10. Program DBSR_DMAT (version 3)

The DBSR_DMAT program prepares the dipole matrix, **d.nnn**, for subsequent use in the DBSR_PHOT program for photoionization calculations, or performs the calculations of oscillator strengths between *B*-spline bound-state solutions. For completeness, DBSR_DMAT also has the option to calculate oscillator strengths between MCHF solutions, and between *B*-spline bound states and MCHF solutions.

10.1.Dipole transition matrix

For calculations of radiative parameters, such as oscillator strengths or photoionization cross sections, we need dipole matrix elements between the initial and final states. Each atomic states is represented in some basis. It is convenient to represent the dipole matrix elements by using the dipole transition matrix, which consists from the dipole matrix elements between the basis states. Suppose we have two sets of solutions of the Hamiltonian matrix in different bases. In our case, it can be either the configuration basis from the MCHF/CI calculations, or a close-coupling *B*-spline expansion from DBSR calculations. Then the matrix element for the given solutions *a* and *b* is

$$< a \mid D^{[\lambda]} \mid b >= \sum_{i,j} a_i d_{ij} b_j = \mathbf{a}^T \mathbf{d}\ \mathbf{b}\,, \tag{10.1}$$

where $\{a_i\}$ and $\{b_i\}$ are the vectors of expansion coefficients in the respective bases, and **d** is the corresponding transition matrix. Once we generate the transition matrix **d** , the matrix elements for any other solutions is simply defined by convoluting **d** with the corresponding expansion vectors. The logical structure of DBSR_DMAT is such that it first generates the relevant dipole transition matrix, and then, if indicated, calculates the corresponding set of radiative parameters. This enables us to use the same code for photoionization and bound-state calculations.

Consider the structure of the transition matrix in the *B*-spline representation. This structure is very similar to the structure of the Hamiltonian matrix considered in the write-up of the DBSR_MAT program in Section 7. For convenience, we repeat some definitions here. The large and small components of the one-electron orbitals are represented as

$$P_i(r) = \sum_{m=1}^{n_p} p_m^i B_m^{k_p}(r), \quad Q_i(r) = \sum_{m=1}^{n_q} q_m^i B_m^{k_q}(r). \tag{10.2}$$

If the atomic state is represented as close-coupling expansion, the *B*-spline solution vector, ***c***, can be then written as

$$\boldsymbol{c} = [\boldsymbol{a}_1,...,\boldsymbol{a}_{N_c},\boldsymbol{b}]^T \tag{10.3}$$

where each $\boldsymbol{a}_i$ is a column vector of *B*-spline coefficients for the given channel functions $\overline{\Phi}_i^{\Gamma}$

$$\mathbf{a}_i = [\,p_1^i,\, p_2^i,...,\, p_{n_p}^i, q_1^i, q_2^i,...,q_{n_p}^i\,]^T \tag{10.3}$$

and $\boldsymbol{b}$ is the column vector of correlation functions coefficients

$$\boldsymbol{b}_j = [b_1, b_2,...,b_{N_p}]^T, \tag{10.5}$$

where N_c is the number of channels, while N_p is the number of correlation functions. Then the transition matrix $\mathbf{d}$ has the form

$$\begin{pmatrix} D(11) & D(12) & \cdots & D(1N_c) & d(1p) \\ D(21) & D(22) & \cdots & D(2N_c) & d(2p) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ D(N_c1) & D(N_c2) & \cdots & D(N_cN_c) & d(N_cp) \\ d(1p)^T & d(2p)^T & \cdots & d(N_cp)^T & d(pp) \end{pmatrix} \tag{10.6}$$

where $d(pp)$ is an $N_p \times N_p$ matrix that comes from the bound-bound interaction, the $d(ip)$ are the $2n_s \times N_p$ matrices, representing the interaction between the *i*-th channel and the bound states, and the $D(ij)$ are the $2n_s \times 2n_s$ matrices for the channel-channel interaction. When we work with MCHF solutions, the transition matrix is reduced just to the $d(pp)$ matrix.

