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Calculation of reduced coefficients and matrix elements in jj-coupling

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Abstract

A program RCFP will be presented for calculating standard quantities in the decomposition of many-electron matrix elements in atomic structure theory. The list of quantities which are supported by the present program includes the coefficients of fractional parentage, the reduced coefficients of fractional parentage, the reduced matrix elements of the unit operator T^k as well as the completely reduced matrix elements of the operator $W^{k_j k_q}$ in jj-coupling. These quantities are now available for all subshells (nj) with $j \leqslant 9/2$ including partially filled $9/2$-shells. Our program is based on a recently developed new approach on the spin-angular integration which combines second quantization and quasispin methods with the theory of angular momentum in order to obtain a more efficient evaluation of many-electron matrix elements. An underlying Fortran 90/95 module can directly be used also in (other) atomic structure codes to accelerate the computation for open-shell atoms and ions.

PROGRAM SUMMARY

Title of program: RCFP

Catalogue identifier: ADNA

Program Summary URL: http://cpc.cs.qub.ac.uk/summaries/ADNA

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland. Users may obtain the program also by dow-loading a tarfile `ratip-rcfp.tar` from our home page at the University of Kassel (http://www.physik.uni-kassel.de/fritzsche/programs.html)

Licensing provisions: None

Computer for which the program is designed and has been tested: IBM RS 6000, PC Pentium II

Installations: University of Kassel (Germany)

Operating systems: IBM AIX 4.1.2+, Linux 6.1+

Program language used in the new version: ANSI standard Fortran 90/95

Memory required to execute with typical data: 100 kB

No. of bits in a word: All real variables are parametrized by a `selected kind parameter` and, thus, can be adapted to any required precision if supported by the compiler. Currently, the `kind`

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parameter is set to double precision (two 32-bit words) as it is for other components of the RATIP package [1]

Peripheral used: Terminal for input/output

No. of bytes in distributed program, including test data, etc: 70 953

Distribution format: tar gzip file

CPC Program Library subprograms required: Catalogue number: to be assigned; Title: REOS99; Ref. [1].

Keywords: Atomic many-body perturbation theory, complex atom, configuration interaction, effective Hamiltonian, energy level, Racah algebra, reduced coefficients of fractional parentage, reduced matrix element, relativistic, second quantization, standard unit tensors, tensor operators, 9/2-subshell

Nature of the physical problem
The calculation of atomic properties and level structures is based on the evaluation of many-particle matrix elements of physical operators. For symmetry-adapted functions, the matrix element for a given tensor operator A^K of rank K can be expressed as $\sum_{j,k} \mathrm{coeff}(j,k)\langle \gamma_j J_j \| A^K \| \gamma_k J_k \rangle$ by using the (reduced) coefficients of fractional parentage and the reduced matrix elements of the (unit) standard tensors T^k or $W^{k_q k_j}$. These reduced coefficients and matrix elements are frequently applied to both the configuration interaction and multi-configuration Dirac–Fock method [2] as well as to many-body perturbation theory [3].

Method of solution
A new combination of second quantization and quasispin methods with the theory of angular momentum and irreducible tensor operators leads to a more efficient evaluation of (many-particle) matrix elements and to faster computer codes [4]. Practical implementations of this new scheme will support not only large-scale computations on open-shell atoms but may even help to develop programs for calculating the angular parts of (effective) one- and two-particle operators for many-body perturbation theory (in higher orders) in the future.

Restrictions onto the complexity of the problem
For jj-coupled subshells states, our module provides coefficients and matrix elements for all subshells (nj) with $j = 1/2$, $3/2$, $5/2$, $7/2$, and $9/2$.

Typical running time
For large computations, the running time depends on the shell structure and the size of the wave function expansion for a given atomic system. However, the program *promptly* responds in its interactive mode if only single coefficients and matrix elements are to be calculated.

Unusual features of the program
The interactive version of RCFP can be used as an "electronic tabulation" of standard quantities for evaluating general matrix elements for jj-coupled functions.

References
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LONG WRITE-UP

1. Introduction

In atomic structure theory, the efficient evaluation of many-electron matrix elements play a crucial role. Typically, such matrix elements have to be evaluated for different one- and two-particle operators which describe the interaction of the electrons with each other or with external particles and fields. By exploiting the techniques of Racah's algebra [1], the evaluation of these matrix elements may often be considerably simplified by carrying out the integration over the spin-angular coordinates analytically. For atoms with open shells, several approaches to this analytic integration were developed in the past. One of the most widely-used computational schemes is from Fano [2,3] and has been implemented in a number of powerful programs [4,5] since that time.

