# THE PROGRAM FOR THE TRANSFORMATION OF ATOMIC STATE FUNCTIONS FROM LS- TO jj-COUPLED BASIS

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#### Abstract

Here we present the program for the transformation of the expansions of the atomic state functions from LS- to jj-coupled bases. The program is a part of the coupling optimization package LARIS and allows to transform the multiconfigurational expansions with the arbitrary number of open shells (including f-electrons) and to identify atomic levels and classify the atomic spectra by means of intermediate quantum numbers of LS- and jj-couplings.

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Keywords: atomic structure, LS-coupling, jj-coupling, LS-jj transformation, optimal coupling scheme, classification of atomic spectra.

#### PROGRAM SUMMARY

Title of program: LSJJ

Program obtainable from: Vilnius University Research Institute of Theoretical Physics and Astronomy, A. Goštauto 12, Vilnius, 2600, Lithuania. E-mail: tomas@mserv.itpa.lt

Computer for which the library is designed and others on which it has been tested: Pentium-based PC 155 MHz. Installations: Vilnius University Research Institute of Theoretical Physics and Astronomy (Lithuania) Operating systems or monitors under which the new version has been tested: LINUX 2.4.5

Programming language used in the new version: ANSI standard Fortran 90/95.

Memory required to execute with typical data: Memory requirements depend on the shell structure and the size of the wave function expansion which is used to represent the atomic levels.

No. of bits in a word: All real variables are parametrized by a selected kind parameter and, thus, can easily be adapted to any required precision as supported by the compiler. Presently, the kind parameter is set to double precision (two 32-bit words) in the module rabs\_constant.

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

Distribution format: compressed tar file

Keywords: atomic structure, LS-coupling, jj-coupling, LS-jj transformation, optimal coupling scheme, classification of atomic spectra.

#### Nature of physical problem:

The set of quantum numbers for the identification of atomic state functions (levels) and the classification of atomic spectra usually are chosen comparing the distributions of the mixing coefficients in the bases corresponding to various coupling schemes. The corresponding mixing coefficients usually are obtained diagonalizing the energy matrix in the basis of the wave functions of certain coupling. Once the secular equation is solved and the mixing coefficients in some coupling scheme are obtained they can be used as a source to get corresponding coefficients for the bases of other coupling schemes if the appropriate transformation matrix is known [1].

#### Method of solution:

For the transformation of the atomic state functions from LS- to jj-coupled basis we use the recently obtained LS-jj transformation matrices for the shells of equivalent electrons [2] as well as the formula for the LS-jj transformation matrices [3].

Restrictions on the complexity of the problem:

The program restricted to the configurations with LS-coupled shells with l=0, 1, 2 and 3.

Unusual features of the program: The LSJJ program is designed as a part of the coupling optimization package LARIS.

#### References:

- [1] Z. Rudzikas, Theoretical Atomic Spectroscopy (Cambridge Univ. Press, Cambridge, 1997).
- [2] G. Gaigalas, T. Žalandauskas and Z. Rudzikas, At. Data Nucl. Data Tables, in print (2002).
- [3] G. Gaigalas, Z. Rudzikas and T. Žalandauskas, Book of Abstracts of XI HCI Conference, 1-6 September, 2002, Caen, France, 48.

### LONG WRITE-UP

## 1 Introduction

In investigating the energy spectra and other characteristics of atoms and ions, the experimentalists most often use the LS-coupling scheme. There a shell of electrons is made of the electron states having the same principal and angular quantum numbers, n and l. Such a shell is additionally characterized by the shell occupation number N and the resulting orbital and spin momenta,  $L_i$  and  $S_i$ . When several shells are present, the state in LS-coupling is additionally characterized by the intermediate resulting momenta  $L_{ij}$ and  $S_{ij}$ , and by the total momenta L, S and J. This coupling scheme is very popular in the theoretical atomic physics when atoms and ions are investigated in the non-relativistic approximation. This, in the first place, is related to the fact that for the light atoms and ions such an approximation produces quite accurate results and the agreement with the experiment is fairly good. Secondly, this coupling scheme is realistic for such systems. Therefore it is convenient for the identifying the energy levels. At the same time, this scheme is convenient to investigate such processes as transitions, whereby the selection rules for electronic transitions are both easily determined and reflect the real situation. But this coupling scheme is for a relatively small number of atoms and ions. The quantum numbers of this scheme are not accurate for highly charged ions and a number of other cases. For the identification of atomic state functions (ASF) and classification of energy spectra the approximate quantum numbers are widely used. Usually such a classification relies on the characteristics of the LS- or jj- coupling scheme. But in a number of cases (for example ions of intermediate ionization degree) the choice of such classification is not trivial and implies the consideration of the expansions of atomic state functions in several bases of pure coupling wave functions. Therefore it is convinient to have the possibility to transform the expansions of atomic state functions between various bases of pure coupling wave functions [1].

