The Library of Subroutines for Calculation of Matrix Elements of Two–particle Operators for Many–Electron Atoms

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Abstract

In this paper a library for spin–angular integration in $LS$–coupling for many–electron atoms is presented. 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 of the relevant methodology to open $f$–shells and leads to faster execution of angular integration codes. The possibility of using some library routines for solving various angular momentum problems in atomic physics is also discussed.

PACS: 31.15.Ne, 31.25.-v, 32.10.-f, 32.30.-r

Keywords: atomic structure, configuration interaction, complex atom, correlation, bound states, $LS$–coupling.
PROGRAM SUMMARY

Title of program : SAI Catalogue identifier:

Program obtainable from: Institute of Theoretical Physics and Astronomy, A. Goštauto 12, 2600 Vilnius, 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, 2600 Vilnius, LITHUANIA.

Programming language used in the new version: FORTRAN 77 [1]

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.: 442 297 bytes

Distribution format: compressed tar file

Additional keywords : atomic structure, configuration interaction, reduced coefficients of fractional parentage, irreducible tensors, angular momentum theory in three spaces (orbital, spin and quasispin), second quantization in the coupled tensorial form, recoupling coefficients, Slater integrals, complex atom, correlation, wave functions, bound states, LS–coupling, f–shell states.

Nature of physical problem
Theoretical determination of atomic orbitals, energy levels and radiative transition data requires the calculation of matrix elements of the relevant physical operators (see the multiconfiguration Hartree–Fock method [2], for example). The matrix elements of arbitrary operator can generally be expressed as
\[ \sum\limits_{i,j} \text{coef}(i,j) \langle \gamma_i L_i S_i | T^{(k_1 k_2)} | \gamma_j L_j S_j \rangle, \]
where \( T^{(k_1 k_2)} \) is a tensorial operator of ranks \( k_1, k_2 \). The program calculates the spin–angular part for matrix elements \( \langle \gamma_i L_i S_i | T^{(k_1)} | \gamma_j L_j S_j \rangle \) of one– and/or two–particle operator \( T^{(k_1 k_2)} \).

Method of solution
This program is created involving the angular methodology of [3–6]. It has been extended to include partially filled f–shells in wave function expansions. The classification of terms is identical to that described in [6].

Restrictions on the complexity of the problem
The non–orthogonal orbitals are not supported.

References
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[3] G. Gaigalas and Z. Rudzikas, J. Phys. B: At. Mol. Phys. 29 (1996) 3303.
[4] G. Gaigalas, Z. Rudzikas and C. Froese Fischer, J. Phys. B: At. Mol. Phys. 30 (1997) 3747.
[5] G. Gaigalas, A. Bernotas, Z. Rudzikas and C. Froese Fischer, Physica Scripta 57 (1998) 207.
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1 Introduction

Models of many-electron atoms and ions require both relativistic and correlation effects to be taken into account for getting very precise characteristics of atoms and ions. This can be done, for example, by using multiconfiguration Hartree–Fock, configuration interaction method, various versions of perturbation theory, or semiempirical methods \[1\]. All of them require the calculation of matrix elements of physical operators or effective operators from perturbation theory. The symmetry properties of atomic states allow the calculation of matrix elements to be divided into the calculation of spin–angular terms and the accompanying radial integrals. The latter are the more straightforward and can be handled by methods such as used in the MCHF atomic structure package (ATSP-MCHF) \[2, 3\]. Such packages have a modular structure, and the modules for calculation of the spin–angular part for matrix elements of any operator can easily be replaced with new one, which is more efficient for large scale computation of open shell atoms.

This paper describes modules of such a sort. The new program (library for integration over spin–angular variables in atomic theory – library SAI) is based on combination of the angular momentum theory, on the concept of irreducible tensorial sets, on a generalized graphical approach, on the second quantization in coupled tensorial form, on the quasispin approach and on standard quantities like the reduced coefficients of fractional parentage, completely reduced matrix elements of the unit tensors as well as a number of other completely reduced matrix elements occurring in various products of electron creation and annihilation operators \[4\]. The program for calculation of standard quantities have been published as library SQ \[5\]. The program presented in this paper uses the library SQ for evaluation of these standard quantities. The new module for the calculation of spin–angular coefficients is faster compared to previous ones and can treat configurations with open \(f^N\) shell.

The theoretical background is presented in Section 2, program organization is outlined in Section 3, the description of the use of this library for other programs is given in Section 4. The program installation is presented in Section 5. Finally, a few examples are given in Section 6.

2 Notations and Methodology of Angular Integrations

2.1 Matrix Elements Between Complex Configurations

According to the approach \[4, 6\], a general expression of a submatrix element for any two–particle operator between functions with \(u\) open shells, can be written as follows:

\[
(\psi_u (LS) | G | \psi_u (L'S')) = \sum_{n,i,n',i'} (\psi_u (LS) | \hat{G} (n_i l_i, n_j l_j, n_i' l_i', n_j' l_j') | \psi_u (L'S'))
\]

\[
= \sum_{n,i,n',i'} (-1)^{\Delta} \Theta' (n_i l_i, n_j l_j, n_i' l_i', n_j' l_j', \Xi) \times T (n_i l_i, n_j l_j, n_i' l_i', n_j' l_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma) R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma),
\]

where \(\lambda \equiv l, s, \Lambda^{bra} \equiv (L_i, L_j, L_i', L_j')^{bra}, \Lambda^{ket} \equiv (S_i, S_j, S_i', S_j')^{bra}\) and \(\Gamma\) refers to the array of coupling parameters connecting the recoupling matrix \(R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)\) to the submatrix element \(T (n_i l_i, n_j l_j, n_i' l_i', n_j' l_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)\). The expression (1) has summation over intermediate ranks \(\kappa_{12}, \sigma_{12}, \sigma_{12}', K_i, K_j\) in \(T (n_i l_i, n_j l_j, n_i' l_i', n_j' l_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)\).

So, to calculate the spin–angular part of a submatrix element of this type, one has to obtain:

1. Recoupling matrix \(R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Gamma)\). This recoupling matrix accounts for the change in going from matrix element \(\langle \psi_u (LS) | G | \psi_u (L'S') \rangle\), which has \(u\) open shells in the \(bra\) and \(ket\) functions, to the submatrix element \(T (n_i l_i, n_j l_j, n_i' l_i', n_j' l_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)\), which has only the shells being acted upon by the two–particle operator in its \(bra\) and \(ket\) functions.
2. Submatrix elements $T (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)$.

3. Phase factor $\Delta$.

4. $\Theta' (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j'; \Xi)$, which is proportional to the radial part. It consists of a submatrix element $(n_i \lambda_i n_j \lambda_j || g^{[\kappa_1 \kappa_2 \kappa_1 \sigma_2 \kappa]} || \psi_u (L'S'))$, and in some cases of simple factors and $3nj$–coefficients (for more details see [6]).

Some important points to note are the following:

1. The recoupling matrices $R (\lambda_j, \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Gamma)$ in our approach are much simpler than in other known approaches. We have obtained their analytical expressions in terms of just $6j$– and $9j$–coefficients. That is why we choose a special form of operator in second quantization, where second quantization operators acting upon the same shell are tensorially coupled together.