Each individual matrix element in (10.5) is expressed by the program DBSR_MULT in the form

$$\sum_{\alpha,\beta} c_{\alpha\beta} R^{\lambda}(\alpha,\beta) \times D(\{n\kappa\};\{n'\kappa'\}) \tag{10.7}$$

where α,β denote the one-electron orbitals involved, $c_{\alpha\beta}$ are numeric coefficients that only depend on the angular symmetry of the CSFs involved, R^{λ} stands for the corresponding one-electron multipole integrals, and $D(\{n\kappa\},\{n'\kappa'\})$ is the overlap factor which depends only on the orthogonality of the radial orbitals used in the construction of the basis CSFs. In general, the overlap factor is the multiplier of determinants of matrices consisting of one-electron overlaps between radial functions in the initial and final states (see Eq. 27, 28 in the DBSR_BREIT write-up).

The channel orbitals can appear in the radial integrals R^{λ}, as well as in the determinant factors. To derive the final expression for the matrix elements in the *B*-spline basis, let us first simplify the overlap factors (7.8) by expanding them over those rows which contain one-electron overlaps with the channel orbitals. At most, there can be two such rows. The residual overlap determinants depend only on the known bound orbitals and they can be calculated in a standard manner. It is convenient to redefine the

angular coefficients $c_{\alpha\beta}$ by multiplying them by these residual overlap factors. As a result, the initial overlap factor $D(\{n\kappa\},\{n'\kappa'\})$ in expression (10.7) is reduced to one-electron or two-electron overlaps of the form

$$\langle k\kappa \,|\, n\kappa\rangle, \quad \langle k\kappa \,|\, k'\kappa\rangle \quad \text{or} \quad \langle k\kappa \,|\, n\kappa\rangle \,\langle n'\kappa' \,|\, k'\kappa'\rangle, \tag{10.8}$$

where $|k\kappa>$ stands for the radial function of the channel orbital in the inner region.

We have different type of the one-electron transition integrals $R^{\lambda}(\alpha,\beta)$:

1. Electric multipole, Babushkin (length) gauge:

$$R^{\lambda}(\alpha\beta) = R^{\lambda}(P_{\alpha},P_{\beta}) + R^{\lambda}(Q_{\alpha},Q_{\beta}) \tag{10.9}$$

2. Electric multipole, Coulomb (velocity) gauge:

$$R^{\lambda}(\alpha\beta) = \frac{c}{\omega}\Big[(\kappa_{\alpha}-\kappa_{\beta}-\lambda)R^{\lambda-1}(P_{\alpha},Q_{\beta}) + (\kappa_{\alpha}-\kappa_{\beta}+\lambda)R^{\lambda-1}(Q_{\alpha},P_{\beta})\Big] \tag{10.10}$$

3. Magnetic multipole:

$$R^{\lambda}(\alpha\beta) = \frac{1}{(\lambda+1)}(\kappa_{\alpha}+\kappa_{\beta})[R^{\lambda}(P_{\alpha},Q_{\beta}) + R^{\lambda}(Q_{\alpha},P_{\beta})] \tag{10.11}$$

where

$$R^{\lambda}(f,g) = \int_0^{\infty} f(r)g(r)r^{\lambda}dr \tag{10.12}$$

For more detailed description of the transition matrix **d**, let us introduce the integrals between individual *B*-splines. Here we should take into account that we use two different *B*-spline bases for the large and small components. For one-electron overlap integrals we introduce matrix

$$B(\bullet\bullet)_{ij} \rightarrow \begin{pmatrix} \mathbf{B}^{pp} & 0 \\ 0 & \mathbf{B}^{qq} \end{pmatrix}, \qquad B_{ij}^{pp} = < B_i^p \,|\, B_j^p >, \quad B_{ij}^{qq} = < B_i^q \,|\, B_j^q > . \tag{10.13}$$