Fano's procedure [2] is based on the coefficients of fractional parentage (cfp). During the last decades, this procedure was applied both to LS- and jj-coupling; in the following, we will restrict ourselves to jj-coupling as appropriate for relativistic calculations. By using the cfp as the basic quantities, however, Fano's procedure does

not exploit the full power of Racah's algebra. Instead of using cfp, it is often more convenient to exploit unit tensors [6,7] which are closer related to the tensorial form of physical operators. But so far, unit tensors have been applied only for evaluating diagonal matrix elements while all non-diagonal matrix elements still have to be evaluated by using the cfp [7,8]. A recently developed approach [9,10] now treats diagonal and non-diagonal matrix elements on a uniform basis. This approach is based on a second quantization and uses a coupled tensorial form for the creation and annihilation operators [11]. It also applies the theory of angular momentum to two different spaces, i.e. the space of orbital angular momentum j and the quasispin space [12]. The basic quantities of this new approach are the so-called reduced coefficients of fractional parentage (rcfp) and the completely reduced matrix elements of the $W^{(k_q k_j)}$ operator.

Obviously, each computational scheme is based on a set of standard quantities to decompose the many-electron matrix elements. These quantities are either the cfp, rcfp, the reduced matrix elements of the unit tensor T^k, the completely reduced matrix elements $W^{k_q k_j}$, depending on the approach. Therefore, very different tabulations of these quantities are found in the literature. For example, numerical values for the cfp are found by de Shalit and Talmi [13] for subshells with $j = 5/2$, $7/2$ and $9/2$ while rcfp for $j = 5/2$ and $7/2$ were first tabulated by Savičius et al. [14]. Matrix elements of T^k are tabulated, for instance, by Slepcov et al. [15] for subshells with $j = 3/2$, $5/2$ and $7/2$; often, however, it is more convenient to express these matrix elements in terms of the completely reduced matrix elements of the operator $W^{(k_q k_j)}$ even though no explicit compilation of these matrix elements yet available. In practical applications, they are instead derived from a sum of products of rcfp and 6-j symbols.

In this paper, we will present the program RCFP for the calculation of the standard quantities both in Fano's and our new approach. These quantities are needed for the integration over the spin-angular variables. Our program not only supports large-scale computations on open-shell atoms but may even help to develope codes for calculating the angular parts of (effective) one- and two-particle operators from many-body perturbation theory (in higher orders) in the future.

The theoretical background will be presented in Section 2. This includes a brief outline of the quasispin concept, the definitions of the rcfp and the reduced matrix elements of the unit tensors $W^{k_q k_j}$ and T^k as well as the proper classification of subshells in jj-coupling. The program organization will be dealt with in Section 3 while, finally, a few examples are given in Section 4.

2. Theoretical background

The theory of angular integration for symmetry-adapted functions has been reviewed in several texts and monographs [3,7,10,16]. As mention above, this theory is usually built on a number of standard quantities like the cfp or the reduced matrix elements of the unit tensor T^k which, in turn, can be applied to lay down the expressions for more complex matrix elements. Other important quantities (which are also provided by our program) are the rcfp and the completely reduced matrix elements of the tensor operators $W^{k_q k_j}$. In the following, we shall not repeat too many details about this angular integration on the spin-angular coordinates; instead, we just list the definition of those quantities which can be obtained from our program along with a number of useful relations among them. For all further details, we ask the reader to refer to the literature given above.

In the literature, several definitions and phase conventions are used for defining the standard quantities for angular integration. Here, we follow the definitions from Savičius [14] and from Kaniauskas and Rudzikas [12]. We also apply the so-called *standard-phase systems*,

$$A_q^{(k)\dagger} = (-1)^{k-q} A_{-q}^{(k)} \tag{1}$$

throughout this paper which were originally introduced by Fano and Racah [17].

