Computer Physics Communications 141 (2001) 73–82

Computer Physics Communications

www.elsevier.com/locate/cpc

Calculation of the matrix elements of the Coulomb interaction involving relativistic hydrogenic wave functions ☆,☆☆

L. Lugosi, L. Sarkadi *

Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), P.O. Box 51, H-4001 Debrecen, Hungary

Received 23 April 2001; accepted 23 May 2001

Abstract

A program is presented for calculation of the matrix elements of the Coulomb interaction between a charged particle and an atomic electron, $\int \psi_f^{\dagger}(\boldsymbol{r})|\boldsymbol{R}-\boldsymbol{r}|^{-1}\psi_i(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}$. Bound-free transitions are considered. Relativistic hydrogenic wave functions are used for the numerical evaluation of the matrix elements. The applied algorithm is based on the multipole series expansion of the Coulomb potential. The radial part of the terms of this series expansion (known as G functions) can also be obtained.

PACS: 34.50.Fa; 34.80.Dp; 34.80.Kw

Keywords: Coulomb interaction; Matrix elements; Ionization; Relativistic hydrogenic wave functions; Dirac–Coulomb functions; Multipole series expansion

PROGRAM SUMMARY

Title of program: MTRDCOUL

Catalogue identifier: ADOX

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

Program Summary URL: http://cpc.cs.qub.ac.uk/summaries/ADOX

Computer for which the program is designed: IBM compatible PC with Pentium processor

Operating system under which the program has been tested: MS-DOS

Programming language used: Fortran 77

Memory required to execute with typical data: 200 kbytes

No. of bits in a word: 8

No. of bytes in distributed program, including test data, etc.: 15 020

Distribution format: gzip file

☆ Work supported by the Hungarian Scientific Research Foundation (OTKA, Grant No. T031833).
☆☆ This program can be downloaded from the CPC Program Library under catalogue identifier: http://cpc.cs.qub.ac.uk/summaries/ADOX
* Corresponding author.
E-mail address: sarkadil@atomki.hu (L. Sarkadi).

0010-4655/01/$ – see front matter
PII: S0010-4655(01)00294-6

CPC Program Library subprograms used: F3Y [1] (catalogue number: AAQQ); DCOUL [2] (catalogue number: ADBP). The subprograms are included in the distributed program

Keywords: Coulomb interaction, matrix elements, ionization, relativistic hydrogenic wave functions, Dirac–Coulomb functions, multipole series expansion

Nature of physical problem
The theoretical description of the excitation and ionization of atoms by charged particle impact often requires the knowledge of the matrix elements of the Coulomb interaction. The program MTRDCOUL calculates the matrix elements between bound and free states represented by relativistic hydrogenic wave functions.

Method of solution
The multipole series expansion of the Coulomb potential is used to solve the problem.

Restrictions on the complexity of the problem
The matrix elements are calculated with the following restrictions. The initial bound states are limited to $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, $3d_{5/2}$. The quantum number l in the final state has a maximum value of 10.

Typical running time
The test run requires about 170 s.

References
[1] A. Liberato de Brito, Comput. Phys. Commun. 25 (1982) 81.
[2] F. Salvat, J.M. Fernández-Varea, W. Williamson Jr., Comput. Phys. Commun. 90 (1995) 151.

LONG WRITE-UP

1. Introduction

This study is an extension of a previous work [1] in which a computer program (called MTRXCOUL) was developed to calculate the matrix elements of the Coulomb interaction between a charged particle and an atomic electron,

$$V_{fi}(\boldsymbol{R}) = \left\langle \psi_f(\boldsymbol{r}) \left| \frac{1}{|\boldsymbol{R}-\boldsymbol{r}|} \right| \psi_i(\boldsymbol{r}) \right\rangle. \tag{1}$$

These quantities are relevant in the theoretical description of the excitation, ionization processes of atoms by impact of charged particles. In Eq. (1) $\boldsymbol{r}$ is the coordinate of the orbital electron and $\boldsymbol{R}$ is that of the incident projectile. The $\psi_j(\boldsymbol{r})$ one-electron wave functions define the dynamical state of the electron in the atom. In MTRXCOUL the initial and final states are represented by *non-relativistic* hydrogenic wave functions. It is known that at low collision velocities and for heavy target atoms the inner-shell ionization cross sections are considerably affected by electronic relativistic effects. Therefore, for an accurate description of the inner-shell processes the use of *relativistic* wave functions is unavoidable. In the present work the program MTRXCOUL was further developed: We replaced the non-relativistic wave functions by one-electron Dirac bispinors. We considered again bound-free transitions. To carry out such calculations one needs accurate Coulomb functions. In the new relativistic code (called MTRDCOUL) the DCOUL subroutine developed by Salvat et al. [2] is used for calculation of the Dirac–Coulomb functions.

