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Maple procedures for the coupling of angular momenta. IV. Spherical harmonics ☆

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Abstract

Spherical harmonics play a crucial role in theoretical physics since they represent a complete and orthonormal set of functions on the unit sphere. The spherical harmonics are therefore applied in many different fields of physics including classical field theory as well as the treatment of quantum many-particle systems. Along with their well-known properties, they are frequently utilized to evaluate one- and many-particle matrix elements from atomic and nuclear structure theory analytically.

In this paper, we present an extension of the RACAH program to incorporate the behaviour and the properties of the spherical harmonics. Our new version also supports various useful expansions for these functions, recursion relations as well as the algebraic evaluation of integrals.

PACS: 3.65Fd; 2.90+p

Keywords: Angular momentum; Clebsch–Gordan expansion; Racah algebra techniques; Spherical harmonic; Spherical tensor operator; Sum rule evaluation; Wigner $n-j$ symbol

PROGRAM SUMMARY

Title of program: RACAH

Catalogue identifier: ADOR

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

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland. Users may obtain the program also by down-loading either the *compress*ed tar-file `racah2000.tgz` (for Unix & Linux) or the zip-file `racah2000-windows.zip` (for Windows & Macintosh) 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 others on which it is operable: 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: AIX, Linux, Windows

Program language used: Maple V, Releases 3, 4, and 5

Memory required to execute with typical data: 6 MB

☆ This program can be downloaded from the CPC Program Library under catalogue identifier: http://cpc.cs.qub.ac.uk/summaries/ADOR

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PII: S0010-4655(01)00218-1

No. of lines in distributed program, etc.: ca. 22 000

No. of bytes in distributed program, including test data, etc.: 541 996

Distribution format: tar gzip file

Nature of the physical problem
Spherical harmonics are applied in many fields of physics. In classical electrodynamics, for instance, the spherical harmonics may be utilized to expand the electro-magnetic field of a charge distribution in terms of its multipoles. The spherical harmonics also provide an important *basis* in quantum mechanics for classifying one- and many-particle states since they are simultaneous eigenfunctions of one component and of the square of the orbital angular momentum operator $-i\mathbf{r} \times \nabla$. In many-particle physics, the properties of these functions (completeness, orthogonality, ...) are frequently applied to evaluate the spin-angular part of the corresponding matrix elements analytically.

Method of solution
In a previous version of the RACAH program [2], we defined data structures and a hierarchy of MAPLE procedures to evaluate and simplify expressions from Racah's algebra. Our revised program now also supports the occurrence of spherical harmonics as well as integrals over the spherical harmonics in such expressions. The evaluation follows similar lines as before by utilizing, in addition, the properties, sum rules, and recursion relations for the spherical harmonics. Several sum rules for these functions lead to (new) Wigner $n-j$ symbols which may be simplified owing to the previous capabilities of the program.

Restrictions onto the complexity of the problem
The definition of the spherical harmonics and the sum rules, which have been implemented in the program, mainly refer to the monograph by Varshalovich et al. [3]. There are literally no other limitations on the complexity of individual expressions than those of the resources and computer time which is needed for their evaluation. Even though a large number of sum rules for the Wigner $n-j$ symbols is now incorporated in the program (including the *graphical loop* rules for the $3-j$ symbols), only a selected set of those sum rules, which involve the $9-j$ symbols, are implemented so far. Also, we do not support higher $n-j$ symbols ($n = 12, 15, \ldots$) since they are defined in rather different ways in the literature.

Unusual features of the program
All commands of the RACAH package are available for interactive work. As explained in Ref. [2] and Appendix A below, the program is based on data structures which are suitable for almost any complexity of Racah algebra expressions. The present version also supports *Clebsch–Gordan expansions* for two or more spherical harmonics (which depend on the same angular coordinates) into a sum of products of a single spherical harmonic and the corresponding number of Wigner $3-j$ symbols. To accelerate the evaluation of Racah expression, the code for most sum rules of the Wigner $n-j$ symbols ($n = 3, 6, 9$), as implemented in the program, have also been improved.

Typical running time
All the examples below take only a few seconds on a Pentium III 450 MHz computer.

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, Comp. Phys. Commun. 111 (1998) 167.
[3] D.A. Varshalovich, A.N. Moskalev, V.K. Khersonskii, Quantum Theory of Angular Momentum, World Scientific, Singapore, 1988.

LONG WRITE-UP

1. Introduction

Spherical harmonics are applied in many research areas, both in classical and quantum physics. In classical field theory, for instance, these functions are often used to approximate the potential of a given charge distribution by its (lowest) multipole moments [1,2]. The spherical harmonics also frequently occur in the quantum mechanics of one- and many-particle systems. For an electron moving in a central potential, the harmonics $Y_{lm}(\vartheta, \varphi) = \langle \vartheta\varphi | lm \rangle$ are known to form simultaneous eigenfunctions of the square of the orbital angular momentum operator and of one of its components [3]. In practical applications of the theory, this gives rise immediately to the *radial–spherical* representation

$$\psi_{nlm_lm_s}(r, \vartheta, \varphi) = R_{nl}(r) Y_{lm}(\vartheta, \varphi) \chi_{m_s} \tag{1}$$

of the total (one-electron) functions. A similar structure as in (1) even appears in relativistic quantum mechanics where one starts from Dirac's equation to describe the motion of spin-1/2 particles. But although several (spinor-)

components need to be distinguished in this case, all of them still separate into products of radial and spherical functions including the Y_{lm}'s.

The radial-spherical representation (1) of the one-particle wave functions also plays a major role in describing (interacting) N-particle systems since it enables one to carry out the integration over the $2N$ angular coordinates of the systems analytically. Such techniques of analytical integration have been established for a long time in the theory of angular momentum (or sometimes called the Racah algebra), but they often result in very complex expressions which are difficult to deal with manually. Therefore, in order to facilitate an (automatically supported) manipulation and transformation of such expressions, we developed the RACAH program [4,5] during the last years which has been found helpful in a number of applications. — In a previous version, this program could be applied already for sum rule evaluations as well as for various numerical computations of standard expressions of Racah's algebra.

Our present work extends the RACAH program to incorporate also the knowledge of the analytic behaviour and properties of the spherical harmonics. To this end, we enlarged our (previous) definition of a *Racah expression* (cf. Fig. 1 in Ref. [4]) for taking into account the spherical harmonics *in addition to* the Wigner $n-j$ symbols. Such expressions, in fact, may now include integrals over products of any number of spherical harmonics (and with different arguments) which will be evaluated and simplified similar to our previous rules. Details on this evaluation process of typical Racah expressions (including the Y_{lm}'s) will be described below in Sections 3 and 4.

