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Maple procedures for the coupling of angular momenta. III. Standard quantities for evaluating many-particle matrix elements

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Abstract

An extension to the RACAH program is presented for calculating standard quantities in the decomposition of many-electron matrix elements in atomic structure theory. These quantities include the coefficients of fractional parentage, the reduced coefficients of fractional parentage as well as reduced and completely reduced matrix elements for several operators within the two most frequently applied coupling schemes, namely *LS*- and *jj*-coupling, respectively. Values for these quantities are available for all (partially-filled) shells (nl) with $l \leqslant 3$ in *LS*-coupling and for all subshells with $j \leqslant 9/2$ in *jj*-coupling. Different notations and classification schemes are supported to characterize the antisymmetrized states of partially-filled shells.

PACS: 3.65F; 2.90+p

PROGRAM SUMMARY

Title of program: RACAH

Catalogue identifier: ADNM

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADNM

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland. Users may obtain the program also by down-loading the file `racah3.src.gz` from our home page at the University of Kassel (http://www.physik.uni-kassel.de/fritzsche/programs.html)

Licensing provisions: None

Computers for which the program is designed: All computers with a license of the computer algebra package MAPLE [1]

Installations: University of Kassel (Germany)

Operating systems under which the program has been tested: Linux, Windows

Program language used: Maple V, Releases 4 and 5

Memory required to execute with typical data: 2 MB

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PII: S0010-4655(00)00234-4

No. of bytes in distributed program, including test data, etc.: 153 140

Distribution format: gzip file

Keywords: Angular momentum, atomic many-body perturbation theory, complex atom, *jj*-coupling, *LS*-coupling, recoupling coefficient, reduced coefficient of fractional parentage, reduced matrix element, standard unit tensor, tensor operator

Nature of the physical problem
In atomic and nuclear structure theory, the evaluation and spin-angular integration of many-particle matrix elements is typically based on standard quantities like the matrix elements of the unit tensor, the (reduced) coefficients of fractional parentage as well as a number of other reduced matrix elements concerning various products of creation and annihilation operators. These quantities arise very frequently both in configuration interaction approaches and the derivation of perturbation expansions for many-particle systems using symmetry-adapted configuration state functions.

Method of solution
In the framework of the RACAH program [2], we provide a set of procedures for the manipulation and computation of such standard quantities in atomic theory. Different classifications of the antisymmetrized (sub-) shell states are supported for both, *LS*- and *jj*-coupling. The currently provided set of entities includes the coefficients of fractional parentage, the reduced coefficients of fractional parentage, and the reduced matrix elements of the operators $U^{(k)}$, $V^{(k1)}$ and $W^{(k_q k_l k_s)}$ in *LS*-coupling and of the operators $T^{(k)}$ and $W^{(k_q k_j)}$ in *jj*-coupling, respectively.

Restrictions onto the complexity of the problem
Coefficients and reduced matrix elements can be obtained for all shells with $l \leqslant 3$ in *LS*-coupling, i.e. including open f-shells, and for all subshells with $j \leqslant 9/2$ in *jj*-coupling (i.e. up to $f_{9/2}$ and $g_{9/2}$ subshells).

Unusual features of the program
The interactive use of the procedures within the RACAH program [2] allows a quick and reliable ‘electronic reference’ to these quantities for evaluating general matrix elements. The concept and functionality of MAPLE can easily be exploited to combine these coefficients in any other (useful) form than supported by the program in order to support the evaluation of complex expressions. The definitions and relations which are relevant for the computation of those quantities are displayed in Appendix A. For quick reference, Appendix B lists the additional or extended commands to the RACAH program.

Typical running time
The program replies promptly on all requests. Even lengthy tabulations of (reduced) coefficients and matrix elements can easily be carried out within a few (tens of) seconds.

References
[1] Maple is a registered trademark of Waterloo Maple Inc.
[2] S. Fritzsche, Comp. Phys. Commun. 103 (1997) 51;
S. Fritzsche, S. Varga, D. Geschke, B. Fricke, Comput. Phys. Commun. 111 (1998) 167 .

LONG WRITE-UP

1. Introduction

During recent years, the RACAH program [1] has been found useful for evaluating expressions from the theory of angular momentum. The interactive and modular design of this package does not only support numerical computations on standard expressions (as other libraries do) but also facilitate current research work which is based on the techniques of Racah’s algebra [2]. The RACAH program is particularly helpful for such (complex) expressions for which the known algebraic and graphical methods start to become tedious and prone to making errors. For details about the design and application of RACAH package, we refer the reader to our previous work [1] and to the web. [1]

Beside of further applications, atomic structure theory is one of the main areas which, traditionally, makes use of the rotational symmetry of free atoms. In this theory, the efficient evaluation of many-electron matrix elements for different one- and two-particle operators plays a very crucial role. These operators can be part of the atomic Hamiltonian or may describe the interaction of the electrons with other particles and fields. By exploiting the techniques of Racah’s algebra in atomic structure (see Ref. [3], for instance), the evaluation of these matrix elements may often be considerably simplified by carrying out the integration over the spin-angular coordinates analytically.

[1] http://www.physik.uni-kassel.de/fritzsche/programs.html.

Different computational schemes have been developed to evaluate many-electron matrix elements, including those for open-shell structures [4–7]. They deal with different couplings of the individual angular momenta as well as different notations for classifying the subshell states of equivalent electrons for open-shell configurations. One of the most popular scheme ist due to Fano [4] which is based on the coefficients of fractional parentage. Typically, each computational method exploits a set of *standard quantities* to decompose the many-electron matrix elements. Quantities which frequently occur are, for example, (i) the coefficients of fractional parentage (CFP), (ii) the reduced coefficients of fractional parentage (RCFP), and (iii) the reduced matrix elements of the unit tensors $U^{(k)}$ and $V^{(k1)}$ in *LS*-coupling or of $T^{(k)}$ in *jj*-coupling, respectively. Often also (iv) the completely reduced matrix elements of the single-particle operator $W^{(k_q k_l k_s)}$ (*LS*-coupling) or $W^{(k_q k_j)}$ (*jj*-coupling) occur in the decomposition. Of course, details in the final evaluation depend on the underlying coupling scheme, phase conventions, and on quite a number of different notations which are found in the literature. For all these quantities is common, however, that they are closely related to angular momentum theory.

Among the standard entities, the RCFPs play a central role in that most of the other quantities above can be represented in terms of these coefficients. The well-known CFPs, for example, can be expressed as a product of Wigner $3 - j$ symbols and corresponding RCFPs which are independent of the occupation number N of the subshell states. Similarly, the (completely) reduced matrix element of the unit tensor can be written as a weighted sum of products of Wigner $6 - j$ symbols and RCFPs where the summation is always finite owing to triangular conditions of the quantum numbers.

In practice, however, the handling and the application of such standard entities in the evaluation of open-shell matrix elements is not always that simple and often requires considerable effort to bring new implementations into work. Compilations of various coefficients and matrix elements can be found (in printed form) in the literature, but their arrangement and notation is often not so suitable for numerical studies. Therefore, in order to facilitate the usage of these (reduced) coefficients and matrix elements, here we describe an extension to the RACAH program [1] which provides the user with a fast and interactive access to these quantities. In the following section, we briefly recall the basic notations for different coupling schemes (as frequently applied in atomic structure). This also includes the classification of all subshell states to which the program can be applied. In Section 3, we outline how this extension is built into our previous work and how the program will be distributed. Finally, Section 4 shows several examples for using the program; this includes the generation of tabulations (or data files) which could immediately be exploited further in numerical investigations.

2. The quasispin concept

In describing the structure of many-particle systems, a significant simplification is typically achieved by using a symmetry-adapted basis for the construction of many particle states. Different classification and coupling schemes have been developed over the years to incorporate the insight into the ‘physical regime’ (concerning the interaction among the particles and with external fields) already in the construction of the basis. The two most popular coupling schemes in defining a symmetry-adapted basis are *LS*- and *jj*-coupling whereby the latter one, in particular, has been applied in the relativistic domain of atomic (as well as nuclear) structure theory. Apart from the well-established seniority scheme for the classification of (antisymmetrized) subshell states, the concept of quasispin [6] shows a number of advantages and has therefore been utilized in recent years.

Below, we briefly recall the most frequently applied classifications of (open) subshell states and their notation. A rather large number of independent subshell states arise in particular for open d and f shells ($l \geqslant 2$) in *LS*-coupling and for subshells (nj) with $j \geqslant 7/2$ in *jj*-coupling, respectively. We also display a compilation of all subshell states which ensure the ‘access’ to the present extension to the RACAH program.

2.1. LS-coupling

In quasispin notation, a subshell state of N equivalent electrons $|nl^N \alpha LS)$ is written as [6]

$$|nl^N \alpha QLS), \tag{1}$$

where Q is the quasispin momentum of the shell nl and α denotes all additional quantum numbers which are needed for an unique classification of these states. In practice, such a quantum number α need to be taken into account only for subshells with orbital angular momenta $l \geqslant 3$. Table 1 lists the classification of the s-, p-, d- and f-subshell states both in quasispin and seniority notation together with their group labels W and U [8].

The quasispin momentum Q of a given shell (nl) and its z-projection M_Q behave like an angular momentum in quasispin space (Q-space). When compared with the *seniority classification*, Q is simply related to the seniority quantum number ν by $Q = (2l + 1 - \nu)/2$ while $M_Q = (N - 2l - 1)/2$ depends on the subshell occupation number N. To facilitate the application of the program to open f-shell states, we also introduce the quantum number w instead of the formal group labels W and U in Table 1 which just provides an (arbitrary) ordering of otherwise degenerate subshell states.