2. Method of solution

Let us consider the stationary Dirac equation of an electron moving with $s = 1/2$ spin in the Coulomb field $V(r) = -Z\mathrm{e}^2/r$ of a nuclear point charge Z:

$$\widehat{H}_{\mathrm{D}} = -\mathrm{i}c\hbar\hat{\boldsymbol{\alpha}}\hat{\boldsymbol{p}} + \hat{\beta}m_e c^2 + V(r), \qquad \widehat{H}_{\mathrm{D}}\psi(\boldsymbol{r}) = (E + m_e c^2)\psi(\boldsymbol{r}). \tag{2}$$

Here $\widehat{H}_{\mathrm{D}}$ is the Dirac Hamiltonian and E is the corresponding total energy eigenvalue minus the rest energy of the electron, $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ are standard 4×4 Dirac matrices in the spinor representation, m_e is the electron mass and c is the speed of light. The $\psi(\boldsymbol{r})$ eigenstate is a four-component function. The total angular momentum vector $\widehat{\boldsymbol{J}}$ for a relativistic electron is given by $\widehat{\boldsymbol{J}} = \widehat{\boldsymbol{L}} + \widehat{\boldsymbol{S}}$, where $\widehat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$ is the orbital angular momentum operator and $\widehat{\boldsymbol{S}} = 1/2\hbar\widehat{\boldsymbol{\Sigma}}$ is the spin angular momentum operator ($\widehat{\boldsymbol{\Sigma}} = \mathrm{diag}(\hat{\boldsymbol{\sigma}}, \hat{\boldsymbol{\sigma}})$). The 2×2 matrices $\hat{\boldsymbol{\sigma}}$ are the Pauli spin matrices. The total angular momentum operator commutes with the central field Dirac Hamiltonian: $[\widehat{\boldsymbol{J}}, \widehat{H}_{\mathrm{D}}] = 0$. One can, therefore construct simultaneous eigenstates of the three commuting operators $\widehat{H}_{\mathrm{D}}$, $\widehat{\boldsymbol{J}}^2$ and $\widehat{J}_z$. The operators $\{\widehat{\boldsymbol{J}}^2, \widehat{J}_z, \widehat{\boldsymbol{L}}^2, \widehat{\boldsymbol{S}}^2\}$ form a complete set of commuting observables (C.S.C.O.). The common eigenstates of these operators are the two-component spherical spinors

$$\Omega_{jlm_j}(\hat{\boldsymbol{r}}) = \sum_{m_s=\pm 1/2} (lm_l sm_s|jm_j) Y_{lm_j-m_s}\chi_{sm_s}, \tag{3}$$

where $j = 1/2, 3/2, 5/2, \ldots$ is the total angular momentum quantum number and $m_j = -j, -j+1/2, \ldots, j-1/2, j$ is its z-projection. In Eq. (3) Y_{lm_l} is a spherical harmonics which is eigenfunction of the $\widehat{\boldsymbol{L}}^2$ and $\widehat{L}_z$ operators with eigenvalues $l(l+1)$ and m_l ($l = 0, 1, 2, \ldots$; $m_l = -l, -l+1, \ldots, l-1, l$), as well as χ_{sm_s} are two-component eigenfunctions of the $\widehat{\boldsymbol{S}}^2$ and $\widehat{S}_z$ operators with eigenvalues $s(s+1) = 3/4$ and $m_s = \pm 1/2$. The quantities $(lm_l sm_s|jm_j)$ are the Clebsch–Gordan coefficients. There are two possible l values in Eq. (3) for each value of j: $l = j + 1/2$ and $l = j - 1/2$. The corresponding spherical spinors have opposite parity. Since for relativistic electron motion the orbital angular momentum is not conserved, the upper and lower components of the Dirac bispinor differ in their orbital angular momentum quantum numbers. The eigenstates $\psi(\boldsymbol{r})$ are usually characterized by the eigenvalue κ of the Dirac angular momentum operator $\widehat{K} = -\hat{\beta}(\widehat{\boldsymbol{\Sigma}} \cdot \widehat{\boldsymbol{L}} + \hbar)$ and by the magnetic quantum number m_j. We note that $\widehat{K}\Omega_{jlm_j} = \kappa\Omega_{jlm_j}$, where $\kappa = -(j+1/2)$ for $j = l + 1/2$, and $\kappa = j + 1/2$ for $j = l - 1/2$. The operator $\widehat{K}$ has integer eigenvalues $\kappa = \pm 1, \pm 2, \ldots$. We introduce the more compact notation $\Omega_{jlm_j}(\hat{\boldsymbol{r}}) \stackrel{\mathrm{def}}{=} \Omega_{\kappa m_j}(\hat{\boldsymbol{r}})$. The oparators $\{\widehat{H}_{\mathrm{D}}, \widehat{\boldsymbol{J}}^2, \widehat{J}_z, \widehat{K}\}$ also form C.S.C.O., thus we can label the common eigenstates with quantum numbers n, j, m_j and κ. Here $n = 0, 1, 2, \ldots$ is the principal quantum number. At the end, the one-electron Dirac orbital $\psi_{n\kappa m_j}(\boldsymbol{r})$ can be expressed in the form

