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Maple procedures for the coupling of angular momenta. IX. Wigner D-functions and rotation matrices ☆

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Abstract

The Wigner D-functions, $D^j_{pq}(\alpha,\beta,\gamma)$, are known for their frequent use in quantum mechanics. Defined as the matrix elements of the rotation operator $\hat{R}(\alpha,\beta,\gamma)$ in $\mathcal{R}^3$ and parametrized in terms of the three Euler angles α, β, and γ, these functions arise not only in the transformation of tensor components under the rotation of the coordinates, but also as the eigenfunctions of the spherical top. In practice, however, the use of the Wigner D-functions is not always that simple, in particular, if expressions in terms of these and other functions from the theory of angular momentum need to be simplified before some computations can be carried out in detail.

To facilitate the manipulation of such Racah expressions, here we present an extension to the RACAH program [S. Fritzsche, Comput. Phys. Comm. 103 (1997) 51] in which the properties and the algebraic rules of the Wigner D-functions and reduced rotation matrices are implemented. Care has been taken to combine the standard knowledge about the rotation matrices with the previously implemented rules for the Clebsch–Gordan coefficients, Wigner $n-j$ symbols, and the spherical harmonics. Moreover, the application of the program has been illustrated below by means of three examples.

Program summary

Title of program: RACAH
Catalogue identifier: ADFv_9_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADFv_9_0
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Catalogue identifier of previous version: ADFW, ADHW, title RACAH
Journal reference of previous version(s): S. Fritzsche, Comput. Phys. Comm. 103 (1997) 51; S. Fritzsche, S. Varga, D. Geschke, B. Fricke, Comput. Phys. Comm. 111 (1998) 167; S. Fritzsche, T. Inghoff, M. Tomaselli, Comput. Phys. Comm. 153 (2003) 424.
Does the new version supersede the previous one: Yes, in addition to the spherical harmonics and recoupling coefficients, the program now supports also the occurrence of the Wigner rotation matrices in the algebraic expressions to be evaluated.
Licensing provisions: None
Computer for which the program is designed and others on which it is operable: All computers with a license for the computer algebra package Maple [Maple is a registered trademark of Waterloo Maple Inc.]
Installations: University of Kassel (Germany)
Operating systems under which the program has been tested: Linux 8.2+
Program language used: MAPLE, Release 8 and 9
Memory required to execute with typical data: 10–50 MB
No. of lines in distributed program, including test data, etc.: 52 653
No. of bytes in distributed program, including test data, etc.: 1 195 346

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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Distribution format: tar.gzip
Nature of the physical problem: The Wigner D-functions and (reduced) rotation matrices occur very frequently in physical applications. They are known not only as the (infinite) representation of the rotation group but also to obey a number of integral and summation rules, including those for their orthogonality and completeness. Instead of the direct computation of these matrices, therefore, one first often wishes to find algebraic simplifications before the computations can be carried out in practice.
Reasons for new version: The RACAH program has been found an efficient tool during recent years, in order to evaluate and simplify expressions from Racah's algebra. Apart from the Wigner $n - j$ symbols ($j = 3, 6, 9$) and spherical harmonics, we now extended the code to allow for Wigner rotation matrices. This extension will support the study of those quantum processes especially where different axis of quantization occurs in course of the theoretical deviations.
Summary of revisions: In a revised version of the RACAH program [S. Fritzsche, Comput. Phys. Comm. 103 (1997) 51; S. Fritzsche, T. Inghoff, M. Tomaselli, Comput. Phys. Comm. 153 (2003) 424], we now also support the occurrence of the Wigner D-functions and reduced rotation matrices. By following our previous design, the (algebraic) properties of these rotation matrices as well as a number of summation and integration rules are implemented to facilitate the algebraic simplification of expressions from the theories of angular momentum and the spherical tensor operators.
Restrictions onto the complexity of the problem: The definition as well as the properties of the rotation matrices, as used in our implementation, are based mainly on the book of Varshalovich et al. [D.A. Varshalovich, A.N. Moskalev, V.K. Khersonskii, Quantum Theory of Angular Momentum, World Scientific, Singapore, 1988], Chapter 4. From this monograph, most of the relations involving the Wigner D-functions and rotation matrices are taken into account although, in practice, only a rather selected set was needed to be implemented explicitly owing to the symmetries of these functions. In the integration over the rotation matrices, products of up to three Wigner D-functions or reduced matrices (with the same angular arguments) are recognized and simplified properly; for the integration over a solid angle, however, the domain of integration must be specified for the Euler angles α and γ. This restriction arose because MAPLE does not generate a *constant of integration* when the limits in the integral are omitted. For any integration over the angle β the range of the integration, if omitted, is always taken from 0 to π.
Unusual features of the program: The RACAH program is designed for interactive use that allows a quick and algebraic evaluation of (complex) expression from Racah's algebra. It is based on a number of well-defined data structures that are now extended to incorporate the Wigner rotation matrices. For these matrices, the transformation properties, sum rules, recursion relations, as well as a variety of special function expansions have been added to the previous functionality of the RACAH program. Moreover, the knowledge about the orthogonality as well as the completeness of the Wigner D-functions is also implemented.
Typical running time: All the examples presented in Section 4 take only a few seconds on a 1.5 GHz Pentium Pro computer.