In the following section, we briefly summarize the properties of the spherical harmonics. The main extensions of the program and how the properties and sum rules of these functions are implemented in the program is then described in Section 3. In the next section, several examples show how the program can be utilized to evaluate integrals and to carry out simple expansions of the spherical harmonics. Two slightly more advanced examples later point towards the application of the RACAH program to atomic and nuclear theory. Finally, Section 5 gives a brief outlook on future developments of the RACAH program. In addition, two appendices below list a rather concise description of the new and extended data structures as well as of all commands at user's level which have been modified or added to the RACAH package.

2. Properties of the spherical harmonics

The most utilized power of the spherical harmonics is to form a *complete* and orthogonal set of functions on the unit sphere. These two properties are used, for instance, for carrying out multipole expansions for classical fields and of quantum-mechanical operators, both in two and three dimensions. Together with the known Clebsch–Gordan expansion for products of spherical harmonics, these properties also facilitate an analytic integration on a sphere. In order to provide the reader with some guidance for the examples below, here we briefly summarize a few important properties of these functions.

For a particle in a central field, the spherical harmonics $Y_{lm}(\vartheta,\varphi)$ are known as the eigenfunctions of the square and of one component of the orbital angular momentum operator $-\mathrm{i}\mathbf{r}\times\nabla_{\mathbf{r}}$. These functions, therefore, simultaneously obey the two eigenvalue equations $\hat{L}_z Y_{lm}(\vartheta,\varphi) = mY_{lm}(\vartheta,\varphi)$ and $\hat{\mathbf{L}}^2 Y_{lm}(\vartheta,\varphi) = l(l+1)Y_{lm}(\vartheta,\varphi)$, or explicitly [1]

$$\frac{\partial}{\partial\varphi} Y_{lm}(\vartheta,\varphi) = \mathrm{i}m Y_{lm}(\vartheta,\varphi), \tag{2}$$

$$\Delta_{(\vartheta,\varphi)} Y_{lm}(\vartheta,\varphi) \equiv \left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right] Y_{lm}(\vartheta,\varphi) = -l(l+1)Y_{lm}(\vartheta,\varphi), \tag{3}$$

where ϑ and φ are the polar coordinates (for the solid angle Ω) and $\Delta_{(\vartheta,\varphi)}$ denotes the angular part of the Laplacian $\Delta \equiv r^{-2}\partial/\partial r(r^2\partial/\partial r) + r^{-2}\Delta_{(\vartheta,\varphi)}$.

[1] Throughout this article we use atomic units, where $e = m_{\mathrm{e}} = \hbar = 1$.

For a given $l \geqslant 0$, there exist $(2l+1)$ functions according to different m's in the range $-l \leqslant m \leqslant l$. Both the spherical harmonics as well as all of their derivatives are single-valued, continuous, and finite functions on the unit sphere.

The normalized (standard) solutions of Eqs. (2) and (3) are

$$Y_{lm}(\vartheta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\,P_l^m(\cos\vartheta)\mathrm{e}^{\mathrm{i}m\varphi}, \tag{4}$$

where the functions $P_l^m(x)$ are the associated Legendre polynomials

$$P_l^m(x) \,=\, (-1)^m\big(1-x^2\big)^{m/2}\frac{d^{l+m}}{dx^{l+m}}\frac{(x^2-1)^l}{2^l l!} = (-1)^m\big(1-x^2\big)^{m/2}\frac{d^m}{dx^m}P_l(x) \tag{5}$$

and $P_l(x)$ denotes a Legendre polynomial of order l. In the definition (4), moreover, the phase has been chosen to fulfill the symmetry $Y_{lm}^*(\vartheta,\varphi) = (-1)^m Y_{l,-m}(\vartheta,\varphi)$. This *phase convention* is in line with many texts on quantum mechanics and, in particular, with the monograph of Varshalovich et al. [6] to who we refer for further details. Unfortunately, however, there are a number of different conventions used in the literature, both for the spherical harmonics and associated Legendre polynomials as discussed in Ref. [7]. Therefore, the user must take care about proper phases if parts of the derivation were obtained *independent* of the RACAH program.

Symmetry properties. Various symmetry relations of the spherical harmonics concern a sign reversal of the magnetic quantum number m and of the angular arguments as well as the periodicity in ϑ and φ. From the explicit form (4), one may find the symmetries

$$\begin{aligned} Y_{lm}(\vartheta,\varphi) \,&=\, (-1)^m\mathrm{e}^{2\mathrm{i}m\varphi}Y_{l,-m}(\vartheta,\varphi) = (-1)^m Y_{lm}(-\vartheta,\varphi) \\ &=\, \mathrm{e}^{2\mathrm{i}m\varphi}Y_{l,-m}(-\vartheta,\varphi) = (-1)^m Y_{l,-m}(\vartheta,-\varphi) \\ &=\, \mathrm{e}^{2\mathrm{i}m\varphi}Y_{lm}(\vartheta,-\varphi) = Y_{l,-m}(-\vartheta,-\varphi) \\ &=\, (-1)^m\mathrm{e}^{2\mathrm{i}m\varphi}Y_{lm}(-\vartheta,-\varphi). \end{aligned} \tag{6}$$

For each of these symmetries, there is another relation due to the complex conjugate of a spherical harmonic: $Y_{lm}(\vartheta,\varphi) = Y_{lm}^*(\vartheta,-\varphi)$.

Orthogonality and completeness. These two properties of the spherical harmonics follow immediately from being the eigenvectors of the Hermitian angular momentum operators $\hat{\mathbf{L}}^2$ and $\hat{L}_z$; they are given by

$$\int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}\mathrm{d}\vartheta\,\sin\vartheta\, Y_{lm}^*(\vartheta,\varphi)Y_{l'm'}(\vartheta,\varphi) = \delta_{ll'}\delta_{mm'}, \tag{7}$$

$$\sum_{l,m} Y_{lm}^*(\vartheta,\varphi)Y_{lm}(\vartheta',\varphi') = \delta(\cos\vartheta-\cos\vartheta')\delta(\varphi-\varphi'). \tag{8}$$

The second relation displays the completeness in the (ϑ,φ)-space.

Addition theorem.

$$\sum_{m=-l}^{l} Y_{lm}^*(\Omega_1)Y_{lm}(\Omega_2) \,=\, \frac{2l+1}{4\pi}P_l(\cos\theta_{12}), \tag{9}$$

where $\Omega_1 \equiv (\vartheta_1,\varphi_1)$ and $\Omega_2 \equiv (\vartheta_2,\varphi_2)$ define two different directions and $\theta_{12} = \angle(\boldsymbol{\Omega}_1,\boldsymbol{\Omega}_2)$ is the angle between them.