The transformation matrices between the different bases of pure coupling wave functions were studied ([2]-[10]), whereas the corresponding software were developed ([11, 12, 13, 14]). Nevertheless until recently there were neither LS-jj transformation matrices for the arbitrary number of open shells available, nor the corresponding software allowing one to transform the ASFs resulted from the large scale calculations. In addition, the software created earlier does not always allow to find the most suitable coupling scheme, as sometimes it appears that no dominating scheme is present and several schemes are equally suitable simultaneously. We present the investigation of the Fluorine isoelectronic sequence as an example [15]. In this case, several coupling schemes are treated in the search for an optimal one. Those are LS, LK, JKand JJ. In all those schemes the LS coupling is valid inside a shell. Using the analysis of the structure of the weights of the ASF or the quantity R, one may notice that in this particular isoelectronic sequence the ions do not have a dominating scheme, or the dominating scheme does not stand out clearly among others. Therefore the above–mentioned methods have been extended [8, 9, 10] in a way providing a possibility to change the LS-coupling scheme into the jj-coupling one inside a shell, when necessary. The recently obtained LS-jj transformation matrices for the shell of equivalent electrons [9] as well as the formulas for the LS-jj transformation matrices [10] enabled us to develop a computer code allowing to transform the ASFs from LS- to jj-coupling for all the configurations practically needed in atomic physics. In the search for an optimal coupling scheme that would allow one to change the coupling scheme inside a shell and to investigate the atoms and ions with ASFs containing open f-shells with arbitrary occupation numbers.

To facilitate such a classification of the atomic levels and wave functions, we present here the program Lsjj. It supports the performance of the LS - jj transformations. This program may be of value as a separate module in solving the physical problems that also need this transformation. However in this case one should bear in mind that the above–mentioned transformation would provide the correct results only if the calculations are performed in the framework of the Racah–Fano phase system [16], and the coefficients of fractional parentage are defined via the quasispin formalism, as described in [17, 18].

A short explanation of the theoretical background is presented in Section 2. The explanation of the usage and the organization of the program with the description of main subroutines are presented in Section 3. The example of the usage of the program and the concluding remarks are presented in Sections 4 and 5 correspondingly.

# 2 Theoretical background

While investigating theoretically various characteristics of atoms and ions (for example using multiconfiguration or configuration interaction approaches) the atomic state functions are used which are either written in terms of a LS-coupled

$$|\Psi_{\tau}(J^P)\rangle = \sum_{r} a_r^{(LS)}(\tau) |\gamma_r L_r S_r JP\rangle$$
 (1)

or jj-coupled basis

$$|\Psi_{\tau}(J^P)\rangle = \sum_{s} a_s^{(jj)}(\tau) |\gamma_s JP\rangle ,$$
 (2)

where  $\tau = 1, 2, ...$  enumerates the atomic states (of the given J and parity P) and  $\gamma_r$ ,  $\gamma_s$  denote the sets of all additional quantum numbers of the LS- and jj-coupled configuration state functions (CSF) correspondingly.

When a pure LS-coupling exists in the atoms or ions under consideration, then r=1 in equation (1). When the jj-coupling exists, then s=1 in equation (2). Therefore such an ASF is identified by an array of quantum numbers  $\gamma_1$ . However, these quantum numbers are exact only for the cases of pure coupling schemes, which is more the exception than a rule.

In the most general case the exact ASF is made up as an infinite sum in (1) or (2). Therefore an ASF consists of an infinite number of CSFs. In the real calculation one attempts to include terms as many as possible in the sum having the maximum coefficients  $a_r^{(LS)}(\tau)$  or  $a_s^{(jj)}(\tau)$ . But in this case it is not clear what array  $\gamma$  to ascribe in identifying the ASF. Bearing in mind that the coefficient modulus squared (weight)  $\left|a_r^{(LS)}(\tau)\right|^2$  or  $\left|a_s^{(jj)}(\tau)\right|^2$  defines the probability for the atomic state to be in a state with the array of quantum numbers  $\gamma_r L_r S_r$  or  $\gamma_s$ , one can easily classify all the energy levels by ascribing the characteristics of the maximum coefficient  $(a_{r_{max}}^{(LS)}(\tau)$  in LS or  $a_{s_{max}}^{(jj)}(\tau)$  in jj-coupling) to the whole ASF.

The situation becomes more complicated when the expansion (1) or (2) has no obviously dominant weight but several approximately equal ones. Most efficient way for such a classification is the transformation of the ASF into another coupling scheme with the suitable distribution of weights (i.e. with only one dominant weight coefficient). For example, the classification of the spectra of complex atoms and ions using the intermediate quantum numbers of LS-coupling quite offen is problematical.

One of the possible solutions is to transform the function (1) into function (2). Then the level is ascribed to the characteristics  $\gamma_{r_{max}}$  that have the maximum weight  $\left|a_{r_{max}}^{(jj)}(\tau)\right|$  at the transformation of CSFs  $|\gamma_{r_{max}}| JP\rangle$ , i.e. the intermediate quantum numbers of jj-coupling are used for the identification of the ASFs. Such transformations and identifications are the tasks of the LSJJ program presented in this paper.