PACS: 3.65.Fd; 2.90.+p

Keywords: Angular momentum; Clebsch–Gordan expansion; Finite rotation matrix; Racah algebra techniques; Reduced rotation matrix; Wigner D-function and rotation matrix; Wigner $n - j$ symbol

1. Introduction

The Wigner D-functions, $D^j_{pq}(\alpha, \beta, \gamma)$, are known to physicists as the matrix elements of the rotation operator $\hat{R}(\alpha, \beta, \gamma)$, taken within a $|jp\rangle$ basis with well defined values for the angular momentum $\mathbf{j}^2$ and its projection j_z. These functions also realize, for instance, the transformation of the (covariant) components of any spherical tensor of rank j under a rotation of the coordinates [1]

$$\psi_{jq}(\vartheta', \varphi', \sigma') = \hat{R}(\alpha, \beta, \gamma)\, \psi_{jq}(\vartheta, \varphi, \sigma) = \sum_{p=-j}^{j} \psi_{jp}(\vartheta, \varphi, \sigma)\, D^j_{pq}(\alpha, \beta, \gamma),$$

where ϑ, φ and ϑ', φ' are the polar angles in the initial and rotated coordinates, respectively, and where σ and σ' refer to the corresponding spin variables. In this expansion of the rotated tensor components, the three Euler angles α, β, and γ denote the (active) rotation of the body-fixed, i.e. the primed coordinates with respect to the original frame. Of course, the Wigner D-functions are known also as the eigenfunctions of the symmetric top [2] and, hence, have played a crucial role in various fields of modern physics including nuclear and molecular physics. Today the Wigner D-functions and the closely related *reduced* rotation matrices $d^j_{pq}(\beta)$ [see below] are certainly one of the most frequently occurring functions in quantum mechanics.

In dealing with the Wigner D-functions the usual aim is to work as long a possible with the *properties* of these functions instead of any of their explicit representations, similar as known, for instance, for the spherical harmonics and various other functions from the theory of angular momentum. For this reason, a great deal of attention has been paid in the literature in order to derive and compile the (algebraic) properties of the rotation matrices, including their symmetries and orthogonality as well as a number of sum and integral rules which have been found useful for the simplification of typical expressions. With the development of modern computer algebra systems such as MAPLE and MATHEMATICA, these properties can now be applied much more efficiently if both the functions as well as their algebraic relations are properly implemented. During the last decade, therefore, we designed and developed the RACAH program [3–5] in order to facilitate the application of the theories of angular momentum and spherical tensor operators as required often for the description of quantum many-particle systems. So far, the RACAH package has been built up