Clebsch–Gordan expansion.

$$Y_{l_1 m_1}(\vartheta,\varphi) Y_{l_2 m_2}(\vartheta,\varphi) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}} \sum_{LM} (-1)^M \sqrt{2L+1} \times \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix} Y_{LM}(\vartheta,\varphi). \tag{10}$$

This expansion provides a means to simplify products of two and more spherical harmonics with the same angles. It relates the spherical harmonics to the Wigner $n-j$ symbols. In the literature, this relationship is frequently expressed also in terms of so-called Gaunt coefficients $\langle l_3 m_3 | l_2 m_2 | l_1 m_1 \rangle$, i.e. of integrals of the product of three spherical harmonics over the unit sphere in 3-dimensional space [8,9].

There are also known a number of other expansions of the spherical harmonics in terms of special functions (Wigner D-functions, Jacobi and Gegenbauer polynomials) as well as of the hypergeometric and trigonometric functions which have been found useful for several applications.

Multipole expansions. The completeness of the spherical harmonics can be used to represent any arbitrary function $f(\vartheta,\varphi)$ in the L^2 Hilbert space of the unit sphere in 3-dimensional space into a series

$$f(\vartheta,\varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} f_{lm} Y_{lm}(\vartheta,\varphi), \tag{11}$$

where the coefficients

$$f_{lm} = \int_0^{2\pi} \mathrm{d}\Phi \int_0^{\pi} \mathrm{d}\Theta\, \sin\Theta\, Y_{lm}^*(\Theta,\Phi) f(\Theta,\Phi)$$

are often called the *multipoles* of this function. Such a representation is useful, in particular, if $f(\vartheta,\varphi)$ is a 'nearly' spherical symmetric function so that it can be replaced approximately by a finite sum over its lowest multipoles: $f(\vartheta,\varphi) \simeq \sum_0^L f_{lm} Y_{lm}(\vartheta,\varphi)$.

Similarly to the 2-dimensional expansion (11), one may define the *spherical multipole moments* a_{lm} for any function $F(r,\vartheta,\varphi)$ in three dimensions

$$a_{lm} \equiv \int \mathrm{d}^3 r'\, r'^l\, Y_{lm}^*(\vartheta',\varphi') F(r',\vartheta',\varphi'). \tag{12}$$

These spherical moments are used, for instance, in electrostatics to describe the potential $V(\mathbf{r})$ *outside* of a localized charge distribution $\rho(\mathbf{r})$. If the potential is taken to satisfy appropriate boundary conditions [i.e. $V(\mathbf{r}\to\infty)\to 0$], it can be written as

$$V(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} \frac{a_{lm}}{r^{l+1}} Y_{lm}(\vartheta,\varphi),$$

where one just need to replace $F(\mathbf{r}) \to \rho(\mathbf{r})$ in the spherical moments (12).

In quantum mechanics, the same expansion is used also to define the multipole operators $\widehat{M}_{kq} = r^k Y_{kq}(\vartheta,\varphi)$ for describing, for instance, the interactions of atoms and molecules with the radiation field.

To complete this section of the properties of the spherical harmonics, we finally give the expansion of the Coulomb repulsion as it occurs in atomic and molecular structure for each pair of electrons. By using the addition theorem from above, the Coulomb operator becomes

$$\frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\vartheta_1,\varphi_1) Y_{lm}(\vartheta_2,\varphi_2) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{r_<^l}{r_>^{l+1}} C_{lm}^*(\vartheta_1,\varphi_1) C_{lm}(\vartheta_2,\varphi_2) \tag{13}$$

with $r_<$ ($r_>$) is the smaller (larger) radius of r_1 and r_2, respectively. The second line *defines* the 'modified' or 'renormalized' spherical harmonics $C_{lm}(\vartheta,\varphi) = \sqrt{4\pi/(2l+1)}\,Y_{lm}(\vartheta,\varphi)$ which are also supported by the RACAH program.

3. Implementation and extensions to the RACAH program

Different lanes were pursued in the past to simplify and evaluate expressions from the theory of angular momentum. With the RACAH program [4,5], we focused on the development of symbolic techniques. By using well defined data structures within the framework of MAPLE V and a hierarchical order for the large set of required procedures, we were able to treat all parts of typical expressions from Racah's algebra as logical objects throughout. The various commands of the RACAH program can be used either for interactive work or as the basic elements in order to built up procedures at some higher level of the hierarchy.

In order to deal with spherical harmonics in Racah expressions and for accelerating their evaluation process, a number of new procedures has been added to the program during the last two years. From the set of procedures, which were already available in the previous version, in particular the two commands `Racah_set()` and `Racah_evaluate()` have been improved considerably. The procedure `Racah_set()`, for instance, now supports to enter a whole Racah expression within a single line and, thus, facilitates the handling of complex expressions. Moreover, to achieve a faster simplification of recoupling coefficients, the user may now also select different 'routes' for the evaluation like a set of 'graphical' *loop* rules as will be described in an accompanying manuscript. The implementation of such graphical rules, however, has accelerated the time for evaluation by more than two orders of magnitude in certain cases.

Apart from modifications on (a few previously) available procedures, several new commands deal with the representation and the properties of the spherical harmonics. Typical Racah expressions, which were first defined for the Wigner $n-j$ symbols only, may now also contain (any product of) the spherical harmonics as well as integrals over these functions, defined on the unit sphere. For this purpose, we specified several new data structures like `Ylm` or `int` in order to handle single spherical harmonics or the domain of integration for a given angle. In the present implementation, the spherical harmonics are now treated equivalently to the Wigner symbols and, thus, the internal `Ylm` lists became part of the `Rproduct` list of a given Racah expression. For details on the definition of all data structures, we refer to Ref. [4] and Appendix A below (new data types). To facilitate the further development of the RACAH program, we already specified the data type `dlmm` for representing the reduced matrix elements of the rotation operator. These functions are not yet supported by most of the procedures but will be treated similar to the other two data types, i.e. `wnj` and `Ylm`.

Of course, the spherical harmonics and their integrals on a unit sphere require also to define (continuous) angles; see the list structure `ang` in Appendix A. In order to specify the integration over a particular domain of such angles, in addition, we specified the structure `int` which occurs — equivalently to any (discrete) summation variable — in the `Rsummationset` of a given Racah expression. The *set* structure of this particular type hereby reflects the overall *assumption* of the program that all sums and integrals can be interchanged with each other.

