

## *SPINS Directives*

**electrons**  $N$

Defines the number of electrons in the system (integer, currently 1 to 12). Should be the first directive in the command file. The **electrons** directive initiates work on a completely new task, i.e. *SPINS* ‘forgets’ any information which may have been supplied beforehand.

**spin**  $S$

Defines the required value of the total spin  $S$ .  $S$  should be compatible with  $N$ , i.e.  $0 \leq S \leq N/2$ , taking integer, or half-integer values when  $N$  is even, or odd, respectively. If the **spin** directive is omitted, the default values of  $S$  for  $N$  even or odd are 0 (singlet) and 0.5 (doublet). The **spin** directive, similarly to the **electrons** directive, instructs *SPINS* to start a new task. The only difference is that it does not cancel a previously defined permutation (see the **permutation** directive).

**input** *Rumer* | *Kotani* | *Serber* | *Rumer\_VB*  $C_{S1}$   $C_{S2}$  ...  $C_{Sf_S^N}$

Defines an input vector of spin-coupling ( $C_{Sk}$ ) coefficients from a spin function expanded in the *Rumer*, *Kotani* or *Serber* spin basis. *Rumer\_VB* should be used in case the Rumer spin functions have the phases defined in Mario Raimondi’s VB program. Should be followed by  $f_S^N$  numbers, forming the input vector of spin-coupling coefficients. The input vector is renormalized and printed out, together with the spin-function designations. If it follows the *Rumer\_VB* conventions, the output vector is of the standard *Rumer* type (i.e. the signs of the spin-factors corresponding to the leading terms are positive in all spin functions). Then, if a permutation has already been defined (see the **permutation** directive), the input vector is transformed so as to correspond to the permuted spin basis.

**permutation**  $p_1$   $p_2$  ...  $p_N$

Defines the permutation

$$\begin{pmatrix} 1 & 2 & \dots & N \\ p_1 & p_2 & \dots & p_N \end{pmatrix}.$$

If an input vector has been defined, it is transformed to match an accordingly permuted spin basis. The permutation stays in effect till the next **electrons** or **permutation** directive, if any, i.e. each new input vector of spin-coupling coefficients will be transformed in a similar way.  $p_1, p_2, \dots, p_N$  should be unique integers.

**transform** *Rumer* | *Kotani* | *Serber*

Transforms the vector of spin-coupling coefficients defined previously by an **input** directive to the spin basis specified. Note that if the initial vector was in the *Rumer* spin basis, then **transform** *Kotani*, followed by **transform** *Serber* leads to the same final vector as **transform** *Serber* only.

**representation** *Rumer* | *Kotani* | *Serber*

Calculates the dual representation matrix of the permutation defined previously by a **permutation** directive in the *Rumer*, *Kotani* or *Serber* spin basis.

```
print Leading_Terms | Kotani_and_Serber_Paths | Rumer_Functions | Rumer_Overlaps |  
      Transformations | Everything | All
```

Modifies the detail of output. *Everything* and *All* are synonyms.

A line with a percentage sign (%) in the first position is considered as a comment line.

There are very few restrictions on the format of the command file. Keywords and numbers should be separated by any non-zero number of blanks. A blank is considered to be one of the characters space ( ), comma (,), semi-column (;), slash (/), as well as the end-of-line separator.