$$\text{Racahexpr} := \sum_{j_1, j_2, l_1, \ldots} (-1)^{2j_1 - j_2 + \cdots} j_1^{3/2} [j_2] \cdots \begin{pmatrix} \cdot & \cdot & j_1 \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{pmatrix} j_1 & j_2 & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \begin{Bmatrix} \cdot & j_3 & \cdot \\ j_1 & \cdot & \cdot \\ J & \cdot & j_2 \end{Bmatrix} \cdots$$
$$\times \int d\Omega_1\, Y_{l_1 m_1}(\Omega_1) Y_{l_2 m_2}(\Omega_2) \int d\beta\, d^{j_3}_{p_3 q_3}(\beta) d^{j_4}_{p_4 q_4}(\beta') \cdots$$

Fig. 1. Structure of Racah expressions which can be simplified by means of the RACAH package.

in several distinct steps, including the definition and algebraic relations about the Clebsch–Gordan coefficients and Wigner $n-j$ symbols [3,4], the efficient evaluation of recoupling coefficients [6] as well as various integral rules for the spherical harmonics [7].

With the present work, we now extent the RACAH program in order to incorporate also the knowledge about the Wigner D-functions and rotation matrices. As previously [4,7], emphasis is placed first of all on the symbolic manipulation and simplification of expressions including the summation over products of the Wigner $n-j$ symbols, spherical harmonics, and (by now) also of the rotation matrices. Fig. 1 displays the general structure of such Racah expressions that can be treated by means of the RACAH program. Less attention, in contrast, has been paid to the efficient computation of these functions which we considered before [5] and for which a great deal of theoretical studies and subroutines are meanwhile available in the literature [8–13]. To outline the present extension of the RACAH program, here we first summarize the properties and basic relations of the rotation matrices in Section 2 and explain in Section 3 how they are implemented into the code. A few test examples later show the use of the current extension including, as a somewhat more advanced example, the group-theoretical derivation of the selection rules for diatomic molecules with respect to the emission or absorption of light.

2. Properties of the Wigner D-functions and rotation matrices

Although the properties of the D-functions and the reduced rotation matrices have been discussed in a large number of texts, see Refs. [1,2], for example, let us briefly compile and review the most useful ones in order to set the *basis* for the manipulations and discussions below. Apart from the explicit definition of the rotation matrices, this concerns in particular their symmetries and orthogonality as well as the completeness of these functions from which most other properties can be derived. In fact, we will restrict ourselves mainly to the properties of the reduced rotation matrices [i.e. the $d^j_{pq}(\beta)$ functions, see below] which are known as the central part of the D-functions and which enable us to reduced the number of 'algebraic rules' considerably. We also display a number of integral rules, including products of two and three rotation matrices, as often utilized in the algebraic simplification of complex expressions. All of these relations are shown in order to explain the implementation of the RACAH program and to guide the reader through the examples in Section 4.

As mentioned before, the Wigner D-functions, $D^j_{pq}(\alpha, \beta, \gamma)$, can be introduced as the matrix elements of the rotation operator $\hat{R}(\alpha, \beta, \gamma)$ in a basis with well-defined values of the angular momentum. For a given set of the Euler angles and any fixed value of j, the $(2j+1) \times (2j+1)$ functions $D^j_{pq}(\alpha, \beta, \gamma)$ with $p = -j, -j+1, \ldots, j$ and $q = -j, -j+1, \ldots, j$ form a unitary matrix

$$\left[D^{+}(\alpha, \beta, \gamma)\right]^j_{pq} \equiv D^{j*}_{pq}(\alpha, \beta, \gamma) = \left[D^{-1}(\alpha, \beta, \gamma)\right]^j_{qp} = D^j_{qp}(-\gamma, -\beta, -\alpha). \tag{1}$$

While for all integer values of j, the Euler angles may take values in the ranges

$$0 \leqslant \alpha \leqslant 2\pi, \quad 0 \leqslant \beta \leqslant \pi, \quad 0 \leqslant \gamma \leqslant 2\pi, \tag{2}$$

the 'double' of the volume of the 3-dimensional rotation group has to be considered for half-integer values of j because, then the period of $D^j_{pq}(\alpha, \beta, \gamma)$ is 4π rather than 2π. Such a doubling of the volume is achieved by taking either $0 \leqslant \alpha \leqslant 4\pi$ or $0 \leqslant \gamma \leqslant 4\pi$ (with a total volume of $16\pi^2$) and ensures that the D-functions, $D^j_{pq}(\alpha, \beta, \gamma)$, are mutually orthogonal with respect to integration for all integer or half-integer j values.