The implementation of the spherical harmonics also affects the hierarchy in evaluating the various parts of a Racah expression. In `Racah_evaluate()`, the simplification now always starts with an analysis of the sum and integration rules for the spherical harmonics. As shown in Section 2, this may result in Kronecker or Dirac *delta* factors as well as in a number of (new) $3-j$ symbols [cf. Eq. (10)]. These additional factors are then simplified in a later step, similar to our previous work. If, moreover, the keyword *loop* is selected for `Racah_evaluate()`, only a special set of *loop rules* for the Wigner $3-j$ symbols will be tested explicitly. The implementation of these rules and their application to complex recoupling coefficients will be discussed in an accompanying paper [10].

A further extension of the Racah program improves the support of sums of (different) Racah expressions. Such Racah sums naturally occur for the derivatives of Racah expressions with respect to angular (and other continuous) variables and for the use of recursion relations for the Wigner $n - j$ symbols and spherical harmonics. To combine two Racah expressions into a single `Racahsum`, i.e. to *add* them in a mathematical sense, the command Racah_plus() can be invoked. The procedure Racah_add(), in contrast, allows to *subjoin* some parts to a previously defined Racah object. For instance, the multiplication of a `Racahsum` with some factor c is simply achieved by invoking Racah_add(*factor*,c,Racahsum).

As previously, the source code of the RACAH program will be distributed in ASCII format; it is mainly based on Release 5 of the MAPLE framework. Although emphasize was paid to preserve the compatibility of the program also to earlier releases of MAPLE, this downward compatibility cannot always be ensured completely. By providing the source code, however, the user may adjust the program to his own needs.

The full package is provided by a compressed tar file `racah2000.tgz` of the `racah` root directory. This directory includes the source, the file `Racah-command.ps` as well as several *help* pages in the subdirectory `lib`. The file `Racah-command.ps` contains a quick reference of all user-relevant commands of the RACAH program similar to Appendix B below. The full source (including the help pages) can be read from the root directory by

```
> read racahload;
```

at the beginning of each MAPLE session. The program currently contains more than 160 procedures from which, however, only about 10 have to be known at user's level.

Although the RACAH program allows a fast and reliable handling of the theory of angular momentum, we shall conclude this section with a brief warning. In standard applications, namely, it often appears difficult to recognize (mathematically) erroneous expressions which, in course of the evaluation, may lead to senseless or even wrong results. Therefore, the user must take care that all angular momentum quantum numbers represent integer or half-integer values and that they fulfill proper coupling conditions. For example, the coupling of two half-integer values always results in an integer angular momentum and according rules have to be valid for the coupling of other angular momenta.

4. Examples

To illustrate the present extension and to provide a few test cases, we show several examples below which do not require to type in much information. These examples concern the analytic integration for a product of spherical harmonics on a unit sphere and their expansion in powers of the sin or cos functions. Two other examples later display how the properties of the spherical harmonics can be utilized to evaluate matrix elements from atomic structure and collision theory.

The symmetries (6) and the orthogonality (7) of the spherical harmonics are the *best* known properties for this set of functions. They are often utilized for the analytic integration over products of such functions. To evaluate an integral like

$$\int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \mathrm{d}\vartheta\ \sin\vartheta\, Y_{lm}(-\vartheta,\varphi) Y_{L,-M}(\vartheta,-\varphi) \tag{14}$$

we simply enter

```
> expr1 := Racah_set(int,phi,0,2*Pi,int,theta,
                0,Pi,factor,sin(theta),
                Ylm(l,m,-theta,phi),Ylm(L,-M,theta,-phi)):
> Racah_print(expr1):
```

```
--->
                              2 Pi           Pi
                             /              /
                            |              |
                            |       dphi   |      dtheta
                            |              |
                           /              /
                             0              0

                                 sin(theta)

                             Y_{l,m} (-theta,phi)

                             Y_{L,-M} (theta,-phi)
```

```
> Racah_evaluate(expr1):
> Racah_print(%):
```

```
--->
                                             M
                                         (-1)

                             delta(l,L)  delta(M,-m)
```

Note that in the expression above we can also omit the boundaries (on the sphere) for the integration over the standard intervals $0 \leqslant \phi \leqslant 2\pi$ and $0 \leqslant \theta \leqslant \pi$. Generally, if the boundaries are omitted or if a solid angle Ω is specified, the integration over these standard intervals is always assumed in the RACAH program. However, to avoid any ambiguity of the expressions, we recommend to specify the boundaries explicitly if the integrals over the (polar) angles ϑ and φ are described separately.

Several applications of the spherical harmonics benefit from the explicit representation of these functions in powers of the sin or cos function. A variety of such expansions are supported by the procedure Racah_expand() as in the following example for $Y_{2,-1}(\vartheta, \varphi)$

```
> Racah_expand(Ylm,2,-1,theta,phi);

                        1/2
                      30    cos(theta) sin(theta) exp(-I phi)
                  1/4 ---------------------------------------
                                         1/2
                                       Pi
```

An equivalent expression in terms of powers of $\sin(\vartheta/2)$ is obtained by

```
> Racah_expand(Ylm,2,-1,theta,phi,half_theta,Sin);

       1/2                                     2                    4
     30    sin(1/2 theta) (1 - 3 sin(1/2 theta)  + 2 sin(1/2 theta) ) exp(-I phi)
 1/2 ----------------------------------------------------------------------------
                              1/2
                            Pi    cos(1/2 theta)
```

The use of other allowed *keywords* for selecting a proper expansion, for instance for products of spherical harmonics, is described in Appendix B.

In applying many-body perturbation theory to atomic and molecular systems, large effort has often to be devoted to the evaluation of the matrix elements of symmetric one- and two-particle operators using the *radial-spherical* representation (1) of the one-electron orbital functions. In the following examples, we use the nonrelativistic notation

$$|a\rangle \equiv |n_a l_a m_a m_a^{(s)}\rangle = \frac{1}{r} P_{n_a l_a}(r) Y_{l_a m_a}(\vartheta, \varphi) \chi_{m_a^{(s)}}$$

to specify *spin-orbitals* with well defined spin and orbital angular momentum quantum numbers.