2. The tensorial part of a two–particle operator is expressed in terms of (products of) operators of the type $A^{(kk)} (n\lambda, \Xi)$, $B^{(kk)} (n\lambda, \Xi)$, $C^{(kk)} (n\lambda, \Xi)$, $D^{(k)} (n\lambda, \Xi)$, $E^{(kk)} (n\lambda, \Xi)$. Their explicit expressions are (2)–(6):

\[
a^{(q)}_{m_q} (a^{(q)}_{m_q} \times a^{(q)}_{m_q})^{(k\sigma_1)} (a^{(q)}_{m_q} \times a^{(q)}_{m_q})^{(k\sigma_2)} \times \left[ a^{(q)}_{m_q} \times \left[ a^{(q)}_{m_q} \times a^{(q)}_{m_q} \right]^{(k\sigma_1)} \times a^{(q)}_{m_q} \right]^{(k\sigma_2)} \times \left[ a^{(q)}_{m_q} \times a^{(q)}_{m_q} \right]^{(k\sigma_1)} \times \left[ a^{(q)}_{m_q} \times a^{(q)}_{m_q} \right]^{(k\sigma_2)}
\]

We denote their submatrix elements by $T (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)$. The parameter $\Gamma$ represents the whole array of parameters connecting the recoupling matrix $R (\lambda_j, \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Gamma)$ to the submatrix element $T (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)$. It is worth noting that each of the tensorial quantities (2)–(6) act upon one and the same shell. So, all the advantages of tensor algebra and the quasispin formalism may be efficiently exploited in the process of their calculation.

We obtain the submatrix elements of operator (2) by using straightforwardly the Wigner–Eckert theorem in quasispin space:

\[
\left( l'^N \alpha QLS || a^{(q\alpha\beta)} || l'' N' \alpha' Q' L'S' \right) = - [Q]^{-1/2} \left( Q' \begin{array}{cc} Q' & 1/2 \\ M_Q & m_q \end{array} Q \begin{array}{cc} Q & 1/2 \\ M_Q & m_q \end{array} \right) \left( l'^N \alpha QLS || a^{(q\alpha\beta)} || l' \alpha' Q' L'S' \right),
\]

where the last multiplier in (7) is the so–called reduced coefficient of fractional parentage (RCFP) and we use a shorthand notation $(2k+1) \ldots \equiv [k, \ldots]$. The details of the use of quasispin approach are discussed in monograph [1].

The value of a submatrix element of operator (3) is obtained by basing ourselves on (33), (34) in [7]. In the other three cases (4), (5), (6) we obtain them by using (5.16) of Rudzikas [1]:

\[
(nl'^N \alpha QLS || F^{(k\sigma_1)} (n\lambda) \times G^{(k\sigma_2)} (n\lambda) || nl'' N' \alpha' Q' L'S') = (-1)^{L+S+L'+S'+k} \sum_{\alpha''} (nl'^N \alpha QLS || F^{(k\sigma_1)} (n\lambda) || nl'' N'' \alpha'' Q'' L'' S'')\times (nl'' N'' \alpha'' Q'' L'' S'') || G^{(k\sigma_2)} (n\lambda) || nl N' \alpha' Q'L'S') \left\{ \begin{array}{c} \kappa_1 \\ L' \end{array} \left\{ \begin{array}{c} \kappa_2 \\ L'' \end{array} \right\} \left\{ \begin{array}{c} k \\ S' \end{array} \right\} \left\{ \begin{array}{c} \sigma_1 \\ S \end{array} \right\} \right\} ,
\]
where $F^{(\kappa_1, \kappa_2)}(n\lambda)$ and $G^{(\kappa_2, \kappa_2)}(n\lambda)$ is one of (2) or (3) and the submatrix elements correspondingly are defined by (7) and (33), (34) in [7]. $N'$ is defined by second quantization operators occurring in $F^{(\kappa_1, \kappa_1)}(n\lambda)$ and $G^{(\kappa_2, \kappa_2)}(n\lambda)$.

As is seen, by using this approach, the calculation of the angular parts of matrix elements between functions with $u$ open shells ends up as a calculation of submatrix elements of tensors (2), (3) within single shell of equivalent electrons. As these completely reduced submatrix elements (reduced in the quasispin, orbital and spin spaces) do not depend on the occupation number of the shell, the tables for them are reduced considerably in comparison with the tables of analogous submatrix elements of tensorial quantities $U^k, V^{k_1 k_2}$ (Jucys and Savukynas [8] or Cowan [9]) and the tables of fractional parentage coefficients (CFP).

That is why the expressions obtained are very useful in practical calculations. This is extremely important for the $f$–shell, where the number of CFPs for $f^1 – f^{14}$ equals 54408 [10], whereas the number of RCFPs, taking into account the transposition symmetry property of RCFP, is only 14161 – of which only 3624 are nonzero [11].

We do not present details on obtaining phase factors $\Delta$ and $\Theta'$ $(n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Xi)$, since no essential generalizations may be made here; those are possible only after a particular operator is chosen (for more details see [6, 12]).

### 2.2 The Electrostatic Electron Interaction, Spin–Spin and Spin–Other–Orbit Operators

The electrostatic (Coulomb) electron interaction operator $H^{\text{Coulomb}}$ itself contains the tensorial structure

$$H^{\text{Coulomb}} \equiv \sum_k H^{(k,k,0,0)}_{\text{Coulomb}}$$

and its submatrix element is:

$$\left( n_i \lambda_i, n_j \lambda_j \right| H^{(k,k,0,0)}_{\text{Coulomb}} \left| n_{i'} \lambda_{i'}, n_{j'} \lambda_{j'} \right) = 2 |k|^{1/2} \left( l_i \right| C^{(k)} \left| l_{i'} \right) \left( l_j \right| C^{(k)} \left| l_{j'} \right) R_k (n_i l_i n_{i'} l_{i'}, n_j l_j n_{j'} l_{j'}) \right).$$

The spin–spin operator $H^{ss}$ itself contains tensorial structure of two different types, summed over $k$:

$$H^{ss} \equiv \sum_k \left[ H^{(k+1,k-12,112)}_{ss} + H^{(k-1,k+12,112)}_{ss} \right].$$

Their submatrix elements are:

$$\left( n_i \lambda_i, n_j \lambda_j \right| H^{(k+1,k-12,112)}_{ss} \left| n_{i'} \lambda_{i'}, n_{j'} \lambda_{j'} \right) = \frac{3}{\sqrt{5}} \sqrt{(2k+3)^5} (l_i \left| C^{(k+1)} \left| l_{i'} \right) \left( l_j \right| C^{(k-1)} \left| l_{j'} \right) N^{k-1} (n_i l_i n_j l_j, n_i' l_i' n_j' l_j'),$$

$$\left( n_i \lambda_i, n_j \lambda_j \right| H^{(k-1,k+12,112)}_{ss} \left| n_{i'} \lambda_{i'}, n_{j'} \lambda_{j'} \right) = \frac{3}{\sqrt{5}} \sqrt{(2k+3)^5} (l_i \left| C^{(k-1)} \left| l_{i'} \right) \left( l_j \right| C^{(k+1)} \left| l_{j'} \right) N^{k-1} (n_j l_j n_i l_i, n_j' l_j' n_i' l_i'),$$

where we use a shorthand notation $(2k+3)^5 = (2k+3)(2k+2)(2k+1)(2k)(2k-1)$ and radial integral (12), (13) is defined as in Glass and Hibbert [13]:

$$N^k (n_i l_i n_j l_j, n_i' l_i' n_j' l_j') = \frac{\alpha^2}{4} \int_0^\infty \int_0^\infty P_1 (r_1) P_3 (r_2) r_1^2 r_2^2 \epsilon(r_1 - r_2) P_{i'} (r_1) P_{j'} (r_2) dr_1 dr_2,$$

where $\epsilon(x)$ is a Heaviside step–function,

$$\epsilon(x) = \begin{cases} 1; & \text{for } x > 0, \\ 0; & \text{for } x \leq 0. \end{cases}$$
The spin–other–orbit operator $H_{\text{soo}}$ itself contains tensorial structure of six different types, summed over $k$:

$$H_{\text{soo}} = \sum_k \left[ H_{\text{soo}}^{(k-1k,101)} + H_{\text{soo}}^{(k-1k,011)} + H_{\text{soo}}^{(k1k,101)} + H_{\text{soo}}^{(k1k,011)} + H_{\text{soo}}^{(k+1k,101)} + H_{\text{soo}}^{(k+1k,011)} \right].$$