2.1. The quasispin concept

In jj-coupling, a wave function for a subshell of N *equivalent* electrons with principal quantum number n and (one-electron) angular momentum j is often written as

$$|nj^N \alpha J), \tag{2}$$

where J denotes the total angular momentum and α all additional quantum numbers as needed for an unique classification of these states. Using the quasispin concept, a further (angular) quantum number Q, the quasispin momentum of the subshell, can be introduced so that the wave function of this subshell (to which we briefly refer to as a *subshell state*) then reads

$$|nj^N \alpha Q J). \tag{3}$$

For any given subshell, the quasispin Q is closely related to the seniority quantum number ν as used in the *seniority scheme*, i.e. $Q = ((2j+1)/2 - \nu)/2$. If compared with the seniority notation the quasispin Q to has the advantage of its projection, M_Q, being related to the occupation number N by $M_Q = (N - (2j+1)/2)/2$. Therefore, when exploring the quasispin concept for classifying the atomic subshell states (3), the Wigner–Eckart theorem can be applied twice, both to the space of quasispin (Q-space) as well as to the total angular momentum (J-space). Hence, any reduced matrix element in J-space can be further reduced also in Q-space [12]

$$\begin{aligned}\left(j^N \alpha Q J M_Q \| A^{(qj)}_{m_q} \| j^{N'} \alpha' Q' J' M'_Q\right) = (-1)^{Q-M_Q} \begin{pmatrix} Q & q & Q' \\ -M_Q & m_q & M'_Q \end{pmatrix} \\ \times \left(j \alpha Q J \| | A^{(qj)} | \| j \alpha' Q' J'\right)\end{aligned} \tag{4}$$

to a so-called *completely reduced* matrix element. In Eq. (4), $A^{(qj)}_{m_q}$ denotes a tensor with rank q and projection m_q in the Q-space. As seen from its notation the completely reduced matrix element $(j \alpha Q J \| | A^{(qj)} | \| j \alpha' Q' J')$ is independent of the occupation number N of the particular subshell states; the occupation number N of these states occurs explicitly only on the left-hand side of Eq. (4) while it is incorporated into Q on the right-hand side. Thus, by applying the quasispin concept, the evaluation of general matrix elements will result in a much smaller number of completely reduced matrix elements which are independent of the occupation of electrons N in this subshell but still allows an unique decomposition.

2.2. Coefficients of fractional parentage

The electron creation $a^{(j)}_{m_j}$ and annihilation $a^{(j)\dagger}_{-m_j}$ operators play a key role in the theory of second quantization and atomic structure [18]. Using the quasispin concept, the operators $a^{(j)}_{-m_j}$ and $\tilde{a}^{(j)}_{m_j} = (-1)^{j-m_j} a^{(j)\dagger}_{-m_j}$ also form components of an irreducible tensor of rank $q = \frac{1}{2}$ in Q-space, i.e.

$$a^{(qj)}_{m_q m_j} = \begin{cases} a^{(j)}_{m_j} & \text{for } m_q = \frac{1}{2}, \\ \tilde{a}^{(j)}_{m_j} & \text{for } m_q = -\frac{1}{2}. \end{cases} \tag{5}$$

Compared with the electron creation and annihilation operators above, the operators $a^{(qj)}_{m_q m_j}$ also act in an additional quasispin space like a tensor component with rank q and a projection $m_q = \pm\frac{1}{2}$. There is the following relation known between the reduced matrix element of a creation operator and the cfp [19]

$$\left(j^N \alpha Q J \| a^{(j)} \| j^{N-1} \alpha' Q' J'\right) = (-1)^N \sqrt{N[J]} \left(j^N \alpha Q J \| j^{N-1} (\alpha' Q' J') j\right) \tag{6}$$

where $[J] \equiv (2J+1)$. Eq. (6) can be used to define the relation between the cfp and its reduced counterpart in Q-space. Introducing the z-projection, M_Q, of the quasispin, this relation is given by [7]

$$\left(j\alpha QJ\|a^{(qj)}\|j\alpha' Q'J'\right) = (-1)^{N+Q-M_Q}\sqrt{N[J]}\begin{pmatrix} Q & 1/2 & Q' \\ -M_Q & 1/2 & M'_Q \end{pmatrix}^{-1} \times \left(j^N\alpha QJ\|j^{N-1}(\alpha' Q'J')j\right). \tag{7}$$

The properties of the rcfp have been summarized by Savičius et al. [14] and Gaigalas et al. [20]. The latter reference also discusses *phase conventions* which are frequently applied in the literature to subshell states with a the same number $N(< j+1/2)$ of electrons or holes, respectively.