Let us first consider the matrix elements of the multipole operator $\widehat{M}_{kq} = r^k Y_{kq}(\vartheta, \varphi)$ which are given explicitly by

$$\langle a|\widehat{M}_{kq}|b\rangle = \delta_{m_a^{(s)} m_b^{(s)}} \cdot \int \mathrm{d}r\, P_{n_a l_a}(r) r^k P_{n_b l_b}(r) \int \mathrm{d}\varphi \int \mathrm{d}\vartheta\, \sin\vartheta\, Y^*_{l_a m_a}(\vartheta, \varphi) Y_{kq}(\vartheta, \varphi) Y_{l_b m_b}(\vartheta, \varphi).$$

We can apply the RACAH program to evaluate the angular part of this matrix element, similar to the example above, and obtain

```
> expr2 := Racah_set(int,Omega,Ylmcc(la,ma,Omega),Ylm(k,q,Omega),
             Ylm(lb,mb,Omega));
> Racah_evaluate(expr2):
> Racah_print(%):

  --->
                                        ma
                                    (-1)

                               1/2            1/2            1/2
                      (2 la + 1)    (2 k + 1)    (2 lb + 1)
                  1/2 ----------------------------------------
                                               1/2
                                             Pi

                           w3j(la,k,lb,0,0,0)

                         w3j(la,k,lb,-ma,q,mb)
```

or, equivalently

$$(-1)^{m_a} \left(\frac{[l_a, k, l_b]}{4\pi} \right)^{1/2} \begin{pmatrix} l_a & k & l_b \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_a & k & l_b \\ -m_a & q & m_b \end{pmatrix}. \tag{15}$$

In this example, we have used the solid angle Ω with its (preassumed) integration domain over the full unit sphere; moreover, the short form `Ylmcc` corresponds to a complex conjugated spherical harmonic. In expression (15), the notation $[a, b, c, \ldots] = (2a + 1)(2b + 1)(2c + 1)\ldots$ is used as often found in the literature about angular momentum theory.

The complexity of the expressions rapidly increases if two-particle operators or products of operators occur in the derivation. For instance, the matrix elements of the instantaneous Coulomb repulsion, Eq. (13), between each pair of electrons is

$$\left\langle ab \left| \frac{1}{r_{12}} \right| cd \right\rangle = \delta_{m_a^{(s)} m_c^{(s)}} \delta_{m_b^{(s)} m_d^{(s)}} \sum_k R^k(ab, cd)$$
$$\times \sum_q \iint \mathrm{d}\Omega_1\, \mathrm{d}\Omega_2\, Y^*_{l_a m_a}(\Omega_1) Y^*_{l_b m_b}(\Omega_2) C_{kq}(\Omega_1) C^*_{kq}(\Omega_2) Y_{l_c m_c}(\Omega_1) Y_{l_d m_d}(\Omega_2), \tag{16}$$

where, again, the radial integral

$$R^k(ab, cd) = \iint \mathrm{d}r_1\,\mathrm{d}r_2\, P_{n_a l_a}(r_1) P_{n_b l_b}(r_2) \frac{r_<^k}{r_>^{k+1}} P_{n_c l_c}(r_1) P_{n_d l_d}(r_2)$$

and the spin contributions can be evaluated separately. Following similar lines for the angular (double) integral of expression (16) as before, we find

```
--->
                                    SUM{q}

                                    (q + mb + ma)
                                (-1)

                 1/2           1/2           1/2           1/2
   (2 lb + 1)     (2 ld + 1)     (2 la + 1)     (2 lc + 1)

                              w3j(k,lb,ld,0,0,0)

                            w3j(k,lb,ld,-q,-mb,md)

                              w3j(k,la,lc,0,0,0)

                             w3j(k,la,lc,q,-ma,mc)
```

or, for the overall angular matrix element

$$\sum_{kq} (-1)^{m_a+m_b+q} [l_a, l_b, l_c, l_d]^{1/2} \begin{pmatrix} k & l_a & l_c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & l_b & l_d \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & l_b & l_d \\ -q & -m_b & m_d \end{pmatrix} \begin{pmatrix} k & l_a & l_c \\ q & -m_a & m_c \end{pmatrix} \quad (17)$$

which can be directly compared with various textbooks on atomic theory [11].

The last two examples can be extended easily also to other operators of nuclear and atomic structure theory. Beside of these two important fields of applications, however, our present extension of the RACAH program may go well beyond these research areas.

5. Summary and outlook

Since its first publication in 1997, the RACAH package [4] has grown extensively over the last few years. Recent developments to this program concerned the analytic evaluation of Racah expressions by exploiting the sum rules and orthogonality properties of the Wigner $n - j$ symbols [5], the implementation of standard quantities for simplifying many-electron matrix elements as well as an implementation of graphical rules [10]. All these developments enlarged the range of applications for the RACAH program and, thus, made it attractive to a broader community. With the present work on spherical harmonics, we now provide a powerful version which may have applications far beyond atomic theory (our own field of interest which motivated these developments originally).

Till now, however, most of the implemented quantities like the Wigner $3 - j$ symbols or the spherical harmonics are *defined* with respect to a given quantization axis. Although this axis can be chosen appropriately for some given task, it must be *specified* for all the subsystems together. But there are many other applications in which different directions need to be *distinguished* from each other. In such cases, one often wishes to rotate the physical states and/or the reference frame before the expressions can be further evaluated. In order to carry out such transformations, the matrix elements of the rotation operator, i.e. the so-called Wigner D-functions are frequently required. These functions can be considered as a generalization of the spherical harmonics and, in fact, may be used as a representation of the rotation group. They depend on three angles (for instance, the Euler angles α, β, γ) as necessary to characterize an arbitrary rotation in space. In the further development of the RACAH program, we intent to incorporate these functions and to make use of their analytically known properties as well as of their close relation to the Wigner $n - j$ symbols and the spherical harmonics.

Another useful concept of theoretical physics, which is built on the spherical harmonics, is the construction of tensor spherical harmonics, $Y_{JM}^{LS}(\Omega)$, of various ranks. These tensor functions have a wide range of applications, particularly in relativistic theory, in order to describe electrons ($S = 1/2$; spin spherical harmonics), photons ($S = 1$; vector spherical harmonics), or other fermions and bosons (with higher spin S). We currently investigate how and to which extent these functions can be incorporated into the RACAH program, of course, including the knowledge about their properties. Similarly, one may also think towards a more efficient use of hyperspherical harmonics [15,16], well beyond their present applications for two- and three-particle systems.