$$\psi_{n\kappa m_j}(\boldsymbol{r}) = \left\{ \begin{array}{c} \mathrm{i} g_{n\kappa}(r)\Omega_{\kappa m_j}(\hat{\boldsymbol{r}}) \\ f_{n\kappa}(r)\Omega_{-\kappa m_j}(\hat{\boldsymbol{r}}) \end{array} \right\}, \tag{4}$$

where $g(r)$ and $f(r)$ are the upper- and lower-component radial wave functions, and the $\Omega_{\kappa m_j}(\hat{\boldsymbol{r}})$, $\Omega_{-\kappa m_j}(\hat{\boldsymbol{r}})$ functions give the angular parts of the eigenstate.

The matrix elements (1) are evaluated using the *multipole series expansion* of the Coulomb potential

$$\frac{1}{|\boldsymbol{R} - \boldsymbol{r}|} = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \frac{4\pi}{2L+1} \frac{(r_<)^L}{(r_>)^{L+1}} Y^*_{LM}(\widehat{\boldsymbol{R}}) Y_{LM}(\hat{\boldsymbol{r}}). \tag{5}$$

Inserting (5) into (1), it follows from the relation

$$\langle \Omega_{\kappa_f m_{j_f}} | Y_{LM} | \Omega_{\kappa_i m_{j_i}} \rangle = \langle \Omega_{-\kappa_f m_{j_f}} | Y_{LM} | \Omega_{-\kappa_i m_{j_i}} \rangle \tag{6}$$

that

$$\begin{aligned} V_{fi}(\boldsymbol{R}) = & \sum_{m_s=\pm 1/2} (l_f, m_{j_f} - m_s, s, m_s | j_f, m_{j_f})(l_i, m_{j_i} - m_s, s, m_s | j_i, m_{j_i}) \\ & \times \sum_{L=L_{\min}}^{L_{\max}} \sum_{M=-L}^{L} \frac{4\pi}{2L+1} G^L_{fi}(R) Y^*_{LM}(\widehat{\boldsymbol{R}}) C^{LM}_{fi}, \end{aligned} \tag{7}$$

where

$$G^L_{fi}(R) = \frac{1}{R^{L+1}}\int_0^R \left[g^*_f(r)g_i(r) + f^*_f(r)f_i(r)\right]r^L r^2\,\mathrm{d}r + R^L\int_R^\infty \left[g^*_f(r)g_i(r) + f^*_f(r)f_i(r)\right]\frac{1}{r^{L+1}}r^2\,\mathrm{d}r \quad (8)$$

is the *form factor* and

$$C^{LM}_{fi} = \int Y^*_{l_f,m_{j_f}-m_s}(\hat{\boldsymbol{r}})Y_{LM}(\hat{\boldsymbol{r}})Y_{l_i,m_{j_i}-m_s}(\hat{\boldsymbol{r}})\,\mathrm{d}\Omega_r \quad (9)$$

is the *geometrical factor*. We use the Wigner–Ekhart theorem to express the integral of the product of three spherical harmonics. It can be given in terms of the Wigner three-j symbols

$$C^{LM}_{fi} = \langle Y_{l_1m_1}|Y_{l_2m_2}|Y_{l_3m_3}\rangle = (-1)^{m_1}\left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right]^{1/2} \times \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (10)$$

The values of C^{LM}_{fi} are obtained using the F3Y subprogram [3]. The Clebsch–Gordan coefficients are evaluated according to the following expressions:

$$(l, m_l, s, m_s = \pm 1/2|j, m_j) = \left(\frac{j \pm m_j}{2j}\right)^{1/2}, \qquad \text{if } j = l + 1/2,$$
$$(l, m_l, s, m_s = \pm 1/2|j, m_j) = \left(\frac{j + 1 \mp m_j}{2j+2}\right)^{1/2}, \quad \text{if } j = l - 1/2. \quad (11)$$

The values of $L_{\min}$ and $L_{\max}$ in Eq. (7) are determined by the properties of C^{LM}_{fi}. In Eq. (10) l_j and m_j should meet the following conditions (otherwise $C^{LM}_{fi} = 0$):

(i) $l_1 + l_2 + l_3$ is even (this ensures the parity conservation),
(ii) $m_1 + m_2 + m_3 = 0$.

