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COMPUTATIONAL PACKAGE FOR ANALYSIS OF THE FINE STRUCTURE OF A FREE ATOM

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Abstract: This work describes some computer programs that are available in compiled form for users of the SGI Power Challenge machine at Poznań Supercomputing and Networking Center. These programs give a possibility to solve very complex problems in the structure of free atoms using experimental data. The procedure of determination of the Slater integrals, spin-orbit parameters and also the parameters representing the effect of virtual excitations (many-body effects) is described. The program gives the propositions of the spectroscopic designations of energy levels. Moreover, the wavefunctions in intermediate coupling scheme in many-configurations approximation for the selected configuration system can be obtained.

1. INTRODUCTION

There are some programs, which are used for semi-empirical calculations of atomic structure. The excellent compilation of fine structure (fs) analyses carried out by the least-squares fitting method have been done by Judd [1] and Biittgenbach [2], However, the used codes don't solve some atomic problems satisfactorily in the cases of the interpretation of very precise experiments [3-5], There are several reasons of difficulties in interpretation;

1) too small basis, in which energy matrix is constructed, limited to the configurations with one or two open shells only,

2) neglect of some important interaction effects (e.g. electrostatically correlated spin-orbit interaction effects, many-body effects) or use of not quite correct formulae for the parametrization of configuration interactions.

This induced us to develop the method of fs-analysis in a large multi-configuration basis, in which all significant interactions are taken into account [6-9]. In this work the last version of the computational package used to study the above problems is presented.

2. PHYSICAL BACKGROUND

In the analysis of energy level structure in a complex atom the method of perturbation theory is used and the following model of interactions is assumed:

- every electron moves in a certain effective field of spherical symmetry produced by the nucleus and other electrons. In this approximation (zero-order approximation of the perturbation theory) the energy depends on n and l quantum numbers only and is called configuration-average energy E_{av}.

— Coulomb repulsion of the electrons leads to the term structure, the energies of the terms differ according to the v, S, L quantum numbers.

- spin-orbit interaction produces the fine structure spilitting and the energy of a level depends (besides *v, S, L)* on the total angular-momentum quantum number *J*.

The two latter effects are treated as the first-order perturbations of the central field and they lead to energy levels dependent on the quantum numbers *v, S, L, J*. The energy spectrum resulting from the interactions of electrons is called fine structure. The other interactions: spin-other orbit, spin-spin and orbit-orbit interactions do not cause any further level splittings; they only change the energy of the levels only.

Hamiltonian of a complex atom can be written in the well known form [1] as:

$$H = \sum_{i=1}^{N} [(-\hbar^2/2m)\nabla_i^2 - Ze^2/r_i)] + \sum_{i>j} e^2/r_{ij} + \sum_{i=j}^{N} \zeta(r_i) s_i l_i \tag{1}$$

In this expression the first term describes the motion of the electrons in the central field independent of interactions between electrons. Coulomb interaction of electrons is represented by the second sum in the formula. This consists of cental and non-central part, where the latter can be considered as perturbation of the central field. The third sum is responsible for fine-splitting of the terms. For such Hamiltonian the one-electron eigenfunctions can be separated into their radial and angular parts dependent on *n, l*- and *s, m_s, l, m_l* - quantum numbers, respectively. This separation of the wavefunctions allows to calculate the angular part using the theory of angular momentum of a complex atom. As a result the energy of the interactions is expressed in terms of radial integrals multiplied by their angular parts. The angular coefficients are the combinations of quantum numbers *SLJ* which represent respective angular momenta. They may be calculated exactly (by group-theoretical and tensorial methods using operator symmetry); the radial integrals may be evaluated by solution of the radial wave equation or left as parameters to be determined experimentally in the level-fitting procedure, where the calculated energy values are fitted to the experimental energies of the levels.

The state of the electronic shell in an atom is described explicitly by the total angular-momentum quantum number *J* and the energy and it can be written as follows:

$$\Psi(J, energy) = \sum_i c(i)\,\Phi(i)\,, \tag{2}$$

where: *i* - configuration and set of quantum numbers *vSLJ,*

c(*i*) - eigenvector amplitude in the basis of "pure" states $\Phi(i)$ of the *SL*-coupling.

The summation extends usually over all states of the configuration under study but if strong configuration mixing effects appear, the basis consists of states belonging to many configurations with the same parity.

3. METHOD

After choice of the set of the basis states and after the definition of the Hamiltonian, the energy matrix is constructed. The matrix elements H_{ij} are written as:

$$H_{ij} = \langle \Phi(i) \,|\, \hat{H}_{fs} \,|\, \Phi(j) \rangle \tag{3}$$

and they may be expressed by linear combinations of the well known radial parameters: F^k G^k, α,β,ζ,R^k [10], The matrix elements are diagonal in J and therefore the energy matrix can be split into separate, independent, submatrices for each possible J. For any particular J value the dimension of the submatrix is given by the number of possible levels of that J. For a total matrix H the problem to find the eigenvalues E^i_j together with the corresponding eigenvectors Ψ^i *(J, energy)* may be resolved by numerical diagonalization of the Hamiltonian matrix H. This is accomplished by supplying numerical values of the matrix elements H_{ij} to a computer and finding the matrix T by tri-diagonalization of H via a sequence of Hauseholder transformations and then using the QR algorithm. The i-th diagonal element of the diagonalized matrix is the eigenvalue E^i,

$$T^{-1}HT = \{E^i\delta_{ij}\} \tag{4}$$

and the i-th column of T represents the corresponding eigenvector Ψ^i *{J, energy)*.