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Appendix A. New and extended data structures

The definition of proper data structures may facilitate an efficient symbolic manipulation of complex (mathematical) objects. Similar as in Ref. [4], here we provide a short description of the new and extended structures as they are utilized for the internal representation of Racah expressions. In order to specify the integration over a (continuous) *domain* of an angle, we now provide the particular list structure `int` as an additional component of `Rsummationset`. For this definition, we assume that all summations and integrations commute with each other and, therefore, can be carried out independently. Moreover, two derived data types for spherical harmonics and for the Wigner $d_{mm'}^{(j)}(\beta)$ functions have been introduced which became part of the `Rproduct` list of `Racahexpr`. In order to facilitate internally the recognition of the different substructures of a Racah expression, these logical objects typically start with an *identifier* to which a ‡ is attached.

ang Short-hand notation for describing appropriate coordinates on a unit sphere, i.e. either the (polar) angles ϑ and φ, or the solid angle Ω [$\equiv (\vartheta, \varphi)$], or a single (polar) angle β. The internal list representation is

ang$_1$:= [*ang*‡, theta, phi],

ang$_2$:= [*ang*‡, Omega], or

ang$_3$:= [*ang*‡, beta].

dmm Short-hand notation for the reduced matrix elements $d_{mm'}^{(j)}(\beta)$. The internal list representation is

dmm := [*djmm*‡, j, m, m', ang].

int Notation to specify the integration over a continuous variable as well as the domain of integration. The integration variable must not appear to be constant or as a discrete index in any of the Wigner $n - j$ symbols in the corresponding Racahexpr. Moreover, the domain of integration must not depend on other integration variables nor summation indices.

int$_1$:= [*int*‡, variable, lower_limit, upper_limit] or

int$_2$:= [*int*‡, variable].

The second form may be used either if the boundaries of the integration follow uniquely from the structure of the Racah expression or in order to denote a symbolic integration over the full range of this (angular) variable.

tdelta A short-hand notation to describe either a Kronecker delta δ_{j_1,j_2}, a Dirac delta function $\delta(\varphi - \varphi')$, or a triangular delta $\delta(j_1, j_2, j_3)$ which depend on two variables or two or three angular momenta, respectively. The triangular delta reflects proper coupling conditions and is $\delta(j_1, j_2, j_3) = 1$, if j_1, j_2, and j_3 fulfill the *triangular condition*, and evaluates to zero otherwise. All of these delta factors are internally represented by a list where a keyword as first operand characterizes the particular specification.

$$\text{tdelta}_1 := [\mathit{delta}\ddagger, j_1, j_2],$$
$$\text{tdelta}_2 := [\mathit{dirac}\ddagger, \varphi, \varphi'], \quad \text{or}$$
$$\text{tdelta}_3 := [\mathit{triangle}\ddagger, j_1, j_2, j_3].$$

Ylm Short-hand notation for a spherical harmonic $Y_{lm}(\vartheta, \varphi)$ or $Y_{lm}(\Omega)$. The internal list representation is

$$\text{Ylm} := [\mathit{ylm}\ddagger, l, m, \text{ang}].$$

See the data structure `ang` above for the internal specification of the angles ϑ and φ (or Ω, respectively).

Appendix B. New commands to the RACAH package

In this appendix, we describe all new and revised procedures of the RACAH program which are of interest for the user and which support an efficient work. Again, we follow the style of the *Maple Handbook* by Redfern [12] which provides not only a quick reference but also sufficient information about the individual commands. For the most important commands, help pages are now available and are incorporated within the framework of MAPLE.

Racah_animate3d(*Ylm*, l, m)

Plots the real part of the spherical harmonic $Y_{lm}(\vartheta, \varphi)$ in polar coordinates and rotates it around the z-axis.

Output: A Maple PLOT3D data structure is returned.

Additional information: The procedure plots $Y_{lm}(\vartheta, \varphi)$ in polar coordinates for all integer arguments $|m| \leqslant l$. ♣ Additional arguments from the Maple plot() procedure (like `numpoints`, `style`, ...) are also allowed.

See also: Racah_plot(), Racah_plot3d().

Racah_diff(wexpr, var)

Calculates the derivative of wexpr with respect to var.

Output: A Racahexpr or a Racahsum is returned if the differentiation was successful and an empty [NULL] list otherwise.

Argument options: `(wexpr,var,n)` to calculate the nth derivative with respect to the variable var.

Additional information: wexpr can be either of type Ylm, Racahexpr, or Racahsum. ♣ A differentiation with respect to a discrete variable (quantum number) is not allowed; the procedure terminates with an appropriate ERROR message in this case. Also, derivatives $\frac{\mathrm{d}^n}{\mathrm{X}^n}\delta(x - x_0)$ of Dirac's delta function are not supported by the present version. ♣ If, mathematically, the differentiation yields zero, a message is printed and a NULL expression returned.

Racah_evaluate(wexpr)

Attempts to simplify wexpr which can be either of type wnj, Ylm, Racahexpr, or Racahsum.

Output: A Racahexpr (or Racahsum) is returned if the simplification was successful and a [NULL] list otherwise.

Argument options: `(wexpr, loop)` to apply only the subset of the fast (graphical) loop rules and the sum rules which are known for the spherical harmonics. ♣ `(wexpr, full)` to evaluate wexpr until no further simplification can be achieved by the program. ♣ `(wexpr, ..., Regge)` to enforce the procedure to utilize the extended set of symmetries of the Wigner $n-j$ symbols due to Regge. ♣ `(wexpr, ..., specialvalues)` to look, in addition, for *special values* of the Wigner $n-j$ symbols or spherical harmonics within wexpr.

Additional information: A Racahexpr is considered to be *simplified* if the number of summation indices, index range equations, Wigner $n-j$ symbols and/or the number of spherical harmonics is reduced in the overall expression. ♣ One or several of the keywords above may occur at the same time as suitable for the user. ♣ If wexpr is of type wnj or Ylm, it is first converted to a Racahexpr for which then the procedure Racah_evaluateRacahexpr() is invoked. ♣ If no simplification was possible, an empty [NULL] list is returned. However, if the keyword *full* is applied or if wexpr is of type Racahsum, the procedure always returns an equivalent expression. ♣ When wexpr is of type Racahsum, the procedure evaluates each term individually. No attempt is presently made to recognize equivalent or similar terms of the Racahsum which could be combined into a single term. ♣ In practice, the procedure attempts three main 'routes' of simplification:

(i) Use of the graphical loop rules for all (sums of) products of Wigner $3-j$ symbols.
(ii) Use of various (additional) sum and integration rules for the Wigner $n-j$ symbols and the spherical harmonics which are found in the literature.
(iii) Check for *special values* for the Wigner $n-j$ symbols if the keyword *specialvalues* is provided.

♣ While *special values* always apply to individual Wigner $n-j$ symbols and spherical harmonics, the methods in steps (i) and (ii) require to analyze the whole Racahexpr carefully, including the summation indices and integration variables, the overall phase as well as dependencies of the remaining parts of a Racahexpr. ♣ A list of important special values can be found in Refs. [6,13]. ♣ The simplification of complex Racahexpr can be both, very time- and memory-consuming.

See also: Racah_usesumrules().