For practical purposes and especially for an efficient transformation the program treats the CSF in a  $standard\ order$ , i.e. it is assumed that the LS-coupled functions are couped consequently

$$|\gamma_r \ LS \ JP\rangle \equiv \left| (...(((l_1^{N_1}\alpha_1L_1S_1, l_2^{N_2}\alpha_2L_2S_2)L_{12}S_{12}, l_3^{N_3}\alpha_3L_3S_3)L_{123}S_{123})...)LS \ J\rangle \right|$$
(3)

as well as the jj-coupled CSFs

where  $\kappa$  is the relativistic (angular momentum) quantum number  $\kappa_i = l_i$  and  $\kappa_i = -l_i - 1$ .

If both subshells with common  $l_i$ , i.e.  $\kappa_i$  and  $\kappa_i$  appear in the expansion, these two subshells always occur successively in the sequence  $(\kappa_i^{N_i} \bar{\nu}_i J_i, \kappa_i^{N_i} \bar{\nu}_i J_i) J_i$ . Formally, we can use this sequence even for the subshell

states with zero occupation if we interpret  $|\kappa^0 \nu = 0 \ J = 0\rangle \equiv 1$ ; in this case, the full Clebsch–Gordan expansion remains valid due to the orthonormality properties of the Clebsch–Gordan coefficients.

For the LS-jj transformation of the configuration states we further assume in a standard order that  $l_1 = \bar{\kappa}_1 = -(\bar{\kappa}_1 + 1)$ ,  $l_2 = \bar{\kappa}_2 = -(\bar{\kappa}_2 + 1)$ , ..., i.e. that the sequence of (sub-)shell states is the same on both sides of the transformation matrix.

The program presented in this paper is based on the methodics [8] where mixing coefficients  $a_r^{(LS)}(\tau)$  are transformed to  $a_s^{(jj)}(\tau)$  using the following relation:

$$a_s^{(jj)}(\tau) = \sum_r \langle \gamma_s JP | \gamma_r L_r S_r JP \rangle a_r^{(LS)}(\tau), \tag{5}$$

where  $\langle \gamma_s JP | \gamma_r L_r S_r JP \rangle$  is the LS - jj transformation matrix.

In general, the performing of the transformations (5) with the matrix  $\langle \gamma_s JP | \gamma_r L_r S_r JP \rangle$  requires the LS-jj transformation matrices for the shell of equivalent electrons [10]. The numerical values of the matrices for the shell of equivalent electrons are presented in [9], nevertheless it is necessary to ensure the compatibility of the coefficients of fractional parentage (CFP) used to form (3) and (4) with the ones used in the transformation matrices. In this program the usage of the CFP obtained from the reduced coefficients (subcoefficients) of fractional parentage (RCFP) is assumed [1] (such CFPs were used for the calculation of LS-jj matrix elements). The program is based on quasisipin formalism and therefore the appropriate data are required. The data could be generated using the popular package [19, 20] with the angular parts [21].

# 3 Description of the Program

The program is written in Fortran 90 programming language. The main part of the program consists of several subroutines collected into the module rabs\_lsjj (file rabs\_lsjj.f90). The program is designed in the way similar to RATIP [22] package. Some of the RATIP features are used and the overall program includes the additional modules rabs\_angular, rabs\_constant, rabs\_csl, rabs\_determinant, rabs\_dirac\_orbital, rabs\_naglib, rabs\_nucleus, rabs\_rcfp, rabs\_utilities, rabs\_lsj\_data [23, 24] (the corresponding files named as the module\_name.f90).

#### 3.1 Installation of the program

The program was designed and tested on the PC with the Linux OS. Nevertheless it can be easily adopted to any Unix-Linux based platforms (including IBM RS/6000, Sun OS). The installation of the program is similar to RATIP components. First, the script make-environment which declares the global variables for the compilation and linkage of the program should be run via statement source make-environment. Then, the make-file (make-lsjj in this case) should be executed via comand make -f make-lsjj (both files can be obtained from the authors together with other program files). Then the executable xlsjj is generated.

#### 3.2 Interactive control and output of the program

The principled scheme of the execution of the program is presented in Figure 1. After the initialization of several data arrays at the beginning of the execution (subroutine lsj\_initialization\_LS\_jj() [23]), the control is taken by the procedure lsjj\_control\_transformation(), which reads and interprets all input data, carries out the transformation for all selected levels, and finally prints the results to screen. The example of an interactive dialogue performed through the execution is presented in Figure 2.

#### 3.2.1 Input

The input of data in this version of the program is performed by the subroutine <code>lsjj\_load\_csfs\_from\_MCHF\_files()</code> called from the subroutine <code>lsjj\_control\_transformation()</code>. The input data is assumed to be in the same format as the MCHF [19, 20] output data and can be generated with this package with the angular parts [21] (to ensure the usage of the CFP defined via the quasispin formalism). Two files, one with the CSF basis (configuration list file <code>.inp</code>) and the other with the ASFs expansions (mixing coefficients file <code>.j</code>) should be

Table 1 The subroutines and functions of the rabs\_lsjj module.

