The library of subroutines for calculating standard quantities in atomic structure theory

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Abstract

This library (collection of subroutines) is presented for calculating standard quantities in the decomposition of many–electron matrix elements in atomic structure theory. These quantities include the coefficients of fractional parentage, the reduced coefficients of fractional parentage as well as reduced and completely reduced matrix elements for several operators. So the library is assigned for any computational scheme. The software is an implementation of a methodology based on the second quantization in coupled tensorial form, the angular momentum theory in 3 spaces (orbital, spin and quasispin), and the graphical technique of angular momentum. This implementation extends applications in atomic theory capabilities to partially filled f–shells and has lead to faster execution of angular integration codes.

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Keywords: atomic structure, Clebsch–Gordan coefficient, configuration interaction, complex atom, correlation, bound states, LS–coupling, matrix elements, 3nj–coefficients.
PROGRAM SUMMARY

Title of program : SQ

Catalogue identifier:

Program obtainable from: State Institute of Theoretical Physic and Astronomy, A. Goštauto 12, Vilnius, 2600, LITHUANIA. E-mail: gaigalas@itpa.lt

Computer for which the library is designed and others on which it has been tested:
Computers: Pentium–based PCs

Installations: Institute of Theoretical Physics and Astronomy, A. Goštauto 12, Vilnius, 2600, LITHUANIA

Operating systems or monitors under which the new version has been tested: Sun UNIX, LINUX 2.2.3

Programming language used in the new version: FORTRAN 77

Memory required to execute with typical data: 6000K Bytes

Peripherals used: terminal, disk

No. of bits in a word: 32

No. of processors used: 1

Has the code been vectorised or parallelized?: no

No. of bytes in distributed program, including test data, etc.: 285 000 bytes

Distribution format: compressed tar file

CPC Program Library subprograms used: none

Additional keywords : atomic structure, Clebsch–Gordan coefficient, configuration interaction, Reduced coefficients of fractional parentage, irreducible tensors, angular momentum theory in three spaces (orbit, spin and quasispin), second quantization in the coupled tensorial form, recoupling coefficients, complex atom, correlation, wave functions, bound states, LS coupling, f–shell, matrix elements, 3nj–coefficients.

Nature of physical problem
Accurate theoretical determination of atomic energy levels, orbitals and radiative transition data requires the calculation of matrix elements of physical operators accounting for relativistic and correlation effects (see the multiconfiguration Hartree–Fock method [1], for example). The spin–angular integration of these matrix elements is typically based on standard quantities like the matrix elements of the unit tensor, the (reduced) coefficients of fractional parentage as well as a number of other reduced matrix elements concerning various products of electron creation and annihilation operators [2]. These quantities arise very frequently both in configuration interaction approaches and the derivation of perturbation expansions for many–particle system using symmetry–adapted configuration state functions.

Method of solution
This program is created involving the angular methodology of [2–7]. It has been extended to include partially filled f–subshells in wavefunction expansions. The classification of terms is identical to that described in [6].

Restrictions on the complexity of the problem
For LS–coupling subshells states, the library provides coefficients and matrix elements for all subshells (nl) with \( l = 0, 1, 2 \) and 3, and \( l^2 \) for \( l \geq 3 \).

Unusual features of the program
The library can be used as an “electronic tables” of standard quantities for evaluating general matrix elements for LS–coupled functions.

References
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[6] G. Gaigalas, Z. Rudzikas and C. Froese Fischer, Atomic Data and Nuclear Data Tables 70 (1998) 1.
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LONG WRITE–UP

1 Introduction

In order to obtain accurate values of atomic quantities it is necessary to account for relativistic and correlation effects (see for example [1, 2]). Relativistic effects may be taken into account as Breit–Pauli corrections or in a fully relativistic approach. In both cases for complex atoms and ions, a considerable part of the effort must be devoted to integrations over spin–angular variables, occurring in the matrix elements of the operators under consideration.

Many existing codes for integrating are based on a scheme first proposed by Fano [3]. This approach is based on the coefficients of fractional parentage (CFP) and then the integrations over spin–angular variables constitute a considerable part of the computation, especially when atoms with many open shells are treated, and the operators are non–trivial [4]. Over the last decade, an efficient approach for finding matrix elements of any one– and two–particle atomic operator between complex configurations has been developed (see papers Gaigalas et al [5, 6, 7, 8, 9]). It is free of the shortcomings of previous approaches (see Gaigalas [10]). This approach is based on a second quantization [11] and uses a coupled tensorial form for the electron creation and annihilation operators [12]. It also applies the theory of angular momentum [13, 14] to three different approaches, but may even help to develop codes for calculating the angular parts of effective operators from the completely reduced matrix elements of the $W^{(k\nu k\nu)}$ operator.

Obviously, each computational scheme is based on a set of standard quantities to decompose the many–electron matrix elements. These quantities are either CFP, RCFP, the reduced matrix elements of the unit tensors $U^{(k)}$ and $V^{(k)}$, the completely reduced matrix elements $W^{(k\nu k\nu)}$, the completely reduced matrix elements of some tensorial products of second quantization operators, depending on the approach [1]. In this paper, we will present the library SQ (standard quantities). This library is collection of subroutines for the calculation of abovementioned standard quantities. The same standard quantities arise very frequently in effective Hamiltonian of perturbation theory or effective operator whose matrix elements between the non–relativistic $LS$ coupling states are equal to the matrix elements of the full electronic hamiltonian, between the corresponding $jj$ coupled relativistic states (see Rudzikas [1]), too. So the library not only supports large–scale computations of open–shell atoms using multiconfiguration Hartree–Fock or configuration interaction approaches, but may even help to develop codes for calculating the angular parts of effective operators from many–body perturbation theory and orthogonal operators or for evaluating relativistic hamiltonian in $LS$–coupling as well as for various versions of semi–empirical methods. The code also is intended for approaches and/or calculations presented in [15, 16, 17, 18, 19]. Some very accurate calculations was performed using this library (see for example [20, 21, 22, 23]), too.

The theoretical background of this program will be presented in the section 2. It includes a brief outline of the quasispin concept, the definitions of the RCFP and the reduced matrix elements of $W^{(k\nu k\nu)}$. The library is presented in section 3.

2 Theoretical background

The library is based on the irreducible tensorial form of the second quantization operators and on a quasispin technique. In this section we briefly describe this approach.

In the quasispin representation, for a wave function of the shell of equivalent electrons $|n l^N \alpha LS \rangle$ a label $Q$ – quasispin momentum of the shell – is introduced, which is related to the seniority quantum number $\nu$, namely, $Q = (2l + 1 – \nu)/2$, and its projection, $M_Q = (N – 2l – 1)/2$. Here $\alpha$ denotes all additional quantum numbers needed for the one–to–one classification of the energy levels. Then, we can rewrite the wavefunction of equivalent electrons as

$$|n l^N \alpha Q LS M_Q \rangle. \quad (1)$$

Making use of the Wigner–Eckart theorem in quasispin space of a shell $l^N$,

$$\left( l^N \alpha Q LS M_Q \langle T_{m_y}^{(k\nu k\nu)} | l'^N \alpha' Q' L'S'M'_Q \right)$$


\[ = (-1)^{2q_s} [Q]^{-1/2} \left[ \begin{array}{ccc} Q' & k_q & Q \\ M'_Q & m_q & M_Q \end{array} \right] \left( l \alpha Q L S ||| T^{(k_q k_s)} ||| l \alpha' Q' L' S' \right) \] (2)

it is possible to define the notions of a completely reduced matrix element \((l \alpha Q L S ||| T^{(k_q k_s)} ||| l \alpha' Q' L' S')\). In (2) \(T^{(k_q k_s)}\) is any tensor with rank \(k_q\) and its projection \(m_q\) in quasispin space and on the right–hand side of this equation only the Clebsch–Gordan coefficient \[ \left[ \begin{array}{ccc} Q' & k_q & Q \\ M'_Q & m_q & M_Q \end{array} \right] \]

depends on the number \(N\) of equivalent electrons.