(16)

Their submatrix elements are:

$$\left( n_i \lambda_i n_j \lambda_j \left| H_{\text{soo}}^{(k-1k,1,\sigma_1,\sigma_2)} \right| n_{i'} \lambda_{i'} n_{j'} \lambda_{j'} \right)$$

$$= 2 \cdot 2^{s_2} (2k - 1) (2k + 1) (l_i + l_{i'} - k + 1) (k - l_i + l_i') (k + l_i - l_i') (k + l_i + l_i' + 1)^{1/2}$$

$$\times (k)^{-1/2} \left( l_i \left| C^{(k)} \right| l_{i'} \right) \left( l_j \left| C^{(k)} \right| l_{j'} \right) N^{k-2} (n_j l_j n_i l_i, n_{j'} l_{j'} n_{i'} l_{i'}) ,$$

(17)

$$\left( n_i \lambda_i n_j \lambda_j \left| H_{\text{soo}}^{(k+1k,1,\sigma_1,\sigma_2)} \right| n_{i'} \lambda_{i'} n_{j'} \lambda_{j'} \right)$$

$$= 2 \cdot 2^{s_2} (2k + 1) (2k + 3) (l_i + l_{i'} - k) (k - l_i + l_i' + 1) (k + l_i - l_i' + 1) (k + l_i + l_i' + 2)^{1/2}$$

$$\times (k + 1)^{-1/2} \left( l_i \left| C^{(k)} \right| l_{i'} \right) \left( l_j \left| C^{(k)} \right| l_{j'} \right) N^k (n_j l_j n_i l_i, n_{j'} l_{j'} n_{i'} l_{i'}) .$$

(18)

$$\left( n_i \lambda_i n_j \lambda_j \left| H_{\text{soo}}^{(k1k,1,\sigma_1,\sigma_2)} \right| n_{i'} \lambda_{i'} n_{j'} \lambda_{j'} \right)$$

$$= -2 \cdot 2^{s_2} (2k + 1)^{1/2} \left( l_i \left| C^{(k)} \right| l_{i'} \right) \left( l_j \left| C^{(k)} \right| l_{j'} \right) \left\{ (k (k + 1))^{-1/2} \right.\right.$$

$$\times (l_i (l_i + 1) - k (k + 1) - l_{i'} (l_{i'} + 1)) \left\{ (k + 1) N^{k-2} (n_j l_j n_i l_i, n_{j'} l_{j'} n_{i'} l_{i'}) \right.$$

$$\left.- k N^k (n_j l_j n_i l_i, n_{j'} l_{j'} n_{i'} l_{i'}) \right\} - 2 (k (k + 1))^{1/2} V^{k-1} (n_i l_i n_j l_j, n_{i'} l_{i'} n_{j'} l_{j'}) \right\} .$$

(19)

The radial integrals in (17)–(19) are defined by (14) and below (see Glass and Hibbert [13]):

$$V^k (n_i l_i n_j l_j, n_{i'} l_{i'} n_{j'} l_{j'}) = \frac{\alpha^2}{4} \int_0^\infty \int_0^\infty P_1 (r_1) P_2 (r_2) r_{k+2}^{k-1} r_2 \frac{\partial}{\partial r_2} P_{i'} (r_1) P_{j'} (r_2) dr_1 dr_2 .$$

(20)

Now we have all we need (the operators with tensorial structure and their submatrix elements) for obtaining the values of a matrix element of these operators for any number of open shells in bra and ket functions. This lets us exploit all advantages of the approach by [6].

The spin–spin and spin–other–orbit operators themselves generally contain tensorial structure of several different types. Therefore the expression (1) must be used separately for each possible tensorial structure for performing spin–angular integrations according to [6]. Each type of tensorial structure is associated with a different type of recoupling matrix $R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}}, \Gamma)$ and with different matrix elements of standard tensorial quantities $T (n_i \lambda_i, n_j \lambda_j, n_{i'} \lambda_{i'}, n_{j'} \lambda_{j'}, \Lambda^{\text{bra}}, \Lambda^{\text{ket}}, \Xi, \Gamma)$.

The one–particle operators are treated in a similar manner. Their expressions are much simpler and therefore we do not present them here, for brevity. They may be found in [14].

3 Description of the Library

The library SAI presented in this paper is aimed at the spin–angular integration for any one– and two–particle operator. It is a separate unit and can easily be adapted to existing codes such as the MCHF atomic structure package (ATSP-MCHF) [2, 3] or can easily be used to create a new one. It contains four modules – SAI.RECLS, SAI.SQ, SAI.NORE and SAI.DUDU. They are classified according to the methodology presented in papers [4, 6, 7, 12], and adhere to the principles of modular programming (although FORTRAN 77 does not fully support this).
The module SAI was published separately [5]. In this paper we will discuss briefly the new modules and subroutines contained therein. The author does not attempt to describe in detail all the subroutines belonging to separate libraries. In order to give the reader a more complete view of the implementation of methodology, published in papers [4, 6, 7, 11, 12, 15], only the main subroutines are described. Special attention is given to the description of subroutines that other programs must call for use of this library. The subroutines described in more detail can easily be used separately from the complete library SAI, too. These subroutines are useful for creating new programs or modifying old ones, even those based on the traditional methodology of angular calculations described by Fano [16].

3.1 SAI_RECLS

This library contains 20 routines for calculation of recoupling matrices

\[
R \left( \lambda_i, \lambda_j, \lambda'_i, \lambda'_{j}, \lambda^{bra}, \lambda^{ket}, \Gamma \right) = R \left( l_i, l_j, l'_i, l'_j, \lambda^{bra}, \lambda^{ket}, \Gamma_i \right) R \left( s, s, s, \lambda^{bra}, \lambda^{ket}, \Gamma_s \right).
\]  

(21)

For more details see [6] (Section 4). Most of the subroutines from this module use common blocks CONSTS and MEDEFN from ATSP_MCHF [2, 3].

DLSAn, n=1, 2, ..., 6, evaluates respectively coefficients \(C_1, C_5, C_2, C_4, C_3, C'_6\), defined in equations (15), (16), (23), (21), (17), (25) of [6].

RECOUP0 checks the angular momentum selection rules for the recoupling coefficients. For example, it uses the expression (18) in one interacting shell case (see [6]).