General purpose	
	<pre>lsjj_control_transformation()</pre>
	<pre>lsjj_load_csfs_from_MCHF_files()</pre>
	<pre>lsjj_form_csf_basis_jj()</pre>
	<pre>lsjj_transformation_ASF()</pre>
	<pre>lsjj_get_subshell_term_jj()</pre>
Output facilities	
	lsjj_print_MCHF_data()
	<pre>lsjj_print_csfs_LS_MCHF()</pre>
	<pre>lsjj_print_coefficients_LS_MCHF()</pre>
	<pre>lsjj_print_single_configuration_jj2()</pre>
	<pre>lsjj_print_coefficients_jj()</pre>
	<pre>lsjj_print_configuration_scheme_jj()</pre>
	<pre>lsjj_print_detailed_info_csf_set_LS()</pre>
Utilities	
	lsjj_lval()
	lsjj_lvalr()
	<pre>lsjj_largest_coeff()</pre>
	<pre>lsjj_deallocate_asf_basis_jj()</pre>

provided. The configuration list file may be generated using the GENCLF and the mixing coefficients file using the CI program from the MCHF package [19]. The fragments of the input files are presented in Figures 3, 4. The detailed specification of the format of these files is avialable at the description of the popular MCHF package (mentioned above) therefore we will not go into details.

#### **3.2.2** Output

The output of the program, namely the jj-coupled CSFs and the expansions of the selected ASFs are performed either directly from the subroutine  $lsjj\_control\_transformation()$  or from the specific data output subroutines called from it.

The direct "onscreen" output includes the quantum numbers and weights of several CSFs with the greatest weights as well as the sum of the squares of the mixing coefficients (in the output of the program denoted as Total sum of weights), serving as the numerical criteria of the accuracy of the expansions 1, 2.

The procedures  $lsjj\_print\_configuration\_scheme\_jj()$ ,  $lsjj\_print\_coefficients\_jj()$  also print a full expansions of all ASFs in jj-coupled basis to the files  $lsjj\_out\_csfs.jj$  and  $lsjj\_out\_coeff.jj$  in the manner similar to the LS-coupled data. The fragments of the output files are presented in Figures 5, 6.

#### 3.3 Description of the module rabs\_lsjj

In this section we will introduce the main procedures of the module and explain some details of their usage because the main module of the program rabs\_lsjj is assumed to be used within the Lsjj as well as in other programs (for example in other programs of the coupling optimization package Laris). The module collects the procedures and functions in an alphabetic order; they are briefly explained in the header of the module. Further information about the methods, data structures, etc. and their implementation can be found in many in–line comments in the headers of the individual procedures/functions or directly inside the source code. The names of the subroutines/functions in the module begin with the "lsjj\_" and are followed by the rest of the names explaining the purpose of the procedure. Table 1 lists the procedures and functions grouped according to their purpose. The detailed description of the subroutines/functions is presented below.

#### The subroutine lsjj\_control\_transformation()

The main subroutine is controling the flow of the execution. The subroutine performs an interactive dialogue with the user, reads the specification parameters for the calculation, opens and closes input and output streams, calls other subroutines of data input, the proceeding and the output. No direct input arguments should be specified. All the dinamically allocated arrays are deallocated at the end of the execution of the subroutine.

#### The subroutine lsjj\_load\_csfs\_from\_MCHF\_files()

This subroutine loads the data on ASFs and corresponding expansions in terms of *LS*-coupled CSFs from the files. The input files are assumed to be formated like MCHF output files [20]. Two input arguments stream\_nr and stream\_nr\_j specify the input streams for the configuration list file and for mixing coefficient file. The output argument ierr is designed for error handling and is assigned to 0 in case of failure. The data read are placed to the public variable asf\_set\_LS%csf\_set\_LS.

#### The subroutine lsjj\_form\_csf\_basis\_jj()

This subroutine generates the jj-coupled CSFs corresponding to the LS-coupled ones stored in the public variable asf\_set\_LS%csf\_set\_LS. No direct input arguments should be specified. The data generated are placed to the public variable asf\_set%csf\_set. The algorithm of the generation is designed in a way that the subroutine can deal with the wave functions of the configurations with the arbitrary number of open shells. The algorithm is implemented using the utility of recursive subroutines. Two internal recursive subroutines are used. The first one lsjj\_form\_csf\_basis\_jj\_fill\_occupations() is meant for the definition of the number of jj-coupled shells (and occupation numbers  $N_i, N_i$ ) for the given LS coupled shell  $l_i^{N_i}$ . And the second one lsjj\_form\_csf\_basis\_jj\_job\_count() is for the the calculation of the number of CSFs in jj-coupling and corresponding intermediate quantum numbers  $J'_{i,j}, J_{i,j}$  (4).

#### The subroutine lsjj\_transformation\_ASF()

The subroutine transforms the atomic state function, represented in a LS-coupling CSF basis into a basis of jj-coupling CSF. Namely the expansion coefficients  $a_s^{(jj)}(\tau)$  are calculated and placed to the array asf\_set%asf(level\_LS)%eigenvector. The input argument level\_LS specifies a serial number of the state to be considered. The LS - jj matrix elements  $\langle \gamma_s JP | \gamma_r LS JP \rangle$  for the transformation (5) are taken from module rabs\_lsj\_data via the subroutine lsj\_transformation\_LS\_jj\_general() [23].