2.2. jj-coupling

An alternative classification of the subshell states of open-shell systems exploits the quasispin concept in *jj*-coupling. In this representation, a subshell state of N equivalent electrons $|nj^N \alpha J)$ with total angular momentum J is written as

$$|nj^N \alpha QJ). \tag{2}$$

Again, the quasispin momentum $Q = (\frac{2j+1}{2} - \nu)/2$ is related to the seniority quantum number ν while its z-component $M_Q = (N - \frac{2j+1}{2})/2$ depends on the subshell occupation number N. For subshells with angular momenta $j = 1/2$, $3/2$, $5/2$, and $7/2$, a set of two quantum numbers, either Q and J *or* ν and J is sufficient to classify the subshell states for all allowed occupation numbers N unambiguously. An additional quantum number α only occurs for the subshell states with $j \geqslant 9/2$. For subshells with $j = 9/2$, we use a quantum number $w = 0, 1$, or 2 similar as for f-shells in *LS*-coupling. Table 2 lists the allowed subshell states for $j = 1/2, 3/2, 5/2, 7/2$, and $9/2$.

The classification of the subshell states plays a *key role* in using our present extension to the RACAH program. In Tables 1 and 2, we therefore provide a complete reference to this classification schemes; (reduced) coefficients and matrix elements can be computed for all of these states as discussed below. These tables also enable the user to make cross reference between different notations or to transfer the group labels W and U (for open f-shell states in *LS*-coupling) to the quantum number w as applied in our quasispin or seniority notation.

2.3. Completely reduced matrix elements

The concept of quasispin enables us to exploit the Wigner–Eckart theorem in Q-space for subshell states $|n\gamma^N \alpha Q\Gamma)$ in much the same way as for the total angular momenta J in *jj*-coupling ($\Gamma \equiv J$, $\gamma \equiv j$) or for L and S in *LS*-coupling ($\Gamma \equiv LS$, $\gamma \equiv ls$). Let $A_m^{(q\gamma)}$ denote any spherical tensor with rank q and projection m_q in the Q-space, then the corresponding matrix element between any pair of subshell states can be rewritten as

$$\begin{aligned}
&(\gamma^N \alpha Q \Gamma M_Q || A_{m_q}^{(q\gamma)} || \gamma^{N'} \alpha' Q' \Gamma' M'_Q) \\
&\quad = (-1)^{Q-M_Q} \begin{pmatrix} Q & q & Q' \\ -M_Q & m_q & M'_Q \end{pmatrix} (\gamma \alpha Q \Gamma ||| A^{(q\gamma)} ||| \gamma \alpha' Q' \Gamma').
\end{aligned} \tag{3}$$

Eq. (3) represents the relation between the (standard) reduced matrix element on the left-hand side and its *completely* reduced counterpart $(\gamma \alpha Q \Gamma ||| A^{(q\gamma)} ||| \gamma \alpha' Q' \Gamma')$ of the operator $A^{(q\gamma)}$. As seen from this notation,

Table 1
Classification of states $[l]^N$ of N *equivalent* electrons in shells with $l = 0, 1, 2, 3$. The (total) subshell orbital angular momentum L, spin momentum S, seniority quantum number ν, quasispin Q and the group labels W and U are shown. For open f-shell states, the last column lists the additional quantum number w as presently be used for a unique classification of the corresponding subshell states

subshell	^{2S+1}L	ν	Q	W	U	w
s^0 or s^2	^{1}S	0	1/2			
s^1	^{2}S	1	0			
p^0 or p^6	^{1}S	0	3/2			
p^1 or p^5	^{2}P	1	1			
p^2 or p^4	^{3}P	2	1/2			
	^{1}S	0	3/2			
	^{1}D	2	1/2			
p^3	^{4}S	3	0			
	^{2}P	1	1			
	^{2}D	3	0			
d^0 or d^{10}	^{1}S	0	5/2			
d^1 or d^9	^{2}D	1	2			
d^2 or d^8	^{3}P	2	3/2			
	^{3}F	2	3/2			
	^{1}S	0	5/2			
	^{1}D	2	3/2			
	^{1}G	2	3/2			
d^3 or d^7	^{4}P	3	1			
	^{4}F	3	1			
	^{2}P	3	1			
	^{2}D	1	2			
	^{2}D	3	1			
	^{2}F	3	1			
	^{2}G	3	1			
	^{2}H	3	1			
d^4 or d^6	^{5}D	4	1/2			
	^{3}P	2	3/2			
	^{3}P	4	1/2			
	^{3}D	4	1/2			
	^{3}F	2	3/2			
	^{3}F	4	1/2			
	^{3}G	4	1/2			
	^{3}H	4	1/2			
	^{1}S	0	5/2			
	^{1}S	4	1/2			
	^{1}D	2	3/2			
	^{1}D	4	1/2			
	^{1}F	4	1/2			
	^{1}G	2	3/2			
	^{1}G	4	1/2			
	^{1}I	4	1/2			
d^5	^{6}S	5	0			
	^{4}P	3	1			
	^{4}D	5	0			
	^{4}F	3	1			
	^{4}G	5	0			
	^{2}S	5	0			
	^{2}P	3	1			
	^{2}D	1	2			
	^{2}D	3	1			
	^{2}D	5	0			
	^{2}F	3	1			
	^{2}F	5	0			
	^{2}G	3	1			
	^{2}G	5	0			
	^{2}H	3	1			
	^{2}I	5	0			
subshell f^0 or f^{14}						
	^{1}S	0	7/2	(000)	(00)	1
subshell f^1 or f^{13}						
	^{2}F	1	3	(100)	(10)	1
subshell f^2 or f^{12}						
	^{3}P	2	5/2	(110)	(11)	1
	^{3}F	2	5/2	(110)	(10)	1
	^{3}H	2	5/2	(110)	(11)	1
	^{1}S	0	7/2	(000)	(00)	1
	^{1}D	2	5/2	(200)	(20)	1
	^{1}G	2	5/2	(200)	(20)	1
	^{1}I	2	5/2	(200)	(20)	1
subshell f^3 or f^{11}						
	^{4}S	3	2	(111)	(00)	1
	^{4}D	3	2	(111)	(20)	1
	^{4}F	3	2	(111)	(10)	1
	^{4}G	3	2	(111)	(20)	1
	^{4}I	3	2	(111)	(20)	1
	^{2}P	3	2	(210)	(11)	1
	^{2}D	3	2	(210)	(20)	1
	^{2}D	3	2	(210)	(21)	2
	^{2}F	1	3	(100)	(10)	1
	^{2}F	3	2	(210)	(21)	2
	^{2}G	3	2	(210)	(20)	1
	^{2}G	3	2	(210)	(21)	2
	^{2}H	3	2	(210)	(11)	1
	^{2}H	3	2	(210)	(21)	2
	^{2}I	3	2	(210)	(20)	1
	^{2}K	3	2	(210)	(21)	1
	^{2}L	3	2	(210)	(21)	1
subshell f^4 or f^{10}						
	^{5}S	4	3/2	(111)	(00)	0
	^{5}D	4	3/2	(111)	(20)	1
	^{5}F	4	3/2	(111)	(10)	1
	^{5}G	4	3/2	(111)	(20)	1
	^{5}I	4	3/2	(111)	(20)	1
	^{3}P	2	5/2	(110)	(11)	1
	^{3}P	4	3/2	(211)	(11)	2
	^{3}P	4	3/2	(211)	(30)	3
	^{3}D	4	3/2	(211)	(20)	1
	^{3}D	4	3/2	(211)	(21)	2
	^{3}F	2	5/2	(110)	(10)	1
	^{3}F	4	3/2	(211)	(10)	2
	^{3}F	4	3/2	(211)	(21)	3
	^{3}F	4	3/2	(211)	(30)	4
	^{3}G	4	3/2	(211)	(20)	1
	^{3}G	4	3/2	(211)	(21)	2
	^{3}G	4	3/2	(211)	(30)	3
	^{3}H	2	5/2	(110)	(11)	1
	^{3}H	4	3/2	(211)	(11)	2
	^{3}H	4	3/2	(211)	(21)	3
	^{3}H	4	3/2	(211)	(30)	4
	^{3}I	4	3/2	(211)	(20)	1
	^{3}I	4	3/2	(211)	(30)	2
	^{3}K	4	3/2	(211)	(21)	1
	^{3}K	4	3/2	(211)	(30)	2
	^{3}L	4	3/2	(211)	(21)	1
	^{3}M	4	3/2	(211)	(30)	1
	^{1}S	0	7/2	(000)	(00)	1
	^{1}S	4	3/2	(220)	(22)	2
	^{1}D	2	5/2	(200)	(20)	1
	^{1}D	4	3/2	(220)	(20)	2
	^{1}D	4	3/2	(220)	(21)	3
	^{1}D	4	3/2	(220)	(22)	4
	^{1}F	4	3/2	(220)	(21)	1
	^{1}G	2	5/2	(200)	(20)	1
	^{1}G	4	3/2	(220)	(20)	2
	^{1}G	4	3/2	(220)	(21)	3
	^{1}G	4	3/2	(220)	(22)	4
	^{1}H	4	3/2	(220)	(21)	1
	^{1}H	4	3/2	(220)	(22)	2
	^{1}I	2	5/2	(200)	(20)	1
	^{1}I	4	3/2	(220)	(20)	2
	^{1}I	4	3/2	(220)	(22)	3
	^{1}K	4	3/2	(220)	(21)	1
	^{1}L	4	3/2	(220)	(21)	1
	^{1}L	4	3/2	(220)	(22)	2
	^{1}N	4	3/2	(220)	(22)	1
subshell f^5 or f^9						
	^{6}P	5	1	(110)	(11)	0
	^{6}F	5	1	(110)	(10)	0
	^{6}H	5	1	(110)	(11)	0
	^{4}S	3	2	(111)	(00)	1
	^{4}P	5	1	(211)	(11)	1
	^{4}P	5	1	(211)	(30)	2
	^{4}D	3	2	(111)	(20)	1
	^{4}D	5	1	(211)	(20)	2
	^{4}D	5	1	(211)	(21)	3
	^{4}F	3	2	(111)	(10)	1
	^{4}F	5	1	(211)	(10)	2
	^{4}F	5	1	(211)	(21)	3
	^{4}F	5	1	(211)	(30)	4
	^{4}G	3	2	(111)	(20)	1

Table 1
(Continued.)