The electron creation \(a_{m_{l_s} m_s}^{(l_s)}\) and annihilation \(a_{-m_{l_s} -m_s}^{(l_s)}\) operators play a key role in the theory of second quantization and atomic structure [11]. Using the quasispin concept, the operators \(a_{m_{l_s} m_s}^{(l_s)}\) and \(\tilde{a}_{m_{l_s} m_s}^{(l_s)} = (-1)^{l + m_{l_s} - m_s} \cdot a_{-m_{l_s} -m_s}^{(l_s)}\) also form components of an irreducible tensor of rank \(q = \frac{1}{2}\) in \(Q\)–space, i.e.

\[
a_{m_{q(s)} m_{l_s} m_s}^{(q(l_s))} = \begin{cases} a_{m_{l_s} m_s}^{(l_s)} & \text{for } m_q = \frac{1}{2}, \\ \tilde{a}_{m_{l_s} m_s}^{(l_s)} & \text{for } m_q = -\frac{1}{2}. \end{cases} \tag{3}
\]

Compared with the electron creation and annihilation operators above, the operators \(a_{m_{q(s)} m_{l_s} m_s}^{(q(l_s))}\) also act in an additional quasispin space like a tensor component with rank \(q\) and a projection \(m_q = \pm \frac{1}{2}\). There is the following relation known between the reduced matrix element of a creation operator and the CFP [24]:

\[
(l^N \alpha Q L S ||| a^{(l_s)} ||| l^{N-1} \alpha' Q' L' S') = (-1)^N \sqrt{N} [J, L, S] (l^N \alpha Q L S ||| l^{N-1} (\alpha' Q' L' S') ||| l), \tag{4}
\]

where \([L, S] \equiv (2L + 1)(2S + 1)\). Eqs. (4) and (2) can be used to define the relation between the CFP and its reduced counterpart in \(Q\)–space. Introducing the \(z\)–projection, \(M_Q\), of the quasispin, this relation is given by [1]

\[
(l^N \alpha Q L S ||| l^{N-1} (\alpha' Q' L' S') ||| l) = (-1)^{N-1} (N [Q, L, S])^{-1/2} \times \left[ \begin{array}{ccc} Q' & 1/2 & Q \\ M'_Q & 1/2 & M_Q \end{array} \right] \left( l \alpha Q L S ||| a^{(q(l_s))} ||| l \alpha' Q' L' S' \right). \tag{5}
\]

Tables of numerical values of \((l \alpha Q L S ||| a^{(q(l_s))} ||| l \alpha' Q' L' S')\) are presented in Rudzikas and Kaniauskas [12] when \(l = 0, 1, 2\). For the tensorial product of two one–electron operators, the submatrix element equals

\[
\left[ n^N \alpha Q L S \right] \left[ a_{m_{q_1} m_{q_2}}^{(q_1)} \times a_{m_{q_2} m_{q_3}}^{(q_2)} \right] \left( ^{(k_1 k_2)} \right) ||| n^N' \alpha' Q' L' S' \] = \sum_{\epsilon, m_{\epsilon}} [Q]^{-1/2} \left[ q \ k_{q_1} \ q \ m_{q_2} \ m_{\epsilon} \right] \left[ Q' \ \epsilon \ Q \ M'_Q \ m_{\epsilon} \ M_Q \right] \times (n^N \alpha Q L S ||| W^{(\epsilon k_1 k_2)} ||| n^N' \alpha' Q' L' S'). \tag{6}
\]

On the right–hand side of equations (5) and (6) only the Clebsch–Gordan coefficient \[ \left[ \begin{array}{ccc} Q' & \epsilon & Q \\ M'_Q & m_{\epsilon} & M_Q \end{array} \right] \]

depends on the number \(N\) of equivalent electrons.

\((n^N \alpha Q L S ||| W^{(\epsilon k_1 k_2)} ||| n^N \alpha' Q' L' S')\) denotes reduced in quasispin space submatrix element (completely reduced matrix element) of the triple tensor \(W^{(\epsilon k_1 k_2)} = [a^{(q(l_s))} \times a^{(q(l_s))}]^{(\epsilon k_1 k_2)}\). It is related to the RCFP in a following way:

\[
(n^N \alpha Q L S ||| W^{(\epsilon k_1 k_2)} ||| n^N \alpha' Q' L' S') = \left( (-1)^{Q+L+S+Q'+L'+S'+\epsilon+k_1+k_2 \ [\epsilon, k_1, k_2]} \right)^{1/2} \times \sum_{\alpha'' Q'' L'' S''} \left( l \alpha Q L S ||| a^{(q(l_s))} ||| l \alpha'' Q'' L'' S'' \right) \times \left( l \alpha'' Q'' L'' S'' ||| a^{(q(l_s))} ||| l \alpha' Q' L' S' \right) \times \left\{ q \ q \ \epsilon \right\} \left\{ \begin{array}{ccc} l \ l \ k_1 \ l' \ L' \ l'' \ \{ s \ s \ k_2 \ \{ s' \ s' \ S' \ S' \} \right\}. \tag{7}
\]

So, by applying the quasispin method for calculating the matrix elements of any operator, we can use the RCFP or the completely reduced matrix elements of \(W^{(\epsilon k_1 k_2)}(n^N, n^N)\), which are independent of the
occupation number of the shell. The main advantage of this approach is that the standard data tables in such a case will be much smaller in comparison with tables of the usual coefficients and, therefore, many summations will be less time-consuming. Also one can see that in such an approach the completely reduced matrix elements of standard tensors and RCFP actually can be treated in a uniform way as they all are the completely reduced matrix elements of the second quantization operators. Hence, all methodology of calculation of matrix elements will be much more universal in comparison with the traditional one.

3 Description of the Library

3.1 SAI SQLS1

The section SQLS1, (standard quantities in LS coupling, part one) is a collection of utilities for calculation of standard quantities as:

- Clebsh–Gordan coefficients of type
  \[
  \begin{bmatrix}
  Q & \frac{1}{2} & C \\
  m_Q & m_S & m_C
  \end{bmatrix},
  \begin{bmatrix}
  Q & 1 & C \\
  m_Q & 0 & m_C
  \end{bmatrix}
  \] and
  \[
  \begin{bmatrix}
  Q & 1 & C \\
  m_Q & 1 & m_C
  \end{bmatrix}.
  \]

- The 6j– and 9j– coefficients.

- The RCFP (\(l QLS \Vert \| a^{(qls)} \| l Q' L'S'\)).

- Reduced matrix element (\(l QLS \Vert \| a^{(qls)} \times a^{(qls)} \| (k_1 k_2 k_3) \Vert l Q' L'S'\)).