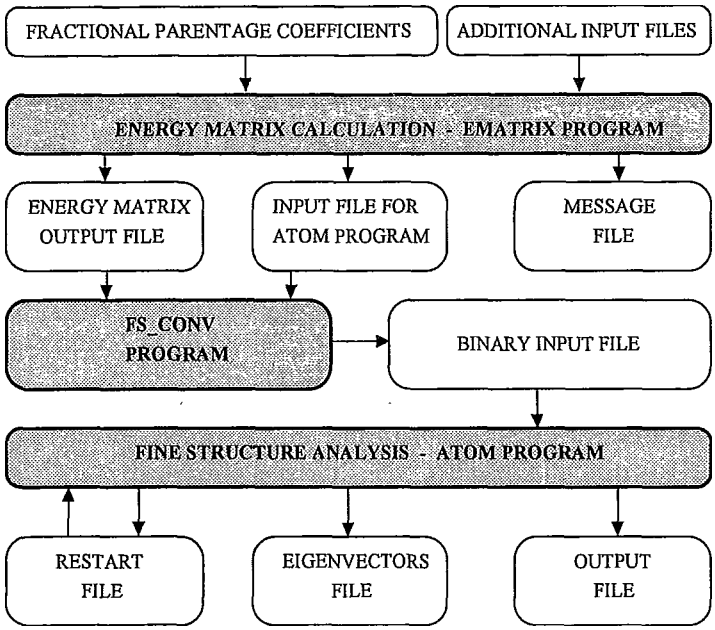

Fig. 1. The structure of the package

In the fitting-procedure the values of parameters are chosen to minimize the root-mean-square deviation between the calculated eigenvalues and the experimental ones. The residuum R of such calculation is defined by

$$R = \sum_{J,i}\left[E^i_J - E^i_{J\,obs}\right]^2 = min\,, \tag{5}$$

where the sum over J extends over all J-submatrices and the i designates the summation over all levels with given J. The "mean error" δ of the calculations is defined by

$$\delta = [R/(n-m)]^{1/2}, \tag{6}$$

where n is the number of the energy levels E_{Jobs} known from experiment, m is the number of free parameters. Small value of δ under the condition $n \gg m$ indicates the proper consideration of interactions between electrons in the atom. All important interactions within configuration system under study have been taking into account in the first-order of perturbation theory and the effects caused by the states belonging to the far configurations have been considered in the second-order. However, the fitting procedure of energy levels cannot be regarded as a purely statistical problem. It is not enough to obtain any fit of the energies of the levels. A correct theoretical description should also yield eigenfunctions that can be used to calculate other physical observables with a comparable precision.

If the matrix elements H_{ij} and the eigenvalues E_j are known, the eigenvector amplitudes $c(i)$ can be obtained. Using the equation (2) one can determine the wavefunctions in intermediate coupling

$$\Psi^i(J, energy) = \sum_i c(i).$$

Comparison of the experimental Landé g_j-factors and the ones calculated using the amplitudes $c(i)$ can also provide a useful test of the eigenvector compositions and thus for the fitting-procedure. The structure of the computer package is shown in Fig. 1.

4. DESCRIPTION OF THE PROGRAMS

4.1. Program EMATRIX

The computer program EMATRIX has been constructed to generate energy matrix in many-configuration approximation. This program calculate angular coefficients corresponding to fine structure radial parameters, which represent the following interactions:

- within each configuration: Coulomb-, spin-orbit-, orbit-orbit-, spin-other-orbit- and electrostatically correlated spin-orbit interaction, within the model space $(d+s)^{N+2}$: the T2, T3, Ts, Γ and Ω parameters,
- between configurations: Coulomb- and spin-orbit-interaction, for the $(l+s)^{N+2}$ configurations - electrostatically correlated spin-orbit interaction, in the model space $(d+s)^{N+2}$ - parameter Γ.

The EMATRIX program consists of 4 blocks of statements: EMATRIX, EMDIA, EMOFF and EMSUB. The scheme of the program is shown in Fig. 2.

Specifications of the program:

The calculations can be performed for the configurations of the type:

$nl^N n_1 l^2_1$, $nl^{N+1} n_1 l_1$, nl^{N+2}, $nl^N n_1 l_1 n_2 l_2$, $nl^{N-1} n_1 l^2_1 n_2 l_2$ and $nl^{N-1} n_1 l_1 n_2 l_2 n_3 l_3$;

where $l = p, d, f$ and l_1, l_2, l_3 are unrestricted.

Sizes of the particular segments are defined by the parameters given in the PARAMETER statements:

- max. no. of configurations: PNK
- max. no. of submatrices: PJ
- max. no. of terms in the l^N core: PNT0
- max. no. of parent terms: Pcfp
- max. no. of terms: PNT

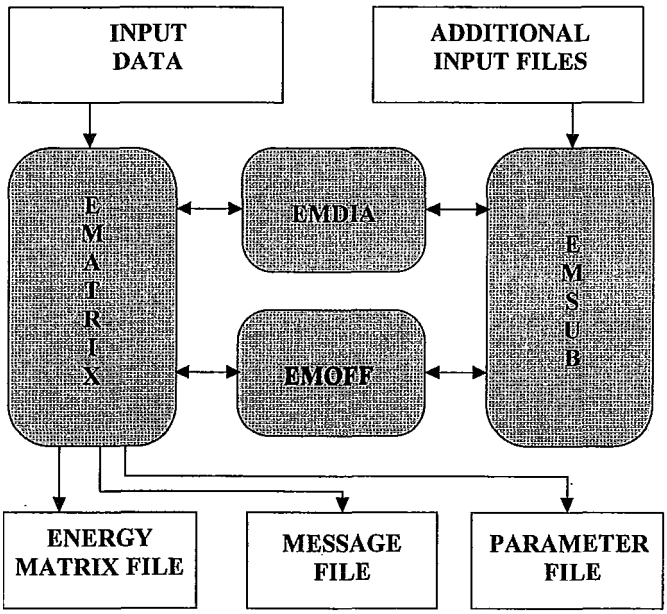

Fig. 2. The structure of EMATRIX program

4.1.1. Block EMATRIX

The EMATRIX block consists of the main program and 3 subprograms. In the main program the configurations, for which the energy matrix is generated, are read in the spectroscopic description e.g. *3d2*, *4s2*. The program analyses these data (the number of electrons and their *l* quantum number, configuration parity) and then transforms the initial description for the calculations purposes. After reading all configuration descriptions the matrix elements of interactions within every configuration is generated. The main program turns to the subprogram from the EMDIA block, which is adequate for a given type of configuration. At the end of the calculations for each configuration, information of numeration of parameters and terms is written to the "Message" file.