Starting from the parametrization of a rotation in terms of the Euler angles, the D-functions may be represented also as a product of three functions, where each function is known to depend only on one of the angles α, β, or γ,

$$D^j_{pq}(\alpha, \beta, \gamma) = \langle jp| e^{-i\alpha j_z} e^{-i\beta j_y} e^{-i\gamma j_z} |jq\rangle = e^{-i\alpha p} d^j_{pq}(\beta) e^{-i\gamma q}, \tag{3}$$

where $d^j_{pq}(\beta) = \langle jp| e^{-i\beta j_y} |jq\rangle$ is chosen to be real and is called the reduced (or sometimes Wigner) rotation matrix. It is *this* relation between the D-functions and the rotation matrices that enables us very easily to re-write all expressions in terms of the reduced matrices (and some additional exponential functions) and to utilize only these reduced functions for all algebraic manipulations. In the following, therefore, we preferably display the properties and relations for the reduced matrix elements and will show the analogue relations for the D-functions only if appropriate.

Symmetry properties. As most of the ‘algebraic relations’ are displayed in some *standard form* in the literature, the symmetries of the symbols and functions, which are involved in some expression, are of crucial importance for all manipulations. In fact, these symmetries need often to be applied before any simplification due to a particular rule becomes obvious. For the Wigner rotation matrices, various symmetries are known by allowing a change of the sign in one of the *magnetic* quantum numbers p or q

$$d^j_{pq}(\beta) = (-1)^{p-q} d^j_{-p-q}(\beta) = (-1)^{p-q} d^j_{qp}(\beta) = d^j_{-q-p}(\beta) \tag{4}$$

or changes in the angular arguments

$$d^j_{pq}(-\beta) = (-1)^{p-q} d^j_{pq}(\beta) = d^j_{qp}(\beta), \tag{5}$$

$$d^j_{pq}(\pi-\beta) = (-1)^{j-q} d^j_{-pq}(\beta) = (-1)^{j+p} d^j_{p,-q}(\beta). \tag{6}$$

Two other symmetries arise, moreover, from the periodicity of rotations in space

$$d^j_{pq}(\beta \pm 2\pi n) = (-1)^{2jn} d^j_{pq}(\beta), \tag{7}$$

$$d^j_{pq}\big(\beta \pm (2n+1)\pi\big) = (-1)^{\pm(2n+1)j-q} d^j_{p,-q}(\beta), \tag{8}$$

where n as usual is an integer. In the RACAH program, the symmetry of a function is taken into account by generating all the symmetric forms of an expression and by comparing them with the standard representation of the rules as known internally.

Orthogonality relations. If written in terms of the reduced rotation matrices, the unitary condition of the Wigner D-functions

$$\sum_{p=-j}^{j} D^j_{pq}(\alpha,\beta,\gamma) D^{j*}_{pr}(\alpha,\beta,\gamma) = \delta_{qr}, \tag{9}$$

$$\sum_{q=-j}^{j} D^{j*}_{pq}(\alpha,\beta,\gamma) D^j_{rq}(\alpha,\beta,\gamma) = \delta_{pr} \tag{10}$$

simply states that the reduced matrices are orthogonal and unimodular, that is, the rows and columns of these matrices form orthonormal vectors

$$\sum_{p=-j}^{j} d^j_{pq}(\beta) d^j_{pr}(\beta) = \delta_{qr}, \qquad \sum_{q=-j}^{j} d^j_{pq}(\beta) d^j_{rq}(\beta) = \delta_{pr}. \tag{11}$$

Apart from these relations, of course, there is another orthogonality for the rotation matrices with respect to an integration over the β-angle

$$\int_0^{\pi} \mathrm{d}\beta \, \sin\beta \, d^j_{pq}(\beta) d^k_{pq}(\beta) = \frac{2}{2j+1}\delta_{jk} \tag{12}$$

which reflects the fact, that the rotation matrices are (parts of) the irreducible representation of the SO_3 rotation group.