#### The subroutine lsjj\_get\_subshell\_term\_jj()

This procedure returns all allowed subshell terms (j, w, Q, J) for given  $j^N$  which must be 1/2, 3/2, 5/2, 7/2 or 9/2. Two input arguments namely j\_shell and N define the value of the angular momentum and the occupation. The number of corresponding terms as well as their quantum numbers are given by the output arguments number and jj correspondingly.

There are a number of subroutines for the data output in various forms. All the names for all subroutines begin with the <code>lsjj\_print\_</code> and are followed by the rest of the names explaining the content and type of the output.

#### The subroutine lsjj\_print\_MCHF\_data()

The subroutine prints the data in the manner of MCHF program. The input arguments  $streamnr\_inp$  and  $streamnr\_j$  specify the output streams for the MCHF mixing coefficients (.j) and configuration list (.inp) files correspondingly. The argument  $asf\_set\_LS$  specifies the variable where the LS-coupled data are stored. The subroutine first generates the temporary set of CSFs not coupled to J (as it is in MCHF files), prescribes the mixing coefficients to this set of CSFs and stores this data in temporary variable  $asf\_set\_LS\_MCHF$ . Then the subroutine calls  $lsjj\_print\_csfs\_LS\_MCHF$ () and  $lsjj\_print\_coefficients\_LS\_MCHF$ () for the output of CSFs and ASFs with the corresponding mixing coefficients from this temporary variable.

#### The subroutine lsjj\_print\_csfs\_LS\_MCHF()

The subroutine prints the configuration state functions to the file in the form similar to MCHF configuration list file (.inp). The argument streamnr specifies the output stream and the csf\_set\_LS specifies the CSFs in LS-coupling (not coupled to J).

#### The subroutine lsjj\_print\_coefficients\_LS\_MCHF()

The subroutine prints the data on ASFs with expansion coefficients to the file in the form similar to MCHF mixing coefficients .j file. The argument streamnr specifies the output stream and the asf\_set\_LS specifies the ASFs and the mixing coefficients in LS-coupling (for the list of CSFs not coupled to J).

#### The subroutine lsjj\_print\_single\_configuration\_jj2()

The subroutine prints all information about a single CSF in jj-coupling. The input argument stream specifies the output stream, the csf\_set specifies the variable of type csf\_basis where information on jj-coupled CSFs is stored and csf\_number the serial number of CSF to be printed. The subroutine is similar to the lsjj\_print\_single\_configuration\_jj() defined in module rabs\_lsj.

#### The subroutine lsjj\_print\_coefficients\_jj()

The subroutine prints expansion coefficients in jj-coupling to the file in the form similar to MCHF mixing coefficients (.j) file. The input argument streamnr specifies the output stream and the asf\_set specifies the variable where the jj-coupled data are stored.

#### The subroutine lsjj\_print\_configuration\_scheme\_jj()

The subroutine prints information about the CSFs in jj-coupling. The input argument stream specifies the output stream and the csf\_set specifies variable where the data on jj-coupled CSFs are stored.

#### The subroutine lsjj\_print\_detailed\_info\_csf\_set\_LS()

The subroutine prints detailed info about the LS-coupled CSFs. The input argument stream specifies the output stream and the  $csf_set_LS$  specifies variable where the data on LS-coupled CSFs are stored.

The module rabs\_lsjj contains a number of auxiliary subroutines and functions.

#### The function lsjj\_lval()

The function returns the integer value of an orbital quantum number given as a character. The range of an argument 1 should be from s to q (or from S to Q), i.e. the corresponding angular momentum l from 0 to 12.

#### The function lsjj\_lvalr()

The function returns the character value of an orbital quantum number given as an integer. The range of an argument 1 should be from 1 to 12. The subroutine is inverse to the lsjj\_lval().

#### The function lsjj\_largest\_coeff()

The function defines the serial number of the largest element in an array. The argument array specifies the dinamically allocated array and size - it's size.

#### The subroutine lsjj\_deallocate\_asf\_basis\_jj()

The subroutine deallocates the dinamically allocated data arrays within the variable  $sf_set$  (i.e. the jj-coupled data). The variable is defined in the module  $rabs_lsj$ . No direct input arguments should be specified.

# 4 Example

Here we present the example of the transformation of the atomic state function and classification in terms of quantum numbers of LS- and jj-coupling schemes. The example considers the excited state of Ne II. The interactive dialogue performed in the process of the execution of the program is presented in Figure 7.

First the names of configuration list file (Ne.inp) and mixing coefficients file Ne.j) are specified (the fragments of the input files presented in Figures 3 and 4). Then the program proceeds the input and asks to specify the ASFs to consider.

After the specification of the ASFs the corresponding jj-coupled CSF basis is formed (144 CSFs in this case) and the mixing coefficients  $a_s^{(jj)}(\tau)$  of the MCHF expansion (2) are calculated. The resultant CSF basis and mixing coefficients of the specified ASF are printed to the files lsjj-out-csfs.jj

and lsjj-out-coeff.jj correspondingly. The fragments of the output files are presented in Figures 5 and 6. In addition the LS- and jj-coupled CSFs with the greatest weights (squares of the mixing coefficients) useful for the identification and classification of ASFs under the consideration presented interactively. In our case the considered ASF may be identified by means of the quantum numbers of the LS-coupled CSF  $\left|\left(((2s^2)^1S,(2p^4)^3P)\ ^3P,(3s^1)^2S\right)\ ^4P_{\frac{5}{2}}\right\rangle$  or by means of the quantum numbers of jj-coupled CSF  $\left|\left(((2s^2)^0,(2p-2)^0)\ 0,(2p^2)^2\right)\ 2,(3s^1)^{\frac{1}{2}}\right)\ ^{\frac{5}{2}}\right\rangle$ .