In the next step matrix elements of the interactions between configurations are calculated. For any pair of interacting configurations the parameter "Code" is established (detailed description in Appendix). This parameter is used to describe the type of the configurations and to initiate

suitable procedure in the EMOFF block. At the end of these calculations information of numeration of configuration interaction parameters is written to the "Message" file. Finally the PARAM procedure checks out uniqueness of the parameter numeration. This procedure also verifies the consistence of the system, especially when new parameters are taken into account. If there are some inconsistencies, errors are written to EMATRIX.ERR file. The next procedure DIVIDE arrange matrix elements according to quantum number *J* into separate submatrices and writes the data to the output file specified in "Matrix elements output file" prompt. The procedure PREPARE adds to the mentioned above output file the g_J-factors and terms descriptions set in order according to *J*. The same procedure forms matrices to be filled up with corresponding values of radial parameters and experimental energy levels.

4.1.2. Block EMDIA

Block EMDIA consists of subprograms calculating the matrix elements of interactions within single configuration. The structure of the block is shown in Fig. 3.

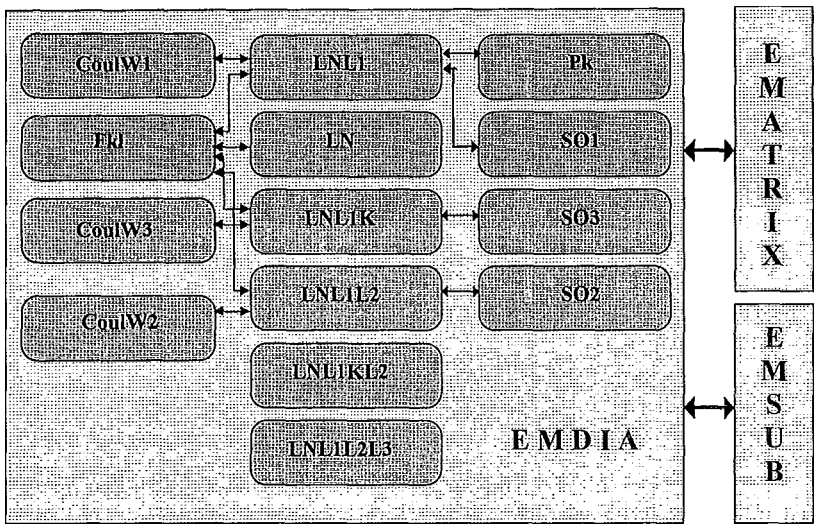

Fig. 3. The structure of EMDIA block

The following subprograms correspond with the types of configurations:

– configuration nl^{N+2} and $nl^N n_1 s^2$ - -subprogram LN
– configuration $nl^{N+1} n_1 l_1$ – subprogram LNL1
– configuration $nl^N n_1 l_1 n_2 l_2$ – subprogram LNL1L2
– configuration $nl^N n_1 l_1^2$ – subprogram LNL1K
– configuration $nl^{N-1} n_1 l_1^2 n_2 l_2$ – subprogram LNL1KL2
– configuration $nl^{N-1} n_1 l_1 n_2 l_2 n_3 l_3$ – subprogram LNL1L2L3

The structure of the subprogram LNL1L2 is shown in Fig. 4.

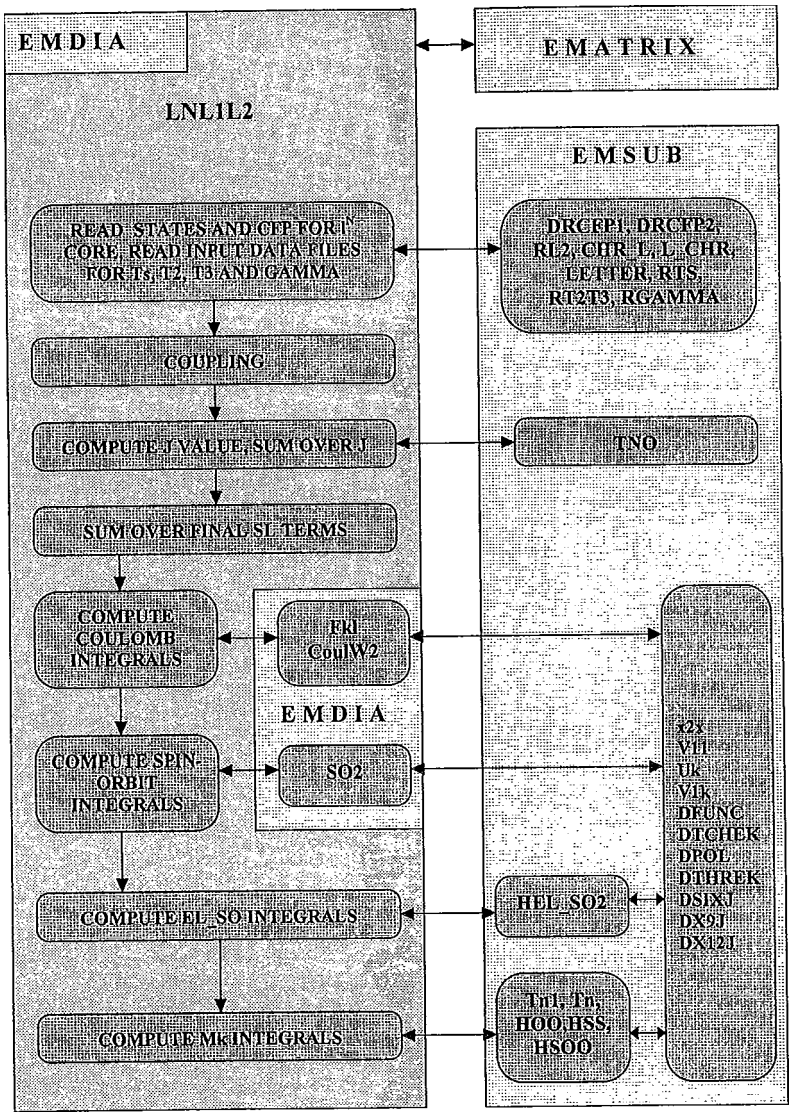

Fig. 4. The structure of LNL1L2 subroutine

The block EMDIA includes also the following subprograms and functions:

- Fkl - calculation of the Slater integrals F^k of the l^Ncore,
- CoulWl - calculation of the direct and exchange Slater integrals F^k and G^k for the configuration of the type $nl^{N+1}n_1l_1$
- SO 1 - calculation of the spin-orbit parameter ζ for the configuration $nl^{N+1}n_1l_1$
- Pk - calculation of the electrostatically correlated spin-orbit parameter $P(l_1)$ for the configurations of the type $n^{lN+1}n_1l_1$

- CoulW2 - calculation of the direct and exchange Slater integrals F^k and G^k for the configuration of the type $nl^N n_1 l_1 n_2 l_2$
- S02 - calculation of the spin-orbit parameter ζ for the configuration $nl^N n_1 l_1 n_2 l_2$
- CoulW3 - calculation of the direct and exchange Slater integrals F^k i G^k for the configuration of the type $nl^N n_1 l^2_1$
- S03 - calculation of the spin-orbit parameter ζ for the configuration $nl^N n_1 l^2_1$
- S15JW - calculation of the 15-j Wigner coefficients

4.1. 3. Block EMOFF

Block EMOFF consists of subprograms calculating the matrix elements of interconfiguration interactions. The following subprograms correspond to the pairs of interacting configurations:

– LL_2L1L2	l^{N+2}	$\leftrightarrow$	$l^N l_1^2$	Code = 1320, 6320,
	l^{N+2}	$\leftrightarrow$	$l^N l_1 l_2$	Code = 1330, 6330
– LNLN_1L1	l^{N+2}	$\leftrightarrow$	$l^{N+1} l_1$	Code = 1220, 6220
– LNL1LNL	$l^{N+1} l_1$	$\leftrightarrow$	$l^{N+1} l_2$	Code = 2102
– L1L_1L23	$l^{N+1} l_1$	$\leftrightarrow$	$l^N l_1 l_2$	Code = 2201, 7201
	$l^{N+1} l_1$	$\leftrightarrow$	$l^N l_2 l_1$	Code = 2202, 7202
	$l^{N+1} l_1$	$\leftrightarrow$	$l^N l_2 l_3$	Code = 2203, 7203
– L1KLN1L2	$l^N l_1^2$	$\leftrightarrow$	$l^{N+1} l_1$	Code = 2021, 2211
	$l^N l_1^2$	$\leftrightarrow$	$l^{N+1} l_2$	Code = 2022, 2222
– L1KL2L3	$l^N l_1^2$	$\leftrightarrow$	$l^N l_1 l_2$	Code = 2121, 7121
	$l^N l_1^2$	$\leftrightarrow$	$l^N l_2 l_1$	Code = 2122, 7122
	$l^N l_1^2$	$\leftrightarrow$	$l^N l_2 l_3$	Code = 2123, 7123
– L1L2L3L4	$l^N l_1 l_2$	$\leftrightarrow$	$l^N l_1 l_3$	Code = 3109
	$l^N l_1 l_2$	$\leftrightarrow$	$l^N l_3 l_4$	Code = 3106
	$l^N l_2 l_1$	$\leftrightarrow$	$l^N l_3 l_1$	Code = 3105
– L1KL2K	$l^N l_1^2$	$\leftrightarrow$	$l^N l_2^2$	Code = 2111
– L1KL2L1K	$l^N l_1^2$	$\leftrightarrow$	$(l^{N-1} l_2) l_1^2$	Code = 2262, 7262
– L1KL1L2K	$l^N l_1^2$	$\leftrightarrow$	$(l^{N-1} l_1) l_2^2$	Code = 2261, 7261
– L12L1L3K	$l^N l_1 l_2$	$\leftrightarrow$	$(l^{N-1} l_1) l_3^2$	Code = 3219, 3029
	$l^N l_2 l_1$	$\leftrightarrow$	$(l^{N-1} l_1)_3^2$	Code = 3214, 3023
– L12L3L1K	$l^N l_1 l_2$	$\leftrightarrow$	$(l^{N-1} l_3) l_1^2$	Code = 3213, 3024
	$l^N l_2 l_1$	$\leftrightarrow$	$(l^{N-1} l_3) l_1^2$	Code = 3215, 3025
– L1L2L1K	$l^{N+1} l_1$	$\leftrightarrow$	$(l^{N-1} l_2) l_1^2$	Code = 2342, 7342
– L1L1L2K	$l^{N+1} l_1$	$\leftrightarrow$	$(l^{N-1} l_1) l_2^2$	Code = 2341, 7341
– L12L1L2K	$l^N l_1 l_2$	$\leftrightarrow$	$(l^{N-1} l_1) l_2^2$	Code = 3211, 3021
	$l^N l_2 l_1$	$\leftrightarrow$	$(l^{N-1} l_1) l_2^2$	Code = 3212, 3022
– L1KSL1SK	$l^{N-1} l_1^2 s$	$\leftrightarrow$	$l^{N-1} l_1 s^2$	Code = 3151, 3121
– L1KL2L23	$l^{N-1} l_1^2 l_2$	$\leftrightarrow$	$l^N l_1 l_2$	Code = 3041, 3201