Completeness of the rotation matrices. For the D-functions, the completeness is given by [1]

$$\sum_{j=0,1/2,1,\ldots}^{\infty} \sum_{p=-j}^{j} \sum_{q=-j}^{j} \frac{2j+1}{16\pi^2} D^{j*}_{pq}(\alpha_1,\beta_1,\gamma_1) D^j_{pq}(\alpha_2,\beta_2,\gamma_2) = \delta(\alpha_1-\alpha_2)\delta(\cos\beta_1-\cos\beta_2)\delta(\gamma_1-\gamma_2), \tag{13}$$

with a summation over all the Wigner D-functions having integer and half-integer quantum numbers j. For the rotation matrices, this relation simplifies to

$$\sum_{j=0,1/2,1,\ldots}^{\infty} \frac{2j+1}{2} d^j_{pq}(\beta_1) d^j_{pq}(\beta_2) = \delta(\cos\beta_1-\cos\beta_2) \tag{14}$$

independently of the particular values of p and q.

To evaluate algebraic expressions, which include products of the Wigner D-functions and/or the rotation matrices, strategies along several lines may be followed. Apart from the test of the expressions *against* special values and the orthogonality and completeness of these functions, products of the rotation matrices can first be expanded into a Clebsch–Gordan series. Often, integrals over such products can be evaluated explicitly by means of known integration rules if the integrals are taken over the full domain of the corresponding Euler angles.

To simplify the presentation of formulas below, from now on we always assume

$$\sum_p \equiv \sum_{p=-j}^{+j}, \qquad \sum_{pq} \equiv \sum_{p=-j_1}^{+j_1} \sum_{q=-j_2}^{+j_2}, \tag{15}$$

unless indicated otherwise; moreover, a summation over a j quantum number is typically restricted by other j-values of the individual terms in the product due to the coupling rules of angular momenta.

Clebsch–Gordan expansion. Products of two Wigner rotation matrices with equal argument β can be expanded [1]

$$d^{j_1}_{p_1 q_1}(\beta) d^{j_2}_{p_2 q_2}(\beta) = \sum_{JPQ} (-1)^{-2J+2j_2-p_2-q_2}(2j_2+1) \begin{pmatrix} J & j_2 & j_2 \\ P & p_2 & -p_2 \end{pmatrix} \begin{pmatrix} J & j_2 & j_2 \\ Q & q_2 & -q_2 \end{pmatrix} d^J_{PQ}(\beta) \tag{16}$$

in terms of a restricted summation over such matrices by using the Wigner $3-j$ symbol (or equivalently the Clebsch–Gordan coefficients). Similar as for the spherical harmonics $Y_{lm}(\vartheta, \varphi)$, Eq. (16) represents in fact a transformation of the basis, i.e. the change from a *uncoupled* to a *coupled* representation for systems consisting out of two or more subsystems.

As a special case of the Clebsch–Gordan expansion, the product of two rotation matrices at $\beta = \pi/2$ can be evaluated to (by setting $j_1 = j_2 = j$, $p_1 = p_2 = p$, and $q_1 = q_2 = q$)

$$\left(d^j_{pq}\left(\frac{\pi}{2}\right)\right)^2 = \sum_{J=0,2,4,\ldots} (-1)^{J+2j+2p}(2j+1)\frac{(J-1)!!}{J!!} \begin{pmatrix} J & j & j \\ 0 & p & p \end{pmatrix} \begin{pmatrix} J & j & j \\ 0 & q & q \end{pmatrix}. \tag{17}$$

Both expansions provide a means of simplifying products of two or more Wigner rotation matrices with same angular arguments as they relate these matrices to the Wigner $n-j$ symbols for which the algebraic rules are known already to the RACAH program.