For electric multipole integrals in length form we need matrix

$$R^{\lambda}(\bullet\bullet)_{ij} \rightarrow \begin{pmatrix} \mathbf{R}^{\lambda,pp} & 0 \\ 0 & \mathbf{R}^{\lambda,qq} \end{pmatrix}, \qquad R_{ij}^{\lambda,pp} = < B_i^p \,|\, r^{\lambda} \,|\, B_j^p >, \quad R_{ij}^{\lambda,qq} = < B_i^q \,|\, r^{\lambda} \,|\, B_j^q > . \tag{10.14}$$

For electric multipole integrals we introduce matrix

$$R^{\lambda}(\bullet\bullet)_{ij} \rightarrow \begin{pmatrix} 0 & \mathbf{R}^{\lambda,pq} \\ \mathbf{R}^{\lambda,qp} & 0 \end{pmatrix}, \qquad R_{ij}^{\lambda,pq} = < B_i^p \,|\, r^{\lambda} \,|\, B_j^q >, \quad R_{ij}^{\lambda,qp} = < B_i^q \,|\, r^{\lambda} \,|\, B_j^p > . \tag{10.15}$$

Similar matrix is used to describe electric multipole integrals in velocity form. These matrices are used to construct the $D(ij)$ channel-channel blocks in full transition matrix (10.6).

To describe the channel-bound interaction, we introduce the following vectors with elements

$$B(\,.\,a)_i = \sum_{j=1}^{2n_s} a_j B_{ij}, \qquad R^\lambda(\,.\,a)_i = \sum_{j=1}^{2n_s} a_j R_{ij}\,, \tag{10.16}$$

Finally, for bound-bound interaction we have

$$R^\lambda(ab) = \sum_{i,j=1}^{2n_s} a_i R^\lambda_{ij} b_j\,. \tag{10.17}$$

With this notation, table 10.1 represents the contributions of the different terms from the matrix element expression (10.6), which usually produces the angular integration codes, to the transition matrix (10.5), along with an indication of its structure.

Table 10.1. Contribution of different terms (without indication of angular coefficients) in the transition matrix. The symbols *a*,*b* stand for the bound orbitals, while the symbol k_i indicates the channel orbitals in *B*-spline basis.

Term	Contribution	Remarks
Channel-channel interaction		
$R^\lambda(k_i, k_j)$	$R^\lambda(\,.\,.)$	banded matrix
$\langle k_i \mid a\rangle \langle b \mid k_j\rangle R^\lambda$	$B(\,.\,a) \bullet B(\,.\,b) * R^\lambda$	Full matrix, contribution due to non-orthogonality
$\langle k_i \mid k_j\rangle R^\lambda$	$B(\,.\,.) * R^\lambda$	Banded matrix,
$R^\lambda(k_i,a) \langle b \mid k_j\rangle$	$L(\,.\,a) \bullet B(\,.\,b)$	full matrix, contribution due to non-orthogonality
Channel-bound interaction		
$R^\lambda(k_i,a)$	$R^\lambda(\,.\,a)$	vector
$\langle k_i \mid a\rangle R^\lambda$	$B(\,.\,a) * R^\lambda$	vector, contribution due to non-orthogonality
Bound-bound interaction		
$R^\lambda(a, b)$		scalar

10.2. Oscillator strengths and decay probabilities

For completeness of the description, we provide below the main formulae used in the present code for the calculation of radiative properties. The line strength for a given transition is defined as

$$S_{ij} = S_{ji} = |< \gamma_i J_i \,||\, D^{[\lambda]} \,||\, \gamma_j J_j >|^2 \tag{10.18}$$

where the reduce matrix element can be determined from the transition matric according expression (10.1). The transition probability can then be found as:

$$A_{ji} = \frac{2(2\lambda+1)(\lambda+1)}{\lambda[(2\lambda+1)!!]^2}\frac{1}{g_i}\frac{1}{\hbar}\left(\frac{E_j - E_i}{\hbar c}\right)^{2\lambda+1} S_{ij}\,. \tag{10.19}$$

The oscillator strength (unitless) is related to the transition probability by

$$g_i f_{ij} = \frac{mc}{8\pi^2 e^2} g_j A_{ij}\lambda^2 = \frac{mc^3}{2e^2}\frac{g_j A_{ji}}{\omega^2}, \tag{10.20}$$

independent of the nature of the radiative transition.