Condition (i) determines the range of multipole order ($L = L_{\min}, L_{\min} + 2, \ldots, L_{\max}$), condition (ii) reduces the summation over L and M to terms with $|j_f - j_i| \leqslant L \leqslant |j_f + j_i|$ and $M = m_{j_f} - m_{j_i}$, respectively.

3. Radial Dirac wave functions

Introducing the fine-structure constant $\alpha = \mathrm{e}^2/\hbar c = 1/137.036$, as well as the $\zeta = \alpha Z$ and $\lambda = \sqrt{\kappa^2 - \zeta^2}$ variables, the Sommerfeld formula for the *bound* hydrogenic eigenenergies can be written as

$$W_{n\kappa} = m_e c^2 \cdot w_{n\kappa}, \quad w_{n\kappa} = \left[1 + \left(\frac{\zeta}{n_r + \lambda}\right)^2\right]^{-1/2}, \quad (12)$$

where the radial quantum number $n_r = 0, 1, 2, \ldots$ is related to the principal quantum number by $n = n_r + |\kappa|$. Furthermore, we introduce the notations $\lambda_c = \hbar/m_e c$ (the electron Compton wavelength divided by 2π) and $\nu_{n\kappa} = \sqrt{1 - w^2_{n\kappa}}/\lambda_c$ (the bound-state wave number). With these notations the radial bound wave functions $g(r)$ and $f(r)$ can be expressed by the confluent hypergeometric functions ${}_1\mathrm{F}_1(a, c; x)$ as

$$\left.\begin{matrix} g(r) \\ f(r) \end{matrix}\right\} = \left.\begin{matrix} N_g \\ N_f \end{matrix}\right\} (2\nu r)^{\lambda-1}\mathrm{e}^{-\nu r}\left[\left(\frac{\zeta}{\nu\lambda_c} - \kappa\right){}_1\mathrm{F}_1(-n_r, 2\lambda+1; 2\nu r) \mp n_r\,{}_1\mathrm{F}_1(1-n_r, 2\lambda+1; 2\nu r)\right] \quad (13)$$

with the normalization factors

$$\left.\begin{matrix} N_g \\ N_f \end{matrix}\right\} = (-1)^{\epsilon} \frac{\sqrt{2}\nu^{5/2}\lambda_c}{\Gamma(2\lambda+1)} \left[\frac{(1\pm w)\Gamma(2\lambda+1+n_r)}{\zeta(\zeta-\kappa\nu\lambda_c)n_r!}\right]^{1/2}. \tag{14}$$

(The definition of the parameter ϵ will be given later.) In Eqs. (13) and (14) we omitted the indices n, κ from the variables $\nu_{n\kappa}$ and $w_{n\kappa}$.

Introducing the quantities

$$k = \frac{1}{\lambda_c}\sqrt{w^2-1}, \qquad \eta = \frac{\zeta w}{k\lambda_c}, \qquad \mathrm{e}^{2\mathrm{i}\Delta_\kappa} = \frac{-\kappa+\mathrm{i}\eta/w}{\lambda+\mathrm{i}\eta}, \tag{15}$$

the radial hydrogenic *continuum* wave functions belonging to electron energy $W = m_e c^2 \cdot w$ has the following form:

$$\left.\begin{matrix} g(r) \\ f(r) \end{matrix}\right\} = (-1)^{\epsilon} \sqrt{\frac{k}{\pi E}} \sqrt{\frac{w\pm 1}{w+1}} \mathrm{e}^{\frac{1}{2}\eta\pi} \frac{|\Gamma(\lambda+\mathrm{i}\eta)|}{\Gamma(2\lambda+1)} \frac{(2kr)^{\lambda}}{r}$$

$$\times \begin{matrix} \mathrm{Re} \\ \mathrm{Im} \end{matrix} \left\{\mathrm{e}^{-\mathrm{i}kr+\mathrm{i}\Delta_\kappa}(\lambda+\mathrm{i}\eta)\cdot {}_1\mathrm{F}_1(\lambda+1+\mathrm{i}\eta, 2\lambda+1; 2\mathrm{i}kr)\right\}. \tag{16}$$

Methods to construct analytical expression for the bound- and free-state solutions of the Dirac-equation in central field have been described in detail by Greiner [4] and Rose [5]. For numerical calculation of the radial continuum Dirac–Coulomb functions we use a program developed by Salvat et al. [2].