RECOUPn, n=2, 3, 4, evaluates the Kronecker delta functions or calculates the recoupling coefficients respectively for the scalar operator

\[
\left[ A^{(k)} (n_1 l_1) \times B^{(k)} (n_2 l_2) \right]^{(0)},
\]

(22)

\[
\left[ A^{(k_1)} (n_1 l_1) \times B^{(k_2)} (n_1 l_2) \right]^{(k)} \times C^{(k)} (n_m l_m) \right]^{(0)},
\]

(23)

\[
\left[ A^{(k_1)} (n_1 l_1) \times B^{(k_2)} (n_2 l_2) \right]^{(k)} \times \left[ C^{(k_3)} (n_3 l_3) \times D^{(k_4)} (n_4 l_4) \right]^{(k)}
\]

(24)

defined in equations (22), (26), (33) of [6]. The \(A^{(k)}, B^{(k_2)}, C^{(k_3)}\) and \(D^{(k_4)}\) may be simple or composite tensorial operators.

RLSP0 evaluates the Kronecker delta functions \(\delta (L_i, L'_i)\) for one and two interacting shells (see (14) and (19) in [6]).

RLSP00 evaluates the Kronecker delta functions \(\delta (L_i, L'_i)\) for three and four interacting shells (see (24) and (27) in [6]).

RLSPn, n=1, 2, 3 evaluates the Kronecker delta functions or calculates the recoupling coefficients respectively for the non–scalar operator

\[
A^{(k)} (n_1 l_1),
\]

(25)

\[
\left[ A^{(k_1)} (n_1 l_1) \times B^{(k_2)} (n_2 l_2) \right]^{(k)},
\]

(26)

\[
\left[ A^{(k_1)} (n_1 l_1) \times B^{(k_2)} (n_j l_j) \right]^{(k_3)} \times C^{(k_4)} (n_m l_m) \right]^{(k)},
\]

(27)
defined in equations (14), (19), (24) of [6]. This routine evaluates the Kronecker delta functions or calculates respectively the first or second part of recoupling coefficients for the non–scalar operator

$$\left[ A^{(k_1)} (n_1 l_1) \times B^{(k_2)} (n_2 l_2) \right]^{(k_3)} \times \left[ C^{(k_4)} (n_3 l_3) \times D^{(k_5)} (n_4 l_4) \right]^{(k_1)} \times \left( k \right).$$

in the case n=4a, 4b.

3.2 SALNORE

This library is for calculating the spin–angular parts of matrix elements for a scalar two–particle operator. It contains 18 subroutines. Most of the subroutines from this module use common blocks \texttt{CONSTS} and \texttt{MEDEFN} from \texttt{ATSP\_MCHF} [2, 3].

From (1) we see that the matrix element of any two–particle operator can be written as a sum over all possible sets of active shell quantum numbers $n_i l_i$. The systematic analysis of [6] aims to minimize the number of distributions, which is necessary to obtain the matrix elements of any two–electron operator, when the bra and ket functions consist of arbitrary number of shells. Table 1 lists all these distributions and at the same time the expressions used by each of the subroutines \texttt{NONRELAT1}, \texttt{NONRELAT2}, \texttt{NONRELAT31}, \texttt{NONRELAT32}, \texttt{NONRELAT33}, \texttt{NONRELAT41}, \texttt{NONRELAT51}, \texttt{NONRELAT52}, \texttt{NONRELAT53}. The numbering of expressions is the same as in paper [6], where all these expressions are presented. As the structure of all the subroutines mentioned earlier is the same, and only different expressions are used and different subroutines are called, we will discuss in more detail only one of these subroutines.

\texttt{NONRELAT1} is meant for finding spin–angular coefficients for the distributions $\alpha\alpha\alpha\alpha$, $\alpha\beta\alpha\beta$ and $\beta\alpha\beta\alpha$.

In the $\alpha\alpha\alpha\alpha$ case, the program uses expression (5) from [6]. In this case

$$\hat{G}^I \sim \sum_{\kappa i_2, \sigma i_2} \sum_p \left[ \Theta_{IIa} (n\lambda, \Xi) A^{(00)} (n\lambda, \Xi) + \Theta_{IIb} (n\lambda, \Xi) A^{(kk)} (b)p,\sigma (n\lambda, \Xi) \right],$$

where

$$A^{(00)} (n\lambda, \Xi) = \left[ a^{(l_{a}s)} \times a^{(l_{a}s)} \right]^{(\kappa_1 \sigma_1)} \times \left[ a^{(l_{a}s)} \times a^{(l_{a}s)} \right]^{(\kappa_2 \sigma_2)}^{(00)},$$

$$A^{(kk)} (b)p,\sigma (n\lambda, \Xi) = \left[ a^{(l_{a}s)} \times a^{(l_{a}s)} \right]^{(kk)} (n\lambda, \Xi),$$

and

$$\Theta_{IIa} (n\lambda, \Xi) = \Theta_{IIa} \left( n\alpha\lambda\lambda, n\alpha\lambda\lambda, n\alpha\lambda\lambda, n\alpha\lambda\lambda, \Xi \right)$$

$$= \frac{1}{2} (-1)^{k-p} \left[ \kappa_1, \sigma_1, \kappa_2, \sigma_2 \right]^{-1/2} \left( n\alpha\lambda\lambda n\alpha\lambda\lambda \right),$$

and

$$\Theta_{IIb} (n\lambda, \Xi) = \Theta_{IIb} \left( n\alpha\lambda\lambda, n\alpha\lambda\lambda, n\alpha\lambda\lambda, n\alpha\lambda\lambda, \Xi \right)$$

$$= (-1)^{k-p+1} \left( n\alpha\lambda\lambda n\alpha\lambda\lambda \right) \left\{ \kappa_1 \begin{array}{ccc} \kappa_2 & k & \kappa_2 \end{array} \right\},$$

The value of the reduced matrix element of operator (30) is found by subroutine \texttt{WWLS1}, and that of (31) by \texttt{W1} (see module \texttt{SAL\_SQ} in [5]). The value of coefficient $\Theta_{IIa} (n\lambda, \Xi)$ is calculated by \texttt{COULOMBSLS} subroutine, because this coefficient, to the accuracy of a factor and a phase, is equal to that part of the two–electron submatrix elements of electrostatic interaction, which this subroutine is calculating. The coefficient $\Theta_{IIb} (n\lambda, \Xi)$ is found by \texttt{COULOMBSLS} and \texttt{SIXJ}, and the recoupling matrix is investigated by \texttt{RECOUP0} (see section \texttt{SAL\_RECLS}).
Table 1: Scheme of the expressions for matrix elements of two–particle scalar operator (like Coulomb interaction).