2.3. Reduced matrix elements of standard operators

The unit tensors $W^{k_q k_j}$ and T^k are other standard quantities in atomic spectroscopy. Many texts on the evaluation of matrix elements in many-particle physics frequently refer to these quantities [6,7]. The tensor $W^{k_q k_j}$, for example, is defined as the tensorial product of two creation operators in second quantization

$$W^{k_q k_j}_{m_q m_j} = \left[a^{(qj)} \times a^{(qj)}\right]^{k_q k_j}_{m_q m_j}. \tag{8}$$

Following Savičius et al. [14], the operators T^k and $W^{k_q k_j}$ obey the relation

$$T^k_m = \begin{cases} -(2[k])^{-1/2} W^{0k}_{0m} & \text{if } k \text{ is odd,} \\ -(2[k])^{-1/2} W^{1k}_{0m} & \text{if } k \text{ is even.} \end{cases} \tag{9}$$

The reduced matrix elements of T^k can be represented in terms of a sum over 6-j symbols and cfp's

$$\left(j^N\alpha J\|T^k\|j^N\alpha' J'\right) = N\sqrt{[J,J']}\sum_{\alpha'' J''}(-1)^{J''+j+J+k}\begin{Bmatrix} j & J & J'' \\ J' & j & k \end{Bmatrix} \times \left(j^N\alpha J\|j^{N-1}(\alpha'' J'')j\right)\left(j^{N-1}(\alpha'' J'')j\|j^N\alpha' J'\right). \tag{10}$$

The completely reduced matrix elements of the operator $W^{(k_q k_j)}$ is related to the rcfp in the following way

$$\begin{aligned}&\left(nj\alpha QJ\|W^{k_q k_j}\|nj\alpha' Q'J'\right) \\ &\quad = (-1)^{Q+J+Q'+J'+k_q+k_j}\sqrt{[k_q,k_j]}\sum_{\alpha'' Q'' J''}\begin{Bmatrix} q & q & k_q \\ Q' & Q & Q'' \end{Bmatrix}\begin{Bmatrix} j & j & k_j \\ J' & J & J'' \end{Bmatrix} \\ &\qquad \times \left(j\alpha QJ\|a^{(qj)}\|j\alpha'' Q'' J''\right)\left(j\alpha'' Q'' J''\|a^{(qj)}\|j\alpha' Q'J'\right).\end{aligned} \tag{11}$$

Thus, a close relationship between the completely reduced matrix elements of $W^{k_q k_j}$ and the reduced matrix elements of the unit tensor T^k is given by

$$\left(nj\alpha QJ\|W^{1k}\|nj\alpha' Q'J'\right) = (-1)^{1+Q-M_Q}\sqrt{2[k]}\begin{pmatrix} Q & 1 & Q' \\ -M_Q & 0 & M'_Q \end{pmatrix}^{-1} \times \left(j^N\alpha QJM_Q\|T^k\|j^N\alpha' Q'J'M'_Q\right)$$

if $k_q = 1$ and k is even (12)

and

$$\left(nj\alpha QJ\|W^{0k}\|nj\alpha' Q'J'\right) = -\sqrt{2[Q,k]}\left(j^N\alpha QJM_Q\|T^{(k)}\|j^N\alpha' Q'J'M'_Q\right)$$

if $k_q = 0$ and k is odd. (13)

Since the completely reduced matrix elements $(nj\alpha QJ\|W^{k_q k_j}\|nj\alpha' Q'J')$ of the operator $W^{k_q k_j}$ are, again, independent of the occupation number, they allow for a more compact representation (tabulation) in atomic

Table 1
Allowed couplings $[j]^N$ of N *equivalent* electrons for subshells with $j = 1/2, \ldots, 9/2$. The seniority quantum number v, the subshell angular momentum J, the subshell quasispin Q and the number Nr (for subshells with $j = 9/2$ only) are shown

