11. Program DBSR_POL

This program calculates the polarized pseudo-states of order k in B-spline representation for the given atomic state. Structure of pseudo-state is defined by close-coupling expansion for the given partial wave. The input for DBSR_POL contains the corresponding Hamiltonian matrix in B-spline representation, obtained with DBSR_MAT, and the multipole interactions matrix, obtained with DBSR_DMAT. Additional orthogonality constraints can be implied. The resulting pseudo-state is recording into **pol.nnn** file in the same format as bound states, obtained with program DBSR_HD and recorded in the **dbound.nnn** files..

11.1 Definition of polarized pseudo-states.

It is well known that the elastic scattering of low energy electrons by atoms is strongly influenced by the long-range polarization potential. The close-coupling expansion usually takes into account only part of the polarizability of the ground state states due to limited number of target states which can be included into close-coupling expansion. In many cases, considerable part of polarization arises from the continuum, which usually is neglected in actual CC expansions due to computational difficulties. In the case of the rare gases, typically 50% or more of the polarizability comes from the continuum, and the error arising from this source can be serious.

One solution to this problem was given by Damburg and Karule (1967). They pointed out that it was possible to define a pseudo-state which could be included in the close coupling expansion in the same way as an atomic eigen-state but which allowed for the full polarizability of the ground state. We will refer to this state as a polarized pseudo-state to distinguish it from pseudo-states which have been widely used to represent other aspects of the collision process. For example, in the RMPS (R-matrix pseudo-state, Bartschat et al 1996) or CCC (convergent close-coupling, Bray et al 2002) methods, pseudo-states are used to mimic the target continuum and they are usually determined from diagonalization of the atomic Hamiltonian in the bases of L^2 integrable wavefunctions.

First attempt to employ polarized pseudo-states in scattering problem has been made by Burke and Mitchell (1974), who obtained the polarized pseudo-states as linear combinations of configurations based on analytic orbitals. Further development of using polarized pseudo-states in the multiconfigurational approach for calculation of atomic polarizabilities has been reported in series of work by Hibbert et al (1977). In the present calculations we follow these developments but employ the different numerical technique which is based on the B-spline expansions.

The static dipole polarizability of an atomic system in atomic units, is defined by the equation

$$\alpha^{(1)} = 2\sum_k \int dk \frac{|<\phi_0 \mid D^{(1)} \mid \phi_k>|^2}{E_k - E_0} \qquad (1)$$

The summation and integration in this equation are taken over all states ϕ_k including the continuum which are coupled to the ground state ϕ_0 by the dipole operator $D^{(1)}$. The polarized pseudo-state ϕ_p is defined by the requirement that the summation and integration in equation (1) is replaced by a single term

$$\alpha^{(1)} = 2\frac{|<\phi_0 \mid D^{(1)} \mid \phi_p>|^2}{E_p - E_0} \tag{4}$$

where ϕ_p is normalized

$$<\phi_p \mid \phi_p >= 1 \tag{5}$$

and E_p is defined by

$$<\phi_p \mid H \mid \phi_p >= E_p \tag{6}$$

As shown by Burke and Mitchell (1974), the ϕ_p can be written as

$$\phi_p = N^{-1/2}\tilde{\phi}_p \tag{7}$$

where $\tilde{\phi}_p$ is a solution of the equation

$$(H - E_o)\tilde{\phi}_p = D_0^{(1)}\phi_0 \tag{8}$$

and the factor $N^{-1/2}$ ensures that equation (5) is satisfied.