10.3. Structure and data flow

The block diagram of the program DBSR_DMAT, along with the data flow, is given in Fig. 10.1. First, the program read all input data related to the given case. It includes input parameters from the command line, subroutine **read_arg**, the list of configurations, **read_conf_jj**, the target states and channel information, routines **read_target** and **read_channels**, B-spline basis, **read_knot_dat**, and the list of one-electron radial functions involved in description of the initial and final states, routine **read_bsw**. The orbitals in the initial and final sets are supposed to be non-orthogonal. All one-electron radial functions should be in the *B*-spline representation. They can be either the user-prepared **name1.bsw** files, or the **bound.nnn** files generated by the BSR_HD program (in this case the program requires the **target** file with a description of the relevant close-coupling expansions). The above programs also generate all needed working arrays to keep the input information. These arrays are automatically allocated in accordance with the input data. At these stage, the program also generate multipole integrals between individual B-splines, routine **gen_dbs** (see Eq.10.13-10.15).

The **check_mult_bnk** routine analyses the information contained in the databank **mult_bnk**, and determines whether the data bank contains all angular coefficients needed for the given case. If not, the program stops, suggesting to rerun DBSR_MULT program. Note that the multipole index and the type of transition under consideration are recorded in **mult_bnk.**

The **d_matr** routine controls the calculation of the transition matrix (10.6). First, the program reads all overlap factors $D(\{n\kappa\},\{n'\kappa'\})$ from data bank in routine **read_dets.** These overlap factors are presented in the symbolic form, without indication of the specific one-electron orbitals involves. Then the program reads and processes, one by one, all one-configurational matrix elements presented in the **mult_bnk**, see Eq.(10.7). It first determines if the given matrix elements is relevant to the given

transition. If so, the overlap factor $D(\{n\kappa\},\{n'\kappa'\})$ is reduced to one-electron or two-electron overlaps of the form (10.8) by the routine **det_fact** for specific one-electron orbitals. The integrals are then sorted according to their structure (see table 10.1) and stored in the module **cmdata** in different ordered blocks, routine **add_coef.** When all coefficients from **mult_bnk** are exhausted, or when all blocks are full, they are processed by **gen_matrix** to get the transition matrix (10.6). The *B*-spline representation for specific integrals is controls by routine **d_data** (this may require preliminary merging different blocks in the large-scale case, routine **merge_cdata**). The corresponding contributions are then added (using **updates** routines) to the transition matrix (10.6), located in the module **dmatrix**.

The next step of the calculation depends on the input/output mode, defined by parameters **ctype2**. For calculations of oscillator strengths, the program calls the routine **gen_gf** for processing transitions between all input states. The resulting line strengths, oscillator strengths, transition energies, and transition probabilities are recorded in the file **zf_res** (see section 10.7 below). In photoionization calculations, the dipole matrix (10.6) is calculated on the base of the *R*-matrix solutions placed in the file **rsol.nnn**, and then is recorded in the file **d.nnn**. The present version 3 also contain two additional output options **ctype2=q**, where we prepare the transition matrix, **dv.nnn**, needed for polarization calculations in program DBSR_POL.