Subshell	v	J	$2Q$	Nr	Subshell	v	J	$2Q$	Nr
$[1/2]^0$ or $[1/2]^2$	0	0	1			3	5/2	2	
$[1/2]^1$	1	1/2	0			3	7/2	2	
						3	9/2	2	
$[3/2]^0$ or $[3/2]^4$	0	0	2			3	11/2	2	
$[3/2]^1$ or $[3/2]^3$	1	3/2	1			3	13/2	2	
$[3/2]^2$	0	0	2			3	15/2	2	
	2	2	0			3	17/2	2	
						3	21/2	2	
$[5/2]^0$ or $[5/2]^6$	0	0	3		$[9/2]^4$ or $[9/2]^6$	0	0	5	
$[5/2]^1$ or $[5/2]^5$	1	5/2	2			2	2	3	
$[5/2]^2$ or $[5/2]^4$	0	0	3			2	4	3	
	2	2	1			2	6	3	
	2	4	1			2	8	3	
$[5/2]^3$	1	5/2	2			4	0	1	
	3	3/2	0			4	2	1	
	3	9/2	0			4	3	1	
						4	4	1	1
$[7/2]^0$ or $[7/2]^8$	0	0	4			4	4	1	2
$[7/2]^1$ or $[7/2]^7$	1	7/2	3			4	5	1	
$[7/2]^2$ or $[7/2]^6$	0	0	4			4	6	1	1
	2	2	2			4	6	1	2
	2	4	2			4	7	1	
	2	6	2			4	8	1	
$[7/2]^3$ or $[7/2]^5$	1	7/2	3			4	9	1	
	3	3/2	1			4	10	1	
	3	5/2	1			4	12	1	
	3	9/2	1		$[9/2]^5$	1	9/2	4	
	3	11/2	1			3	3/2	2	
	3	15/2	1			3	5/2	2	
$[7/2]^4$	0	0	4			3	7/2	2	
	2	2	2			3	9/2	2	
	2	4	2			3	11/2	2	
	2	6	2			3	13/2	2	

Table 1
(Continued)

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

structure calculations. This fact becomes important, in particular, when calculating atoms with open d- and/or f-shells. So far, no detailed analysis or tabulation of these completely reduced matrix elements in jj-coupling has been published in the literature or has been implemented in any atomic structure code.

2.4. Classification of subshells in jj-coupling

A unique classification of the atomic states and, hence, the subshell states is required for all structure computations. For subshells with $j = 1/2, 3/2, 5/2$, and $7/2$, two quantum numbers Q and J (respectively v and J in the seniority notation) are sufficient to classify the subshell states for all allowed occupation numbers N unambiguously. For these subshells, no additional quantum numbers α are then needed to be specified in (3). By contrast, some additional number(s) are required for classifying the subshell states for $j \geqslant 9/2$ (cf. de Shalit and Talmi [13] or Grant [3]). For $j = 9/2$, there are two doublets (pairs of subshell states) with $v = 4$, $J = 4$ and $v = 4$, $J = 6$ in the $[9/2]^4$ and $[9/2]^6$ configurations which require an additional "number" in order to classify these states uniquely. To distinguish the individual subshell states of these two pairs, we use the number $Nr = 1$ or $Nr = 2$ beside of the standard quantum numbers Q and J, respectively, v and J. Table 1 lists all (jj-coupled) subshell states for j = 1/2, 3/2, 5/2, 7/2 and 9/2, starting for each j with the lowest occupation number.

3. Program organization

3.1. Overview to program

The program RCFP supports the computation of the cfp, the rcfp, the (completely) reduced matrix elements of the operator $W^{k_q k_j}$ as well as the matrix elements of the unit tensor T^k. It can be applied interactively, for instance,

for calculating a few individual coefficients or matrix elements in some theoretical derivation but also, by *using* the underlying module `rabs_rcfp`, in any relativistic atomic structure calculations in order to evaluate all required (many-electron) matrix elements automatically. RCFP is written in Fortran 90/95 and is designed as additional component of the RATIP package [21] as will be explained in Section 3.3. By exploiting the advantages of the new Fortran 90/95 standard, we defined several derived data types which facilitate the work and which shall enable us to incorporate this module in our present developments on large-scale computations for open-shell atoms and ions. The definition of the various derived structures can be found in the header of the module `rabs_rcfp` but will not be explained here.