${}^{2S+1}L$	v	Q	W	U	w	${}^{2S+1}L$	v	Q	W	U	w	${}^{2S+1}L$	v	Q	W	U	w
${}^4G$	5	1	(211)	(20)	2	${}^2K$	5	1	(221)	(31)	4	${}^3G$	6	1/2	(221)	(20)	4
${}^4G$	5	1	(211)	(21)	3	${}^2K$	5	1	(221)	(31)	5	${}^3G$	6	1/2	(221)	(21)	5
${}^4G$	5	1	(211)	(30)	4	${}^2L$	3	2	(210)	(21)	1	${}^3G$	6	1/2	(221)	(30)	6
${}^4H$	5	1	(211)	(11)	1	${}^2L$	5	1	(221)	(21)	2	${}^3G$	6	1/2	(221)	(31)	7
${}^4H$	5	1	(211)	(21)	2	${}^2L$	5	1	(221)	(31)	3	${}^3H$	2	5/2	(110)	(11)	1
${}^4H$	5	1	(211)	(30)	3	${}^2M$	5	1	(221)	(30)	1	${}^3H$	4	3/2	(211)	(11)	2
${}^4I$	3	2	(111)	(20)	1	${}^2M$	5	1	(221)	(31)	2	${}^3H$	4	3/2	(211)	(21)	3
${}^4I$	5	1	(211)	(20)	2	${}^2N$	5	1	(221)	(31)	1	${}^3H$	4	3/2	(211)	(30)	4
${}^4I$	5	1	(211)	(30)	3	${}^2O$	5	1	(221)	(31)	0	${}^3H$	6	1/2	(221)	(11)	5
${}^4K$	5	1	(211)	(21)	1	subshell f^6 or f^8						${}^3H$	6	1/2	(221)	(21)	6
${}^4K$	5	1	(211)	(30)	2	${}^7F$	6	1/2	(100)	(10)	0	${}^3H$	6	1/2	(221)	(30)	7
${}^4L$	5	1	(211)	(21)	1	${}^5S$	4	3/2	(111)	(00)	0	${}^3H$	6	1/2	(221)	(31)	8
${}^4M$	5	1	(211)	(30)	0	${}^5P$	6	1/2	(210)	(11)	0	${}^3H$	6	1/2	(221)	(31)	9
${}^2P$	3	2	(210)	(11)	1	${}^5D$	4	3/2	(111)	(20)	1	${}^3I$	4	3/2	(211)	(20)	1
${}^2P$	5	1	(221)	(11)	2	${}^5D$	6	1/2	(210)	(20)	2	${}^3I$	4	3/2	(211)	(30)	2
${}^2P$	5	1	(221)	(30)	3	${}^5D$	6	1/2	(210)	(21)	3	${}^3I$	6	1/2	(221)	(20)	3
${}^2P$	5	1	(221)	(31)	4	${}^5F$	4	3/2	(111)	(10)	1	${}^3I$	6	1/2	(221)	(30)	4
${}^2D$	3	2	(210)	(20)	1	${}^5F$	6	1/2	(210)	(21)	2	${}^3I$	6	1/2	(221)	(31)	5
${}^2D$	3	2	(210)	(21)	2	${}^5G$	4	3/2	(111)	(20)	1	${}^3I$	6	1/2	(221)	(31)	6
${}^2D$	5	1	(221)	(20)	3	${}^5G$	6	1/2	(210)	(20)	2	${}^3K$	4	3/2	(211)	(21)	1
${}^2D$	5	1	(221)	(21)	4	${}^5G$	6	1/2	(210)	(21)	3	${}^3K$	4	3/2	(211)	(30)	2
${}^2D$	5	1	(221)	(31)	5	${}^5H$	6	1/2	(210)	(11)	1	${}^3K$	6	1/2	(221)	(21)	3
${}^2F$	1	3	(100)	(10)	1	${}^5H$	6	1/2	(210)	(21)	2	${}^3K$	6	1/2	(221)	(30)	4
${}^2F$	3	2	(210)	(21)	2	${}^5I$	4	3/2	(111)	(20)	1	${}^3K$	6	1/2	(221)	(31)	5
${}^2F$	5	1	(221)	(10)	3	${}^5I$	6	1/2	(210)	(20)	2	${}^3K$	6	1/2	(221)	(31)	6
${}^2F$	5	1	(221)	(21)	4	${}^5K$	6	1/2	(210)	(21)	0	${}^3L$	4	3/2	(211)	(21)	1
${}^2F$	5	1	(221)	(30)	5	${}^5L$	6	1/2	(210)	(21)	0	${}^3L$	6	1/2	(221)	(21)	2
${}^2F$	5	1	(221)	(31)	6	${}^3P$	2	5/2	(110)	(11)	1	${}^3L$	6	1/2	(221)	(31)	3
${}^2F$	5	1	(221)	(31)	7	${}^3P$	4	3/2	(211)	(11)	2	${}^3M$	4	3/2	(211)	(30)	1
${}^2G$	3	2	(210)	(20)	1	${}^3P$	4	3/2	(211)	(30)	3	${}^3M$	6	1/2	(221)	(30)	2
${}^2G$	3	2	(210)	(21)	2	${}^3P$	6	1/2	(221)	(11)	4	${}^3M$	6	1/2	(221)	(31)	3
${}^2G$	5	1	(221)	(20)	3	${}^3P$	6	1/2	(221)	(30)	5	${}^3N$	6	1/2	(221)	(31)	0
${}^2G$	5	1	(221)	(21)	4	${}^3P$	6	1/2	(221)	(31)	6	${}^3O$	6	1/2	(221)	(31)	0
${}^2G$	5	1	(221)	(30)	5	${}^3D$	4	3/2	(211)	(20)	1	${}^1S$	0	7/2	(000)	(00)	1
${}^2G$	5	1	(221)	(31)	6	${}^3D$	4	3/2	(211)	(21)	2	${}^1S$	4	3/2	(220)	(22)	2
${}^2H$	3	2	(210)	(11)	1	${}^3D$	6	1/2	(221)	(20)	3	${}^1S$	6	1/2	(222)	(00)	3
${}^2H$	3	2	(210)	(21)	2	${}^3D$	6	1/2	(221)	(21)	4	${}^1S$	6	1/2	(222)	(40)	4
${}^2H$	5	1	(221)	(11)	3	${}^3D$	6	1/2	(221)	(31)	5	${}^1P$	6	1/2	(222)	(30)	0
${}^2H$	5	1	(221)	(21)	4	${}^3F$	2	5/2	(110)	(10)	1	${}^1D$	2	5/2	(200)	(20)	1
${}^2H$	5	1	(221)	(30)	5	${}^3F$	4	3/2	(211)	(10)	2	${}^1D$	4	3/2	(220)	(20)	2
${}^2H$	5	1	(221)	(31)	6	${}^3F$	4	3/2	(211)	(21)	3	${}^1D$	4	3/2	(220)	(21)	3
${}^2H$	5	1	(221)	(31)	7	${}^3F$	4	3/2	(211)	(30)	4	${}^1D$	4	3/2	(220)	(22)	4
${}^2I$	3	2	(210)	(20)	1	${}^3F$	6	1/2	(221)	(10)	5	${}^1D$	6	1/2	(222)	(20)	5
${}^2I$	5	1	(221)	(20)	2	${}^3F$	6	1/2	(221)	(21)	6	${}^1D$	6	1/2	(222)	(40)	6
${}^2I$	5	1	(221)	(30)	3	${}^3F$	6	1/2	(221)	(30)	7	${}^1F$	4	3/2	(220)	(21)	1
${}^2I$	5	1	(211)	(31)	4	${}^3F$	6	1/2	(221)	(31)	8	${}^1F$	6	1/2	(222)	(10)	2
${}^2I$	5	1	(221)	(31)	5	${}^3F$	6	1/2	(221)	(31)	9	${}^1F$	6	1/2	(222)	(30)	3
${}^2K$	3	2	(210)	(21)	1	${}^3G$	4	3/2	(211)	(20)	1	${}^1F$	6	1/2	(222)	(40)	4
${}^2K$	5	1	(221)	(21)	2	${}^3G$	4	3/2	(211)	(21)	2	${}^1G$	2	5/2	(200)	(20)	1
${}^2K$	5	1	(221)	(30)	3	${}^3G$	4	3/2	(211)	(30)	3	${}^1G$	4	3/2	(220)	(20)	2

Table 1
(Continued.)