The generalization to any higher multipole k is straightforward by using multipole operator $\mathbf{D}^{(k)}$. The equation (8) becomes

$$(H - E_o)\tilde{\phi}_p = D_0^{(k)}\phi_0 - <\phi_0 \mid D^{(k)} \mid \phi_0 > \phi_0 \ , \tag{12}$$

where second term appears only for even multipoles. From equation (12) we also see that any function

$$\varphi_p = \tilde{\phi}_p + \gamma\phi_0 \tag{13}$$

is also solution of equation (9). Therefore in order to obtain a unique solution it is necessary to impose the condition

$$<\phi_p \mid \phi_0 >= 0 \tag{14}$$

which is automatically satisfied for odd multipoles. Orthogonality ϕ_p to any function ϕ_i can be imposed with Lagrange multipliers and final equation for polarized pseudo-orbitals is

$$(H - E_o)\tilde{\phi}_p + \sum_i \lambda_i\phi_i = D_0^{(k)}\phi_0 - <\phi_0 \mid D^{(k)} \mid \phi_0 > \phi_0 \ . \tag{15}$$

Let's supposed that all atomic states are represented in B-spline bases as shown in DBSR_MAT write-up, and vectors $\mathbf{c}_0$, $\mathbf{c}_p$ or $\mathbf{c}_i$ represent the functions φ_o, φ_p, and φ_i, respectively. Then Eq.(12) in the B-spline basis has the form

$$(\mathbf{H}-E_0\mathbf{S})\mathbf{c}+\sum_i \lambda_i \mathbf{S}\mathbf{c}_i = \mathbf{D}\mathbf{c}_0 - <\mathbf{c}_0\,|\,\mathbf{D}\,|\,\mathbf{c}_0>\mathbf{S}\mathbf{c}_0 \qquad (16)$$

where **H**, **S** and **D** are the Hamiltonian, overlap and dipole matrixes between the basic functions. We may consider **c** together with Lagrange multipliers as new unknown vector and introducing

$$\mathbf{d} = \mathbf{D}\mathbf{c}_0 - <\mathbf{c}_0\,|\,\mathbf{D}\,|\,\mathbf{c}_0>\mathbf{S}\mathbf{c}_0\,, \qquad (17)$$

we may rewrite (13) as

$$\begin{vmatrix} \mathbf{H}-E_0\mathbf{S} & \mathbf{S}\mathbf{c}_1 & \dots \\ \mathbf{c}_1^T\mathbf{S} & 0 & 0 \\ \dots & 0 & 0 \end{vmatrix} \begin{pmatrix} \mathbf{c} \\ \lambda_1 \\ \dots \end{pmatrix} = \begin{pmatrix} \mathbf{d} \\ 0 \\ 0 \end{pmatrix} \qquad (18)$$

where … stands for additional orthogonal conditions if any. In actual calculations, we do not need the **D**-matrix and $\mathbf{c}_0$ vector explicitly, but rather their product $\mathbf{d}=\mathbf{D}\mathbf{c}_0$ which can be obtained by using DBSR_DMAT program with option **ctype2=q**. Note that BSR_DMAT can employ both B-spline (DBSR) and standard configurational (MCHF) representation for the ground state, φ_o .

11.2. Structure and data flow

The block diagram of the program DBSR_POL, along with the data flow, is given in Fig. 11.1. The program has simple structure. We first read all relevant data, concerning the close-coupling expansions and one-electron radial functions in B-spline basis, subroutine **read_data**. Then we download the Hamiltonian and dipole matrixes, routines **read_bsr_mat** and **read_dipmat**. Then we define the additional orthogonal constraints if any, routine **read_nortb**. Finally, the program solves the equation (18), determine the polarizability and output the polarized pseudo-state in file **pol.nnn**.