| Dis. | $G$ | $G(T)$ | $\beta$ | $\gamma$ | $\delta$ | $\Theta$ | $R$ | $\Delta$ |
|------|-----|--------|--------|--------|--------|--------|----|--------|
| NONRELAT1 |   |        |        |        |        |        |    |        |
| $\alpha\alpha\alpha$ | (47) | (5) | (38),(35) | $\alpha\alpha\alpha$ | (48),(49) | (18) | (41) |
| $\beta\alpha\beta$ | (50) | (6) | (35) | (35) | $\alpha\alpha\beta$ | (51) | (22) | (41) |
| $\beta\alpha\beta$ | (50) | (6) | (35) | (35) | $\beta\alpha\beta$ | (51) | (22) | (41) |
| $\alpha\beta\alpha$ | (54) | (6) | (35) | (35) | $\alpha\beta\alpha$ | (55) | (22) | (41) |
| $\beta\alpha\beta$ | (54) | (6) | (35) | (35) | $\beta\alpha\beta$ | (55) | (22) | (41) |
| NONRELAT2 |   |        |        |        |        |        |    |        |
| $\alpha\alpha\beta$ | (52) | (6) | (35) | (35) | $\alpha\alpha\beta$ | (53) | (22) | (41) |
| NONRELAT31 |   |        |        |        |        |        |    |        |
| $\beta\alpha\alpha$ | (56) | (6) | (36) | (34) | $\alpha\beta\alpha$ | (58) | (22) | (42) |
| $\alpha\beta\alpha$ | (56) | (6) | (36) | (34) | $\alpha\beta\alpha$ | (59) | (22) | (42) |
| NONRELAT32 |   |        |        |        |        |        |    |        |
| $\beta\beta\alpha$ | (60) | (6) | (34) | (34) | $\beta\beta\alpha$ | (62) | (22) | (42) |
| $\beta\beta\alpha$ | (60) | (6) | (34) | (34) | $\beta\beta\alpha$ | (63) | (22) | (42) |
| NONRELAT33 |   |        |        |        |        |        |    |        |
| $\beta\gamma\gamma$ | (50) | (7) | (34) | (34) | (35) | (51) | (26) | (42) |
| $\gamma\beta\gamma$ | (50) | (7) | (34) | (34) | (35) | (51) | (26) | (42) |
| $\gamma\beta\gamma$ | (54) | (7) | (34) | (34) | (35) | (55) | (26) | (42) |
| $\beta\gamma\gamma$ | (54) | (7) | (34) | (34) | (35) | (55) | (26) | (42) |
| NONRELAT41 |   |        |        |        |        |        |    |        |
| $\gamma\gamma\alpha$ | (52) | (7) | (34) | (34) | (35) | (53) | (26) | (42) |
| $\gamma\gamma\alpha$ | (52) | (7) | (34) | (34) | (35) | (53) | (26) | (42) |
| $\alpha\beta\gamma$ | (52) | (7) | (34) | (34) | (35) | (53) | (26) | (42) |
| $\beta\beta\gamma$ | (52) | (7) | (34) | (34) | (35) | (53) | (26) | (42) |
| NONRELAT51 |   |        |        |        |        |        |    |        |
| $\alpha\beta\gamma$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\beta\alpha\gamma$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\alpha\beta\gamma$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\beta\alpha\gamma$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\gamma\delta\alpha$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\gamma\delta\alpha$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\delta\gamma\alpha$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| $\delta\gamma\alpha$ | (52) | (8) | (34) | (34) | (34) | (34) | (53) | (33) | (43) |
| NONRELAT52 |   |        |        |        |        |        |    |        |
| $\alpha\gamma\beta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\alpha\gamma\beta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\alpha\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\alpha\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\alpha\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\alpha\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| NONRELAT53 |   |        |        |        |        |        |    |        |
| $\alpha\delta\beta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\alpha\delta\beta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\alpha\delta\beta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\alpha\delta\beta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\beta\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\beta\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\beta\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\beta\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\beta\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
| $\gamma\beta\delta$ | (50) | (8) | (34) | (34) | (34) | (34) | (51) | (33) | (43) |
For the distributions $\alpha\beta\alpha\beta$ and $\beta\alpha\beta\alpha$ the subroutine NONRELAT1 uses (6) of [6], keeping in mind that $\Theta(n_\alpha, n_\beta, \lambda, \Xi)$ is expressed as (51) of [6] and tensorial parts $B^{(\kappa_1, \sigma_1, \Omega)}(n_\alpha, \lambda, \Xi)$, $C^{(\kappa_2, \sigma_2, \Omega)}(n_\beta, \lambda, \Xi)$ are equal to (35) from [6]. The coefficients $\Theta(n_\alpha, n_\beta, \lambda, \Xi)$ are investigated by COULOMBS, the coefficients $B^{(\kappa_1, \sigma_1, \Omega)}(n_\alpha, \lambda, \Xi)$ and $C^{(\kappa_2, \sigma_2, \Omega)}(n_\beta, \lambda, \Xi)$ are found by W1W2LS from the SAILSQ library [5], and the recoupling matrix is calculated by RECoup2.

For the distributions $\alpha\beta\alpha\beta$ and $\beta\alpha\beta\alpha$ the subroutine NONRELAT1 uses (6) of [6], keeping in mind that $\Theta(n_\alpha, n_\beta, \lambda, \Xi)$ is expressed as (55) of [6] and tensorial parts $B^{(\kappa_1, \sigma_1, \Omega)}(n_\alpha, \lambda, \Xi)$, $C^{(\kappa_2, \sigma_2, \Omega)}(n_\beta, \lambda, \Xi)$ are equal to (35) from [6]. The coefficients $\Theta(n_\alpha, n_\beta, \lambda, \Xi)$ are investigated by COULOMBS and SIXJ, the coefficients $B^{(\kappa_1, \sigma_1, \Omega)}(n_\alpha, \lambda, \Xi)$ and $C^{(\kappa_2, \sigma_2, \Omega)}(n_\beta, \lambda, \Xi)$ are found by W1W2LS from the SAILSQ library [5], and the recoupling matrix is calculated by RECoup2.

COULOMBS Investigates the two–electron submatrix elements of electrostatic interaction
\[
\left(n_i \lambda_i n_j \lambda_j \right) || g_{\text{Coulomb}}^{(k, k, 0, 0)} || n_i' \lambda_i' n_j' \lambda_j',
\]
according to the formula (9) of [7]. The values of these matrix elements are needed because of (see [6])
\[
\Theta(\Xi) \sim \left(n_i \lambda_i n_j \lambda_j || g \right) \left(n_i' \lambda_i' n_j' \lambda_j' \right).
\]

The value of the output parameter $AA$ of this subroutine is:
\[
AA = 2 \beta^1/2 \left(L_i || C^{(k)} || L_i' \right) \left(L_j || C^{(k)} || L_j' \right).
\]

### 3.3 SAILDUDU

This library is meant for the calculation of matrix elements of any one– or two–particle operator. It contains 44 subroutines. Most of the subroutines from this module use common blocks CONSTS and MEDEFN from package ATSP.MCHF [2, 3]. Similar to the SAILDUDU library, it uses the methodology described in paper [6]. Therefore the arrangement of library SAILDUDU is analogous to that of library SAILDUDU. Therefore we will not go into computational details of spin–angular parts of one– or two–particle operator matrix elements, but instead will reserve all the attention to a demonstration of connection of the Breit–Pauli operators to the general algorithm of one– or two–particle operator calculation.

#### 3.3.1 Spin–own–orbit interaction

The subroutine SPINOR investigates the submatrix elements of the spin–own–orbit interaction operator
\[
\left(n_i \lambda_i || J^{(11)} || n_i' \lambda_i' \right),
\]
according to the formula (5) of [11].

#### 3.3.2 Spin–spin interaction

The subroutine SSC investigates the spin–spin operator, which has the tensorial form (11) and finds the submatrix element of this operator between functions with any number of open shells. This subroutine is used for all distributions except $aaaa$, $\alpha\beta\alpha\beta$, $\beta\alpha\beta\alpha$, $\alpha\beta\beta\alpha$, $\beta\alpha\alpha\beta$ and $\alpha\alpha\beta\beta$. In the latter cases, instead of subroutine SSC the subroutines SS1111, SS1212, SS1212, SS1221, SS1221 and SS1122 are used.