	$l^{N-1}l_1^2l_2$	$\leftrightarrow$	$l^N l_2 l_3$	Code = 3044, 3203
– L2KL123	$l^{N+1}l_2^2$	$\leftrightarrow$	$l^N l_1 l_2 l_3$	Code = 4222, 9222
– L12L123	$l^{N+1}l_1 l_2$	$\leftrightarrow$	$l^N l_1 l_2 l_3$	Code = 4201, 9201
– L32L123	$l^{N+1}l_3 s^2$	$\leftrightarrow$	$l^N l_1 l_2 l_3$	Code = 4125, 9125
– L1L2KL1	$l^N l_1$	$\leftrightarrow$	$l^{N-2}(l_2^2 l_1)$	Code = 2312, 7312
– L1L1KL2	$l^N l_1$	$\leftrightarrow$	$l^{N-2}(l_1^2 l_2)$	Code = 2311, 7311
– L1KL2KL1	$l^N l_1^2$	$\leftrightarrow$	$l^{N-1}(l_2^2 l_1)$	Code = 2232, 7232
– L2KL3L2	$(l^N l_1)l_2^2$	$\leftrightarrow$	$l^N(l_3^2 l_2)$	Code = 3125, 3155
– L1KL1KL2	$l^N l_1^2$	$\leftrightarrow$	$l^{N-1}(l_1^2 l_2)$	Code = 2231, 7231
– L1SL1SK	$l^N l_1^2 s$	$\leftrightarrow$	$(l^{N-1}l_1^2)s^2$	Code = 3251, 3061
– L1KL1LSK	$l^N l_1^2$	$\leftrightarrow$	$(l^{N-2}l_1^2)s^2$	Code = 2371, 7371
– L1KL3L12	$l^{N-1}(l_1^2 l_3)$	$\leftrightarrow$	$l^N l_1 l_2$	Code = 3049, 3209
– L1K2L1K3	$l^N(l_1^2 l_2)$	$\leftrightarrow$	$l^N(l_1^2 l_3)$	Code = 3149
– L1KSKL2	$l^N(l_1^2 l_2)$	$\leftrightarrow$	$(l^{N-1}l_1^2)s^2$	Code = 3259, 3069

The structure of the subprogram L1KL2L3 is shown in Fig. 5.

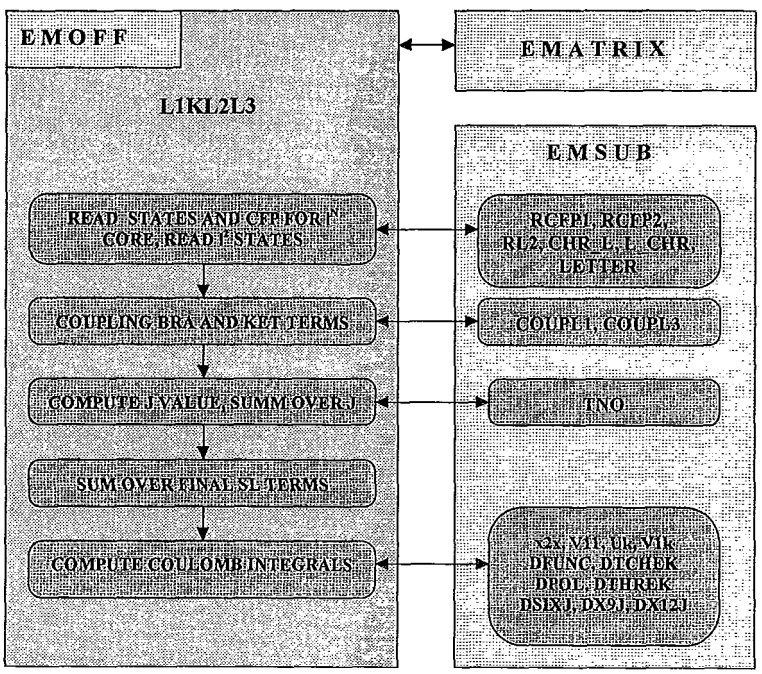

Fig. 5. The structure of L1KL2L3 subroutine

4.1.4. Block EMSUB

Blok EMSUB includes the following subprograms and functions:

-T11 calculation of the reduced matrix element $< l^2 \| T^{11} \| l^2 >$

- Tnl calculation of the reduced matrix element $< l^2 \| T^{N(11)} \| l^N >$
- T22 calculation of the reduced matrix element $< l^2 \| T^{2(\varkappa k)} \| l^2 >$
- Tn calculation of the reduced matrix element $< l^N \| T^{N(\varkappa k)} \| l^N >$
- HOO calculation of the interconfiguration orbit-orbit parameter for the configurations nl^{N+2} and $nl\ {}^{N}n_1s^2$
- HSS calculation of the interconfiguration spin-spin parameter for the configurations nl^{N+2} and $nl^N n_1 s^2$
- HSOO calculation of the interconfiguration spin-otherorbit parameter for the configurations nl^{N+2} and $nl^N n_1 s^2$
- HEL_SO calculation of the electrostatically correlated interconfiguration spin-orbit parameter for the configurations nl^{N+2} and $nl^N n_1 s^2$
- HEL_S01 calculation of the electrostatically correlated spin-orbit parameter for the configuration $nl^{N+1} n_1 l_1$
- HELS02 calculation of the electrostatically correlated spin-orbit parameter for the configuration $nl^N n_1 l_1 n_2 l_2$
- LETTER block DATE with the spectroscopic descriptions corresponding to the quantum number l
- CHR_L conversion from the spectroscopic description into numerical value of l
- L_CHR conversion from numerical value of l into relevant spectroscopic description
- DRCFP1 reading of one-electron coefficients of fractional parentage in the block EMDIA
- DRCFP2 reading of two-electron coefficients of fractional parentage in the block EMDIA
- RL2 reading of the states for the pair of eqivalent electrons $l2$
- RGAMMA reading of the configuration parameter Γ
- RT2T3 reading of the configuration parameters T2 i T3
- RTS reading of the configuration parameter Ts
- RCFP1 reading of one-electron coefficients of fractional parentage in the block EMOFF
- RCFP2 reading of two-electron coefficients of fractional parentage in the block EMOFF
- RGAMIC reading of the interconfiguration parameter Γ
- COUPL1 coupling of angular momenta $(l_1 l_2)\ S_2 L_2$
- COUPL2 coupling of angular momenta $(l^N S_0 L_0,\ l_1)$ SL
- COUPL3 coupling of angular momenta $(l^N S_0 L_0, l^2{}_1 S_2 L_2)$ SL $(l^N S_0 L_0, l_1 l_2 S_2 L_2)$ SL
- COUPL4 coupling of angular momenta $((l^N S_0 L_0, l,)\ S_4 L_4, l^2{}_2 S_2 L_2)$ SL
- COUPL5 coupling of angular momenta $((l^N S_0 L_0,\ l_1)\ S_4 L_4, l, l_2 S_2 L_2)$ SL
- TNO determination of the number of terms for given J
- OUT1÷OUT7 print out the values of configuaration interactions parameters
- x2x calculation of [x] 2x + 1