The bound-state wave functions are normalized to unity. The normalization of the free states is such that the upper component oscillates with unit amplitude in the asymptotic region apart from the energy normalization factor $(k/(\pi E))^{1/2}$. It is a natural expectation that in the non-relativistic limit the upper component reduces to the non-relativistic Coulomb function, and the lower component vanishes. For calculation of the bound-state wave functions we adopted the normalization condition determined by Salvat et al. [2] which gives correct sign for this limit. This is ensured by the factor $(-1)^{\epsilon}$ in Eqs. (14) and (16): ϵ equals 0 when $\kappa < 0$, or equals 1 when $\kappa > 0$ (for an attractive potential, i.e. for $\zeta > 0$).

4. Code description

Since MTRDCOUL is the relativistic extension of MTRXCOUL [1], here we discuss only the differences between the two programs.

The matrix element V_{fi} for the eigenstates of the total angular momentum j is determined by the function VJ according to Eq. (7). The value of VJ is obtained with the help of the function VK that calculates the Coulomb matrix element for eigenstates of the Dirac angular momentum $\kappa = (2j+1)(l-j)$ (the term with the sum over L and M in Eq. (7)). This function was named by VL in MTRXCOUL. Taking into account that the Dirac radial wave functions depend on the j quantum number, the parameter list of VK includes also the j_i and j_f quantum numbers in the relativistic version.

Before using the function VJ or VK, one has to call the subroutine PREPARE. This program unit calculates the values of $G^L_{fi}(R)$ and stores them in the array GMTRX. PREPARE also includes the j_i quantum number in its parameter list. In the relativistic case the radial wave function has two components, accordingly the two integrands in expression (8) of the $G^L_{fi}(R)$ function consists of two terms. Therefore, we modified the integration subroutine QGAUS, too.

The final orbital angular momentum l varies in the range from 0 to $l_{f\max}$ defined by the user. The quantum numbers l and κ are related by

$$l = \begin{cases} \kappa, & \text{if } \kappa > 0 \\ -\kappa - 1, & \text{if } \kappa < 0. \end{cases} \tag{17}$$

So, the first index of array GMTRX now corresponds to the value of κ_f which is changing between $-l_{f\max} - 1$, $-l_{f\max}, \ldots, -1, 1, \ldots, l_{f\max} - 1, l_{f\max}$ according to Eq. (17). For more details of the program description, see Sarkadi [1].

The components of the bound and continuum radial wave functions (see Eqs. (13) and (16)) are generated by the RINIT and RFINAL subroutines. For the K, L and M shells the bound wave functions g and f can be written in the following simple forms:

$$\left.\begin{matrix} g_i(\rho) \\ f_i(\rho) \end{matrix}\right\} = (-1)^{\epsilon} N_i (1 \pm w_i)^{1/2} \rho^{\lambda_i - 1} \mathrm{e}^{-\mu_i \rho} \left\{\begin{matrix} a_0 + a_1\rho + a_2\rho^2 \\ c_0 + c_1\rho + c_2\rho^2 \end{matrix}\right\}, \tag{18}$$

where $\rho = Zr$ and $\mu_i = \nu_i/Z$. For the K shell and the L subshells the coefficients a_k and c_k were taken from Rose [5], while for the M subshells they were derived in the present work.

For the free states the radial wave functions are as follows:

$$\left.\begin{matrix} g_{E\kappa_f}(\rho) \\ f_{E\kappa_f}(\rho) \end{matrix}\right\} = \frac{Z}{\rho}\left(\frac{k}{\pi E}\right)^{1/2} \left\{\begin{matrix} F^{(u)}_{\lambda_f}\left(\eta, \frac{k\rho}{Z}\right) \\ F^{(l)}_{\lambda_f}\left(\eta, \frac{k\rho}{Z}\right) \end{matrix}\right\}. \tag{19}$$

The regular Dirac–Coulomb functions $F^{(u,l)}_{\lambda}(\eta, x)$ are provided by the code DCOUL [2] for $E \neq 0$. DCOUL is called as

CALL DCOUL(−Z, E, K, R, FU, FL, GU, GL, ERR).