^{2S+1}L	v	Q	W	U	w	^{2S+1}L	v	Q	W	U	w	^{2S+1}L	v	Q	W	U	w
^1G	4	3/2	(220)	(21)	3	^4F	5	1	(211)	(30)	4	^2F	7	0	(222)	(40)	10
^1G	4	3/2	(220)	(22)	4	^4F	7	0	(220)	(21)	5	^2G	3	2	(210)	(20)	1
^1G	6	1/2	(222)	(20)	5	^4G	3	2	(111)	(20)	1	^2G	3	2	(210)	(21)	2
^1G	6	1/2	(222)	(30)	6	^4G	5	1	(211)	(20)	2	^2G	5	1	(221)	(20)	3
^1G	6	1/2	(222)	(40)	7	^4G	5	1	(211)	(21)	3	^2G	5	1	(221)	(21)	4
^1G	6	1/2	(222)	(40)	8	^4G	5	1	(211)	(30)	4	^2G	5	1	(221)	(30)	5
^1H	4	3/2	(220)	(21)	1	^4G	7	0	(220)	(20)	5	^2G	5	1	(221)	(31)	6
^1H	4	3/2	(220)	(22)	2	^4G	7	0	(220)	(21)	6	^2G	7	0	(222)	(20)	7
^1H	6	1/2	(222)	(30)	3	^4G	7	0	(220)	(22)	7	^2G	7	0	(222)	(30)	8
^1H	6	1/2	(222)	(40)	4	^4H	5	1	(211)	(11)	1	^2G	7	0	(222)	(40)	9
^1I	2	5/2	(200)	(20)	1	^4H	5	1	(221)	(21)	2	^2G	7	0	(222)	(40)	10
^1I	4	3/2	(220)	(20)	2	^4H	5	1	(221)	(30)	3	^2H	3	2	(210)	(11)	1
^1I	4	3/2	(220)	(22)	3	^4H	7	0	(220)	(21)	4	^2H	3	2	(210)	(21)	2
^1I	6	1/2	(222)	(20)	4	^4H	7	0	(220)	(22)	5	^2H	5	1	(221)	(11)	3
^1I	6	1/2	(222)	(30)	5	^4I	3	2	(111)	(20)	1	^2H	5	1	(221)	(21)	4
^1I	6	1/2	(222)	(40)	6	^4I	5	1	(211)	(20)	2	^2H	5	1	(211)	(30)	5
^1I	6	1/2	(222)	(40)	7	^4I	5	1	(211)	(30)	3	^2H	5	1	(221)	(31)	6
^1K	4	3/2	(220)	(21)	1	^4I	7	0	(220)	(20)	4	^2H	5	1	(221)	(31)	7
^1K	6	1/2	(222)	(30)	2	^4I	7	0	(220)	(22)	5	^2H	7	0	(222)	(30)	8
^1K	6	1/2	(222)	(40)	3	^4K	5	1	(211)	(21)	1	^2H	7	0	(222)	(40)	9
^1L	4	3/2	(220)	(21)	1	^4K	5	1	(211)	(30)	2	^2I	3	2	(210)	(20)	1
^1L	4	3/2	(220)	(22)	2	^4K	7	0	(220)	(21)	3	^2I	5	1	(221)	(20)	2
^1L	6	1/2	(222)	(40)	3	^4L	5	1	(211)	(21)	1	^2I	5	1	(221)	(30)	3
^1L	6	1/2	(222)	(40)	4	^4L	7	0	(220)	(21)	2	^2I	5	1	(221)	(31)	4
^1M	6	1/2	(222)	(30)	1	^4L	7	0	(220)	(22)	3	^2I	5	1	(221)	(31)	5
^1M	6	1/2	(222)	(40)	2	^4M	5	1	(211)	(30)	0	^2I	7	0	(222)	(20)	6
^1N	4	3/2	(220)	(22)	1	^4N	7	0	(220)	(22)	0	^2I	7	0	(222)	(30)	7
^1N	6	1/2	(222)	(40)	2	^2S	7	0	(222)	(00)	1	^2I	7	0	(222)	(40)	8
^1Q	6	1/2	(222)	(40)	0	^2S	7	0	(222)	(40)	2	^2I	7	0	(222)	(40)	9
subshell f^7						^2P	3	2	(210)	(11)	1	^2K	3	2	(210)	(21)	1
^8S	7	0	(000)	(00)	0	^2P	5	1	(221)	(11)	2	^2K	5	1	(221)	(21)	2
^6P	5	1	(110)	(11)	0	^2P	5	1	(221)	(30)	3	^2K	5	1	(221)	(30)	3
^6D	7	0	(200)	(20)	0	^2P	5	1	(221)	(31)	4	^2K	5	1	(221)	(31)	4
^6F	5	1	(110)	(10)	0	^2P	7	0	(222)	(30)	5	^2K	5	1	(221)	(31)	5
^6G	7	0	(200)	(20)	0	^2D	3	2	(210)	(20)	1	^2K	7	0	(222)	(30)	6
^6H	5	1	(110)	(11)	0	^2D	3	2	(210)	(21)	2	^2K	7	0	(222)	(40)	7
^6I	7	0	(200)	(20)	0	^2D	5	1	(221)	(20)	3	^2L	3	2	(210)	(21)	1
^4S	3	2	(111)	(00)	1	^2D	5	1	(221)	(21)	4	^2L	5	1	(221)	(21)	2
^4S	7	0	(220)	(22)	2	^2D	5	1	(221)	(31)	5	^2L	5	1	(221)	(31)	3
^4P	5	1	(211)	(11)	1	^2D	7	0	(222)	(20)	6	^2L	7	0	(222)	(40)	4
^4P	5	1	(211)	(30)	2	^2D	7	0	(222)	(40)	7	^2L	7	0	(222)	(40)	5
^4D	3	2	(111)	(20)	1	^2F	1	3	(100)	(10)	1	^2M	5	1	(221)	(30)	1
^4D	5	1	(211)	(20)	2	^2F	3	2	(210)	(21)	2	^2M	5	1	(221)	(31)	2
^4D	5	1	(211)	(21)	3	^2F	5	1	(221)	(10)	3	^2M	7	0	(222)	(30)	3
^4D	7	0	(220)	(20)	4	^2F	5	1	(221)	(21)	4	^2M	7	0	(222)	(40)	4
^4D	7	0	(220)	(21)	5	^2F	5	1	(221)	(30)	5	^2N	5	1	(221)	(31)	1
^4D	7	0	(220)	(22)	6	^2F	5	1	(221)	(31)	6	^2N	7	0	(222)	(40)	2
^4F	3	2	(111)	(10)	1	^2F	5	1	(221)	(31)	7	^2O	5	1	(221)	(31)	0
^4F	5	1	(211)	(10)	2	^2F	7	0	(222)	(10)	8	^2Q	7	0	(222)	(40)	0
^4F	5	1	(221)	(21)	3	^2F	7	0	(222)	(30)	9						

Table 2
Classification of subshell states $[j]^N$ of N *equivalent* electrons with $j = 1/2,\ 3/2, 5/2, 7/2,$ and $9/2$. The seniority quantum number ν, the subshell angular momentum J, the subshell quasispin Q and the additional quantum number w (for subshells with $j = 9/2$ only) are displayed

subshell	ν	J	Q	w
$[1/2]^0$ or $[1/2]^2$	0	0	1/2	
$[1/2]^1$	1	1/2	0	
$[3/2]^0$ or $[3/2]^4$	0	0	1	
$[3/2]^1$ or $[3/2]^3$	1	3/2	1/2	
$[3/2]^2$	0	0	1	
	2	2	0	
$[5/2]^0$ or $[5/2]^6$	0	0	3/2	
$[5/2]^1$ or $[5/2]^5$	1	5/2	1	
$[5/2]^2$ or $[5/2]^4$	0	0	3/2	
	2	2	1/2	
	2	4	1/2	
$[5/2]^3$	1	5/2	1	
	3	3/2	0	
	3	9/2	0	
$[7/2]^0$ or $[7/2]^8$	0	0	2	
$[7/2]^1$ or $[7/2]^7$	1	7/2	3/2	
$[7/2]^2$ or $[7/2]^6$	0	0	2	
	2	2	1	
	2	4	1	
	2	6	1	
$[7/2]^3$ or $[7/2]^5$	1	7/2	3/2	
	3	3/2	1/2	
	3	5/2	1/2	
	3	9/2	1/2	
	3	11/2	1/2	
	3	15/2	1/2	
$[7/2]^4$	0	0	2	
	2	2	1	
	2	4	1	
	2	6	1	
	4	2	0	
	4	4	0	
	4	5	0	
	4	8	0	
$[9/2]^0$ or $[9/2]^{10}$	0	0	5/2	0
$[9/2]^1$ or $[9/2]^9$	1	9/2	2	0
$[9/2]^2$ or $[9/2]^8$	0	0	5/2	0
	2	2	3/2	0
	2	4	3/2	0
	2	6	3/2	0
	2	8	3/2	0
$[9/2]^3$ or $[9/2]^7$	1	9/2	2	0
	3	3/2	1	0
	3	5/2	1	0
	3	7/2	1	0
	3	9/2	1	0
	3	11/2	1	0
	3	13/2	1	0
	3	15/2	1	0
	3	17/2	1	0
	3	21/2	1	0
$[9/2]^4$ or $[9/2]^6$	0	0	5/2	0
	2	2	3/2	0
	2	4	3/2	0
	2	6	3/2	0
	2	8	3/2	0
	4	0	1/2	0
	4	2	1/2	0
	4	3	1/2	0
	4	4	1/2	1
	4	4	1/2	2
	4	5	1/2	0
	4	6	1/2	1
	4	6	1/2	2
	4	7	1/2	0
	4	8	1/2	0
	4	9	1/2	0
	4	10	1/2	0
	4	12	1/2	0
$[9/2]^5$	1	9/2	2	0
	3	3/2	1	0
	3	5/2	1	0
	3	7/2	1	0
	3	9/2	1	0
	3	11/2	1	0
	3	13/2	1	0
	3	15/2	1	0
	3	17/2	1	0
	3	21/2	1	0
	5	1/2	0	0
	5	5/2	0	0
	5	7/2	0	0
	5	9/2	0	0
	5	11/2	0	0
	5	13/2	0	0
	5	15/2	0	0
	5	17/2	0	0
	5	19/2	0	0
	5	25/2	0	0

the completely reduced matrix element is independent of the occupation number N of the corresponding subshell state; the dependence on N is contained in M_Q and occurs on the right-hand side as projection of the quasispin only within the Wigner $3-j$ symbol $\begin{pmatrix} Q & q & Q' \\ -M_Q & m_q & M'_Q \end{pmatrix}$. Thus, by applying the quasispin method to the calculation of matrix elements of tensor operators between different subshell states, it is often more efficient to exploit the completely reduced matrix elements instead of the reduced ones. For these quantities, the size of the tabulations are typically much smaller if compared with those of the standard coefficients and reduced matrix elements [9,10].