The sums of the squares of the mixing coefficients in LS- and jj-couplings equal to 1 with the precision of the input coefficients in LS-coupling (0.0000001). The fact that the sums in LS- and jj-couplings match up to the thirteenth digit reveals the accuracy of the performation of the transformation (5).

#### 5 Conclusions and outlook

The program LSJJ enables us to transform the multiconfigurational expansions of the atomic state functions from LS- to jj-coupled bases. The input data in the current version of the program are supposed to be in the form of MCHF [20] output files, but the structure of the program enables to add more data input interfaces easily. The module rabs\_lsjj together with the earlier constructed rabs\_lsj [23] extends the possibility of comparison of ASFs expansions in various bases. This extent combined together with the program for the changing coupling scheme between the LS-coupled shells of equivalent electrons and evaluation of the suitability of the intermediate quantum numbers for the identification and classification of atomic spectra under consideration [13] will serve as a tool for the search of the optimal set of quantum numbers for the classification of spectra of atoms and ions.

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

#### References

- [1] Z. Rudzikas, Theoretical Atomic Spectroscopy (Cambridge Univ. Press, Cambridge, 1997).
- [2] R. D. Cowan and K. L. Andrew, Coupling considerations in two-electron spectra, J. Opt. Soc. Am., 55, 502 (1965).
- [3] I. Kičkin, A. Slepcov, V. Sivcev, Z. Rudzikas, Correlation between wave functions of many-electron atoms in various coupling schemes, Liet. Fiz. Rink., 16, 217-229 (1976) [in Russian].
- [4] R.D. Cowan, The Theory of Atomic Structure and Spectra (Berkeley, CA: University of California Press 1981).
- [5] J. B. Calvert and E. R. Tuttle, The jj-LS transformation matrices for three or more equivalent p or d electrons, Il nuovo cimento 54 B, 413 (1979)
- [6] K. G. Dyall and I. P. Grant, Phase conventions, quasi-spin and the jj-LS transformation coefficients, J. Phys. B., 15, L371-L373 (1982).
- [7] W. J. Childs, Matrix elements of hyperfine structure operators in the SL and jj representations for the  $s, p^N$ , and  $d^N$  configurations and the SLjj transformation, At. Data Nucl. Data Tables, **67**, 1 (1997)
- [8] G. Gaigalas, T. Žalandauskas and Z. Rudzikas, Analytical expressions for special cases of LS jj transformation matrices for a shell of equivalent electrons, Lithuanian Journal of Physics, **41**, 226 (2001).
- [9] G. Gaigalas, T. Žalandauskas and Z. Rudzikas, LS-jj transformation matrices for a shell of equivalent electrons, At. Data Nucl. Data Tables, in print (2003).
- [10] G. Gaigalas, Z. Rudzikas and T. Žalandauskas, On the Optimization of Classification of HCI Spectra, Book of Abstracts of XI HCI Conference, 1-6 September, 2002, Caen, France, 48.
- [11] R. D. Cowan, Theoretical calculation of atomic spectra using digital computers, J. Opt. Soc. Am., **50**, 808 (1968).
- [12] J. V. Čiplys, The program for the optimization of the coupling scheme of angular momenta, A Collection of Programs on Mathematical Supply of Atom Calculations, Ed. 16 (Institute of Physics of the Academy of Sciences of the Lithuanian SSR, 1986).
- [13] T. Žalandauskas, The computer program for the optimization of the coupling scheme, Book of Abstracts of EGAS 34, 9-12 July, 2002, Sofia, Bulgaria, 123.
- [14] G. Gaigalas, and S. Fritzsche, Maple procedures for the coupling of angular momenta. VI. LS-jj transformations, Comput. Phys. Commun., 149, 39 (2002).
- [15] G. Gaigalas, R. Karpuškiene and Z. B. Rudzikas, Optimal classification of HCI spectra, Physica Scripta, T80, 472 (1999).
- [16] G. Gaigalas, Z. Rudzikas and Ch. Froese Fischer, J. Phys. B 30 (1997) 3747.
- [17] G. Gaigalas, Z. Rudzikas and Ch. Froese Fischer, At. Data Nucl. Data Tables, 70 (1998) 1.
- [18] G. Gaigalas, T. Zalandauskas and Z. Rudzikas, At. Data Nucl. Data Tables, in print (2003).
- [19] C. Froese Fischer, A general multi-configuration Hartree-Fock program, Comput. Phys. Commun., 14, 145 (1978).
- [20] C. Froese Fischer, T. Brage and P. Jönsson, Computational Atomic Structure. An MCHF Approach (Institute of Physics Publishing, Bristol/Philadelphia, 1997).
- [21] G. Gaigalas, The library of subroutines for calculation of matrix elements of two-particle operators for many-electron atoms, Lithuanian Journal of Physics, **42**, 73 (2002).
- [22] S. Fritzsche, J. Elec. Spec. Rel. Phenom., 114–116, 1155 (2001).