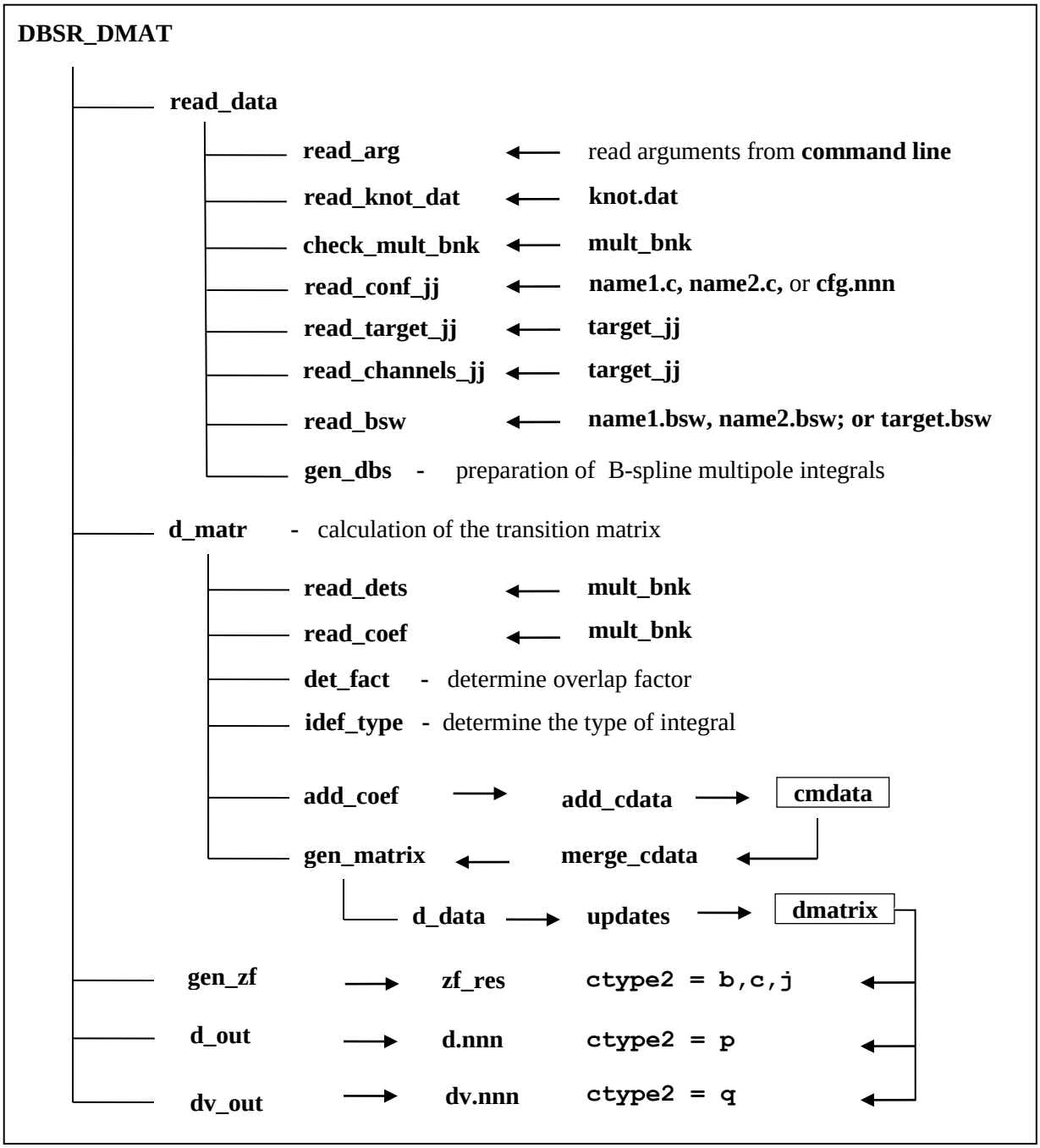

Fig. 10.1. Block diagram for the program DBSR_DMAT and data flow (see text).