Here Z is the atomic number, E is the kinetic energy, K $= \kappa$, R is the radial distance. FU, FL and GU, GL are the upper- and lower-components of the regular and irregular Dirac–Coulomb functions, ERR is the accuracy of the computed functions.

At limit of zero kinetic energy the relativistic continuum wave functions in the Coulomb field have the following form [6]:

$$g_{E=0,\kappa_f}(\rho) = (-1)^{\epsilon}\sqrt{\frac{2Z}{\rho}}\left[J_{2\lambda_f - 1}\left(\sqrt{8\rho}\right) - \frac{\lambda_f + \kappa_f}{\sqrt{2\rho}} J_{2\lambda_f}\left(\sqrt{8\rho}\right)\right], \tag{20}$$

$$f_{E=0,\kappa_f}(\rho) = (-1)^{\epsilon}\frac{Z^{1/2}}{\rho}\zeta J_{2\lambda_f}\left(\sqrt{8\rho}\right), \tag{21}$$

where $J_z(x)$ is the fractional order Bessel function. For calculation of $J_z(x)$ we use the relationship

$$J_z(x) = \sqrt{\frac{2}{\pi x}} F_{z-1/2}(0, x). \tag{22}$$

Here $F_{\upsilon}(\eta, x)$ is the regular Schrödinger–Coulomb function which is calculated by the subroutine FCOUL [2] with the following parameters:

CALL FCOUL(ETA, RLAMB, X, F, FP, G, GP, ERR)

ETA $= \eta = 0$, RLAMB $= z - 1/2$, X $= (8\rho)^{1/2}$, F and G are the regular and irregular Schrödinger–Coulomb functions, FP and GP are their derivatives, ERR is the relative numerical uncertainty.

5. Check of the program

For bound-free transitions, in the special case of $E_f = 0$, the limits $G^L_{fi}(R = 0)$ and $G^L_{fi}(R \to \infty)$ can be expressed analytically, therefore the numerically computed values can be checked for these G functions. In this section we present some examples for the calculation of the G matrix. First we consider the $2p_{3/2}$ initial state and the $E_f = 0$ final state with $\kappa_f = 1$. In this case the parameters in Eq. (18) are as follows: $N = Z^{3/2}/[2\Gamma(2\lambda_i + 1)]^{1/2}$, $w_i = \lambda_i/2$, $\mu_i = 1/2$, $a_0 = c_0 = 1$, $a_1 = a_2 = c_1 = c_2 = 0$. Using expressions (20) and (21) for the initial and final states, as well as applying the integral formula of Ref. [7], the integration (8) of the G the function can be performed analytically for large values of R in the quadrupole order:

$$G^2_{fi}(R \to \infty) = \frac{C^\infty}{(Z \cdot R)^3}, \tag{23}$$

where

$$\begin{aligned} C^\infty = & -2^{2\lambda_f+\lambda_i+3}\frac{\Gamma(\lambda_i+\lambda_f+3)}{[2\Gamma(2\lambda_i+1)]^{1/2}}\left(1+\frac{\lambda_i}{2}\right)^{1/2} \\ & \times\left\{\frac{1}{\Gamma(2\lambda_f)}\,{}_1\mathrm{F}_1(\lambda_i+\lambda_f+3,2\lambda_f;-4)\right. \\ & \left.+\left[\left(\frac{2-\lambda_i}{2+\lambda_i}\right)^{1/2}\zeta-\lambda_f-\kappa_f\right]\frac{1}{\Gamma(2\lambda_f+1)}\,{}_1\mathrm{F}_1(\lambda_i+\lambda_f+3,2\lambda_f+1;-4)\right\}. \end{aligned} \tag{24}$$

As a second example, let us consider the G functions values at $R = 0$ for different final states (with $E_f = 0$) and multipole orders. As initial state, the $2p_{3/2}$ orbital was chosen again. The analytical term of the G function at the origin is:

$$G^L_{fi}(R \to 0) = C^0(Z \cdot R)^L, \tag{25}$$

where

$$\begin{aligned} C^0 = & -\mathrm{sgn}(\kappa_f)2^{2\lambda_f+\lambda_i-L}\frac{\Gamma(\lambda_i+\lambda_f-L)}{[2\Gamma(2\lambda_i+1)]^{1/2}}\left(1+\frac{\lambda_i}{2}\right)^{1/2} \\ & \times\left\{\frac{1}{\Gamma(2\lambda_f)}\,{}_1\mathrm{F}_1(\lambda_i+\lambda_f-L,2\lambda_f;-4)\right. \\ & \left.+\left[\left(\frac{2-\lambda_i}{2+\lambda_i}\right)^{1/2}\zeta-\lambda_f-\kappa_f\right]\frac{1}{\Gamma(2\lambda_f+1)}\,{}_1\mathrm{F}_1(\lambda_i+\lambda_f-L,2\lambda_f+1;-4)\right\}. \end{aligned} \tag{26}$$

