypergeom([-2.], [2.4822692600484958419], 65.198486534462221484 r) -
```

```
2. hypergeom([-1.], [2.4822692600484958419], 65.198486534462221484 r))
```

Having the $3s$ radial wave functions from the nonrelativistic and relativistic theory, we can plot them by using the standard MAPLE procedures `plot()`. Physically more important than the wave function, however, is the ‘contraction’ in the charge distribution as given by the *radial distribution functions* $|P_{n=3,l=0}(r)|^2$ and $|P_{n=3,\kappa=-1}(r)|^2$, respectively.

```
> plot([(P_3s(r))^2, abs(P_3s_r(r))^2], r=0..0.3, linestyle=[DASH, SOLID]);
```

As expected, a clear contraction of the relativistic function (solid line) is found when compared with the nonrelativistic radial wavefunction (dashed line) (see Fig. 1).

4.3. Evaluation of the relativistic radial integrals

Until now, we have demonstrated the use of the DIRAC program by simple ‘textbook examples’ such as the computation of the level energies or the hydrogenic wave functions. The DIRAC procedures, however, are able to help the user with much advanced studies concerning the excitation and decay properties or the dynamical behavior of the hydrogen-like ions. For such investigations, we need to compute *transition matrix elements* including the wavefunctions from above and the corresponding (transition) operators. The exact relativistic treatment of the *photoionization* of hydrogen-like ions, for instance, can be traced back to the computation of the bound–free transition amplitude [3]

$$M_{f,b}^{\text{PI}} = \langle \psi_{E_f \kappa_f m_f} | \alpha \mathbf{u}_\lambda e^{i\mathbf{k}r} | \psi_{n_b \kappa_b l_b} \rangle, \quad (32)$$

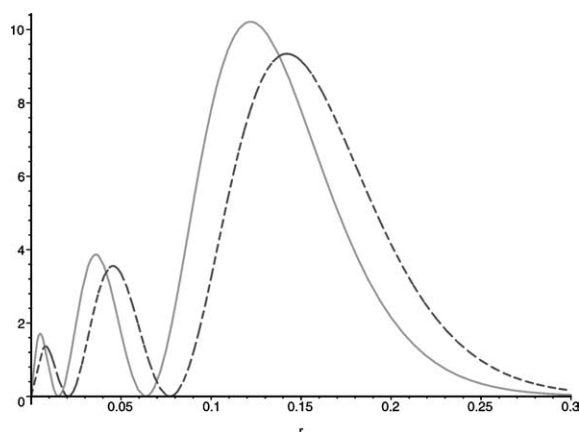


Fig. 1.

where $\psi_{n_b \kappa_b \mu_b}(\mathbf{r})$ and $\psi_{E_f \kappa_f m_f}(\mathbf{r})$ are the (relativistic) wavefunctions for the initially bound and the final continuum electron, respectively, and where the operator $\mathbf{u}_\lambda e^{i\mathbf{k}\cdot\mathbf{r}}$ describes the electron–photon interaction.

The simplification of the transition amplitude (32) requires elements from the algebra of angular momentum and has been discussed elsewhere [3,14]. In particular, it was shown that this amplitude can be factorized into radial and angular parts where the latter ones evaluate to Wigner 3- j and 6- j symbols and a constant factor, while the radial part is reduced to the integrals (27)–(29). Below, we therefore discuss how the DIRAC package can be utilized to compute these radial integrals. We start with the straightforward numerical integration of the radial integral $I_{L=1}^0(q; a, b)$, which arises if a $1s_{1/2}$ electron ($n_b = 1$, $\kappa_b = -1$) is ionized by a photon with energy $E_\gamma = 70$ eV into a $s_{1/2}$ continuum state (partial s-wave; $\kappa_f = -1$). For this particular choice of the parameters and quantum numbers, we may simply enter

```
> Dirac_settings(charge, 1):
> Dirac_settings(framework, relativistic):
> Pa(r) := Dirac_evalf(Dirac_radial_component(large, 1, -1, r)):
> Qb(r) := Dirac_evalf(Dirac_radial_component(small, 2.072432345, -1, r, free)):
> int(Pa(r)*Dirac_spherical_j(1,0.01877198124*r)*Qb(r),r=0..70.);
```

-5
-0.23633058961153019500 10

where the keyword *free* in the procedure `Dirac_radial_component()` is used to generate the small component of a continuum state with (kinetic) energy $E_f = 2.072432345$ (a.u.) and where most of the intermediate printout has been suppressed by using a colon to terminate the first 5 lines. Both the energy E_f and the momentum transfer $q = 0.01877198124$ (a.u.) are easily derived from the conservation of energy, assuming $I = 0.5$ (a.u.) as the ionization potential for the $1s$ electron of atomic hydrogen. In the last input line, moreover, the procedure `Dirac_spherical_j()` is used to return the spherical Bessel function $j_L(qr)$.

The (direct) numerical computation of the integrals (27)–(29) is typically reliable but also very *time consuming*. For the integral above, for instance, MAPLE requires about 145 s at a 1 GHz processor. An alternative and (much) faster computation is achieved by using the *analytical* expressions for the radial integrals (27)–(29) in terms of the special hypergeometric functions [28]. Within the DIRAC program, such a (analytical) integration algorithm is supported by means of the procedure `Dirac_IJ_radial()` which can be invoked with the same parameters as above to determine the $I_{L=1}^0(q; a, b)$ integral

```
> Dirac\_IJ\_radial(IL0, 0.01877198124, 1, 1, -1, 2.072432345, -1, free):
```


-5

`-0.23633058961153083452 10`

Although, of course, the integral is the same for using both, the numerical or analytical integration scheme (at least up to the 16th decimal digit), the procedure `Dirac_IJ_radial()` is faster by almost two orders of magnitude when compared to MAPLE's numerical integration. It is also more accurate as found by increasing the number of digits to `Digits := 30`.

5. Summary and outlook

The DIRAC program has been presented to facilitate a fast and consistent access to the basic elements and properties of the hydrogen-like ions. In its present form, this program consists out of a set of MAPLE procedures for the numerical and analytical evaluation of the Coulomb wave and Green's functions, both within the nonrelativistic and relativistic framework. Apart from these functions, moreover, the computation of radial integrals (as they frequently arise in the evaluation of transition amplitudes for various types operators) is supported by means of the DIRAC program by implementing the analytic formulas.

Of course, the procedures above can be seen also as the *technical basis* for more advanced studies concerning the behavior of the hydrogen-like ions or, more generally, applications of the atomic shell model. In the future, therefore, several lines are possible (and desirable) for the further development of the DIRAC program. In a first step, we want to extend the present set of procedures towards the interaction of hydrogen-like ions with the radiation field as it occurs in the ionization or capture of electrons by high-Z ions or in laser fields. Examples of very desirable procedures refer to a simple access to the decay rates, angular distributions, or to the polarization of the emitted radiation. Having collaborations with the atomic physics community at GSI and elsewhere for many years, we know that these developments will make the DIRAC package attractive to both, experimental and theoretical investigations on energetic ion–atom and ion–electron collisions.

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