The subroutine SSA investigates the submatrix elements of the spin–spin interaction operator
\[
\left(n_i \lambda_i n_j \lambda_j || H_{ss}^{(k+1, k-12, 112)} || n_i' \lambda_i' n_j' \lambda_j' \right)
\]
and
\[
\left(n_i \lambda_i n_j \lambda_j || H_{ss}^{(k-1, k+12, 112)} || n_i' \lambda_i' n_j' \lambda_j' \right)
\]
respectively. This subroutine is used for all distributions except $aaaa$, $\alpha\beta\alpha\beta$, and $\beta\alpha\beta\alpha$. In the latter cases, instead of subroutine SSA the subroutine SS1 is used.
3.3.3 Spin–other–orbit interaction

The subroutine SOOC investigates the spin–other–orbit operator (16). This subroutine is used for all distributions except $aaa$, $\alpha\beta\beta$, $\beta\alpha\beta$, $\alpha\beta\alpha$ and $\alpha\alpha\beta$. For distributions $aaa$, $\alpha\beta\beta$ and $\beta\alpha\beta$, according to (34), (39) and (40) of [12], the tensorial form

$$H^{soo}_{12} = \sum_k \left\{ H^{(k-1)l,1} + H^{(k-1)l,011} + H^{(k+1)l,1} + H^{(k+1)l,011} \right\}$$

is valid. Therefore instead of subroutine SSC the subroutines SOO1111, SOO1212, SOO1212 respectively are used. The distribution $\alpha\beta\beta$, $\beta\alpha\beta$ and $\alpha\alpha\beta$ are also calculated according to separate expressions. These are treated by the subroutines SOO1221P, SOO1221P and SOO1122P.

The subroutines SOOA and SOOB investigate the submatrix elements of the spin–other–orbit interaction operator

$$\left( n_i \lambda_i n_j \lambda_j || H^{(k-1)l,011} || n'_i \lambda'_i n'_j \lambda'_j \right), \quad \left( n_i \lambda_i n_j \lambda_j || H^{(k-1)l,111} || n'_i \lambda'_i n'_j \lambda'_j \right),$$

$$\left( n_i \lambda_i n_j \lambda_j || H^{(k+1)l,1} || n'_i \lambda'_i n'_j \lambda'_j \right), \quad \left( n_i \lambda_i n_j \lambda_j || H^{(k+1)l,011} || n'_i \lambda'_i n'_j \lambda'_j \right)$$

according to the formulas (26), (27) and (28) of [12] respectively. These subroutines are used for all distributions except $aaa$. In the latter case instead of subroutines SOOA and SOOB the subroutine SOO1 is used.

4 The Library usage for other programs

There are different versions of ATSP_MCHF [2, 3, 17], which support non–relativistic atomic structure calculations. Each of them has some specific disparity. But it is possible to implement the library SAI in all of them and in other programs as well. The one example of such connection between ATSP_MCHF and SAI is shown for the program Breit from [3] in Table 2. The modify package ATSP_MCHF [3] which is fit to the module SAI is coming with the distribution of the library SAI.

For writing the similar interface for other programmes like [18] we need to fill in the Common block MEDEFN from ATSP_MCHF, to write similar program as is presented in the Table 2 and to make some other subroutines similar as is presented in this distribution (the files breit.f, savenon.f and setupgg.f in the directory /dudu/breit).

Table 2. THE MODIFY PROGRAM BREIT FOR CONNECTION BETWEEN ATSP_MCHF AND SAI.

| PROGRAM BREIT |
|---------------|
| IMPLICIT DOUBLE PRECISION(A-H,O-Z) |
| PARAMETER (XWD=60,NCD=1000,NCD2=2+*NCD) |
| CHARACTER A*N+2, NAME(2)*24 |
| COMMON/DBUG/IBUG1,IBUG2,IBUG3,IBUG4,NBUG,NBUG7,IFULL |
| COMMON/CONS/T/ZEK, TENTH, HALF, ONE, TWO, THREE, FOUR, SEVEN, ELEVEN, EPS |
| COMMON/DIAG/E, IDIQ, JA, JB |
| COMMON/FOUT/NOV(2), IOLAP(10,2), NF, NG, NR, NL, NZ, NN, NV, NS, IPLAQ, NIJ |
| COMMON/IMAG/CONST, CONSDD, CONSS, ISPORB, ISOGAB, IPSPEX, |
| : IRE, IPRF, IZOUT, ISEL, ITEINF |
| COMMON/ISFORM/IREAB, IWRITE, IOUT, ISC(8) |
| COMMON/MEDIINF/IBRH,NJ(16),IJ(16),NOSH(16),NOSH2(16),J1QW(31,3), |
| : J1QW(31,3),IJ1QW |
| COMMON/PHASES/SIGNF(NCD2), ICSTAS |
| COMMON/STATES/KCFS, NOCSSH(NCD2), NOCORB(5, NCD2), NELCSSH(5, NCD2), |
| : JIQORB(9, NCD2), MAIORB, JCOMP(NCD), IAJCOMP(NCD) |
| COMMON /OPERAT/ ICOLOM, ISOTOP, ISOGAB |
| COMMON /BREIT/ ISPORB, ISOGRB, ISPEX |
| COMMON/STEED/IX, IGGD, IRAND, ISIC, IRHSP, ISIGP |
| DIMENSION XPLD(20), IRPSK(NCD2), NCOUNT(8) |

11
EQUIVALENCE (NCOUNT(1),NF)
LOGICAL 10I

105 FORMAT (49H ISPORB=0 AND ISOORB=1 CAUSES THE PROGRAM TO FAIL,/
: 34H BECAUSE THE BLUME WATSON FORMULAE,/)

11 FORMAT(49H THE TYPE OF CALCULATION IS DEFINED BY ',/
: 'THE FOLLOWING PARAMETERS - /
: 5X,22H BREIT-PAULI OPERATORS,13X,8IHERL =,I2/
: 5X,27H PHASE CONVENTION PARAMETER,8X,8ICSTAS =,I2/
: IT (,11,22H), SPIN-OTHER-ORBIT (,I1,15H), SPIN-SPIN (.I1,1H)/)

24 FORMAT(56H INITIAL DEBUG: IN 1-ELECTRON PART =,I2,2H,,5X,/
: IN 2-ELECTRON PART=,I2/16X,23H IN RECOUPLING PACKAGE =,I2/)
IF(ISPORB.EQ.0.AND.ISOORB.NE.0) THEN
  WRITE (IWRITE,105)
END IF
END IF

IBUG1 = 0
IBUG2 = 0
IBUG3 = 0
IBUG6 = 0
IBUG7 = 0
WRITE(IWRITE,11) IREL,ICSTAS
ISPORBG = ISPORB
ISOORBG = ISOORB
ISPSPNG = ISPSPN
CALL FACTRL(32)

* --- READ IN THE SET OF CONFIGURATIONS
CALL ACNFIG(NAME(1))
IDG = 0
NZERO = NCFG
NEW = NCFG
DO 554 I = 1,NZERO
  IRFST(I) = 1
  ISTART = 1
  WRITE(0,'(A)') ' All Interactions? (Y/N): '
  READ (5,'(A2)') ANS
  IF (ANS .NE. 'Y' .AND. ANS .NE. 'y') THEN
    DO 553 I = 1,(20)
      NFLG(I) = 0
      WRITE(0,*) ' Define your reference set : FORM(20I3)'
    READ (5,'(20I3)') (NFLG(I),I=1,(20))
    DO 551 I = 1,(ISTART-1)
      IRFST(I) = 0
      DO 552 J = 1,(20)
        IF (NFLG(J) .EQ. I) THEN
          IRFST(I) = 1
          GO TO 552
        ENDIF
      552 CONTINUE
    551 CONTINUE
  ENDIF
  NZERO = NZERO - NEW
  IF (NZERO .eq. 0) NZERO = NEW
  DO 554 I = 1,NZERO
    PRINT 554
  554 DO 554 I = 1,NZERO
      IRFST(I) = 0
      NEW = NEW + 1
  554 CONTINUE
ENDIF