- The matrix elements of type (\(l^N QLS \Vert \| a^{(qls)} \times a^{(qls)} \| (k_1 k_2) \Vert l^N' Q' L'S'\)),
  \(l^N QLS \Vert \| a^{(qls)} \times a^{(qls)} \| (k_1 k_2) \times a^{(qls)} \| (k_1 k_2) \Vert l^N' Q' L'S'\),
  \(l^N QLS \Vert \| a^{(qls)} \times a^{(qls)} \| (k_1 k_2) \times a^{(qls)} \| (k_1 k_2) \Vert l^N' Q' L'S'\),
  \(l^N QLS \Vert \| a^{(qls)} \times a^{(qls)} \| (k_1 k_2) \times a^{(qls)} \| (k_1 k_2) \Vert l^N' QLS\) and
  \(l^N QLS \Vert \| a^{(qls)} \times a^{(qls)} \| (k_1 k_2) \times a^{(qls)} \| (k_1 k_2) \Vert l^N' QLS\).

The subroutines presented in this section are independent and may be useful for other programs. 67 subroutines are contained in this library. Was created the library [25] on the low–powered computers BESM–6 of the 1980s for some similar quantities for the s–, p– and d– shells. It was written in Fortran 4 and had 17 subroutines. It was based on the approach [26] and assign for calculation submatrix elements of the nonrelativistic effective Hamiltonian of atom in the first two orders of stationary perturbation theory in the case of configuration of two open–shells \(n_1 l_1^{N_1}, n_2 l_2^{N_2}\). The present library is more general and has more future because it is useful for different approaches with any number of open shells with \(l = 0, 1, 2 \) and 3, and \(l^2\) for \(l \geq 3\).

3.1.1 Common Blocks

Most of the subroutines use common block GLCONS from MCHF atomic structure package [2, 27]. The parameters contained in this block are defined in BLOCK DATA GLCONS.

The Common blocks /MT/ and /MT67/ are important, too. The first one has the array MT(40), which contains all the term characteristics of s–, p– and d– shells, that are needed while calculating matrix elements in the quasispin formalism (see Table 1). An element of the MT array is indicated in the column No of Table 1, and the Term column indicates the characteristics of a term contained in that element of MT array. In other words, for all the s–, p– and d– shells, the terms are numbered from 1 to 40. The terms are marked as \((2s+1)L(2Q+1)\) in the table.

All the terms for f– shell (see Table 2) are similarly placed in the Common block /MT67/. The No column of Table 2 indicates the term number. The TERM column has \((2s+1)L^N\) in it, the 2Q column has the quasispin momentum \(Q\) multiplied by two. See [8, 28] for the details of the classification of f– shell terms.

The Common block /MT/ is defined in BLOCK DATA TERMLS. Meanwhile the /MT67/ is defined in BLOCK DATA TRMF from the library SAI_SQLS2 (see below). BLOCK DATA TERMLS defines COMMON /SKMT2/, which contains term characteristics for special cases, i.e. for shells \(l = 3 − 9\) and shell occupation numbers \(N = 1, 2\).

Single shell data are stored in the two arrays I and B. The former consists of
Table 1: Allowed couplings of \( l^N \) states for \( l = 0 \) to \( 2 \). The subshell quasispin angular momentum \( Q \), spin angular momentum \( S \), the subshell angular momentum \( L \) and seniority quantum number \( \nu \) are denoted \( (2S+1)I(2Q+1) \).

| No | Term | No | Term | No | Term | No | Term |
|----|------|----|------|----|------|----|------|
| subshell s | subshell d | subshell s | subshell d | subshell s | subshell d | subshell s | subshell d |
| 1. | \( \frac{1}{2} \)S\(^1\) | 9. | \( \frac{3}{2} \)S\(^1\) | 19. | \( \frac{3}{2} \)F\(^1\) | 30. | \( \frac{1}{2} \)D\(^2\) |
| 2. | \( \frac{1}{2} \)S\(^2\) | 10. | \( \frac{3}{2} \)S\(^1\) | 20. | \( \frac{1}{2} \)G\(^3\) | 31. | \( \frac{1}{2} \)D\(^4\) |
| subshell p | subshell p | subshell p | subshell p | subshell p | subshell p | subshell p | subshell p |
| 3. | \( \frac{3}{2} \)S\(^1\) | 12. | \( \frac{3}{2} \)P\(^3\) | 22. | \( \frac{1}{2} \)G\(^1\) | 33. | \( \frac{3}{2} \)F\(^4\) |
| 4. | \( \frac{1}{2} \)P\(^3\) | 13. | \( \frac{1}{2} \)D\(^5\) | 24. | \( \frac{3}{2} \)P\(^1\) | 35. | \( \frac{1}{2} \)F\(^2\) |
| 5. | \( \frac{5}{2} \)D\(^1\) | 14. | \( \frac{3}{2} \)D\(^3\) | 25. | \( \frac{1}{2} \)S\(^6\) | 36. | \( \frac{1}{2} \)C\(^2\) |
| 6. | \( \frac{1}{2} \)S\(^4\) | 15. | \( \frac{1}{2} \)D\(^1\) | 26. | \( \frac{1}{2} \)S\(^2\) | 37. | \( \frac{1}{2} \)G\(^4\) |
| 7. | \( \frac{3}{2} \)P\(^2\) | 16. | \( \frac{3}{2} \)D\(^1\) | 27. | \( \frac{3}{2} \)P\(^4\) | 38. | \( \frac{1}{2} \)C\(^2\) |
| 8. | \( \frac{3}{2} \)D\(^2\) | 17. | \( \frac{3}{2} \)F\(^3\) | 28. | \( \frac{3}{2} \)P\(^2\) | 39. | \( \frac{3}{2} \)H\(^2\) |
| 9. | \( \frac{3}{2} \)F\(^3\) | 29. | \( \frac{5}{4} \)D\(^2\) | 40. | \( \frac{1}{4} \)P\(^2\) |

**Notes:**

- I(1) is the state number of the shell (see Tables 1, 2).
- I(2) is the principal quantum number \( n \).
- I(3) is the orbital quantum number \( l \).
- I(4) is the number of electrons in the subshell.
- I(5) is the shell total angular momentum \( L \) multiplied by two.
- I(6) is the shell total angular momentum \( S \) multiplied by two.
- I(7) is the shell total quasispin \( Q \) multiplied by two.

The array \( B \) contains:

- B(1) is the shell quasispin \( Q \).
- B(2) is the shell total angular momentum \( S \).
- B(3) is the shell quasispin projection \( M_Q \).

These arrays are placed in Common blocks /TRK/ and /TRK2/. In particular, these are:

**/TRK/**

| Name | Dimension | Function |
|------|-----------|----------|
| BDS1 | 3         | The data of the orbitals for first two shells | the array \( B \) for the first shell of the ket function |
| BDS2 | 3         | the array \( B \) for the second shell of the ket function |
| BKS1 | 3         | the array \( B \) for the first shell of the bra function |
| BKS2 | 3         | the array \( B \) for the second shell of the bra function |
| IBDS1 | 7     | the array \( I \) for the first shell of the ket function |
| IBDS2 | 7     | the array \( I \) for the second shell of the ket function |
| IBKS1 | 7     | the array \( I \) for the first shell of the bra function |
| IBKS2 | 7     | the array \( I \) for the second shell of the bra function |