The results of these calculations are shown in the sample program. The convergence of the matrix elements for $E_f = 0$ to those for small and nonzero ($E_f \neq 0$) energy has been checked.

As a further check of MTRDCOUL, we calculated K-, L- and M-shell ionization probabilities and cross sections for proton on gold collisions within the framework of relativistic version (R) of the semiclassical approximation (SCA) theory [8]. According to this RSCA model the ionization amplitude a_{fi} is given by

$$a_{fi} = -\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\, V_{fi}(t)\mathrm{e}^{\mathrm{i}(E_f-E_i)t}, \tag{27}$$

where

$$V_{fi}(t) = \int \mathrm{d}\boldsymbol{r}\,\psi_f^\dagger(\boldsymbol{r})\frac{-Z_P}{|\boldsymbol{r}-\boldsymbol{R}(t,b)|}\psi_i(\boldsymbol{r}). \tag{28}$$

Here Z_P is the charge of the projectile, b is the impact parameter. The V_{fi} matrix elements are obtained from our program MTRDCOUL. For the description of the states of the inner-shell electrons, an effective Slater-screened nuclear charge Z of the target atom was used in conjuction with the experimental binding energy.

The transition amplitudes allow us to calculate the ionization probability as a function of the impact parameter

$$P_i(b) = \sum_f |a_{fi}|^2, \tag{29}$$

where the sum is taken over all continuum states (including integration over E_f). The total ionization cross section is given by

$$\sigma_i = 2\pi \int_0^\infty \mathrm{d}b\, b P_i(b). \tag{30}$$

The calculated values of the K-shell ionization cross sections were compared with the results of the relativistic plane-wave Born approximation (RPWBA) [9] in the energy range 1–5 MeV. For the L_1, L_2 and L_3 subshells the check was made at 0.4 MeV. The obtained cross sections were compared again with the predictions of the RPWBA model [10]. For the $M_1, M_2, \ldots, M_5$ subshells we could not compare our results with other theories in lack of relativistic M-shell ionization calculations in the literature (with use of hydrogenic Dirac wave functions). Since the relativistic effects are small for the M shell, here we could make a comparison with the non-relativistic SCA model. In the latter calculations the matrix elements were computed with MTRXCOUL [1]. The check for the M shell was made at 0.5 MeV proton energy. For each shells (subshells) the present RSCA calculations were found in satisfactory agreement with the other theoretical data. The above calculations were made assuming straight-line for the projectile trajectory. As a further test, the K-shell ionization cross sections were also computed with a more realistic version of the RSCA model, in which the projectile moves on a hyperbolic trajectory (H), and the increase of the binding energy of the electron is taken into account in the united-atom approximation (UA). The latter model, denoted by HRSCA-UA, resulted in cross section values in good agreement with the measured data of Kamiya et al. [11].

6. Sample program

The MAIN program of MTRDCOUL includes sample calculations of the matrix elements V_{fi} and the values of the $G^L_{fi}(R)$ function for several initial and final states. These are the following:

- Matrix elements between states of the total angular momentum. The quantum numbers of the initial and final states are: $n_i = 2, l_i = 0, j_i = 1/2, m_{ji} = 1/2$; $E_f = 0.1$, $j_f = 1/2, m_{jf} = 1/2$. The values of l_f are 0 and 1, because of the relationship $j_f = l_f \pm 1/2$. The polar coordinates R, θ of the vector $\boldsymbol{R}$ was chosen that R varies between $0 \ldots 10$ in steps 1 and $\theta = 0.5$ radian.
- Comparison of numerically computed $G^L_{fi}(R \to \infty)$ values with the corresponding analytical ones for large values of R. Initial state: $n_i = 2$, $j_i = 3/2$, $l_i = 1$. Final state: $E_f = 0$, $j_f = 3/2$, $l_f = 1$. Multipole order: $L = 2$. The analytical result: C^∞/R^3.
- The numerically computed $G^L_{fi}(R \to 0)$ values are compared with the analytical results at the origin for different multipole orders ($L = 2, 0, 1, 0, 3$) and final states. Initial state: $n_i = 2$, $j_i = 3/2$, $l_i = 1$. Final states: $E_f = 0$, $j_f = 1/2, 1/2, 1/2, 3/2, 3/2$; $l_f = 1, 1, 0, 1, 2$. The analytical results: 0, $C^0_{E_f=0,\kappa_f=1}$, 0, $C^0_{E_f=0,\kappa_f=-2}$, 0.