IF (NZERO .ne. 0) NZERO = NCFG
IF (IINTERNAL .NE. 0 .AND. NZERO .NE. NCFG) THEN
  WRITE(0,'(A)') ' Rel interaction with all the zero block? '
  READ (5,'(A2)') ANS
  IF (ANS .NE. 'Y' .AND. ANS .NE. 'y') THEN
    DO 553 I = 1,(20)
      NFLG(I) = 0
      WRITE(0,*) ' Define your reference set : FORM(20I3)'
    READ (5,'(20I3)') (NFLG(I),I=1,(20))
    DO 551 I = 1,(ISTART-1)
      IRFST(I) = 0
      DO 552 J = 1,(20)
        IF (NFLG(J) .EQ. I) THEN
          IRFST(I) = 1
          GO TO 552
        ENDIF
      552 CONTINUE
    551 CONTINUE
  ENDIF
  IINTERNAL = IINTERNAL + 1
ENDIF

ISTRICT = 1
WRITE(0,*) ' Restricted Two-body interactions? (Y/N); '
READ (5,'(A2)') ANS
IF (ANS .NE. 'Y' .AND. ANS .NE. 'y') ISTRICT = 0

ISTRICT = 1
WRITE(0,*) ' Diagonal rel corrections ? (Y/N): '
READ (5,'(A2)') ANS
IF (ANS .EQ. 'Y' .OR. ANS .EQ. 'y') IDG = 1

ISTRICT = 1
WRITE(0,*) ' Restricted Two-body interactions? (Y/N); '
READ (5,'(A2)') ANS
IF (ANS .NE. 'Y' .AND. ANS .NE. 'y') ISTRICT = 0

END IF

*... Start the calculation
DO 6 JA = ISTART, NCFG
  ICOUNT = 0
  *... Set up defining quantum numbers for each matrix element.
  CALL SETUP(JA,JB)
  IF(IBUG1.HGE.0 OR IBUG2.HGE.0) CALL VIJOUT(JA,JB)
  IF(INSTHOUT.GE.MAXINSTH) STOP

*... Test on possible recoupling orthogonality.
  CALL ORTHOG(LET,INCL)
  IF(LET .NE. 0) THEN
    CALL SETUPGG
    IF (IX .LE. 4) THEN
      IF(IFULL .NE. 0) WRITE(IWRITE,77)
      FORMAT(///30X,'MULTIPLYING FACTOR',11X,'TYPE OF INTEGRAL')
      CALL NONBP
      IF(IFLAG .NE. 0) NIJ = NIJ + 1
    ENDIF
  ENDIF

  NTOTAL = ((2*NCFG - NEW +1)*NEW)/2
END
5 Installation of the Library

The library SAI will be distributed as compressed tar archive file. On a UNIX (or compatible) workstation, the commands `uncompress tar_lib_SAI` and `tar xvf tar_lib_SAI` reconstruct the file structure. The directory LIBRARY_SAI contains the source code (subdirectories dudu, nore, recls, sqlsf1 and sqlsf2) as well as makefile `make_lib_SAI`. It also includes a modify package ATSP_MCHF [3] which is fitted to the module SAI.

The command `make_lib_SAI` creates the libraries `libdudu.a`, `libnore.a`, `librecls.a`, `libsqlsf1.a` and `libsqlsf2.a` in directory `bin`.

6 Examples

The way to determine the ionization potential for Ce is demonstrated in this section. For this, one needs to calculate the ground state energy of Ce atom ($^1G$), the ground state of a Ce$^+$ ion ($^2G$), and find the difference. It has been shown in [19, 20, 21] that the non–relativistic Hartree–Fock ionization potential of singly ionized lanthanides follows the observed trends. Therefore we have chosen the non–relativistic approximation, and find the energy values by solving the multi–configuration Hartree–Fock equations. For brevity, we present only the Ce$^+$ test cases. The energy for Ce is found in the same way.

In Table 3 we present an example of generating a set of configurations where the ground state energy of the Ce$^+$ ion is to be calculated by the multiconfiguration Hartree–Fock method. The configurations are obtained by taking the singles and doubles excitations from \{4f, 5d, 6s\} to the active set \{5f, 5g\} (since neither 5d nor 6s are filled shells, better accuracy would be obtained if these orbitals were also included in the active set) [21]. In this case the program `GENCL` [22] generates a `cfg.out` file with 40 configuration states.

### Table 3. TEST RUN OUTPUT

```
>>genclf
---------------------------------------------------------------------
You are under the program GENCL
    which GENERates a Configuration List
Type H (Help) to obtain information about the input format
Type <RETURN> if you already know
---------------------------------------------------------------------
Header ?
> Ce+ ground state
   Closed Shells ?
   1s 2s 2p 3s 3p 3d 4s 4p 4d 5s 5p
   Reference Set ?
   4f(1)5d(1)6s(1)
   2 ?
> Active Set ?
>
> Replacements ?
> sd
Virtual Set ?
> 5f,5g
   From which shell ?
> 1
```
To which shell ?
> 3
Final Terms ?
> 2

*************** I N P U T D A T A **************
Header : Ce+ ground state
Closed shell : 1s 2s 2p 3s 3p 3d 4s 4p 4d 5s 5p
Reference Set : 4f(1)5d(1)6s(1)
Active Set : 
Replacements : sd
Virtual Set : 5f,5g
From which shell : 1
To which shell : 3
Final Terms : 2G

GENERATE ALL COUPLINGS FOR EACH MEMBER OF THE REFERENCE SET
--------- Ce+ ground state ---------
Closed Shells : 1s 2s 2p 3s 3p 3d 4s 4p 4d 5s 5p
Reference Set : 4f(1)5d(1)6s(1)
Virtual Set : 5f,5g
S-Replacement : 4f = 5f
Configuration : 5d(1) 6s(1) 5f(1)
Their couplings : 2D1 2S1 2F1 1G0 2G0
2D1 2S1 2F1 3D0 2G0

FOR VIRTUAL SET, GENERATE CONFIGURATION STATES FOR S-REPLACEMENT
--------- Ce+ ground state ---------
Closed Shells : 1s 2s 2p 3s 3p 3d 4s 4p 4d 5s 5p
Reference Set : 4f(1)5d(1)6s(1)
Virtual Set : 5f,5g
S-Replacement : 4f = 5f
Configuration : 5d(1) 6s(1) 5f(1)
Their couplings : 2D1 2S1 2F1 1G0 2G0
2D1 2S1 2F1 3D0 2G0

OK!
List of configurations and their couplings
is in the file cfg.inp

The generating of the angles file int.lst is demonstrated in Table 4 with the modify package ATSP_MCHF [3] which is fitted to the module SAI and presented in the distribution. It will be needed for calculating the energy of \( ^2 \)G state of Ce\(^+\) with the MCHF program [23]. The program input file cfg.inp is taken with the help of renaming cfg.out to cfg.inp.