**/TRK2/**

| Name | Dimension | Function |
|------|-----------|----------|
| BDS3 | 3         | The data of the orbitals for last two shells | the array \( B \) for the third shell of the ket function |
| BDS4 | 3         | the array \( B \) for the fourth shell of the ket function |
| BKS3 | 3         | the array \( B \) for the third shell of the bra function |
| BKS4 | 3         | the array \( B \) for the fourth shell of the bra function |
| IBDS3 | 7     | the array \( I \) for the third shell of the ket function |
Table 2: Allowed couplings of $f^N$. The subshell spin angular momentum $S$, number $N_r$ and the subshell angular momentum $L$ are denoted $(2S+1)L^{N_r}$. The quasispin angular momentum is denoted $Q$.

| No | Term | 2Q | No | Term | 2Q | No | Term | 2Q |
|----|------|----|----|------|----|----|------|----|
| 1  | $^8S^0$ | 0  | 35 | $^4I^1$ | 4  | 69 | $^2F^8$ | 0  |
| 2  | $^6P^0$ | 2  | 36 | $^4I^2$ | 2  | 70 | $^2F^9$ | 0  |
| 3  | $^6D^0$ | 0  | 37 | $^4I^3$ | 2  | 71 | $^2F^4$ | 0  |
| 4  | $^6F^0$ | 2  | 38 | $^4I^4$ | 0  | 72 | $^2G^1$ | 4  |
| 5  | $^6G^0$ | 0  | 39 | $^4I^5$ | 0  | 73 | $^2G^2$ | 1  |
| 6  | $^6H^0$ | 2  | 40 | $^4K^3$ | 2  | 74 | $^2G^3$ | 2  |
| 7  | $^6I^0$ | 0  | 41 | $^4K^2$ | 2  | 75 | $^2G^4$ | 2  |
| 8  | $^4S^1$ | 4  | 42 | $^4K^3$ | 0  | 76 | $^2G^5$ | 2  |
| 9  | $^4S^2$ | 0  | 43 | $^4L^1$ | 2  | 77 | $^2G^6$ | 2  |
| 10 | $^4P^1$ | 2  | 44 | $^4L^2$ | 0  | 78 | $^2G^7$ | 0  |
| 11 | $^4P^2$ | 2  | 45 | $^4L^3$ | 0  | 79 | $^2G^8$ | 0  |
| 12 | $^4D^1$ | 4  | 46 | $^4M^0$ | 2  | 80 | $^2G^9$ | 0  |
| 13 | $^4D^2$ | 2  | 47 | $^4N^0$ | 0  | 81 | $^2G^4$ | 0  |
| 14 | $^4D^3$ | 2  | 48 | $^2S^1$ | 0  | 82 | $^2H^1$ | 4  |
| 15 | $^4D^4$ | 0  | 49 | $^2S^2$ | 0  | 83 | $^2H^2$ | 4  |
| 16 | $^4D^5$ | 0  | 50 | $^2P^1$ | 4  | 84 | $^2H^3$ | 2  |
| 17 | $^4D^6$ | 0  | 51 | $^2P^2$ | 2  | 85 | $^2H^4$ | 2  |
| 18 | $^4F^1$ | 4  | 52 | $^2P^3$ | 2  | 86 | $^2H^5$ | 2  |
| 19 | $^4F^2$ | 2  | 53 | $^2P^4$ | 2  | 87 | $^2H^6$ | 2  |
| 20 | $^4F^3$ | 2  | 54 | $^2P^5$ | 0  | 88 | $^2H^7$ | 2  |
| 21 | $^4F^4$ | 2  | 55 | $^2D^1$ | 4  | 89 | $^2H^8$ | 0  |
| 22 | $^4F^5$ | 2  | 56 | $^2D^2$ | 4  | 90 | $^2H^9$ | 0  |
| 23 | $^4G^1$ | 4  | 57 | $^2D^3$ | 2  | 91 | $^2I^1$ | 4  |
| 24 | $^4G^2$ | 2  | 58 | $^2D^4$ | 2  | 92 | $^2I^2$ | 2  |
| 25 | $^4G^3$ | 2  | 59 | $^2D^5$ | 2  | 93 | $^2I^3$ | 2  |
| 26 | $^4G^4$ | 2  | 60 | $^2D^6$ | 0  | 94 | $^2I^4$ | 2  |
| 27 | $^4G^5$ | 0  | 61 | $^2D^7$ | 0  | 95 | $^2I^5$ | 2  |
| 28 | $^4G^6$ | 0  | 62 | $^2F^1$ | 6  | 96 | $^2I^6$ | 0  |
| 29 | $^4G^7$ | 0  | 63 | $^2F^2$ | 4  | 97 | $^2I^7$ | 0  |
| 30 | $^4H^1$ | 2  | 64 | $^2F^3$ | 2  | 98 | $^2I^8$ | 0  |
| 31 | $^4H^2$ | 2  | 65 | $^2F^4$ | 2  | 99 | $^2I^9$ | 0  |
| 32 | $^4H^3$ | 2  | 66 | $^2F^5$ | 2  | 100 | $^2K^1$ | 4  |
| 33 | $^4H^4$ | 0  | 67 | $^2F^6$ | 2  | 101 | $^2K^2$ | 2  |
| 34 | $^4H^5$ | 0  | 68 | $^2F^7$ | 2  | 102 | $^2K^3$ | 2  |
Table 2 (continued)

| No | Term | 2Q | No | Term | 2Q | No | Term | 2Q |
|----|------|----|----|------|----|----|------|----|
| 137 | $^3F^1$ | 5 | 171 | $^3H^6$ | 1 | 205 | $^1D^6$ | 1 |
| 138 | $^3F^2$ | 3 | 172 | $^3H^9$ | 1 | 206 | $^1G^9$ | 1 |
| 139 | $^3F^6$ | 1 | 173 | $^3I^1$ | 3 | 207 | $^1G^7$ | 1 |
| 140 | $^3F^8$ | 1 | 174 | $^3I^2$ | 3 | 208 | $^1G^8$ | 1 |
| 141 | $^3D^1$ | 3 | 175 | $^3I^3$ | 1 | 209 | $^1D^3$ | 3 |
| 142 | $^3D^2$ | 3 | 176 | $^3I^4$ | 1 | 210 | $^1G^4$ | 3 |
| 143 | $^3D^3$ | 1 | 177 | $^3I^5$ | 1 | 211 | $^1H^1$ | 3 |
| 144 | $^3D^4$ | 1 | 178 | $^3I^6$ | 1 | 212 | $^1H^2$ | 3 |
| 145 | $^3F^3$ | 3 | 179 | $^3K^1$ | 3 | 213 | $^1P^0$ | 1 |
| 146 | $^3F^5$ | 1 | 180 | $^3K^2$ | 3 | 214 | $^1H^3$ | 1 |
| 147 | $^3G^1$ | 3 | 181 | $^3K^3$ | 1 | 215 | $^1H^4$ | 1 |
| 148 | $^3G^2$ | 3 | 182 | $^3K^4$ | 1 | 216 | $^1S^1$ | 7 |
| 149 | $^3G^4$ | 1 | 183 | $^3K^5$ | 1 | 217 | $^1I^1$ | 5 |
| 150 | $^3G^5$ | 1 | 184 | $^3K^6$ | 1 | 218 | $^1S^2$ | 3 |
| 151 | $^3D^5$ | 1 | 185 | $^3L^1$ | 3 | 219 | $^1I^2$ | 3 |
| 152 | $^3F^4$ | 3 | 186 | $^3L^2$ | 1 | 220 | $^1I^3$ | 3 |
| 153 | $^3F^7$ | 1 | 187 | $^3L^3$ | 1 | 221 | $^1S^3$ | 1 |
| 154 | $^3F^9$ | 1 | 188 | $^3M^1$ | 3 | 222 | $^1I^4$ | 1 |
| 155 | $^3G^3$ | 3 | 189 | $^3M^2$ | 1 | 223 | $^1I^5$ | 1 |
| 156 | $^3G^6$ | 1 | 190 | $^3M^3$ | 1 | 224 | $^1S^4$ | 1 |
| 157 | $^3G^7$ | 1 | 191 | $^3N^0$ | 1 | 225 | $^1I^6$ | 1 |
| 158 | $^3P^1$ | 5 | 192 | $^3O^0$ | 1 | 226 | $^1I^7$ | 1 |
| 159 | $^3P^2$ | 3 | 193 | $^1F^2$ | 1 | 227 | $^1K^3$ | 3 |
| 160 | $^3P^3$ | 3 | 194 | $^1F^3$ | 1 | 228 | $^1K^2$ | 1 |
| 161 | $^3H^1$ | 5 | 195 | $^1F^4$ | 1 | 229 | $^1K^3$ | 1 |
| 162 | $^3H^2$ | 3 | 196 | $^1D^1$ | 5 | 230 | $^1L^1$ | 3 |
| 163 | $^3H^3$ | 3 | 197 | $^1D^2$ | 3 | 231 | $^1L^2$ | 3 |
| 164 | $^3H^4$ | 3 | 198 | $^1D^3$ | 3 | 232 | $^1L^3$ | 1 |
| 165 | $^3P^4$ | 1 | 199 | $^1F^1$ | 3 | 233 | $^1L^4$ | 1 |
| 166 | $^3H^5$ | 1 | 200 | $^1G^1$ | 5 | 234 | $^1M^1$ | 1 |
| 167 | $^3H^6$ | 1 | 201 | $^1G^2$ | 3 | 235 | $^1M^2$ | 1 |
| 168 | $^3P^5$ | 1 | 202 | $^1G^3$ | 3 | 236 | $^1N^3$ | 3 |
| 169 | $^3P^6$ | 1 | 203 | $^1D^5$ | 1 | 237 | $^1N^2$ | 1 |
| 170 | $^3H^7$ | 1 | 204 | $^1G^5$ | 1 | 238 | $^1Q^5$ | 1 |
IBDS4 7 the array I for the fourth shell of the ket function
IBKS3 7 the array I for the third shell of the bra function
IBKS4 7 the array I for the fourth shell of the bra function