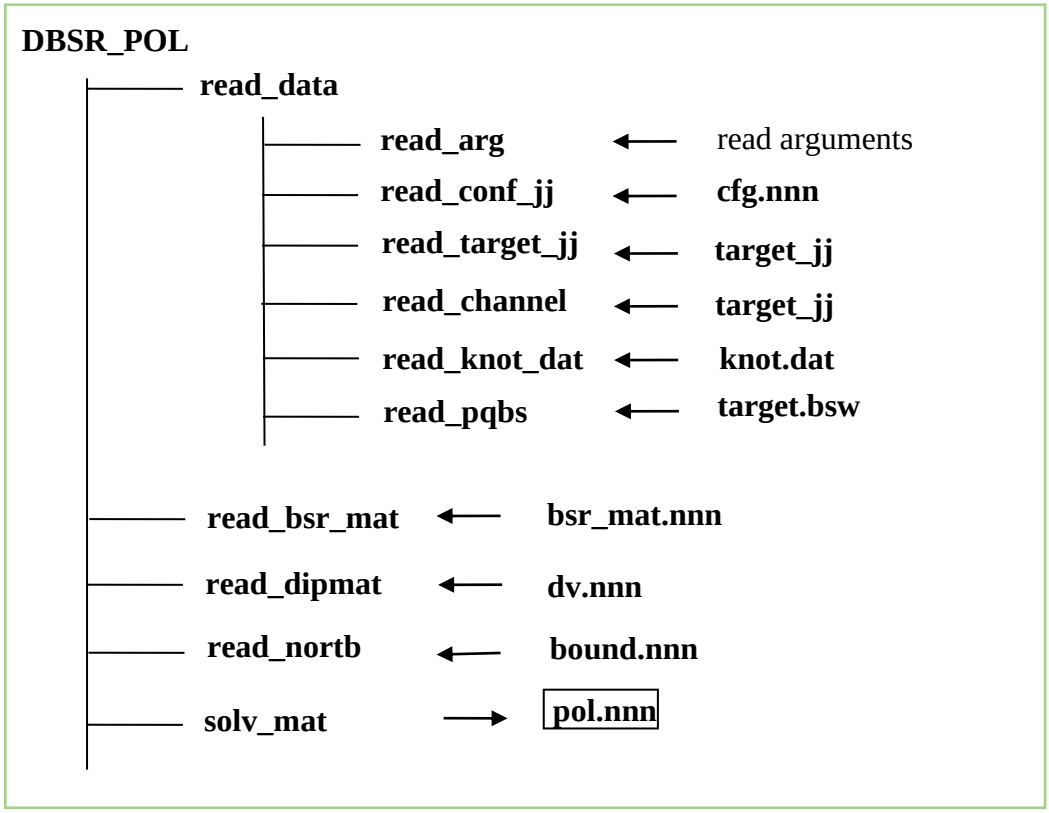

Fig. 11.1. Block diagram for the program DBSR_POT3 and data flow (see text).

11.3 Input parameters

klsp	index of partial wave, **nnn,** for polarized pseuo-state
ilzero [1]	number of initial B-splines to be excluded from orbital expansions
ibzero [1]	number of final B-splines to be excluded from orbital expansions
nortb [0]	number of additional orthogonal conditions
inorb	indexes of solutions in **dbound.nnn** file which will be used for orthogonality (if **nortb** > 0)

11.4. Data files

dbsr_par	File type: formatted sequential input. Written by user. Read by routine **read_arg**. Description: input parameters for given run.
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, optional.

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

cfg.nnn File type: formatted sequential input.
Created DBSR_CONF programs.
Read by routine **read_conf_jj**.
Description: contains the configuration expansion for the polarized pseudo-state

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

bsr_mat.nnn File type: unformatted sequential input
Created by program DBSR_MAT.
Description: Overlap/Hamiltonian matrix in B-spline basis.

dv.nnn File type: formatted sequential input.
Written by program DBSR_DMAT**.**
Read by DBSR_POL.
Description: dipole vector between given initial state and partial wave **nnn**.

bsr_pol.nnn File type: formatted sequential input.
Written by program DBSR_POL**.**
Read by user.
Description: running information.

pol.nnn File type: formatted sequential output **(main result)**.
Written by program DBSR_POL**.**
Read by **bound_bsw** utility.
Description: bound-state solutions for given pseudo-state in the *B*-spline close-coupling representation (8.2).