- V11 calculation of the reduced matrix elements V^{11}
- Uk calculation of the reduced matrix elements U^k
- V1k calculation of the reduced matrix elements V^{1k}
- DFUNC, DTCHEK, DPOL, DTHREK, DSIXJ
  procedure for calculation of the 3-j and 6-j Wigner-coefficients
- DX9J procedure for calculation of the 9-j Wigner-coefficients
- DX12J procedure for calculation of the 12-j Wigner-coefficients

4. 1. 5. Calculation process

The program requires the following input data:

Number of configurations > number of configurations

Conf. No. 1 > spectroscopic description of the first configuration, e. g. $3d^3\ 4s^2$ has to be written in the form 3d3 4s2, where the subsequent subshells are separated by spaces from each other

Conf. No. 2 > the same procedure for the second configuration etc.

Start value for parameter > ordinal number of the first parameter; usually number 1

Matrix elements output file > name of matrix elements file

Message file > name of the message file

Input file for ATOM program > name of parameters input file

Which interaction compute?

all = *1*

without EL-SO and Mk integrals = *2*

without Mk integrals = *3*

option "1" indicates calculations of all possible interactions

option "2" in the calculation electrostatically correlated spin-orbit interactions, magnetic spin-spin, orbit-orbit and spin-other-orbit interactions are omitted,

option "3" in the calculation magnetic spin-spin, orbit-orbit and spin-other-orbit interactions are omitted,

(the options mentioned above refer to the interactions within a given configuration)

Print zero elements ? y/n >

option "y" - all calculated matrix elements are written into matrix elements file

option "n" - only non-zero matrix elements are written into matrix elements file

The files necessary for calculations (**cpfl.***, **cpf2.*** - one- and two-electron coefficients of fractional parentage, sdld.* - states of two equivalent electrons l^2, **t2t3.*** - parameters T2 i T3, **ts.*** and ***.sts** - parameters Ts and **gam.***, **gamic.*** - parameters Γ) should be accessible during the calculations. These files are read automatically.

4. 1. 6. Compilation

SGI POWER CHALLENGE - compiler F77

4. 1. 7. Input files - data structures

One-electron coefficients of fractional parentage - cpfl.*

Name: cpfl.*, where * denotes spectroscopic description of the core l^N

File for N ≤ 2*l*+ 1:

- record 1: Lc spectroscopic description of the core l^N A1
  mult number of the core electrons I2
  nst number of terms of the core I4

format A1,I2,I4

- record 2: sen seniority number of the core term I2
  mult multiplicity (2*S*+1) I3
  Lcc spectroscopic description of the core term A1
  si quantum number α I2
  ncfp number of parent terms I4
  m1, m2 data for calculation of the parameter Ω (valid only for the core l^N with *l*= *d)* I1,I2

format I2,I3, A1,I2,I4, T20,I1,I2

- record 3 : sen3 seniority number of the parent term I2
  mult multiplicity of the parent term I3
  Lcc spectroscopic description of the parent term A1
  si3 quantum number a of the parent term I2
  a0 phase of the coefficient of fractional parentage I3 (I6 for *l* = *f*)
  ai notation of the coefficient of fractional parentage in form of prime numbers 11A2

format I2,I3, A1, I2,I3, IX, 4A2, 1X, 4A2, 1X, 3A2 (for *l* = *s,p,d)*
I2,I3,A1, I2,4X, 16, 1X, 4A2, 1X, 4A2, 1X, 3A2 (for *l* =*f)*

File for N > 2*l*+ 1:

- record 1 : Lc spectroscopic description of the core l^N Al
  mult number of the core electrons I2
  nst number of terms of the core I4

format A1,I2,I4

- record 2: i ordinal number of the term in the core l^N I4
  ncfp . number of the parent terms I4
  m1, m2 data for calculation of the parameter Ω
  (valid only for the core l^N with *l* = *d)* I1,I2

format 2I4, T20, I1, I2

- record 3 : sen seniority number of the core terms I1
  mult multiplicity (2*S*+1) I1
  Lcc spectroscopic description of the core term Al

si	quantum number α	I1
sen3	seniority number of the parent term	I1
multPT	multiplicity of the parent term	I1
Lc1	spectroscopic description of the parent term	A1
si3	quantum number α of the parent term	I1
CFP	the value of the coefficient of fractional parentage	F13.10

format 2X, I1, 1X, I1, A1, I1, 3X, I1, 1X, I1, A1, I1, 4X, F13.10

In each file cpf.* the data for the core l^N and l^{N-1} are included.