In this library, the common blocks /MEDEFN/ and /FACT/ from the earlier version of the MCHF atomic–structure package [2, 27], and the newly created auxiliary COMMON blocks /KAMPAS/, /RIBOLS/, /RIBOLSF/, /RIBOF/, /RIBOLS3/, are used.

The authors would like to draw attention at the ordering of terms in Table 2, which is tuned to simplifying the placement of tables of $f$–shell reduced coefficients of fractional parentage into DATA blocks.

3.1.2 Subroutines

The subroutine NUMTER

FUNCTION NUMTER has several modes of operation, but only one of these is possible while using it in other programs. If the input values are the shell’s total quasispin $Q$ multiplied by two (input argument I2Q), the shell’s total spin $S$ multiplied by two (input argument I2S), the shell’s total angular momentum $L$ multiplied by two (input argument I2L) and the quantum number $l$, it will find the number of the $s$, $p$–$d$–shell’s term, as numbered in Table 1. The other arguments of this subroutine, $NK$ and $ND$, should be set to 3. In this mode, a COMMON block /MT/, is needed by the program, which is defined in BLOCK DATA TERMLS.

The subroutine RUMT

The subroutine RUMT has several modes of operation, but only one of these is possible while using it in other programs. For an input of the orbital quantum number $l$ (input argument $LL$) and the term number from Table 1 (input argument $KNT$), it finds the shell’s total quasispin $Q$ multiplied by two (output argument $LQ$), the shell’s total spin $S$ multiplied by two (output argument $LS$) and the shell’s total angular momentum $L$ multiplied by two (output argument $L$). It finds these characteristics for $s$, $p$– and $d$–shells. A COMMON blocks /MT/ is needed by this program, which is defined in BLOCK DATA TERMLS.

The subroutine C0T5S

This subroutine determines the value of the Clebsch–Gordan coefficients:

$$\begin{bmatrix} Q \\ QM \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ SM \end{bmatrix} \begin{bmatrix} C \\ CM \end{bmatrix}. \quad (8)$$

The subroutine has the input arguments $Q$, $QM$, $SM$, $C$, $CM$ and output argument $A$. The subroutine performs its calculations by employing analytical expressions from Varshalovich et al [29].

The subroutine C1E0SM

This routine determines the value of the Clebsch–Gordan coefficients:

$$\begin{bmatrix} Q \\ QM \end{bmatrix} = \begin{bmatrix} 1 \\ C \end{bmatrix} \begin{bmatrix} C \\ CM \end{bmatrix}. \quad (9)$$

The subroutine has the input arguments $Q$, $QM$, $C$, $CM$ and output argument $A$. The subroutine performs its calculations by employing analytical expressions from Varshalovich et al [29].

The subroutine C1E1SM

This subroutine determines the value of the Clebsch–Gordan coefficients:

$$\begin{bmatrix} Q \\ QM \end{bmatrix} = \begin{bmatrix} 1 \\ C \end{bmatrix} \begin{bmatrix} 1 \\ CM \end{bmatrix}. \quad (10)$$

The subroutine has the input arguments $Q$, $QM$, $C$, $CM$ and output argument $A$. The subroutine performs its calculations by employing analytical expressions from Varshalovich et al [29].
The subroutine SIXJ

This routine determines the value of the $6j$–coefficients:

\[
\begin{bmatrix}
  I/2 & J/2 & K/2 \\
  L/2 & M/2 & N/2
\end{bmatrix}.
\] (11)

The subroutine has the input arguments $I, J, K, L, M, N, ITIK$ and output argument $SI$. If the parameter $ITIK = 0$, the subroutine does not check the triangular conditions for $6j$–coefficient. In other cases it checks these. If any of the parameters of $6j$–coefficient is equal to $0, 1, 2, 3, 4$, the subroutine calculates the $6j$–coefficients according to analytical formulas [29, 14]. Otherwise, the customary calculations are performed. In that case, the COMMON block /FACT/ must be defined. This is done by addressing the SUBROUTINE FACTRL from the library MCHF_LIB_COM [2, 27].

The subroutine NINE

\[
\begin{bmatrix}
  J_1/2 & J_2/2 & J_3/2 \\
  L_1/2 & L_2/2 & L_3/2 \\
  K_1/2 & K_2/2 & K_3/2
\end{bmatrix}.
\] (12)

The subroutine has the input arguments $J_1, J_2, J_3, L_1, L_2, L_3, K_1, K_2, K_3, I$ and output arguments $IN$ and $AA$. If the parameter $I = 1$, the subroutine only checks the triangular conditions of a $9j$–coefficient. If these are not satisfied, then $IN = 0$, and $IN = 1$ otherwise. At other values of $I$, the subroutine calculates the value of $9j$–coefficient and assigns it to the output parameter $AA$.