In the formalism of second quantization, it is possible to express the CFP by the completely reduced matrix elements of the electron creation and annihilation operators [cf. Eqs. (9) and (13) in Appendix A]. These completely reduced matrix elements of the operator $a^{(q\gamma)}$ in second quantization are often called the reduced coefficients of fractional parentage (RCFP). The reduced matrix elements of the double tensor $W^{(k_q k_j)}$ in *jj*-coupling or of the triple tensor $W^{(k_q k_l k_s)}$ in *LS*-coupling can also be represented as a weighted sum of Wigner $6-j$ symbols and the RCFPs, including a summation over all the intermediate terms of the corresponding shells. Moreover, the RCFPs are closely related to the submatrix elements of the unit tensors $T^{(k)}$ or $U^{(k)}$ and $V^{(k1)}$, respectively. The given reduced coefficients and matrix elements are therefore useful also for the traditional approaches which are based on the CFPs and the submatrix elements of the unit tensors $U^{(k)}$ and $V^{(k1)}$.

3. Additional procedures to the RACAH package

The RACAH package [1] has been designed originally for simplifying expressions from the theory of angular momentum. Emphasize was paid for developing an interactive and user-friendly tool which neither requires a detailed knowledge about the group-theoretical background which leads to these expressions nor about techniques for their simplification. Our previous set of RACAH procedures concerned both, numerical computations as well as the simplification of complex expressions due to the use of graphical and sum rules where a *simplification* means to reduce the number of summation variables, integrals, and/or Wigner $n-j$ symbols. In the future, moreover, we will consider also the properties of the spherical harmonics and of further entities from the angular momentum theory. In this work, we extent the features of the RACAH program by *adding* the knowledge about a number of important standard quantities in the evaluation of matrix elements.

Table 3
Additional commands to the RACAH package. A detailed description of these procedures are listed in Appendix B below. See Section 3 and in-line commands for further information about the internal representation of the RCFP and the individual subshell states for open shells

Racah_cfp()	Calculates a CFP in *LS*- or *jj*-coupling.
Racah_rcfp()	Returns a RCFP in *LS*- or *jj*-coupling.
Racah_reduced_T()	Calculates a reduced matrix element of the operator $T^{(k)}$ in *jj*-coupling.
Racah_reduced_U()	Calculates a reduced matrix element of the operator $U^{(k)}$ in *LS*-coupling.
Racah_reduced_V()	Calculates a reduced matrix element of the operator $V^{(k1)}$ in *LS*-coupling.
Racah_reduced_W()	Calculates a completely reduced matrix element of either the operator $W^{(k_q k_l k_s)}$ in *LS*-coupling or $W^{(k_q k_j)}$ in *jj*-coupling.
Racah_set_coupling_scheme()	*Defines* the current classification and coupling scheme for the evaluation of the standard quantities in this program.

As discussed above, the reduced coefficients and matrix elements of spherical tensor operators are closely related to the theory of angular momentum. This stimulated the present extension which creates a fast access to these quantities in different classification and coupling schemes. We currently support the computation of the RCFP and the completely reduced matrix elements of $W^{(k_q k_j)}$ and $W^{(k_q k_l k_s)}$ as well as of the CFP and the reduced matrix elements of $T^{(k)}$, $U^{(k)}$ and $V^{(k1)}$. Table 3 shows a brief overview of the additional procedures which are relevant to the user; these procedures are based on our previous developments [1]. In total, 18 new procedures have been added to the RACAH program in the present work. Since all coefficients are evaluated directly to their numerical (algebraic and floating-point) values, no additional data structures had to be defined for the present work.

One procedure, namely Racah_set_coupling_scheme(), differs from our previous rules [1] in that it 'assigns' a (string) value to the global variable `Racah_save_coupling_scheme` which specifies the currently defined coupling scheme and the choice of quantum numbers to classify the individual subshell states. The 'value' of this variable also specifies how the quantum numbers for the reduced coefficients and matrix elements are to be *interpreted* to ensure a large flexibility of the program. The command Racah_set_coupling_scheme() must therefore be invoked before any other quantity can be evaluated. In the present version, we support the classification schemes *LS_quasispin*, *LS_seniority*, *jj_quasispin*, and *jj_seniority*; the current selection can be overwritten interactively at any time by a call to this procedure.

The RACAH program will be distributed as the source file `racah3` which contains both, the full source of the program as well as the RCFPs and the subshell terms from Tables 1 and 2 in a compact format. The two commands Racah_set_rcfp_jj() and Racah_set_rcfp_LS() are available to return individual RCFPs, which form the basic elements of the present extension, in *jj*- and *LS*-coupling, respectively. These coefficients are stored internally in MAPLE lists using the format

```
[Q_1, J_1, Q_2, J_2, weight, nom, den]
```

for subshells with $j \leqslant 7/2$ and

```
[w_1, Q_1, J_1, w_2, Q_2, J_2, weight, nom, den]
```

for subshells with $j = 9/2$ in *jj*-coupling as well as

```
[Q_1, L_1, S_1, Q_2, L_2, S_2, weight, nom, den]
```

for all shells with $l \leqslant 2$ and

```
[w_1, Q_1, L_1, S_1, w_2, Q_2, L_2, S_2, weight, nom, den]
```

for f shells in *LS*-coupling, respectively. In this representation, the value of a RCFP is simply given by weight $\times \sqrt{\frac{\text{nom}}{\text{den}}}$. Similarly, the required subshell states are returned as (list of) lists from the procedures Racah_set_term_jj() and Racah_set_term_LS().

The source `racah3` presently contains approximately 140 procedures in alphabetic order. To utilize the code interactively, the whole program can be loaded by

```
> read racah3;
```

at the beginning of each MAPLE session. In a later version, we will slightly modify the form of the distribution since we intent to include also a number of help pages and worksheets within the framework of MAPLE.

4. Examples

To illustrate the use of the present extension, we first calculate two reduced matrix elements of the single-particle operator $W^{(k_q k_l k_s)}$. We also show, how a tabulation of all non-zero coefficients of fractional parentage in *jj*-coupling for subshells with $j = 9/2$ can easily be generated for later use in numerical applications.

Let us consider the computation of the completely reduced matrix element $(l\,Q_1 L_1 S_1|||W^{(k_q k_l k_s)}|||l\,Q_2 L_2 S_2)$. We evaluate this matrix element in *LS*-coupling using quasispin notation for the quantum numbers $k_q = 1, k_l = 2, k_s = 0, l = 1, Q_1 = 1, L_1 = 1, S_1 = 1/2, Q_2 = 0, L_2 = 2,$ and $S_2 = 1/2$. For this, we enter

```
> Racah_set_coupling_scheme(LS_quasispin);
> W := Racah_reduced_W(1,2,0,1,1,1,1/2,0,2,1/2);
```

W := 9.486832985.

Note that in order to obtain a different accuracy of this result, it would simply be enough to change the value of the MAPLE variable `Digits`.

Different representations of the final results are supported by the program. For instance, one may wish to use the seniority scheme, instead of quasispin notation, for classifying the subshell states of equivalent electrons and to obtain the results in a prime–number representation. This is achieved by

```
> Racah_set_coupling_scheme(LS_seniority);
> W := Racah_reduced_W(1,2,0,1,1,1,1/2,3,2,1/2,prime);
```

W := [1, 1, 2, 1].

In this representation, the value of the completely reduced matrix element is given due to the integer powers of (up to 11) prime numbers

$[a_0, a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8, a_9, a_{10}, a_{11}]$

which represent the (real) value

$$a_0 \left(\prod_{i=1}^{11} p_i^{a_i} \right)^{1/2}, \tag{4}$$

where $p_1 = 2,\ p_2 = 3,\ p_3 = 5,\ p_4 = 7,\ p_5 = 11,\ p_6 = 13,\ p_7 = 17,\ p_8 = 19,\ p_9 = 23,\ p_{10} = 29,\ p_{11} = 31$. In the MAPLE output, all *trailing* zeros are omitted and need not to be incorporated in the evaluation of expression (4). Thus, the result W := [1, 1, 2, 1] above is just equivalent to the value $3\sqrt{2 \times 5} \equiv 9.486832985$. The same (algebraic) result would be obtained by using the keyword *algebraic* instead of *prime*.

As second example, we 'prove' the relation (13) from Appendix A numerically. For this, we consider the left- and right-hand-side of Eq. (13) separately for the quantum numbers $j = 7/2$, $N = 4$, $nu = 2$, $J = 2$, $\nu' = 1$, and $J' = 7/2$. Again, we use seniority notation for the CFP $(j^N \alpha\nu J||j^{N-1}(\alpha'\nu' Q' J')j)$ on the left-hand side

```
> Racah_set_coupling_scheme(jj_seniority);
> left := Racah_cfp(7/2,4,2,2,1,7/2,algebraic);
```

left := $1/3\sqrt{3}$

To obtain the value from the right-hand side

$$\frac{(-1)^{N+Q-M_Q}}{\sqrt{N[J]}} \begin{pmatrix} Q & 1/2 & Q' \\ -M_Q & 1/2 & M'_Q \end{pmatrix} (j\ \alpha Q J|||a^{(qj)}|||j\ \alpha' Q' J') \tag{5}$$

we have, in addition, the quantum numbers $Q = ((2j+1)/2 - \nu)/2 = 1$, $M_Q = (N - (2j+1)/2)/2 = 0$, $Q' = 3/2$, and $M'_Q = -1/2$.

```
> right := Racah_rcfp(7/2,2,2,1,7/2,algebraic);
> w3jr := Racah_set(w3j,1,1/2,3/2,0,1/2,-1/2);
```

```
j := 9/2;   Racah_set_coupling_scheme(jj_quasispin);
for N from 1 to 5 do
   lprint("CFP for 9/2 subshell with occupation N = ",N);
   MQ1 := (N - 5) / 2;   MQ2 := (N - 6) / 2;
   if type(MQ1,integer)  then
      term1_jj := Racah_subshell_term_jj(j,Q_int);
      term2_jj := Racah_subshell_term_jj(j,Q_halfint);
   elif  not type(MQ1,integer)  then
      term1_jj := Racah_subshell_term_jj(j,Q_halfint);
      term2_jj := Racah_subshell_term_jj(j,Q_int);
   fi;
   #
   for  i  from 1 to nops(term1_jj) do
      for  m  from 1 to nops(term2_jj) do
         w1  := term1_jj[i][2];  Q1 := term1_jj[i][3];  J1 := term1_jj[i][4];
         w2  := term2_jj[m][2];  Q2 := term2_jj[m][3];  J2 := term2_jj[m][4];
         nu1 := (2*j+1) / 2 -2 * Q1;   nu2 := (2*j+1) / 2 - 2 * Q2;
         if not abs(MQ1) > Q1 and not abs(MQ2) > Q2 then
            result_p := Racah_cfp(9/2,N,w1,Q1,J1,w2,Q2,J2,prime);
            result   := Racah_cfp(9/2,N,w1,Q1,J1,w2,Q2,J2);
            if  result_p[1] <> 0  then
                  lprint(w1,nu1,J1,w2,nu2,J2,‘=‘,result,result_p);
            fi;
         fi;
      od;
   od;
od;
```