Two-electron coefficients of fractional parentage – cpf2.*

Name: cpf2.*, where * denotes spectroscopic description of the core l^N

File:

– record 1:	Lc	spectroscopic description of the core l^N	A1
	mult	number of the core electrons	I4

format A1, I4

– record 2:	iwsk	ordinal number of the term in the core l^N	I4
	iww	number of parent terms in the core l^{N-2}	I4
	idd	number for electron pair l^2	I4

format I4, I4, I4

– record 3:	sen	seniority number of the core term l^N	I1
	mult	multiplicity $(2S+1)$	I1
	Lcc	spectroscopic description of the core term	A1
	si	quantum number α	I1
	senww	seniority number of the parent term for l^{N-2}	I1
	multww	multiplicity of the parent term	I1
	Lww	spectroscopic description of the parent term	A1
	siww	quantum number α	I1
	send	seniority number of the parent term for l^2	I1
	multd	multiplicity	I1
	Ld	spectroscopic description of the term l^2	A1
	sid	quantum number α	I1
	ccfp2	the value of the coefficient of fractional parentage	D13.10

format 2X, I1, 1X, I1, A1, I1, 3X, I1, 1X, I1, A1, I1, 3X, I1, 1X, I1, A1, I1, 4X, D13.10

States for electron pair l^2

Name: sdld.*, where * spectroscopic description ofthe electrons pair l^2

File:

- record 1: mult2 multiplicity ($2S+1$) I3
  Lc spectroscopic description of the term A1
  format 2X, I3, A1

Intra configuration parameter Γ

Name: gam*, where * denotes spectroscopic description of configuration (e. g.: d5, d4s or d3s2)

- record 1: cd quantum number l of the core electrons in spectroscopic notation (*d*) A1
  cN number of the core electrons I2
  cs2 spectroscopic notation of the electrons added to the core (*s* or *s2*) *A2*
  nst number of parameters in the file I2
  format A1, I2, 1X, A2, T9,I2
- record 2: i ordinal number of term, which corresponds to the given value of the parameter
  a0 phase factor of the parameter I2
  pm parameter notation in form of prime numbers 11I3
  format I3, T25,I2, 1X, 11I3

Parameters T2 and T3

Name: t2t3.d*, where * denotes number of the core electrons

- record 1: cd quantum number l of the core electrons in spectroscopic notation (d) Al
  cN number of the core electrons I2
  nst number of parameters in the file I2

format A1,I2,T9,I2

- record 2: i "bra" term number I4
  j "ket" term number I4
  valt2 value of the parameter *T2,* corresponding with term coordinates (*i,j*) F12.6
  valt3 value of the parameter *T3,* corresponding with term coordinates (*i, j*) F12.6

format 2I4, T29, F12.6, 2X, F12.6

Parameter Ts

For configurations of the type: $d^N s^2$ i $d^{N+1}s$

Name: ts.d*s, where * denotes the number of core electrons

- record 1: cd quantum number l of the core electrons in spectroscopic notation *(d)* Al

	cN	number of the core electrons	I2
	cs2	spectroscopic description of the electron added to the core (s)	A1
	nst	number of parameters in the file	I2

format A1, I2, 1X, A1, T9,I2

-record 2:	i	ordinal number of the "bra" term	I4
	j	ordinal number of the "ket" term	I4
	valts	value of the parameter *Ts,* corresponding with term coordinates (i,*j)*	F12.6

format 2I4, T30, F12.6

For configurations of the type $d^N l_1\ l_2$ *(l_1* or/and l_2 = *s)*

Name: d*sts, where * denotes the number of core electrons

- record 1 :	nTs0	number of parameters in the file	I6

format : I6

-record 2:	senTl	seniority number of the core in "bra"	I2
	multd	core multiplicity of "bra"	I3
	Ld	spectroscopic description of the term in the core in "bra"	A1
	senTlp	seniority number of the core in "ket"	I2
	multw	core multiplicity of "ket"	I3
	Lw	spectroscopic description of the term in the core in "ket"	A1
	mult	term multiplicity of $i/^N i$	I3
	Lc	spectroscopic description of the term $d^N s$	A1
	TSO	value of the parameter Ts	F12.6

format 12,13, A1, 2X, 12,13, A1, 2X, 13, A1, 2X, F12.6

Interconfiguration parameter Γ

Name : gamic.*, where * denotes the number of electrons in given configuration

- record 1 :	cN	number of electrons in given configuration	I3

format I3

-record 2:	nst	number of parameters in the file	I2

format T15,I2

- record 3 :	i	ordinal number of the "bra" term	I4
	j	ordinal number of the "ket" term	I4
	a0	phase factor of the parameter T	I2
	pm	parameter notation in form of prime numbers	11I3

format 2I4, T30,I2, 1X, 11I3

In every file gamic.* the data of interacting configurations $(d + s)^{N+2}$ are included.

4. 2. Program FS_CONV

Program FS_CONV converts the energy matrix into binary form.

Input data:

- matrix elements file
- matrix to be filled up with corresponding values of radial parameters and experimental energy levels (input file for the ATOM program)

Output file: binary form of energy matrix

Program limitations :

The following parameters given in the directive PARAMETER define the size of the binary energy matrix:

- max. size of submatrix: MSR
- max. number of parameters: MNP
- max. number of off-diagonal energy matrix elements: MND
- parameter IA: IA
- parameter IB: IB

The values of the above parameters can be changed but the following relations must be fulfilled: MSR < IA and MNP < IB. Moreover if the parameters MSR, MNP, IA and IB are large, it is important to keep the condition that MSR + IA*(MNP + IB*MSR) doesn't exceed the INTEGER numbers region allowed by by used FORTRAN compiler implementation (e. g. CF77, INTEGER $< 2^{45}$).

4. 2.1. Calculation process

Program requires the following data:

Matrix elements input file > name of matrix elements input file

Input file for ATOM program > name of input file for ATOM program

Binary output file > name of binary matrix elements output file

4. 2. 2. Compilation

CRAY - compiling system CF77

SGI POWER CHALLENGE - compiler F77.