The subroutine SLS

This subroutine determines the value of the RCFP:

\[
( l QLS \mid | a^{(qls)} \times a^{(qls)} |^{(k_1 k_2 k_3)} ) \mid || l Q' L'S' \).
\] (13)

for $p$–, $d$–, and $f$– shells (see (39) in [6]). The routine uses the table of reduced matrix elements of the $a^{(qls)}$ tensor operator from [8]). The subroutine has the following arguments:

1. L is the orbital quantum number $l$.
2. IT is the state number of the bra function (see Tables 1, 2).
3. LQ is the quasispin $Q$ for the bra function multiplied by two.
4. LL is the total angular momentum $L$ for the bra function multiplied by two.
5. LS is the total angular momentum $S$ for the bra function multiplied by two.
6. ITS is the state number of the ket function.
7. LQS is the quasispin $Q$ for the ket function multiplied by two.
8. LLS is the total angular momentum $L$ for the ket function multiplied by two.
9. LSS is the total angular momentum $S$ for the ket function multiplied by two.
10. S is the value of the reduced matrix element (13) which is returned by the subroutine.

The subroutine RWLS

The routine determines the value of the reduced matrix element:

\[
( l QLS \mid | a^{(qls)} \times a^{(qls)} |^{(k_1 k_2 k_3)} ) \mid || l Q' L'S' \).
\] (14)

The routine uses the tables of reduced matrix elements of the tensor operator $[a^{(qls)} \times a^{(qls)}]^{(k_1 k_2 k_3)}$ for $s$–, $p$– and $d$– subshells (see Spakauskas et al [30]), and for the $f$– shell the expression (34) from paper [5] is used. The subroutine does not calculate the simple case of $k_1 = k_2 = k_3 = 0$, because then the operator is just $[ a^{(qls)} \times a^{(qls)} ]^{(000)} = -(2l+1)^{1/2}$ (expression (15.54) in Rudzikas [1]). The subroutine has the formal arguments:
1. $K_1$ is the rank $k_1$.
2. $K_2$ is the rank $k_2$.
3. $K_3$ is the rank $k_3$.
4. $L$ is the orbital quantum number $l$.
5. $J_1$ is the state number of the bra function (see Tables 1, 2).
6. $J_2$ is the state number of the ket function.
7. $W$ is the value of the reduced matrix element (14) which is returned by the subroutine.

**The subroutine W1**

This subroutine determines the value of the matrix element:

$$
\left( I^N QLS \left\| a^{(qls)}_{m_{q_1}} \otimes a^{(qls)}_{m_{q_2}} \right\| k_{l_1} k_{l_2} \right) \left\| I^{N'} Q'L'S' \right. \right).
$$

While calculating cases where the orbital number $l=0, 1, 2, 3$ and the shell’s occupation number $N > 2$, the program relies on the expression (31) from the paper [5]. In that case, the subroutine finds the Clebsch–Gordan coefficient which gives the dependence on the shell occupation number. If the tensor product (15) consists of either two electron creation or two annihilation operators then C1E1SM is called. Otherwise CLE0SM is called. The subroutine RWLS finds the reduced matrix elements of the operator $a^{(q_{l_1})} \otimes a^{(q_{l_2})} (k_{l_1} k_{l_2})$. In other cases, the program calculates according to the expression (40) from paper [6]. The subroutine has the formal arguments:

1. IK is the array I for the bra function.
2. BK is the array B for the bra function.
3. ID is the array I for the ket function.
4. BD is the array B for the ket function.
5. K2 is the rank $k_1$.
6. K3 is the rank $k_3$.
7. QM1, QM2 are the quasispin projections in (15).
8. $W$ is the value of the reduced matrix element (15) which is returned by the subroutine.

**The subroutine AWP1LS**

The routine determines the value of the matrix elements:

$$
\left( I^N QLS \left\| a^{(qls)}_{m_{q_1}} \otimes a^{(qls)}_{m_{q_2}} \otimes a^{(qls)}_{m_{q_3}} \right\| (k_{l_1} k_{l_2}) (k_{l_3}) \right) \left\| I^{N'} Q'L'S' \right. \right).
$$

While calculating cases where the orbital number $l=0, 1, 2, 3$ and the shell’s occupation number $N > 2$, the program relies on the expression (31) from the paper [5]. In that case, the subroutine IZAS1 checks that the subshell has a state with the specified characteristics. The subroutine ITLS2 finds the first and the last numbers of the state from the running intermediate sum in array MT. RUMT finds the shell’s total angular momentum $LS$ and quasispin $Q$ for each intermediate state. The routine IXJTIK checks all triads. The subroutine C0T5S finds the Clebsch–Gordan coefficient giving the dependence on the shell’s occupation number and SLS finds the reduced matrix element of $a^{(q_{l_1})}$ tensor operator (see in Section 3.1). The second part of the expression is calculated by the routine W1 (see in Section 3.1.2). The routine SIXJ finds $6j$–symbol. In other cases, the program calculates according to the expression (40) from paper [6]. The subroutine has the arguments:

1. IK is the array I for the bra function.
2. BK is the array B for the bra function.
3. ID is the array I for the ket function.
4. BD is the array B for the ket function.
5. K1 is the rank $k_1$.
6. K2 is the rank $k_2$.
7. K3 is the rank $k_l$.
8. BK4 is the rank $k_s$.
9. QM1, QM2 and QM3 are the quasispin projections in (16).
10. AW is the value of the reduced matrix element (16) which is returned by the subroutine.

The subroutine WAP1LS

This subroutine determines the value of the matrix elements:

$$
\left( t^N QLS \right\| \left[ \left\| a^{qls}_{m_{q_1}} \times a^{qls}_{m_{q_2}} \right\|^{(k_1 k_2)} \times a^{qls}_{m_{q_3}} \right\|^{(k_1 k_s)} \right\| t^{N'} Q'L'S' \right) .
$$

(17)

The structure of the routine WAP1LS is the same as that of AWP1LS. The subroutine has the formal arguments:

1. IK is the array I for the bra function.
2. BK is the array B for the bra function.
3. ID is the array I for the ket function.
4. BD is the array B for the ket function.
5. K1 is the rank $k_1$.
6. K2 is the rank $k_2$.
7. K3 is the rank $k_l$.
8. BK4 is the rank $k_s$.
9. QM1, QM2 and QM3 are the quasispin projections in (17).
10. WA is the value of the reduced matrix element (17) which is returned by the subroutine.

The subroutine WWLS1

The routine determines the value of matrix elements:

$$
\left( t^N QLS \right\| \left[ \left\| a^{qls}_{m_{q_1}} \times a^{qls}_{m_{q_2}} \right\|^{(k_1 k_s)} \times a^{qls}_{m_{q_3}} \times a^{qls}_{m_{q_4}} \right\|^{(k_l k_s)} \right\| t^{N'} QLS \right) .
$$

(18)

The routine WWLS1 uses the routines ITLS, RUMT, IZAS1 for calculation of this sort of the matrix element. The subroutine W1 calculates the first and the second parts of the operator calculates. The subroutine has the formal arguments:

1. IK is the array I for the bra function.
2. BK is the array B for the bra function.
3. ID is the array I for the ket function.
4. BD is the array B for the ket function.
5. K2 is the rank $k_1$.
6. K3 is the rank $k_s$.
7. QM1, QM2, QM3 and QM4 are the quasispin projections in (18).
8. WW is the value of the reduced matrix element (18) which is returned by the subroutine.
The subroutine WWPLS1

The routine determines the value of matrix elements:

\[
( l^N QLS || [ a_{m\nu_1}^{(q_1s)} \times a_{m\nu_2}^{(q_2s)} ]^{(k_1k_2)} \times [ a_{m\nu_3}^{(q_3s)} \times a_{m\nu_4}^{(q_4s)} ]^{(k_3k_4)} ]^{(k_lk_s)} || l^{N'} QLS ).
\]

The routine WWPLS1 uses the routines ITLS, RUMT, IZAS1 for calculation of this sort of the matrix element. The subroutine W1 calculates the first and the second parts of the operator calculates. The routine SIXJ finds 6j–symbol. The subroutine uses the COMMON block /TRK/, which contains arrays I and B for the bra and ket function (ID1, IK1,BD1 and BK1). It uses the expression (40) from [6]. The subroutine has the formal arguments:

1. K1 is the rank \( k_1 \).
2. K2 is the rank \( k_2 \).
3. K3 is the rank \( k_3 \).
4. K4 is the rank \( k_4 \).
5. K5 is the rank \( k_l \).
6. K6 is the rank \( k_s \).
7. QM1, QM2, QM3 and QM4 are the quasispin projections in (19).
8. WW is the value of the reduced matrix element (19) which is returned by the subroutine.