Fig. 1. MAPLE code for generating a compilation of all non-zero CFP in *jj*-coupling and quasispin notation for subshells with $j = 9/2$. See the text for explanation and the TEST RUN OUTPUT for the first lines of the results.

```
> right := right * Racah_compute(w3jr,algebraic);
> right := right * (-1)^(4+1+0) / sqrt(4*(2*2+1));
```

$$\text{right} := 1/30\sqrt{10 \times 6 \times 5}.$$

This test case can be seen as a simple example to establish (new) ‘relations’ among the standard quantities in the evaluation of matrix elements for open-shell configurations. Although, of course, such a numerical treatment will not *prove* any analytic relation it may help to obtain further hints on such symmetries. We therefore hope that our present tool will help to point towards *new* relations which have not yet been found by other, group-theoretical studies.

For several entities, as discussed above, extensive compilations have been published over the years and have been implemented in various ways in atomic structure programs. Even though some of these implementations are not very efficient, modification on these standard quantities and their internal use is often very tedious and error-prone. The present extension of the RACAH program now provides a much simpler way to generate just those ‘tables’ which are most appropriate for a given class of applications. To emphasize this *flexibility* in the representation of such quantities, our final example generates a tabulation of all non-zero CFP in *jj*-coupling and quasispin notation for subshells with $j = 9/2$. Fig. 1 shows the MAPLE code which has to be entered interactively; the first few lines of the corresponding output are displayed in the TEST RUN OUTPUT below.

We need not to explain much about this code in Fig. 1. Following the definition of the coupling scheme and the notation in the first line, we initiate a loop $N = 1, \ldots, 5$ to cycle, in turn, through all allowed occupation numbers up to a half-filled shell. In dependence of M_{Q_1} of the daughter states, we assign a list of all appropriate subshell terms in the definition of the CFP to the MAPLE list `term1_jj` and `term2_jj` for the bra- and ket-functions, respectively, These two list then also carry all required quantum numbers to set up the tabulation owing to a call to the procedure Racah_cfp(). The results are printed, along with the quantum numbers, both as floating-point numbers as well as in a prime-number representation. Only non-zero coefficients are printed to screen.

In conclusion, we provide a set of additional procedures to the RACAH program which facilitates the handling of standard entities for evaluating many-particle matrix elements. Special emphasize has been paid to support different notations and coupling schemes as frequently applied in atomic and nuclear structure theory. We hope our developments will encourage further work in finding more efficient computational schemes for open-shell atoms either by our groups or by others. All basic entities are now accessible in the framework of RACAH or can easily be adopted to the needs of the user within a few lines of code. In the past, similar attempts were hampered by a rather tedious access to these reduced coefficients and matrix elements *via* tabulations [8,11] which are often based on different conventions.

Apart from further developments in atomic structure theory, the present extension to the RACAH program may influence also the work in neighboring fields like nuclear structure and the scattering of particles and light at composite systems. In these fields, numerical studies are often based on similar entities which could be incorporated as well in the framework of the RACAH package.

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Appendix A: Definitions and basic relations

All quantities, which we consider in this work, can be defined in terms of the reduced coefficients of fractional parentage $(\gamma\alpha Q\Gamma|||a^{(q\gamma)}|||\gamma\alpha' Q'\Gamma')$ where we have $\gamma \equiv ls$ and $\Gamma \equiv LS$ in *LS*-coupling and $\gamma \equiv j$ and $\Gamma \equiv J$ in *jj*-coupling. Below, we provide the definition of the CFP and of the completely reduced matrix elements $W^{(k_q k_l k_s)}$ and $W^{(k_q k_j)}$. Owing to the presently supported coupling schemes of the individual angular momenta, this appendix is divided into two parts for *LS*- and *jj*-coupling, respectively.

The quasispin momentum Q and its z-component are defined as $Q = \frac{1}{2}(\frac{\Omega}{2} - \nu)$ and $M_Q = \frac{1}{2}(N - \frac{\Omega}{2})$, where N is the number of particles in the given shell and $\Omega \equiv [l, s]$ in *LS*-coupling or $\Omega \equiv [j]$ in *jj*-coupling. Here, the notation $[a, b, \ldots] \equiv (2a + 1)(2b + 1) \cdots$ is used throughout this appendix. In addition to the basic definitions, we also list several important relations which are fulfilled by the reduced and completely reduced matrix elements of the standard operators $T^{(k)}$, $U^{(k)}$, $V^{(k1)}$, and $W^{(k_q k_\gamma)}$, where $k_\gamma \equiv k_l k_s$ in *LS*-coupling and $k_\gamma \equiv k_j$ in *jj*-coupling.

Several phase conventions among the quantities can be found in the literature. Therefore, the user must pay attention to the phase and designation of these quantities if he needs to compare the results from the RACAH program with tabulated data. The CFP and RCFP are defined as in Refs. [9,10], exploiting the quasispin formalism. This definition simplifies the transformation among different coupling schemes, i.e. in going from *LS*- to *jj*-coupling or vice versa [12], particularly if subshell states with occupation numbers $N > j + 1/2$ are involved in the transformation.

Different definitions also appear for the reduced matrix elements of the unit operator $U^{(k)}$. Karazija et al. [11], for instance, tabulate the submatrix elements

$$\left(l^N \alpha SL||U^{(k)}||l^N \alpha' S' L'\right), \tag{6}$$

while Nielson and Koster [8] and Cowan [3] list

$$\left(l^N \alpha L||U^{(k)}||l^N \alpha' L'\right), \tag{7}$$

even though by using the same notation as in expression (6). The relation between these reduced matrix elements is given by

$$\left(l^N \alpha SL||U^{(k)}||l^N \alpha' S' L'\right) = \delta(S,S')\sqrt{(2S+1)}\left(l^N \alpha L||U^{(k)}||l^N \alpha' L'\right). \tag{8}$$

In RACAH, we follow the work of Karazija et al. [11] by exploiting the relation (11) to generate the reduced matrix elements of $U^{(k)}$ from those of the operator $W^{(k_1 k_2 k_3)}$.

For all further details on the quasispin concept and the definition of standard operators in atomic structure theory, we refer the reader to Rudzikas [6] and to Gaigalas et al. [9,10]. These references also summarize the properties of the corresponding coefficients and matrix elements both in *LS*- and *jj*-coupling, respectively.

A.1. LS-coupling

Coefficients of fractional parentage:

$$\begin{aligned}
&(l^N \alpha QLS||l^{N-1}(\alpha' Q' L' S')l) \\
&\quad = \frac{(-1)^{N+Q-M_Q}}{\sqrt{N[L,S]}} \begin{pmatrix} Q & 1/2 & Q' \\ -M_Q & 1/2 & M'_Q \end{pmatrix} (l\alpha QLS|||a^{(qls)}|||l\alpha' Q' L' S').
\end{aligned} \tag{9}$$

Completely reduced matrix elements of $W^{(k_q k_l k_s)}$:

$$\begin{aligned}
&(l\alpha QLS|||W^{(k_q k_l k_s)}|||l\alpha' Q' L' S') \\
&\quad = (-1)^{Q+L+S+Q'+L'+S'+k_q+k_l+k_s}\sqrt{[k_q,k_l,k_s]} \\
&\qquad \times \sum_{\alpha'' Q'' L'' S''} \begin{Bmatrix} q & q & k_q \\ Q' & Q & Q'' \end{Bmatrix} \begin{Bmatrix} l & l & k_l \\ L' & L & L'' \end{Bmatrix} \begin{Bmatrix} s & s & k_s \\ S' & S & S'' \end{Bmatrix} \\
&\qquad \times (l\alpha QLS|||a^{(qls)}|||l\alpha'' Q'' L'' S'')(l\alpha'' Q'' L'' S''|||a^{(qls)}|||l\alpha' Q' L' S').
\end{aligned} \tag{10}$$

Reduced matrix elements of $U^{(k)}$:

$$(l^N \alpha LS||U^{(k)}||l^N \alpha' L' S') = \begin{cases} \dfrac{(-1)^{Q-M_Q+1}}{\sqrt{[k]}} \begin{pmatrix} Q & 1 & Q' \\ -M_Q & 0 & M_Q \end{pmatrix} \\ \quad \times (l\alpha QLS|||W^{(1k0)}|||l\alpha' Q' L' S') & \text{if } k = \text{even}, \\ \dfrac{-1}{\sqrt{[Q,k]}}(l\alpha QLS|||W^{(0k0)}|||l\alpha' Q' L' S') & \text{if } k = \text{odd}. \end{cases} \tag{11}$$

Reduced matrix elements of $V^{(k1)}$:

$$(l^N \alpha LS||V^{(k1)}||l^N \alpha' L' S') = \begin{cases} \dfrac{-1}{2\sqrt{[Q,k]}}(l\alpha QLS|||W^{(0k0)}|||l\alpha' Q' L' S') & \text{if } k = \text{even}, \\ \dfrac{(-1)^{Q-M_Q+1}}{2\sqrt{[k]}} \begin{pmatrix} Q & 1 & Q' \\ -M_Q & 0 & M_Q \end{pmatrix} \\ \quad \times (l\alpha QLS|||W^{(1k0)}|||l\alpha' Q' L' S') & \text{if } k = \text{odd}. \end{cases} \tag{12}$$