10.4. Data files

name1.c or **cfg.nnn** File type: formatted sequential input.
Created by DBSR_CONF, DBSR_HF or DBSR_MCHF programs.
Read by routine **read_conf_jj**.
Description: contains the configuration expansion for the initial state**.**

name2.c or **cfg.nnn** File type: formatted sequential input.
Created by DBSR_CONF, DBSR_HF or DBSR_MCHF programs.
Read by routine **read_conf_jj**.
Description: contains the configuration expansion for the final state**.**

mult_bnk File type: unformatted sequential input.
Written by program DBSR_MULT**.**
Read by routines **check_mukt_bnk, d_matr**.
Description: databank for the angular coefficients of the multipole operator.

dbound.nnn File type: unformatted sequential input.
Created by program DBSR_HD**.**
Description: bound-state solutions for a given partial wave in the *B*-spline representation (10.3).

target_jj File type: formatted sequential input.
Written by user and modified by DBSR_PREP and DBSR_CONF programs.
Read by routine **read_target_jj.**
Description: contains description of the target states and scattering channels.

knot.dat File type: formatted sequential input.
Written by user and modified by DBSR_PREP.
Read by routine **read_knot dat** from DBS library.
Description: input parameters that define the *B*-spline grid.

target.bsw File type: unformatted sequential input.
Created by program DBSR_PREP**.**
Read by routine **read_dbsw.**
Description: target one-electron orbitals in the *B*-spline basis.

pert_nnn.bsw File type: unformatted sequential input (optional).
Created by program DBSR_PREP**.**
Read by routine **read_dbsw.**
Description: perturber one-electron orbitals in the *B*-spline basis.

name1.bsw File type: unformatted sequential input (optional).
Read by routine **read_dbsw.**
Description: one-electron orbitals in the *B*-spline basis for the initial state.

name2.bsw File type: unformatted sequential input (optional).
Read by routine **read_dbsw.**
Description: one-electron orbitals in the *B*-spline basis for the final state, optional.

rsol.nnn File type: unformatted sequential output.
Created by program DBSR_HD
Read by program DBSR_DMAT.

Description: full set of *R*-matrix solutions in the inner region.

d.nnn File type: formatted sequential output.
Written by program DBSR_DMAT**.**
Read by BSR_PHOT.
Description: dipole vector for R-matrix solutions .

dv.nnn File type: formatted sequential output.
Written by program DBSR_DMAT**.**
Read by DBSR_POL.
Description: dipole vector for given initial state.

zf_res File type: formatted sequential output.
Written by program DBSR_DMAT**.**
Read by user.
Description: oscillator strengths for given multi operator given in **mult_bnk**.

bsr_dmat.log File type: formatted sequential output.
Written by program DBSR_DMAT**.**
Read by user.
Description: running information.

10.5. Input parameters

Since DBSR_DMAT requires only a small number of input parameters, all of them must be defined in the command line as arguments. The input parameters for the BSR_DMAT program are the names of the *c*-files with a list of configuration state functions for the initial and final states involved, and the mode of calculation **ctype.** The input *c*-files may be the ordinary *c*-files from MCHF calculations, or **cfg.nnn** files generated in DBSR calculations. The mode of calculation defines whether this is the generation of the transition matrix for subsequent photoionization calculations or the calculation of oscillator strengths between bound states. The **ctype** parameter also defines the representation format for the initial and final states, which can be **name.c**, **name.j** or **dbound.nnn** files. DBSR_DMAT reads a set of input data files. All of them have default names, or names which are directly connected to the names of the input *c*-files. The specific input data files, which are actually used, depend on the input parameters **ctype1** and **ctype2**.

Below we provide the list of possible arguments in the command line. First four parameter are the mandatory position parameters. All other key-words parameters are optional.

name1.c or **cfg.nnn** name of *c*-file for the initial state

name2.c or **cfg.nnn** name of *c*-file for the final state

ctype1 character, denotes the representation mode for the initial state:
c – initial state is defined by *c*-file after DBSR_HF or CI calculations
j - initial state is defined by *j*-file after DBSR_CI calculations
b - initial state is defined by **bound.nnn** file from DBSR calculations

ctype2 character, the same as **ctype1,** but for the final state. These modes assume the calculation of oscillator strengths, with the output put in the file **zf_res**.