In the above sample calculations $Z = 1$ was taken for the nuclear charge of the atom. The C^∞ and C^0 constants were evaluated using the MAPLE mathematical software system [12].

References

[1] L. Sarkadi, Comput. Phys. Commun. 133 (2000) 119.
[2] F. Salvat, J.M. Fernández-Varea, W. Williamson Jr., Comput. Phys. Commun. 90 (1995) 151.
[3] A. Liberato de Brito, Comput. Phys. Commun. 25 (1982) 81.
[4] W. Greiner, Relativistic Quantum Mechanics — Wave Equations, Springer, Berlin, 1990.
[5] M.E. Rose, Relativistic Electron Theory, John Wiley and Sons, New York, 1961.
[6] T. Mukoyama, L. Sarkadi, Bull. Inst. Chem. Res., Kyoto Univ. 66 (1988) 11.
[7] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, Natl. Bur. Stand. (U.S.) Appl. Math. Ser., Vol. 55, U.S. GPO, Washington, DC, 1964, integral formula No. 11.4.28., pp. 486.
[8] J. Bang, J.M. Hansteen, Kgl. Danske Videnskap. Selskab, Mat.-Fys. Medd. 31 (1959), No. 13.
[9] T. Mukoyama, L. Sarkadi, Bull. Inst. Chem. Res., Kyoto Univ. 57 (1979) 1.
[10] T. Mukoyama, L. Sarkadi, Phys. Rev. A 25 (1981) 1411.
[11] M. Kamiya, K. Ishii, K. Sera, H. Tawara, Phys. Rev. A 16 (1977) 2295.
[12] M. Monagan, K. Geddes, K. Heal, G. Labahn, S. Vorkoetter, Maple V Programming Guide for Release 5, Springer, Berlin, 1997.

TEST RUN OUTPUT

```
 Matrix elements between states of the total angular momentum
 n_i =  1   l_i =  0   j_i =  1/2   mj_i =  1/2   j_f =  1/2   mj_f =  1/2
 E_f = 0.10000D+00    theta = 0.50000D+00

   Z*R            V(l_f=0)                  V(l_f=1)

   0.00     0.510150603681870D+00     0.643348846461918D-16
   1.00     0.251310302012083D+00    -0.104795445906079D+00
   2.00     0.623079628296980D-01    -0.944000425736001D-01
   3.00     0.691992348636800D-02    -0.584261981291566D-01
   4.00    -0.205056097180007D-02    -0.331396045444634D-01
   5.00    -0.153499086559949D-02    -0.196686893562784D-01
   6.00    -0.534621795843407D-03    -0.128820869819304D-01
   7.00    -0.110457479251192D-03    -0.923660832344591D-02
   8.00     0.868285167879229D-07    -0.703804296715670D-02
   9.00     0.127773525167063D-04    -0.556832819077795D-02
  10.00     0.757633525158059D-05    -0.451822132300222D-02

 G function values for large R
 n_i =  2   kappa_i = -2   kappa_f =  1
 E_f = 0.00000D+00
   Z*R       G(L=2, numerical)    G(L=2, analyt.)=const./(Z*R)**3

  50.00    -0.245005727643649D-03    -0.245005823050562D-03
  70.00    -0.892878363960091D-04    -0.892878363886889D-04
  90.00    -0.420106006602451D-04    -0.420106006602473D-04
 110.00    -0.230095626456201D-04    -0.230095626456200D-04
 130.00    -0.139397942108877D-04    -0.139397942108877D-04
 150.00    -0.907428974261342D-05    -0.907428974261342D-05

G function values at R=0
E_f = 0.00000D+00

L  kappa_f  n_i  kappa_i        G, numerical             G, analytical

2     1      2     -2      0.107676238637811D-30      0.000000000000000D+00
0     1      2     -2      0.239267242032862D+00      0.239267242032860D+00
1    -1      2     -2      0.299102568323444D-16      0.000000000000000D+00
0    -2      2     -2      0.239276898638137D+00      0.239276898638135D+00
3     2      2     -2      0.119638449319068D-15      0.000000000000000D+00
```