A.2. jj-coupling

Coefficients of fractional parentage:

$$(j^N \alpha Q J || j^{N-1}(\alpha' Q' J') j) = \frac{(-1)^{N+Q-M_Q}}{\sqrt{N[J]}} \begin{pmatrix} Q & 1/2 & Q' \\ -M_Q & 1/2 & M'_Q \end{pmatrix} (j\alpha Q J ||| a^{(qj)} ||| j\alpha' Q' J'). \tag{13}$$

Completely reduced matrix elements of $W^{(k_q k_j)}$:

$$\begin{aligned}(j\alpha Q J ||| W^{(k_q k_j)} ||| j\alpha' Q' J') &= (-1)^{Q+J+Q'+J'+k_q+k_j} \sqrt{[k_q, k_j]} \sum_{\alpha'' Q'' J''} \begin{Bmatrix} q & q & k_q \\ Q' & Q & Q'' \end{Bmatrix} \begin{Bmatrix} j & j & k_j \\ J' & J & J'' \end{Bmatrix} \\ &\quad \times (j\alpha Q J ||| a^{(qj)} ||| j\alpha'' Q'' J'')(j\alpha'' Q'' J'' ||| a^{(qj)} ||| j\alpha' Q' J'). \end{aligned} \tag{14}$$

Reduced matrix elements of $T^{(k)}$:

$$(j^N \alpha J || T^{(k)} || j^N \alpha' J') = \begin{cases} \dfrac{(-1)^{Q-M_Q+1}}{2\sqrt{[k]}} \begin{pmatrix} Q & 1 & Q' \\ -M_Q & 0 & M_Q \end{pmatrix} \\ \quad \times (j\alpha Q J ||| W^{(1k)} ||| j\alpha' Q' J') & \text{if } k = \text{even}, \\ \dfrac{-1}{\sqrt{2[Q,k]}} (j\alpha Q J ||| W^{(0k)} ||| j\alpha' Q' J') & \text{if } k = \text{odd}. \end{cases} \tag{15}$$

Appendix B: Additional commands to the RACAH package

For a quick reference, here we briefly explain the new procedures to the RACAH package. We only present those procedures in detail which are important for interactive work. The description of these procedures follows the style of *The Maple Handbook* by Redfern [13]. All arguments must be given as integers or half–integers as appropriate for the coupling of angular momenta.

- **Racah_cfp**(j,N,Q_1,J_1,Q_2,J_2)

  Returns the coefficient of fractional parentage $(j^N Q_1 J_1 || j^{N-1}(Q_2 J_2) j)$ for subshells with angular momenta $j = 1/2$, $3/2$, $5/2$ and $7/2$ using the quasispin notation in *jj*-coupling.

  Output: A (floating-point) number is returned.

  Argument options: (j,N,Q_1,J_1,Q_2,J_2, {algebraic, ...}) to return the CFP in algebraic form for subshells with $j = 1/2$, $3/2$, $5/2$ and $7/2$. ♣ (j,N,Q_1,J_1,Q_2,J_2, {prime, ...}) to return the CFP in a prime-number representation. ♣ (j,N,ν_1,J_1,ν_2,J_2,{seniority, ...}) to return the CFP $(j^N \nu_1 J_1 || j^{N-1}(\nu_2 J_2) j)$ using the seniority notation if the coupling scheme *jj_seniority* has not been specified explicitly. ♣ (9/2,N,w_1,Q_1,J_1,w_2,Q_2,J_2, {...}) to return the value of the CFP $(j^N w_1 Q_1 J_1 || j^{N-1}(w_2 Q_2 J_2) j)$ for $j = 9/2$ and for the additionally specified quantum numbers $w_{1,2} = 0$, 1, or 2 [cf. Table 2]. ♣ (l,N,Q_1,L_1,S_1,Q_2,L_2,S_2, {...}) to return the CFP $(l^N Q_1 L_1 S_1 || l^{N-1}(Q_2 L_2 S_2) l)$ in *LS*-coupling for subshells with $l = 0$, 1 and 2 using the quasispin notation in *LS*-coupling. ♣ (l,N,ν_1,L_1,S_1,ν_2,L_2,S_2, {...}) to return the CFP $(l^N \nu_1 L_1 S_1 || l^{N-1}(\nu_2 L_2 S_2) l)$ using seniority notation in *LS*-coupling. ♣ (3,N,w_1,Q_1,L_1,S_1,w_2,Q_2,L_2, S_2,{...}) to return the value of the CFP

$(f^N w_1 Q_1 L_1 S_1 || f^{N-1}(w_2 Q_2 L_2 S_2) f)$ for subshell with orbital angular momentum $l = 3$ and for the additionally specified quantum numbers $w_{1,2} = 0, \ldots, 10$ using the quasispin notation in *LS*-coupling [cf. Table 1].

Additional information: The list and number of arguments depend on the definition of the underlying classification and coupling scheme which has to be defined before by calling the procedure `Racah_set_coupling_scheme()`. The current definition of the coupling scheme is kept in the global variable `Racah_save_coupling_scheme`. ♣ A set of keywords can be provided in any order as the last argument; the currently supported *keywords* are *algebraic*, *prime*, and *seniority* where *algebraic* and *prime* must be used exclusively. The keyword *seniority* 'overwrites' the currently defined classification scheme. ♣ The calculation of the CFPs is based on a list of RCFP which is stored internally. ♣ For details of the prime number representation see `Racah_calculate_prime()`.

See also: `Racah_set_coupling_scheme()`.

- **Racah_rcfp**(j,Q_1,J_1,Q_2,J_2)

Returns the reduced coefficient of fractional parentage $(j Q_1 J_1 ||| a^{(qj)} ||| j Q_2 J_2)$ for subshells with angular momenta $j = 1/2$, $3/2$, $5/2$ and $7/2$ in *jj*-coupling.

Output: A (floating-point) number is returned.

Argument options: (j,Q_1,J_1,Q_2,J_2, {algebraic}) to return the RCFP in algebraic form. ♣ (j,Q_1,J_1,Q_2,J_2, {prime}) to return the RCFP in a prime-number representation. ♣ (9/2,w_1,Q_1,J_1,w_2,Q_2,J_2,{...}) to return the RCFP $(j w_1 Q_1 J_1 ||| a^{(qj)} ||| j w_2 Q_2 J_2)$ for subshells with $j = 9/2$ and for the additionally specified quantum numbers $w_{1,2} = 0, \ldots, 2$. ♣ (l,Q_1,L_1,S_1,Q_2,L_2,S_2,{...}) to return the RCFP $(l Q_1 L_1 S_1 ||| a^{(qls)} ||| l Q_2 L_2 S_2)$ for shells with $l = 0, \ldots, 2$ in LS-coupling. ♣ (3,w_1,Q_1,L_1,S_1,w_2,Q_2,L_2,S_2, {...}) to return the RCFP $(f w_1 Q_1 L_1 S_1 ||| a^{(qls)} ||| f w_2 Q_2 L_2 S_2)$ for subshell with orbital angular momentum $l = 3$ and for the additionally specified quantum numbers $w_{1,2} = 0, \ldots, 10$.

Additional information: The list and number of arguments depend on the definition of the underlying coupling scheme which has to be defined before by calling the procedure `Racah_set_coupling_scheme()`. The current definition of the coupling scheme is kept in the global variable `Racah_save_coupling_scheme`. ♣ One of the keywords *algebraic* or *prime* can be provided as last argument given within a set structure.

See also: `Racah_set_coupling_scheme()`.

- **Racah_reduced_T**(k,j,M_Q,Q_1,J_1,Q_2,J_2)

Returns the reduced matrix element $(j Q_1 J_1 M_Q || T^{(k)} || j Q_2 J_2 M_Q)$ for subshells with angular momenta $j = 1/2$, $3/2$, $5/2$ and $7/2$ using the quasispin notation in *jj*-coupling.

Output: A (floating-point) number is returned.

Argument options: (k,j,M_Q,Q_1,J_1,Q_2,J_2, {algebraic, ...}) to return the reduced matrix element in algebraic form. ♣ (k,j,M_Q,Q_1,J_1,Q_2,J_2, {prime, ...}) to return the reduced matrix element in a prime-number representation. ♣ (k,j,N,ν_1,J_1,ν_2,J_2,{seniority, ...}) to return the reduced matrix element $(j^N \nu_1 J_1 || T^{(k)} || j^N \nu_2 J_2)$ using seniority notation if the coupling scheme *jj_seniority* has not been specified explicitly. ♣ (k,9/2,M_Q,w_1, Q_1,J_1,w_2,Q_2,J_2, {...}) to return the reduced matrix element $(j w_1 Q_1 J_1 M_Q || T^{(k)} || j w_2 Q_2 J_2 M_Q)$ for subshells with orbital angular momentum $j = 9/2$ and for the additionally specified quantum numbers $w_{1,2} = 0$, 1, or 2 using quasispin notation in *jj*-coupling.

Additional information: The reduced matrix elements of the operator $T^{(k)}$ are only defined in *jj*-coupling. ♣ The list and number of arguments depend on the definition of the underlying classification and coupling scheme which has to be defined before by calling the procedure `Racah_set_coupling_scheme()`. The current definition of the coupling scheme is kept in the global variable `Racah_save_coupling_scheme`. ♣ A set of keywords can be provided in any order as the last argument; the currently supported *keywords* are *algebraic*, *prime*, and *seniority* where *algebraic* and *prime* must be used exclusively. The keyword *seniority* 'overwrites' the currently defined classification scheme. ♣ The calculation of the CFP is based on a list of RCFP which is stored internally.

See also: `Racah_set_coupling_scheme()`.

- **Racah_reduced_U**(k,l,M_Q,Q_1,L_1,S_1,Q_2,L_2,S_2)

Returns the reduced matrix element $(l^N Q_1 L_1 S_1 M_Q || U^{(k)} || l^N Q_2 L_2 S_2 M_Q)$ of the unit tensor $U^{(k)}$ for subshells with orbital angular momenta $l = 0$, 1, and 2 using quasispin notation in *LS*-coupling.