Table 4. TEST RUN OUTPUT

>>breitf ============ Obtain Expressions for Breit-Pauli Interactions

B R E I T - P A U L I

Indicate the type of calculation
0 => non-relativistic Hamiltonian only;
1 => one or more relativistic operators only;
2 => non-relativistic operators and selected relativistic:
>0
Is full print-out requested? (Y/N)
>Y
Phases:- Condon and Shortley of Fano and Racah ? (CS/RF)
>CS
All Interactions? (Y/N)
>Y
THE TYPE OF CALCULATION IS DEFINED BY THE FOLLOWING PARAMETERS -
BREIT-PAULI OPERATORS IREL = 0
PHASE CONVENTION PARAMETER ICSTAS = 1

---------------------
THE CONFIGURATION SET

15
STATE (WITH 40 CONFIGURATIONS):

THERE ARE 5 ORBITALS AS FOLLOWS:
4f 5d 6s 5f 5g

THERE ARE 11 CLOSED SUBSHELLS COMMON TO ALL CONFIGURATIONS AS FOLLOWS:
1s 2s 2p 3s 3p 3d 4s 4p 4d 5s 5p

CONFIGURATION 1 (OCCUPIED ORBITALS=3):
4f(1) 5d(1) 6s(1)
COUPLING SCHEME: 2F1 2D1 2S1

... Output omitted for brevity ...

CONFIGURATION 40 (OCCUPIED ORBITALS=2):
4f(1) 5g(2)
COUPLING SCHEME: 2F1 3H2

MATRIX ELEMENTS CONSTRUCTED USING THE SPHERICAL HARMONIC PHASE CONVENTION OF CONDON AND SHORTLEY, THEORY OF ATOMIC STRUCTURE

>>cat int.lst ===> Display the int.lst file produced

Ce+ ground state

```
F 0(4f, 5d) 12  R 0(4f 5d, 5f 5d) 14  R 5(5d 5g, 5f 5f) 2008
F 0(4f, 6s) 16  R 0(4f 6s, 5f 6s) 20  R 5(5f 5f, 5g 5g) 2014
F 0(4f, 5f) 22  R 0(4f 5g, 5f 5g) 32  R 6(4f 5d, 5f 5g) 2018
F 0(4f, 5g) 40  R 1(4f 5d, 5d 5f) 46  R 6(4f 5g, 5f 5f) 2082
F 0(5d, 6s) 44  R 1(4f 5d, 5g 5f) 50  R 6(4f 5d, 5g 5f) 2146
F 0(5d, 5f) 56  R 1(4f 5f, 5d 5g) 110  R 6(4f 5g, 5f 5g) 2178
F 0(6s, 5f) 76  R 1(4f 5g, 5d 5f) 124  R 6(5d 5f, 5g 5f) 2182
F 0(6s, 5g) 80  R 1(4f 5g, 5d 5f) 188  R 7(4f 5g, 5g 5f) 2336
F 0(5f, 5f) 80  R 1(5d 5f, 5f 5g) 354  R 7(5f 5f, 5g 5g) 2342
F 0(5f, 5g) 102  R 1(5d 5g, 5f 5f) 356  *R 26 14
F 0(5g, 5g) 108  R 1(5d 5g, 5f 5f) 406  -1.00000000R 22 10
F 0(4f, 5d) 120  R 1(5f 5f, 5g 5f) 412  1.00000000R 21 9
F 0(4f, 5g) 130  R 1(5f 5g, 5g 5f) 414  1.00000000R 20 8
F 0(4f, 6s) 166  R 1(5f 5g, 5g 5f) 428  1.00000000R 19 7
F 0(5d, 5f) 178  R 1(5f 5g, 5g 5f) 430  0.86602540R 18 6
F 0(5d, 5g) 226  R 1(5f 5g, 5g 5g) 434  -1.00000000R 17 5
F 0(5f, 5g) 258  R 1(5f 5g, 5g 5g) 500  1.00000000R 16 4
F 0(5g, 5g) 264  R 1(5f 5g, 5g 5g) 564  -1.00000000R 15 3
F 0(4f, 5d) 276  R 1(5f 5g, 5g 5g) 604  -1.00000000R 14 2
F 0(4f, 5f) 287  R 1(5f 5g, 5g 5g) 610  1.00000000R 13 1
F 0(4f, 6s) 324  R 1(5f 5g, 5g 5g) 610  -0.86602540R 12 1
F 0(5d, 5f) 336  R 1(5f 5g, 5g 5g) 650  0.50000000R 11 1
F 0(5d, 5g) 388  R 1(5f 5g, 5g 5g) 670  -1.00000000R 10 1
F 0(5f, 6s) 394  R 1(5f 5g, 5g 5g) 720  -0.86602540R 9 1
F 0(5g, 5g) 426  R 1(5f 5g, 5g 5g) 736  0.86602540R 8 1
F 0(6s, 5f) 426  R 1(5f 5g, 5g 5g) 736  0.86602540R 7 1
F 0(6s, 5g) 455  R 1(5f 5g, 5g 5g) 736  0.86602540R 6 1
F 0(6f, 5g) 464  R 1(5f 5g, 5g 5g) 742  0.50000000R 5 1
F 0(5f, 6f) 470  R 1(5f 5g, 5g 5g) 744  1.00000000R 4 1
F 0(5f, 5g) 490  R 1(5f 5g, 5g 5g) 748  -1.00000000R 3 1
F 0(6f, 5g) 490  R 1(5f 5g, 5g 5g) 748  -1.00000000R 2 1
F 0(5g, 6f) 496  R 1(5f 5g, 5g 5g) 768  1.00000000R 1 1
F 0(5g, 5g) 502  R 1(5f 5g, 5g 5g) 780  1.00000000R 0 1

* 1.00000000 1 1  R 3(5f 5g, 5g 5g) 1024  1.00000000R 23 11
1.00000000 13 13  R 3(5f 5g, 5g 5g) 1024  1.00000000R 23 11
1.00000000 14 14  R 3(5f 5g, 5g 5g) 1024  1.00000000R 23 11
1.00000000 15 15  R 3(5f 5g, 5g 5g) 1024  1.00000000R 23 11
(cont.)  R 3(5f 5g, 5g 5g) 1024  1.00000000R 23 11
```
The energy of $^2G$ state of Ce$^+$ is found by the multi-configurational Hartree–Fock method. First, the wave functions are obtained by the HF method, using the HF96 program (see Gaigalas and Fischer [24]). These functions are used as starting ones in solving the multi-configurational Hartree–Fock equations. The input files for MCHF program [23] int.lst, and cfg.inp, are taken from the examples described above.

7 Conclusion

The library SAI supports large scale computations of open-shell atoms using multi-configuration Hartree–Fock or configuration interaction approaches and may be useful for developing codes for calculating the spin–angular parts of effective operators from many-body perturbation theory and orthogonal operators or for evaluating the relativistic Hamiltonian in $LS$–coupling as well as for various versions of semi-empirical methods. For example, it expands the use of possibilities of package MCHFASP [2, 3, 17] because the new program is faster and provides coefficients and matrix elements for shells ($nl$) with $l = 0, 1, 2$ and $3$, and $l^2$ for $l \geq 3$. It is important to underline that the use of the library described allows to perform calculations of energy spectra of practical any atom or ion starting with $LS$–coupling and accounting for all relativistic corrections of the order $\alpha^2$.

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

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