Expansions of the rotation matrices in terms of the spherical harmonics. If the absolute value of (at least) one magnetic quantum number is small, say $|p| \leqslant 1$ or $|q| \leqslant 1$, the Wigner rotation matrices can be expressed conveniently in terms of the spherical harmonics. For $p = 0$, for instance, we obtain

$$d^j_{0k}(\beta) = \sqrt{\frac{4\pi}{2j+1}} Y_{j-k}(\beta, \gamma) e^{+i\gamma k} \quad \text{(for arbitrary } \gamma), \tag{18}$$

where the dependence on the second (azimuthal) angle γ appears rather artificial as both sides of this equation basically represent the associated Legendre polynomial

$$Y_{lm}(\vartheta, \varphi) e^{+im\varphi} = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P^m_l(\cos\vartheta).$$

Owing to the symmetry $d^j_{k0} = (-1)^k d^j_{0k}$ from above, of course, a similar expansion as given by Eq. (18) also holds for a rotation matrix with $q = 0$ by including the additional phase factor $(-1)^k$.

For $p \neq 0$ and $q \neq 0$, more complicated expressions arise which may be of less practical use; when $p = \pm 1/2$, the expansion of the rotation matrices in terms of the spherical harmonics becomes

$$d^j_{\pm 1/2,k}(\beta) = \frac{\sqrt{\pi}}{\sqrt{2j+1}\sin\frac{\beta}{2}} e^{+i\gamma(k\pm 1/2)} r \left\{ \pm \sqrt{\frac{j \pm k + 1}{j+1}} Y_{j+1/2, \mp 1/2-k}(\beta, \gamma) \mp \sqrt{\frac{j \mp k}{j}} Y_{j-1/2, \mp 1/2-k}(\beta, \gamma) \right\} \tag{19}$$

and, again, with an additional phase factor $(-1)^{\pm 1/2-k}$ if p and q are reversed, $d^j_{k,\pm 1/2}(\beta)$. For $p = \pm 1$, finally, an analogous expansion is given by

$$\begin{aligned} d^j_{\pm 1,k}(\beta) = e^{+i\gamma k} \sqrt{\frac{4\pi}{j(j+1)(2j+1)}} \Bigg\{ &\mp \sqrt{(j-k)(j+k+1)} \frac{1 \mp \cos\beta}{2} Y_{j,-k-1}(\beta, \gamma) e^{+i\gamma} \\ &+ k \sin\beta Y_{j,-k}(\beta, \gamma) \pm \sqrt{(j+k)(j-k+1)} \frac{1 \pm \cos\beta}{2} Y_{j,-k+1}(\beta, \gamma) e^{-i\gamma} \Bigg\}, \end{aligned} \tag{20}$$

and with an overall phase factor $(-1)^{k+1}$ if $d^j_{k,\pm 1}(\beta)$ is considered.

There are numerous further expansions of the rotation matrices known in terms of special functions such as the Gegenbauer, Jacobi, and (associated) Legendre polynomials as well as in terms of the hypergeometric and trigonometric functions. Several of these expansions have been implemented into the RACAH program; cf. the command Racah_expand( ) and Table 1, but need not to be displayed here explicitly.