Output: A (floating-point) number is returned.

Argument options: (k,l,M_Q,Q_1,L_1,S_1, Q_2,L_2,S_2,{algebraic, ...}) to return the reduced matrix element in algebraic form. ♣ (k,l,M_Q,Q_1,L_1,S_1,Q_2,L_2,S_2,{prime, ...}) to return the reduced matrix element in a prime-number representation. ♣ (k,l,N,ν_1,L_1,S_1,ν_2,L_2,S_2,{seniority, ...}) to return the reduced matrix element $(l^N \nu_1 L_1 S_1 || U^{(k)} || l^N \nu_2 L_2 S_2)$using seniority notation if the coupling scheme; *LS_seniority* has not been specified explicitly. ♣ (k,3,M_Q,w_1, Q_1,L_1,S_1,w_2,Q_2,L_2,S_2,{...}) to return the reduced matrix element $(f^N w_1 Q_1 L_1 S_1 M_Q || U^{(k)} || f^N w_2 Q_2 L_2 S_2 M_Q)$ for shells with orbital angular momentum $l = 3$ and for the additionally specified quantum numbers $w_{1,2} = 0, \ldots, 10$ using quasispin notation.

Additional information: The reduced matrix elements of the operator $U^{(k)}$ are only defined in *LS*-coupling. ♣ The list and number of arguments depend on the definition of the underlying classification and coupling scheme which has to be defined before by calling the procedure `Racah_set_coupling_scheme()`. The current definition of the coupling scheme is kept in the global variable `Racah_save_coupling_scheme`. ♣ A set of keywords can be provided in any order as the last argument; the currently supported *keyword* are *algebraic*, *prime*, and *seniority* where *algebraic* and *prime* must be used exclusively. ♣ The calculation of the CFP is based on a list of RCFP which is stored internally.

See also: `Racah_set_coupling_scheme()`.

- **Racah_reduced_V**(k,l,M_Q,Q_1,L_1,S_1,Q_2,L_2,S_2)

Returns the reduced matrix element $(l^N Q_1 L_1 S_1 M_Q || V^{(k1)} || l^N Q_2 L_2 S_2 M_Q)$ for subshells with orbital angular momenta $l = 0$, 1 and 2 using quasispin notation in *LS*-coupling.

Output: A (floating-point) number is returned.

Argument options: (k,l,M_Q,Q_1,L_1,S_1, Q_2,L_2,S_2,{algebraic, ...}) to return the reduced matrix element in algebraic form. ♣ (k,l,M_Q,Q_1,L_1,S_1,Q_2,L_2,S_2,{prime, ...}) to return the reduced matrix element in a prime-number representation. ♣ (k,l,N,ν_1,L_1,S_1,ν_2,L_2,S_2,{seniority, ...}) to return the reduced matrix element $(l^N \nu_1 L_1 S_1 || V^{(k1)} || l^N \nu_2 L_2 S_2)$ using seniority notation if the coupling scheme; *LS_seniority* has not been specified explicitly. ♣ (k,3,M_Q,w_1,Q_1,L_1,S_1,w_2,Q_2,L_2,S_2 ,{...}) to return the reduced matrix element $(f^N w_1 Q_1 L_1 S_1 M_Q || V^{(k1)} || f^N w_2 Q_2 L_2 S_2 M_Q)$ for subshell with orbital angular momentum $l = 3$ and for the additionally specified quantum numbers $w_{1,2} = 0, \ldots, 10$ using quasispin notation.

Additional information: The reduced matrix elements of the operator $V^{(k1)}$ are only defined in *LS*-coupling. ♣ The number and sequence of arguments depends on the definition of the coupling scheme which has to be defined before by calling the procedure line `Racah_set_coupling_scheme()`. This definition is kept in the global variable `Racah_save_coupling_scheme`. ♣ A set of different *keywords* can be provided as the last argument. The currently supported *keywords* are *algebraic*, *algebraic*, *prime*, and *seniority* where *algebraic* and *prime* must be used exclusively. ♣ The list and number of arguments depend on the definition of the underlying classification and coupling scheme which has to be defined before by calling the procedure `Racah_set_coupling_scheme()`.

See also: `Racah_set_coupling_scheme()`.

- **Racah_reduced_W**(k$_q$,k$_j$,j,Q$_1$,J$_1$,Q$_2$,J$_2$)

  Returns the reduced matrix element $(j\,Q_1 J_1|||W^{(k_q k_j)}|||j\,Q_2 J_2)$ for subshells with angular momenta $j = 1/2$, $3/2$, $5/2$ and $7/2$ using quasispin notation in *jj*-coupling.

  Output: A (floating-point) number is returned.

  Argument options: (k$_q$,k$_j$,j,Q$_1$,J$_1$,Q$_2$,J$_2$, {algebraic, ...}) to return the reduced matrix element in algebraic form. ♣ (k$_q$,k$_j$,j,Q$_1$,J$_1$,Q$_2$,J$_2$, prime, ...) to return this reduced matrix element in a prime-number representation. ♣ (k$_q$,k$_j$,9/2,w$_1$,Q$_1$,J$_1$,w$_2$,Q$_2$,J$_2$, {...}) to return the reduced matrix element $(j\ w_1 Q_1 J_1|||W^{(k_q k_j)}|||j\ w_2 Q_2 J_2)$ for subshells with $j = 9/2$ and for the additionally specified quantum numbers $w_{1,2} = 0$, 1, or 2 using quasispin notation in *jj*-coupling. ♣ (k$_q$,k$_l$,k$_s$,l,Q$_1$,L$_1$,S$_1$,Q$_2$,L$_2$,S$_2$, {...}) to return the reduced matrix element $(l\,Q_1 L_1 S_1|||W^{(k_q k_l k_s)}|||l\,Q_2 L_2 S_2)$ for subshells with $l = 0$, 1 and 2 using quasispin notation in *LS*-coupling. ♣ (k$_q$,k$_l$,k$_s$,3,w$_1$,Q$_1$,L$_1$,S$_1$,w$_2$,Q$_2$,L$_2$,S$_2$,{...}) to return the reduced matrix element $(f\ w_1 Q_1 L_1 S_1|||W^{(k_q k_l k_s)}|||f\ w_2 Q_2 L_2 S_2)$ for subshells with orbital angular momentum $l = 3$ and for the additionally specified quantum numbers $w_{1,2} = 0, \ldots, 10$ using quasispin notation in *LS*-coupling.

  Additional information: The list and number of arguments depend on the definition of the underlying classification and coupling scheme which has to be defined before by calling the procedure `Racah_set_coupling_scheme()`. ♣ A set of different *keywords* can be provided as the last argument. The currently supported *keywords* are *algebraic*, *prime*, and *seniority* where *algebraic* and *prime* must be used exclusively. The keyword *seniority* ‘overwrites’ the currently defined classification scheme.

  See also: `Racah_set_coupling_scheme()`.

- **Racah_set_coupling_scheme**(*jj_quasispin*)

  ‘Defines’ the global framework to use quasispin notation in *jj*-coupling.

  Output: A NULL expression is returned.

  Argument options: (*LS_quasispin*) to set the global framework to use quasispin notation in *LS*-coupling. ♣ (*jj_seniority*) to set the global framework to use seniority notation in *jj*-coupling. ♣ (*LS_seniority*) to set the global framework to use seniority notation in *LS*-coupling.

  Additional information: The currently defined coupling scheme and notation is kept in the global variable `Racah_save_coupling_scheme`. No default value is provided for this variable and, thus, this procedure *must* be called before any of the other procedures can be invoked.

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TEST RUN OUTPUT

```
"CFP for 9/2 subshells with occupation N = "   1
0   1   9/2   0   0   0   =   .9999999998   [1]
"CFP for 9/2 subshells with occupation N = "   2
0   0   0   0   1   9/2   =   .9999999994   [1]
0   2   2   0   1   9/2   =   1.   [1]
0   2   4   0   1   9/2   =   1.   [1]
0   2   6   0   1   9/2   =   .9999999997   [1]
0   2   8   0   1   9/2   =   .9999999996   [1]
"CFP for 9/2 subshells with occupation N = "   3
0   3   3/2   0   2   4   =   .8528028655   [1, 3, 0, 0, 0, -1]
0   3   3/2   0   2   6   =   -.5222329679   [-1, 0, 1, 0, 0, -1]
0   3   5/2   0   2   2   =   .5270462768   [1, -1, -2, 1]
0   3   5/2   0   2   4   =   -.4438126822   [-1, -1, -1, 0, 0, -1, 1]
0   3   5/2   0   2   6   =   -.7247430754   [-1, 2, -2, 0, 0, -1, 1]
0   3   7/2   0   2   2   =   .7247430753   [1, 2, -2, 0, 0, -1, 1]
0   3   7/2   0   2   4   =   .3739787960   [1, 2, 0, 1, 0, -1, -1]
0   3   7/2   0   2   6   =   .4494665749e-1   [1, 0, -2, -1, 0, -1]
0   3   7/2   0   2   8   =   -.5769463865   [-1, 1, 0, -1, 1, -1, -1, 1]
0   1   9/2   0   0   0   =   .5163977794   [1, 2, -1, -1]
0   1   9/2   0   2   2   =   -.2886751345   [-1, -2, -1]
0   1   9/2   0   2   4   =   -.3872983346   [-1, -2, 1, -1]
0   1   9/2   0   2   6   =   -.4654746682   [-1, -2, -1, -1, 0, 0, 1]
0   1   9/2   0   2   8   =   -.5322906475   [-1, -2, -1, -1, 0, 0, 0, 1]
0   3   9/2   0   2   2   =   .1811857689   [1, -2, -2, 0, 0, -1, 1]
0   3   9/2   0   2   4   =   -.6544628930   [-1, -2, 0, 1, 2, -1, -1]
. . .
```