As seen from Section 2, the most basic quantities for evaluating matrix elements among different subshell states are the rcfp and the completely reduced matrix elements of $W^{k_q k_j}$. These quantities are more general than the cfp or the reduced matrix elements of the unit tensor T^k as they do not depend on the occupation number in the corresponding shells. Thus, the rcfp and the completely reduced matrix elements can be tabulated much easier for subshells with $j \leqslant 7/2$ or even $j = 9/2$ and are also applied in the present program. This is in contrast to most earlier atomic structure codes which are built on the cfp. For $j \leqslant 7/2$, the rcfp have been taken from Rudzikas [7] while the corresponding tables for $j = 9/2$ have been created by us using Eq. (7) and the tabulations by de Shalit and Talmi [13] for the cfp. Similarly, a tabulation of the completely reduced matrix elements of $W^{k_q k_j}$ have been obtained from the reduced matrix elements of T^k [15] and from the two relations (12) and (13) for the subshells with $j \leqslant 7/2$. Up to the present, the module `rabs_rcfp` does not contain a full tabulation of the completely reduced matrix elements of $W^{k_q k_j}$ for $j = 9/2$ even though such an implementation might help considerably in the future in order to accelerate structure calculations on atoms having open $g_{9/2}$ and/or $h_{9/2}$ subshells. At present, these coefficients are calculated from Eq. (11) each time they are needed. Also, the values of the cfp and the reduced matrix elements of T^k are calculated from Eqs. (7) or (12) and (13), respectively.

3.2. Interactive work

The program RCFP is typically applied in its interactive mode. In this mode, it replies immediately to the input as typed in by the user. In the next section, we display several short dialogs for calculating individual coefficients and matrix elements. From the main menu of the RCFP component (see Fig. 1), we need first to select the type of the quantity which is to be computed. For example, by entering `1` on the screen the user can calculate any cfp in jj-coupling for subshells with $j \leqslant 9/2$. Similarly, a `2` supports the computation of rcfp, and so on. Finally, a `q` will terminate the program.

The input of the required quantum numbers needed for the computation of any quantity is facilitated by the program. It is only necessary to type those quantum numbers which cannot be derived automatically and which distinguish the individual coefficients and matrix elements. For calculating a cfp or a reduced matrix elements of T^k, for instance, the orbital quantum number j, the subshell occupation number N, the seniority quantum number ν, and the subshell total angular momentum J is needed in order to specify the bra-function uniquely. Only if additional quantum numbers are indeed required for a unique classification of the subshell states, the program will ask for the quantum number Nr. A number of examples will illustrated the usage of RCFP below in Section 4.

3.3. Distribution and installation of the program

RCFP has been developed as (a new) component of the RATIP package [21]. To facilitate the combination with this package, RCFP will be distributed as an archive file of the directory `ratip_rcfp`. From this archive, first of all the file structure is reconstructed by the command `tar -xvf ratip_rcfp.tar` on a UNIX workstation or any compatible environment. The directory `ratip_rcfp` then contains the Fortran 90/95 module `rabs_rcfp.f`, the (main) program `xrcfp.f` as well as the makefile `make-rcfp`. It also includes a number of examples in the subdirectory `test-rcfp` and a short `Read.me` which explains further details about the installation. Since the same file structure is preserved in both cases, the combination of RCFP with RATIP is simply

```
RCFP: Calculation of coefficients of fractional parentage (cfp) and various
 reduced matrix elements in jj-coupling (Fortran 90 version)
 (C) Copyright by G. Gaigalas and S. Fritzsche, Kassel (1999).

Select one issue from the list for calculating:

  1:  coefficients of fractional parentage,
  2:  reduced coefficients of fractional parentage,
  3:  completely reduced matrix elements of the operator W^{k_q k_j},
  4:  reduced matrix elements of unit operator T^{(k)},
  b:  return back to this menue,
  q:  quit.
```

Fig. 1. The main menue of RCFP.

achieved by running the command `cp -r ratip_rcfp/. ratip/.` Inside of the RATIP root directory, then `make -f make-rcfp` will generate the executable `xrcf`, similarly as for the other two components `xcesd99` [22] and `xreos99` [21] of the RATIP package. Like before, the name of the (Fortran 90/95) compiler and special compiler flags can be overwritten in the header of the makefile. Although RCFP makes *use* of four other modules which are part already of RATIP, no further adaptation of the program is needed. At present, the RCFP program has been installed and tested under the operating systems Linux and AIX but, owing to the compliance of the Fortran 90/95 standard, no difficulties should arise on any other platform.

The subdirectory `test-rcfp` lists a number of examples which demonstrate the usage of the program. To each item in the main menu in Fig. 1, a short file displays the full dialog to compute one or several individual coefficients or (completely reduced) matrix elements. The file `show-cfp-dialog`, for instance, reports the calculation of several cfp for subshells with $j = 9/2$ including an example for which the (additional) quantum number *Nr* need to be specified.