Racah_expand(*Ylm*, wexpr)

Expands any spherical harmonic $Y_{lm}(\vartheta, \varphi)$, which is contained in wexpr, into a power series of the trigonometric functions of ϑ.

Output: A Racahexpr is returned.

Argument options: `(Ylm, l, m, theta, phi)` to return the corresponding expansion for a single spherical harmonic $Y_{lm}(\vartheta, \varphi)$. ♣ `(Ylm, l, m, theta, phi, Sin)` to return an expansion in terms of powers of $\sin\vartheta$. ♣ `(Ylm, l, m, theta, phi, half_theta)` to return an expansion in terms of powers of $\cos\frac{\vartheta}{2}$. A similar expansions in terms of $\sin\frac{\vartheta}{2}$ is returned if the keyword *Sin* is given additionally. ♣ `(ClebschGordan, wexpr)` to carry out a full Clebsch–Gordan expansion of all products of spherical harmonics which are contained in wexpr. ♣ `(ClebschGordan, wexpr, n`$_u$`)` to perform a Clebsch–Gordan expansion of all products of spherical harmonics with the same angular dependence (ϑ, φ) until each of these products only contains n_u spherical harmonics. ♣ `(multipole, f, theta, phi)` to carry out the multipole expansion of the scalar function $f(\vartheta, \varphi)$. ♣ `(multipole, f, theta, phi, l`$_{max}$`)` to carry out the multipole expansion of the scalar function $f(\vartheta,\varphi)$ up to the (finite) order $\mathtt{l}_{\max}$. ♣ `(tensor,theta,phi,l1,l2,L,M)` to return the expansion of the irreducible tensor product of two spherical harmonics $\{\mathbf{Y}_{l_1}(\vartheta,\varphi)\otimes\mathbf{Y}_{l_2}(\vartheta,\varphi)\}_{LM}$. ♣ `(tensor,theta,phi,l1,l2,l12,l3, ...,L,M)` to return the expansion of the irreducible tensor product of three or more spherical harmonics $\{\{\mathbf{Y}_{l_1}(\vartheta,\varphi)\otimes\mathbf{Y}_{l_2}(\vartheta,\varphi)\}_{l_{12}}\otimes\cdots\}_{LM}$.

Additional information: The default is an expansion in term of powers of $\cos(\vartheta)$.

Racah_integrate(Racahexpr)

Carries out the analytical integration which only affects the individual factor of the Racahexpr.

Output: A Racahexpr is returned if an analytic integration has been carried out successfully and an empty [NULL] list otherwise.

Argument options: `(Racahsum)` to attempt the angular integration for each term independently. A Racahsum is returned.

Additional information: This procedure is equivalent to invoke the MAPLE procedure int() for the factor of the Racahexpr; it is checked, however, that the integration variables and the boundaries do not occur elsewhere in the overall expression.

Racah_plot(*Ylm*, l, m)

Plots a 2d projection of the spherical harmonic $Y_{lm}(\vartheta,\varphi)$.

Output: A Maple PLOT data structure is returned.

Additional information: The function $Y_{lm}(\vartheta,0)$ is plotted in polar coordinates for all integer arguments $|m|\leqslant l$. ♣ Additional arguments from the Maple plot() procedure (like `numpoints`, `style`, ...) are also allowed. High values of l, for instance, require to increase the number of plot points to about `numpoints=500`. Maple's default for `numpoints` is 49.

See also: Racah_animate3d(), Racah_plot3d().

Racah_plot3d(*Ylm*, l, m)

Plots the real part of the spherical harmonic $Y_{lm}(\vartheta,\varphi)$ in polar coordinates.

Output: A Maple PLOT3D data structure is returned.

Additional information: The real part of the function $Y_{lm}(\vartheta,\varphi)$ is plotted in polar coordinates for all integer arguments $|m|\leqslant l$. ♣ Additional arguments from the Maple plot3d() procedure (like `numpoints`, `style`, ...) are also allowed. High values of l, for instance, require to increase the number of plot points to about `numpoints=2000`. Maple's default for `numpoints` is 625.

See also: Racah_animate3d(), Racah_plot().

Racah_plus(Racahexpr$_1$, ..., Racahexpr$_n$)

Concatenates the expressions Racahexpr$_1$, ..., Racahexpr$_n$ together into a single Racahsum.

Output: A Racahsum is returned.

Argument options: `(Racahsum`$_1$`, ...)` to include one or more Racah expressions of type Racahsum into the concatenation.

Additional information: From a mathematical viewpoint, the returned Racahsum represents the sum of all given Racah expressions.

Racah_recursionforYlm(nrule, Ylm)

Applies a recursion relation to the spherical harmonic Ylm. The type of recursion is specified by the *integer* or *keyword* nrule.

Output: A Racahsum which contains two or more Racahexpr is returned.

Additional information: The parameter nrule, which specifies the type of recursion, can be either an integer $n = 1, 2$ or one of the allowed keywords { *lstep*, *mstep*}. This sequence corresponds to $n = 1$ and $n = 2$, respectively. ♣ The applied recursion relations are based on the monograph of Varshalovich and coworkers (Ref. [6, Eqs. 5.7.1–2]).

Racah_set(*keyword*$_1$(args$_1$), ..., *keyword*$_n$(args$_n$))
Enters one or more Racah expressions or parts of it into the (internal Maple) representation of a Racahexpr.

Output: A Racahexpr is returned.