4. 3. Program ATOM

Program ATOM is used in fine structure analysis of an atom

Input files:

- binary form of the energy matrix
- input file containing the values of radial parameters and experimental values of energy of the levels

Output files:

- output file containing the results of the fitting procedure:
  calculated fine structure radial integrals, eigenvectors and calculated energy values

- output file containing calculated values of fine structure radial integrals and experimental energy values. These data have a form of input data and can be used to restart the fitting procedure.
- output file with eigenvectors

Program limitations:

The following parameters given in the directive PARAMETER define the size of the binary energy matrix:

- max. number of submatrices:	MSM
- max. rank of submatrices:	MSR
- max. number of energy levels (sum of ranks of all submatrices):	NE
- max. number of off-diagonal elements in the energy matrix:	MND
- max. number of parameters:	FNP
- max. number of free parameters:	NP
- parameter I9:	I9
-parameter I15:	I15

The value of the above parameters can be changed, but the following relations must be fulfilled: MSR <I15 and NP < I9. If the parameters: MSR, NP, I9 and I15 are large, it is important to keep the condition that MSR + I15*(NP + I9*MSR) doesn't exceed the INTEGER numbers region allowed by the used FORTRAN compiler implementation (i.e. CF77, INTEGER < 2^{45}).

4. 3.1. Program organization

Program requires the following data:

Binary input file > name of the binary form of energy matrix file

Read parameters from > name of the parameter input file for the ATOM program

Write output to > name of the output file

Write restart parameters to > name of the restart parameters file

Write eigenvectors to > name of the additional output file with calculated eigenvectors

Print parameter rations ? y/n > print parameters ratios in the output file

If the name of restart parameters file is given, the following options are possible:

Print: all eigenvalues - 1
selected - 2
first n eigenvalues - 3

where

option "1" - print in the output file all calculated eigenvalues,

option "2" - only chosen eigenvalues are written into the output file. In this case ordinal number of the eigenvector to be written into the output file together with ordinal number of the submatrix including this eigenvector has to be specified,

option "3" - only *n* first eigenvalues of any submatrix are written into the output file

4. 3. 2. Compilation

CRAY - compiling system CF77

SGI POWER CHALLENGE - compiler F77.

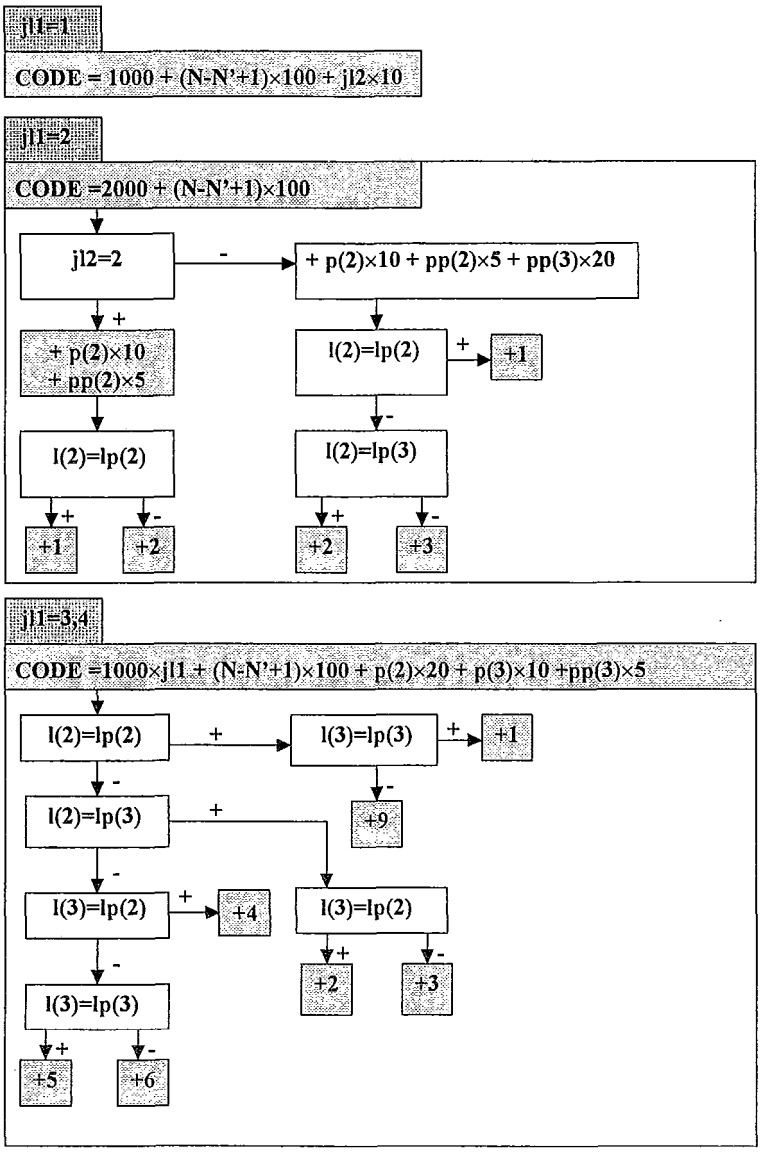

Fig. 6. The scheme of the algorithm for calculation CODE parameter

5. REMARKS

Package of the programs discussed in this paper operates in an interactive or batch mode. The uniform structure of the files permits the efficient transfer of information between programs.

The automatization of data transfer and file generation reduced the risk of errors introduced by manual transformation and proofs of the data. The package contains a standard set of the file structures, which should be available during generation. These files are opened automatically and they possess reserved names. The results of the computation are the values of fine structure parameters, energy eigenvalues and eigenvectors. The eigenvectors constitute an input database for hyperfine structure calculations and analyses.

APPENDIX

Algorithm for calculation of CODE parameter

Description of symbols :

j11, j12: number of shells for "bra" and "ket" configurations

N, N': number of electrons in l^N core for "bra" and "ket" configurations

l(i), lp(i): spectroscopic designations of the *i*-th electron shell for "bra" and "ket"

p(i), pp(i): number of electrons in the *i*-th shell for "bra" and "ket" $i = 1,\ldots, 4$.

Assumption: j11 $\leq$ j12

If *j11* > *j12*: interchange "bra" and "ket' configurations and CODE = CODE + 5000

The scheme of the algorithm is shown in Fig. 6.

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