Apart from the application of `rabs_rcfp` in the RCFP program, this module can be used also in other programs which, in the future, will provide the angular coefficients for general matrix elements of one- and two-particle operators for jj-coupled functions.

4. Examples

To illustrate the use of RCFP in its interactive mode, we show three examples concerning the calculation of rcfp and matrix elements. We will just display the input (which has to be typed in by the user) along with the given reply by the program. In order to support also an occasional usage of the program, the notation of the various coefficients and matrix elements is kept as close as possible with their printed form (cf. Section 2). Moreover, all information which can automatically be deduced by the program is simply provided by typing Enter at input time. For an improper selection of quantum numbers or any incomplete information, a short message is printed explaining the failure before all previous (correct) input is repeated. This saves the user from re-enter all of the previously typed input just because of one single (mistyped) quantum number. In the following examples, we display the user's input in boldface mode while the response of the program is shown in normal text mode.

Our first examples displays the computation of the cfp $([7/2]^4,\ \nu = 2,\ J = 2\{|[7/2]^3,\ \nu = 3,\ J = 3/2,\ \nu = 1,\ j = 7/2)$; from the main menue in Fig. 1, we therefore select the first item

```
1
 Calculate a cfp (j^N  nu J {| j^{N-1} nu' J',  j) :
```

```
(7/2^4 2 2 Enter
7/2^4 2 2 {| 7/2 ^3 3 3/2, Enter
(7/2^4 2 2 {| 7/2 ^3 3 3/2, 1 7/2 ) = 2.53546276E-01
Continue
```

Next, let us calculate the rcfp $(9/2,\ \nu = 5,\ J = 1/2|||a^{(qj)}|||9/2,\ \nu = 4,\ J = 5)$ for which we select item 2 from the main menue

```
2
 Calculate a reduced cfp (j  nu J ||| a^{(1/2 j)} ||| j  nu' J') :
```

```
(9/2 5 1/2 Enter
(9/2 5 1/2 ||| a^{(1/2 j)}||| 9/2 4 5, Enter
Input must either start with symbol '(' or end with symbol ')'; reenter ...
(9/2 5 1/2 ||| a^{(1/2 j)} ||| 9/2 4 5) Enter
(9/2 5 1/2 ||| a^{(1/2 j)} ||| 9/2 4 5) = 3.22490310E+00
Continue
```

In our third example, finally, we ask for the value of one of the completely reduced matrix element of the $W^{(10)}$ operator, i.e. $(j = 9/2,\ \nu = 4,\ J = 6,\ Nr = 2\|\|W^{(10)}\|\|j = 9/2,\ \nu = 4,\ J = 6,\ Nr = 2)$. As mentioned in Section 2, an additional quantum number *Nr* is required for a unique specification of the subshells states with $j = 9/2$. Here, we start by selecting item 3 from the main menue.

```
3
 Calculate a completely reduced matrix element
 (j   nu J ||| W^{k_q k_j} ||| j  nu' J') :
```

```
(9/2 4 6 Enter
Enter the additional state identifier Nr = 1 or 2.
(9/2 4 6 Nr= 2 Enter
(9/2 4 6 Nr= 2 ||| W^{ 1 0 Enter
(9/2 4 6 Nr= 2 ||| W^{1 0 } ||| 9/2 4 6 ) Enter
(9/2 4 6 Nr= 2 ||| W^{ 1 0 } ||| 9/2 Nr= 2 ) Enter
(9/2 4 6 Nr= 2 ||| W^{ 1 0 } ||| 9/2 Nr= 2) = -3.94968353E+00
Continue
```

A very similar dialog occurs for the computation of any other coefficient or reduced matrix element. In conclusion, RCFP has been developed as a new component of the RATIP package which enables the user to calculate standard quantities in the evaluation of many-electron matrix elements explicitly. In the future, the underlying Fortran 90/95 module `rabs_rcfp` will be exploited also to calculate the Hamiltonian matrix and further properties of free atoms from jj-coupled configuration state functions. The definition of the rcfp and the completely reduced matrix elements and further improvements (see Gaigalas et al. [9]) will allow for faster and more convenient computations than it is presently supported by standard atomic structure programs. A module for calculating the angular coefficients for jj-coupled functions with respect to any (given) scalar two-particle operator is currently under development.

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