- [23] G. Gaigalas, T. Žalandauskas and S. Fritzsche, Spectroscopic LSJ notation for atomic levels from relativistic calculations, Comput. Phys. Commun. in print (2003).
- [24] S. Fritzsche, C. F. Fischer and G. Gaigalas, RELCI: A program for relativistic configuration interaction calculations, Comput. Phys. Commun., 148, 103 (2002).

# PROGRAMA ATOMŲ BŪSENŲ FUNKCIJOMS TRANSFORMUOTI IŠ LSĮjjRYŠIO BANGINIŲ FUNKCIJŲ BAZĘ

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#### Santrauka

Eksperimentiškai gaunami atomų ir jonų energetiniai spektrai paprastai identifikuojami ir klasifikuojami naudojant LS ryšio schemos kvantinius skaičius. Ši ryšio schema yra labai populiari ir teorinėje atomo fizikoje, kai atomai ir jonai yra nagrinėjami nereliatyvistiniame artutinume. Bet LS ryšio kvantiniai skaičiai dažnai nėra tinkami sunkių atomų bei didelio ionizacijos laipsnio jonų būsenoms apibudinti. Vienareikšmiam bei tiksliam tokių atomų bei jonų būsenų identifikavimui bei spektrų klasifikavikavimui geriau tinka kitų ryšio shemų (dažnai jj ryšio) kvantiniai skaičiai.

Neseniai gautos LS-jj transformacijos matricos ekvivalentinių elektronų sluoksniams (įskaitant f elektronų sluoksnius su bet kokiu užpildymo skaičiumi) bei LS-jj transformacijos matricų išraiškos konfigūracijoms su bet kokiu atvirų sluoksnių skaičiumi įgalino mus sukurti programą, skirtą atomų bei jonų būsenų funkcijų transformavimui iš LS į jj ryšio banginių funkcijų bazę. Tokio pobūdžio programų, leidžiančių keisti ryšio tipą tiek ekvivalentinių elektronų sluoksnių viduje (įskaitant f elektronų sluoksnius), tiek ir tarp sluoksnių, iki šiol nebuvo.

Programa įgalina atlikti atomų ir jonų spektrų identifikavimą ir klasifikaciją LS ir jj ryšio kvantiniais skaičiais, praplečia kvantinių skaičių rinkinio, optimalaus atominių spektrų identifikavimui ir klasifikavimui, paieškos galimybes.

```
Р
        | lsj_initialization_LS_jj()
R
0
G
R
          lsjj_control_transformation() |
Α
М
            |--- data input
Ε
                      - lsjj_load_csfs_from_MCHF_files()
Х
Ε
C
U
             --- formation of all CSFs in jj coupling
Т
Ι
                      - lsjj_form_csf_basis_jj()
0
N
             --- LS-jj transformation and classification
                  of all selected levels
                      - lsjj_transformation_ASF()
                 data output
                      - lsjj_print_configuration_scheme_jj()
                      - others
```

Figure 1: Schematic flow chart of the LSJJ program.

Transform one or several ASF from a MCHF calculation into a jj-coupled CSF basis. The transformation starts from the given cfg.inp and .j files and is carried out for the n leading CSF in the LS-coupled basis; the new representation in the jj basis is printed as in a standard GRASP92 computation. Enter the name of the MCHF configuration list file: > Enter the name of corresponding .j mixing coefficient file: load\_cfg\_from\_MCHF\_file ... number of core shells = ... total number of shells = ... number of csfs LS = ... reordered there are ... nonrelativistic CSFs (before couplin to J); now couple them to J  $\dots$ now load mixing coefficients and form asf\_set\_LS... end reading j there are  $\dots$  atomic state functions there are ... nonrelativistic CSFs (coupled to J) ... load complete. Maximum number of considered ASF is: ... Enter the level numbers of the ASF which are to be transformed, e.g. 1 3 4 7 - 20 48 69 - 85 :

Program for transformation of atomic states from LS to jj coupling (C) Copyright by T Zalandauskas and G Gaigalas Vilnius (2003).

Figure 2: Interactive dialogue of LSJJ program

```
1s
2s(2)
       2p(4)
               3s(1)
   1S0
          1S0
                   2S1
                           1S
                                   2S
2s(2)
       2p(4)
               3s(1)
   1S0
          3P2
                   2S1
                           ЗР
                                   2P
2s(2)
       2p(4)
               3s(1)
   1S0
          3P2
                   2S1
                           3P
                                   4P
2s(2)
       2p(4)
               3s(1)
   1S0
           1D2
                   2S1
                                   2D
2s(2)
       2p(4)
               3d(1)
   1S0
          1S0
                   2D1
                                   2D
                           1S
2s(2)
       2p(4)
               3d(1)
                   2D1
                                   2P
   1S0
          3P2
                           3P
2s(2)
       2p(4)
               3d(1)
                   2D1
   1S0
          3P2
                                   4P
2s(2)
       2p(4)
               3d(1)
   1S0
          3P2
                   2D1
                                   2D
2s(2)
       2p(4)
               3d(1)
   1S0
          3P2
                   2D1
                           ЗР
                                   4D
2s(2)
       2p(4)
               3d(1)
   1S0
          3P2
                   2D1
                                   4F
2s(2)
       2p(4)
               3d(1)
  1S0
          1D2
                   2D1
                           1D
                                   2P
2s(2)
       2p(4)
               3d(1)
  1S0
          1D2
                   2D1
                           1D
                                   2D
2s(2)
       2p(4) 3d(1)
```