3.2 SAI_SQLS2

The library SAI_SQLS2 is the second part of Standard quantities in \( LS–\) coupling. Everything in it is related to the \( f–\) shells. The tables of CFP for \( f–\) shell (see [8]) and the term characteristics are in this library. This library can be used in other programs to its full extent, by employing programs from SAI_SQLS1 library. These are the subroutines SLS, RWLS, W1, AWP1LS, WAP1LS, WWLS1, WWPLS1. The remaining two subroutines may also be used independently.

The subroutine NUMTERF

The subroutine has several modes of operation. But only one of these is useful while operated independently from the MCHF atomic structure package [2, 27]. In that case, after giving number \( Nr \) from Table 2 (input argument I2N), the values of the shell total spin \( S \) multiplied by two (input arguments I2S and N), the shell total angular momentum \( L \) multiplied by two, (input argument I2L) and the shell total quasispin \( Q \) multiplied by two (input argument I2Q) for the FUNCTION NUMBER, it finds the number of \( f–\) shell term, as numbered in Table 2. The subroutine needs the COMMON block /MT67/, which is defined by BLOCK DATA TERMF.

The subroutine RUMT67

For an input of the term member from Table 2 (input argument KNT), the subroutine RUMT67 finds the number \( Nr \) from Table 2 (output argument NR), the shell total quasispin \( Q \) multiplied by two (output argument LQ), the shell total spin \( S \) multiplied by two (output argument LS) and the shell total angular momentum \( L \) multiplied by two (output argument L). The subroutine needs the COMMON block /MT67/ which is defined by BLOCK DATA TERMF.

4 Examples

A driver program (see Figure 1) accompanying the library SQLSF illustrates three examples.

The examples show that some of the subroutines contained in the libraries may serve as an electronic version of Nielson and Koster [31] or [8] tables. As such they may serve as a basis for extending the capabilities of programs that rely on the principle of calculating the determinants to arbitrarily filled \( f–\) shells (see for example Eissner et al [32] or Zatsarinny [33]).

Here we describe each example separately, the EXAMPLES RUN OUTPUT being shown in Table 4.
IF (ICASE .EQ. 1) THEN
  WRITE(6, '(/A)') ' orbital quantum number l (I1) '
  READ(S, '(/I1)') L
  IF (L .LT. 3) THEN
    WRITE(6, '(/A)') ' 2*Q 2*L 2*S for bra function (3I2) '
    READ(S, '(/3I2)') IQB, ILB, ISB
    JB = NUMTER(IQB, ISB, ILB, L, 3, 3)
    WRITE(6, '(/A)') ' 2*Q 2*L 2*S for ket function (3I2) '
    READ(S, '(/3I2)') IQK, ILK, ISK
    JK = NUMTER(IQK, ISK, ILK, L, 3, 3)
  ELSEIF (L .EQ. 3) THEN
    WRITE(6, '(/A)') ' 2*Q 2*L 2*S Nr for bra function (4I2) '
    READ(S, '(/4I2)') INB, IQB, ISB, ILB
    JB = NUMTERF(INB, ISB, ILB, IQB)
    WRITE(6, '(/A)') ' 2*Q 2*L 2*S Nr for ket function (4I2) '
    READ(S, '(/4I2)') INK, IQK, ISK, ILK
    JK = NUMTERF(INK, ISK, ILK, IQK)
  ENDIF
  CALL SLS(L, JB, IQB, ILB, ISB, JK, IQK, ILK, ISK, S)
  WRITE(6, '(/A,F17.7)') ' Value= ', S
ELSEIF (ICASE .EQ. 2) THEN
  WRITE(6, '(/A)') ' orbital quantum number l (I1) '
  READ(S, '(/I1)') L
  WRITE(6, '(/A)') ' number electrons in the shell N (I1) '
  READ(S, '(/I1)') N
  WRITE(6, '(/A)') ' bra and ket number of term (2I3) '
  READ(S, '(/2I3)') JB, JK
  IF (L .LT. 3) THEN
    CALL RUMT(JB, L, IQB, ISB, ILB)
  ELSEIF (L .EQ. 3) THEN
    CALL RUMT67(JB, NRB, IQB, ISB, ILB)
  ENDIF
  IF (L .LT. 3) THEN
    CALL RUMT(JK, L, IQK, ISK, ILK)
  ELSEIF (L .EQ. 3) THEN
    CALL RUMT67(JK, NRK, IQK, ISK, ILK)
  ENDIF
  CALL SLS(L, JB, IQB, ILB, ISB, JK, IQK, ILK, ISK, S)
  CALL C0T5S(DBLE(IQB)*0.5, DBLE(N-2*L-1)*0.5, DBLE(IQK)*0.5, DBLE(N-2*L-1)*0.5)
  CALL C1E0SM(DBLE(IQB)*0.5, DBLE(N-2*L-1)*0.5, DBLE(IQK)*0.5)
  WRITE(6, '(/A,F17.7)') ' Value= ', DBLE(S)*A/DSQRT(DBLE(N*(IQB+1)*(ILB+1)))
ELSEIF (ICASE .EQ. 3) THEN
  WRITE(6, '(/A)') ' orbital quantum number l (I1) '
  READ(S, '(/I1)') L
  WRITE(6, '(/A)') ' number electrons in the shell N (I1) '
  READ(S, '(/I1)') N
  WRITE(6, '(/A)') ' first and last number of term for bra (2I3) '
  READ(S, '(/2I3)') JFB, JLB
  WRITE(6, '(/A)') ' first and last number of term for ket (2I3) '
  READ(S, '(/2I3)') JFK, JLK
  WRITE(6, '(/A)') ' the ranks K1 K2 K3 (3I1) '
  READ(S, '(/3I1)') K1, K2, K3
  WRITE(6, '(/A)') ' number for bra : number for ket : value ', JTB, JFK, VK
  DO 2 JTB = JFB, JLB
    CALL RUMT(JTB, L, IQB, ISB, ILB)
    CONTINUE
  2 CONTINUE
ELSEIF(L .EQ. 3) THEN
  CALL RUMT(JTB, L, IQB, ISB, ILB)
ELSEIF(L .EQ. 3) THEN
  CALL RUMT(JTB, NRK, IQK, ISK, ILK)
ENDIF
DO 3 JTB = JFB, JLB
  IF (L .LT. 3) THEN
    CALL RUMT(JTB, L, IQB, ISB, ILB)
  ELSEIF (L .EQ. 3) THEN
    CALL RUMT67(JTB, NRB, IQB, ISB, ILB)
  ENDIF
  CALL RUMT(JTB, L, IQK, ISK, ILK)
  CALL RWLS(K1, K2, K3, L, JTB, JFK, W)
  VK = -0.5*W*A/DSQRT(DBLE((IQB+1)*(2*K2+1)))
  WRITE(6, '(/A,F17.7)') ' number for bra : number for ket : value ', JTB, JFK, VK
ENDIF

Figure 1: The program for three examples
Case 1. Finding the RCFP

In this case the subroutine finds the value of a RCFP \( f^8 S^0 \| a_{lq(s)} \| f^7 F^0 \). From Table IV of [8] we see that the value of this coefficient is equal to

\[
( f^8 S^0 \| a_{lq(s)} \| f^7 F^0 ) = -4\sqrt{7}.
\]

This is in accordance with the result obtained with SLS subroutine (see in Section 3.1).