An additional modes:

p - the dipole transition vector for given initial state will be generated in the output file **d.nnn** for subsequent photoionization calculations, BSR_PHOT.

q - the dipole transition vector for given initial state will be generated in the output file **dv.nnn** for subsequent DBSR_POL calculations.

gf (g|f) defines output of gf- or f-values in **zf_res** file

mstates1 [0]
mstates2 [0] if /= 0, restricts the number of initial/final states from the input files in calculations of oscillator strengths

istate1 [0]
istate2 [0] if /=0, indicate specific initial/final state to be considered

ialfa [0] if /=0, for dipole transitions, **zf_res** will contain additional information: dipole matrix element, contribution of the given transition in the polarizability of the initial state, and the sum of all contribution for the initial state defined by **istate1** parameter.

debug [0] if \= 0, provides additional information in the **bsr_dmat.log** file.

10.6. Output of dipole matrix in **d.nnn**.

1. **2J,parity,Etarg(1),nstate2 -** term and number of final states.
2. **2J, parity, E1, Label -** term and energy of the initial state.
3. **(cl(i),cv(i),i=nstate2,-1) -** dipole matrix in length and velocity form.

10.7. Output of dipole matrix in **dv.nnn**.

1. **kdm2,nch2,npert2,E1,jot1,kpol,ktype**
   kdm2 - number of final states (=ms*nch2+npert2)
   nch2 - number of channels
   npert2 - number of perturbers
   E1 - energy if first target states
   jot1 - total 2J-values for the final state
   kpol - multipole index
   ktype - transition type (E|M)
2. **(cl(i),i=1,kdm2) -** dipole matrix in length form.
3. **(cv(i),i=1,kdm2) -** dipole matrix in velocity form.

10.6. Output of radiative data in **zf_res.**

The output format in **zf_res** is the same as in the MCHF Atomic Structure Package (Froese Fischer et al 1997). An example of output is given in Fig.10.2. Each transition is represented by a block, which consists of two empty lines as a delimiter, two lines with a description of the initial and final atomic states, one line with the transition energy in cm^{-1} and Angstroms, and finally a line with the line strength, the oscillator strength, and the transition probability in the length form. For E1 transitions, there is an additional line with the results in the velocity form.

Each atomic state is represented by its spectroscopic label, its absolute energy in a.u., and the value of 2*J*. The f-values are always for transitions from the lower to the higher state, whereas the transition probabilities are always reported from the higher to the lower state. The default output is the gf-values which does not depends on order of initial and final states (see parameter **gf**).

The file **zf_res** is opened in the DBSR_DMAT program with access mode *append*. Hence, the results from different calculations can be accumulated.

```
- 1 -5880.47384280  5p-.1/2*
+ 1 -5879.98893118  5s.5p.1_7p.1/2
  106425.29 CM-1       939.63 ANGS(VAC)       939.63 ANGS(AIR)
 E1   S =  2.77200D-03   FIK=  4.48058D-04   AKI =  3.38507D+06
           8.30219D-04         1.34194D-04         1.01383D+06

- 1 -5880.47384280  5p-.1/2*
+ 1 -5879.98276976  5s.5p.2_kp.1/2
  107777.56 CM-1       927.84 ANGS(VAC)       927.84 ANGS(AIR)
 E1   S =  3.00419D-03   FIK=  4.91759D-04   AKI =  3.81024D+06
           8.56961D-04         1.40277D-04         1.08689D+06

- 1 -5880.47384280  5p-.1/2*
+ 1 -5879.98059840  5s.5p-.0_kp-.1/2
  108254.12 CM-1       923.75 ANGS(VAC)       923.75 ANGS(AIR)
 E1   S =  2.41521D-03   FIK=  3.97096D-04   AKI =  3.10405D+06
           1.20094D-03         1.97453D-04         1.54346D+06

- 1 -5880.47384280  5p-.1/2*
+ 1 -5879.97803268  5s.5p.1_8p-.1/2
  108817.22 CM-1       918.97 ANGS(VAC)       918.97 ANGS(AIR)
 E1   S =  5.36249D-04   FIK=  8.86259D-05   AKI =  7.00002D+05
           3.50463D-04         5.79210D-05         4.57483D+05
```

Fig. 10.2. Example of the output zf_res file with gf=f mode.