Figure 3: Fragment of MCHF configuration list file Ne.inp

Figure 4: Fragment of MCHF mixing coefficients file Ne.j

```
is defined as follows:
Number of electrons: 9
Number of (relativistic) subshells: 9
Core shells:
 1s
Peel shells:
 2s
        2p-
               2p
                      3s
                                    Зр
                                           3d-
                                                   3d
144
    CSF(s):
           1) 2s (2)
                        2p-(1)
                                  2p (3)
                                            3s (1)
                           1/2
                                     3/2
                                                1/2
                              1/2
                                         2
                                                   5/2
                                  2p (2)
           2) 2s (2)
                        2p-(2)
                                            3s (1)
                                     2
                                                1/2
                                                   5/2
           3) 2s (2)
                        2p (4)
                                  3d (1)
                                     5/2
                                        5/2
           4) 2s (2)
                        2p-(1)
                                  2p (3)
                                            3d (1)
                           1/2
                                     3/2
                                                    5/2
                              1/2
                                         1
           5) 2s (2)
                        2p-(1)
                                  2p (3)
                                            3d (1)
                                     3/2
                                         2
                                                    5/2
                              1/2
           6) 2s (2)
                        2p-(1)
                                  2p (3)
                                            3d-( 1)
                                     3/2
                           1/2
                                                    5/2
                              1/2
                                         1
```

. . .

The current configuration scheme with 144 CSF in jj coupling

Figure 5: Fragment of output file lsjj-out-csfs.jj of jj coupled CSFs

```
-126.95806136
 0.5638947 0.8200464
                      -.0140585 0.0254398
                                            0.0123155 -.0067862 -.0061464
                      -.0084857
                                                      0.0440080 -.0234300
 0.0103721
            0.0170042
                                 0.0230858
                                            -.0169735
                      -.0002857
                                                                 -.0016268
 0.0355732
            0.0514159
                                 -.0018696
                                            0.0043991
                                                      0.0004125
 0.0049082 0.0044622
                      -.0028572 -.0023440 0.0025700 0.0059582 0.0018875
. . .
```

Figure 6: Fragment of output file lsjj-out-coeff.jj of the ASFs expansions in jj-coupling

```
Enter the name of the MCHF configuration list file:
Enter the name of corresponding .j mixing coefficient file:
Ne.j
load_cfg_from_MCHF_file ...
 number of core shells = 1
 total number of shells = 6
 number of csfs LS
                    = 224
 there are 224 nonrelativistic CSFs (before coupling to J);
 now couple them to J \dots
 now load mixing coefficients and form asf\_set\_LS...
 end reading j
 there are 1 atomic state functions
 there are 144 nonrelativistic CSFs (coupled to J)
  ... load complete.
Maximum number of considered ASF is: 1
Enter the level numbers of the ASF which are to be transformed,
 e.g. 1 3 4 7 - 20 48 69 - 85 :
1
number_of_levels, levels(:) = 1 1
 start formation of CSFs in jj coupling...
   number of shells in jj coupling = 9
   number of core shells in jj coupling = 1
   number of configuration state functions in jj coupling = 144
 finish formation of CSFs in jj coupling...
Weights of major contributors to ASF in LS-coupling:
 Level J Parity
                   CSF contributions
   1 5/2
                   0.99028 of
                                      0.00391 of
                                                         0.00331 of 11
                                                  15
Definition of leading CSF:
               2s(2)
                        2p(4)
        1)
                                 3s(1)
                                                      4P
                                                              5/2
                  1SO
                           3P2
                                    2S1
                                             3P
 Total sum of weights is: 0.9999999614146498
Weights of major contributors to ASF in jj-coupling:
 Level J Parity
                  CSF contributions
   1 5/2 +
                   0.67248 of
                                 2
                                      0.31798 of
                                                    1
                                                         0.00264 of
                                                                     16
 Total sum of weights is: 0.9999999614146532
Definition of leading CSF:
           1) 2s (2)
                        2p-(1)
                                  2p (3)
                                            3s (1)
                                     3/2
                           1/2
                                               1/2
                              1/2
                                  2p (2)
           2) 2s (2)
                        2p-(2)
                                            3s (1)
                                               1/2
                                         2
                                                   5/2
           16) 2s (1)
                                  2p (2)
                        2p-(2)
                                            3s (2)
                 1/2
                                     2
                              1/2
                                         5/2
                                                   5/2
LS-jj complete ... .
```

Figure 7: Interactive dialogue of LSJJ program for the transformation of state function of excited Ne