Argument options: `(`*Racahexpr*`(wnj`$_1$`, ...,wnj`$_n$`,Ylm`$_1$`, ...,Ylm`$_m$`),...)` to enter the Wigner $n - j$ symbols `wnj`$_i$ and the spherical harmonics `Ylm`$_i$ into a single Racahexpr.
♣ `(`*ClebschGordan*`(j`$_1$`,m`$_1$`,j`$_2$`,m`$_2$`,j`$_3$`,m`$_3$`),...)` to enter the Clebsch–Gordan coefficient $\langle j_1m_1, j_2m_2|j_3m_3\rangle$.
♣ `(`*recoupling*`('<(...((j`$_1$`,j`$_2$`)j`$_{12}$`,j`$_3$`)j`$_{123}$`...)j|(...(j`$'_1$`,j`$'_2$`)j`$'_{12}$`...) j`$'$`>'),...)` to enter a recoupling coefficient. ♣ `(`*w3j*`(j`$_1$`,j`$_2$`,j`$_3$`,m`$_1$`,m`$_2$`,m`$_3$`), ...)` to enter a Wigner $3 - j$ symbol.
♣ `(`*w6j*`(j`$_1$`,j`$_2$`,j`$_3$`,j`$_4$`,j`$_5$`,j`$_6$`), ...)` to enter a Wigner $6 - j$ symbol.
♣ `(`*w9j*`(j`$_1$`,j`$_2$`,j`$_3$`,j`$_4$`,j`$_5$`,j`$_6$`,j`$_7$`,j`$_8$`,j`$_9$`),...)` to enter a Wigner $9 - j$ symbol.
♣ `(`*Ylm*`(l,m,theta,phi),...)` or `(`*Ylm*`(l,m,Omega),...)` to enter a spherical harmonic $Y_{lm}(\vartheta, \varphi)$ or $Y_{lm}(\Omega)$. ♣ `(`*Clm*`(l,m,theta,phi),...)` or `(`*Clm*`(l,m,Omega),...)` to enter a modified spherical harmonic $C_{lm}(\vartheta, \varphi)$ or $C_{lm}(\Omega)$. ♣ The keywords *Ylm**, *Clm**, *Ylmcc*, *Clmcc*, *conjugateYlm*, or *conjugateClm* may be used to enter the complex conjugate of a Y_{lm} or C_{lm} function, respectively. ♣ `(`*phase*`(p),...)` to add a phase $(-1)^p$. ♣ `(`*delta*`(m,n),...)`, `(`*dirac*`(x,X),...)`, or `(`*triangle*`(j`$_1$`,j`$_2$`,j`$_3$`),...)` to enter a Kronecker delta δ_{mn}, a Dirac delta function $\delta(x - X)$, or a triangular delta factor $\delta(j_1, j_2, j_3)$.
♣ `(`*integration*`(variable,lower_limit,upper_limit),...)` to enter a domain of integration; the boundaries may also be omitted. ♣ `(`*summation*`(ndx`$_1$`, ...,ndx`$_m$`),...)` to enter summation indices (the names ndx$_i$ must not be equal to one of the allowed keywords). ♣ `(`*factor*`,` f`,...)` to append a factor f.

Additional information: A notation like `wnj`$_1, \ldots,$`wnj`$_n$ indicates that there can be any number of these data structures in the parameter list. ♣ Above all the explained argument options may also be given as (*keyword*$_1$, args$_1$, ..., *keyword*$_n$, args$_n$). ♣ To combine two or several Racah objects together, one may use the argument sequence: (Racahobject$_1$, ...,Racahobject$_n$). Allowed Racah objects are the data types int, Racahexpr, tdelta, wnj, or Ylm. ♣ For Clebsch–Gordan coefficients, we use the phase convention of Condon and Shortley for the conversion into $3 - j$ symbols, i.e.

$$\langle j_1m_1, j_2m_2|j_3m_3\rangle = (-1)^{j_1-j_2+m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.$$

♣ All j_i and m_i must be integer or half-integer constants or expressions and have to fulfill the conditions of angular coupling.

Racah_usesumrules(Racahexpr)

Attempts to simplify `Racahexpr` by using various sum rules which are known for products of Wigner $n - j$ symbols ($n = 6, 9$) in this expression.

Output: A Racahexpr is returned if the simplification was successful and a [NULL] list otherwise.

Argument options: `(Racahexpr, Regge)` to apply also all symmetric forms due to Regge [14] to the Wigner $n - j$ symbols. This optional argument, however, can result in a very time- and memory-consuming evaluation process.

Additional information: The command invokes a set of procedures which classify the *sum rules* due to groups of products of Wigner $n - j$ symbols as indicated by the names of the corresponding subprocedures. ♣ This modular structure easily allows to add further rules for simplification. ♣ The procedure considers all basic symmetric forms of the Wigner $n - j$ symbols and 'compares' them with the internal representation of the corresponding sum rule. ♣ If a simplification due to one of the sum rules is found, this rule is applied and the simplified Racahexpr is returned. The procedure does not automatically search for further simplifications by the same rule, but this could be easily done by applying the same procedure again to the result of the previous step. ♣ Sum rules for Wigner $3 - j$ symbols are applied by the procedure Racah_usesumrulesloop() while those for the spherical harmonics are treated by Racah_usesumrulesYlm().

See also: Racah_evaluate(), Racah_usesumrulesloop(), Racah_usesumrulesYlm().

Racah_usesumrulesloop(Racahexpr)

Attempts to simplify `Racahexpr` by utilizing a selected set of *loop* rules which frequently occur for products of two or more Wigner $3 - j$ symbols.

Output: A Racahexpr is returned if the simplification was successful and a [NULL] list otherwise.

Argument options: `(Racahexpr, Regge)` to apply also all symmetric forms due to Regge [14] for the Wigner $3 - j$ symbols. This optional argument, however, can result in very time- and memory-consuming evaluation process.

Additional information: The command invokes a set of individual procedures which classify the *loop rules* by the number of Wigner $3 - j$ symbols (the so-called n-loops with $n = 1, \ldots, 6$) as indicated by the names of the corresponding subprocedures. ♣ This modular structure easily allows to add further rules for simplification. ♣ The procedure considers all basic symmetric forms of the Wigner $3 - j$ symbols and 'compares' them with the internal representation of the corresponding sum rule. ♣ If a simplification due to one of these rule is found, this rule is applied and the simplified Racahexpr is returned. Before the procedure looks for further loop rules, the expression is simplified by calling the procedure Racah_simplifydeltas(). ♣ The procedure calls the subprocedures Racah_searchforloopof$n$w3j() to check whether a loop rules might be applicable and Racah_usesumrulesfor$n$w3jloop() to simplify the Racah expression. At present, loop rules of $n = 1$, 2, 3, 4, 5, or 6 Wigner $3 - j$ symbols can be recognized and simplified properly. ♣ Due to the rapidly growing complexity, the present version does not look for Regge symmetries for n-loops with $n \geqslant 5$.

See also: Racah_evaluate(), Racah_usesumrules(), Racah_evaluate().

Racah_usesumrulesYlm(Racahexpr)

Attempts to simplify `Racahexpr` by using a selected set of frequently occurring sum and integration rules for products of two or more spherical harmonics.

Output: A Racahexpr is returned if the simplification was successful and a [NULL] list otherwise.

Additional information: The command invokes a set of procedures which classify the *sum rules* due to the number of spherical harmonics in the products as indicated by the names of the corresponding subprocedures. ♣ This modular structure easily allows to add further rules for simplification. ♣ The procedure considers all basic symmetric forms of the spherical harmonics and 'compares' them with the internal representation of the corresponding sum rule. ♣ If a simplification due to one of the sum rules is found, this rule is applied and the simplified Racahexpr is returned. Before the procedure looks for further sum rules, the expression is simplified by calling the procedure Racah_simplifydeltas().

See also: Racah_evaluate(), Racah_usesumrules(), Racah_evaluate().

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