It is necessary to mention that in the calls to this and some other subroutine, the input of a term number and term characteristics is needed. In this case the user indicates only the term characteristics, and finds the term number by using the subroutine NUMTER (see in Section 3.1) or NUMTERF (see in Section 3.2). In other examples we will present a way, showing how to call subroutines of analogous type, by defining just the term number by the user.

Case 2. Calculating the CFP

This case illustrates the finding of a CFP value, using the SLS program. It may be useful for programs that are based on the tables of CFP, which are much more extended than the tables of RCFP. The values of CFP are found by programming the expression (5).

The value of a CFP \( ( f^7 6 D^0 \| f^6 5 P^0 f ) \) is found in the example. We see from Nielsen and Koster [31] that the value of this CFP is equal to

\[
( f^7 6 D^0 \| f^6 5 P^0 f ) = -\frac{\sqrt{3}}{7}.
\]

This is in accordance with the result obtained with SLS subroutine.

See [8, 28] for details of the encoding of the \( f - \) shell terms. See [8] for a more extensive use of the tables of RCFP in finding the CFP. In that paper, also the problems related to that task are discussed and the ways to solve these are indicated.

Case 3. Calculating the matrix elements of \( V^k \) operator

In this section it is demonstrated how to calculate the \( V^{11} \) operator, using the subroutine RWLS (see in Section 3.1), which calculates the reduced matrix elements (14). For that purpose the relation (16.34) from Rudzikas [1] is used. While using the \( U^k \) and \( V^{k1} \) tables, one must pay attention to various phase conventions used in the literature. In addition, small differences in the definitions of \( U^k \) occur. Some authors, Karazija et al [34] among them, tabulate the submatrix elements

\[
(l^N \alpha SL || U^k || l^N \alpha' S' L'),
\]

others, like Nielsen and Koster [31] or Cowan [35], tabulate

\[
(l^N \alpha L || U^k || l^N \alpha' L'),
\]

although they use the notation of (20). Meanwhile, the relation between these two coefficients is:

\[
(l^N \alpha SL || U^k || l^N \alpha' S' L') = \delta(S, S') \sqrt{2S + 1} (l^N \alpha L || U^k || l^N \alpha' L').
\]

The submatrix elements are defined as (20) if we use the relations between matrix elements of \( W^{(k_1 k_2 k_3)} \) and \( U^k \) as presented in the Rudzikas monograph [1]. Reduced matrix elements of the operator \( V^{11} ( f^7 6 P^0 || V^{11} || f^7 4 S^1 ) \) are calculated in the example. The numerical value of this reduced matrix element is taken from the Nielsen and Koster [31] tables

\[
(f^7 6 P^0 || V^{11} || f^7 4 S^1 ) = -\sqrt{\frac{2}{7}}
\]

and agree with our value.
Table 4. EXAMPLES RUN OUTPUT

Case 1. Finding a reduced coefficient of fractional parentage

>> Example

| orbital quantum number l (I1) |
|-------------------------------|
| bra (number l 2*Q 2*L 2*S N)  |
| ket (number l 2*Q 2*L 2*S)    |

| Value= | -10.583005244258363 |

END OF CASE 1

Case 2. Calculation of the coefficient of fractional parentage

>> Example

| orbital quantum number l (I1) |
|-------------------------------|
| bra (number l 2*Q 2*L 2*S N)  |
| ket (number l 2*Q 2*L 2*S)    |

| Value= | -0.247435829652697 |

END OF CASE 2

Case 3. Calculation of the matrix elements of operator \( V^k \)

>> Example

| orbital quantum number l (I1) |
|-------------------------------|
| bra (number l 2*Q 2*L 2*S N)  |
| ket (number l 2*Q 2*L 2*S)    |

| Value= | -0.534522483824849 |

END OF CASE 3
5 Conclusion

Accurate theoretical determination of atomic energy levels, orbitals and radiative transition data requires the calculation of matrix elements of physical operators accounting for relativistic and correlation effects. The spin–angular integration of these matrix elements is typically based on standard quantities like the matrix elements of the unit tensor, the (reduced) coefficients of fractional parentage as well as a number of other reduced matrix elements concerning various products of electron creation and annihilation operators. These quantities arise very frequently in large–scale computations of open–shell atoms using multiconfiguration Hartree–Fock or configuration interaction approaches, in calculating the angular parts of effective operators from many–body perturbation theory or for evaluating relativistic hamiltonian in $LS$–coupling as well as in various versions of semiempirical methods. The library SQ is assigned for the calculation of all these standard quantities. It can be used as "electronic tables" of standard quantities for evaluating general matrix elements for $LS$–coupled functions, too.

The library SQ is created involving the angular methodology of [5, 6, 7, 8, 9, 10]. For $LS$–coupling subshells states, the library provides coefficients and matrix elements for all subshells (nl) with $l = 0, 1, 2$ and 3, and $l^2$ for $l \geq 3$.

Program is obtainable from State Institute of Theoretical Physic and Astronomy, A. Goštauto 12, Vilnius, 2600, LITHUANIA. E-mail: gaigalas@itpa.lt.

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Santrauka

Straipsnyje pateikta biblioteka (paprogramių rinkinys), parašyta Fortran 77 programavimo kalba. Ji skirta standartinių dydžių skaičiavimui, su kuriais susiduriame atomo teorijoje nagrinėjant fizikinių bei efektyvinių operatorių matricinius elementus LS ryšyje. Visu pirma, tai kilminiai koeficientai bei vienetinių tenzorių $U^k$ ir $V^{k1}$ matriciniai elementai, kurie paprastai pasirodo nagrinėjant matricinius elementus klasikiniais metodus. Be to biblioteka skirta ir tokių standartinių dydžių nagrinėjimui, kurie pasirodo naudojant kvazisukinio formalizmų. Tai subkilminiai koeficientai, bei redukuotiniai kvazisukinio erdvėje, vienetiniai tenzoriai $W^{(k_{vi}k_{i}s_{i})}$. Taigi darbe pateikta biblioteka yra bendro pobūdžio ir skirta matricinių elementų skaičiavimui bet kokia mokslinėje literatūroje žinoma metodika. Pati biblioteka yra parašyta remiantis antrinio kvantavimo suriūstame tenzoriiniame pavidale formalizmu, judesio kiekio momento teorija trijose erdvėse (orbitinėje, sukūrinėje ir kvazisukininiame) ir grafine judesio kiekio momento teorija. Ši biblioteka išplečia atomo teorijos galimybės, kadangi joje yra pilnai ištraukti f sluoksniai su bet kokių sluoksnio užpildymo skaičiumi, bei leidžia pagreitinti jau esamas programas.