Table 1
Optional arguments for the command Racah_expand() which, for various quantities from Racah's algebra, help to carry out Clebsch–Gordan and other expansions

Argument options	Brief description of execution
(*ClebschGordan*,*Ylm*,l$_1$,m$_1$,l$_2$,m$_2$,theta,phi)	Carries out a Clebsch–Gordan expansion on the product $Y_{l_1 m_1}(\vartheta,\varphi) Y_{l_2 m_2}(\vartheta,\varphi)$ of two spherical harmonics.
(*ClebschGordan*,*dmatrix*,j$_1$,p$_1$,q$_1$, j$_2$,p$_2$,q$_2$,beta)	Carries out a Clebsch–Gordan expansion on the product $d^{j_1}_{p_1 q_1}(\beta) d^{j_2}_{p_2 q_2}(\beta)$ of two rotation matrices (16).
(*ClebschGordan*,wexpr)	Expands all products of spherical harmonics and rotation matrices (with the same angular dependence) in terms of a Clebsch–Gordan series. Here, wexpr can be of type Racahexpr or Racahsum.
(*CG_dsquared*,j,p,q) or (*CG_Dsquared*,j,p,q,alpha,gamma1)	Expands the square of either a rotation matrix $[d^j_{pq}(\frac{\pi}{2})]^2$ or a Wigner D-function $[D^j_{pq}(\alpha, \frac{\pi}{2}, \gamma)]^2$ for the fixed angle $\beta = \pi/2$, cf. Eq. (17) and Ref. [1], Eq. (4.16:9).
(*dmatrix*,*Ylm*,l,m,theta,phi)	Expands the spherical harmonic $Y_{lm}(\vartheta,\varphi)$ in terms of the rotation matrices.
(*dmatrix*,wexpr)	Expands all spherical harmonics Ylm in wexpr in terms of the rotation matrices; wexpr can be either of type Racahexpr or Racahsum.
(*Gegenbauer*,*Ylm*,l,m,theta,phi) or (*Gegenbauer*,*dmatrix*,j,p,q,beta) or (*Gegenbauer*,*Dmatrix*,j,p,q,alpha,beta,gamma1)	Expands either the spherical harmonic $Y_{lm}(\vartheta,\varphi)$, the rotation matrix $d^j_{pq}(\beta)$, or the Wigner D–function in terms of the Gegenbauer polynomials.
(*hypergeom*,*Ylm*,l,m,theta,phi) or (*hypergeom*,*dmatrix*,j,p,q,beta) or (*hypergeom*,*Dmatrix*,j,p,q,alpha,beta,gamma1)	To carry out the same expansion but in terms of the hypergeometric function.
(*Jacobi*,*Ylm*,l,m,theta,phi) or (*Jacobi*,*dmatrix*,j,p,q,beta) or (*Jacobi*,*Dmatrix*,j,p,q,alpha,beta,gamma1)	To carry out the same expansion but in terms of the Jacobi polynomials.
(*Legendre*,*Ylm*,l,m,theta,phi) or (*Legendre*,*dmatrix*,j,p,q,beta) or (*Legendre*,*Dmatrix*,j,p,q,alpha,beta,gamma1)	To carry out the same expansion but in terms of the Legendre polynomials.
(*multipole*,f,theta,phi[,lmax]))	Performs a multipole expansion of the scalar function $f = f(\vartheta,\varphi)$. A series in terms of the spherical harmonics $Y_{lm}(\vartheta,\varphi)$ is returned with values $l = 0, \ldots, l_{\max}$ and $m = -l, \ldots, +l$.
(*tensor*,theta,phi,l$_1$,l$_2$,L,M) or (*tensor*,theta,phi,l$_1$,l$_2$,l$_{12}$, ..., L,M)	To return the components of the irreducible tensor product of two or more spherical harmonics, i.e. $\{\mathbf{Y}_{l_1}(\vartheta,\varphi) \otimes \mathbf{Y}_{l_2}(\vartheta,\varphi)\}_{l_{12}}$ or $\{\{\mathbf{Y}_{l_1}(\vartheta,\varphi) \otimes \mathbf{Y}_{l_2}(\vartheta,\varphi)\}_{l_{12}} \otimes \cdots\}_{LM}$, respectively.
(*trig*,*Ylm*,l,m,theta,phi)	Expands the spherical harmonic, $Y_{lm}(\vartheta,\varphi)$ in terms of a power series in $\sin\vartheta$.
(*trig*,*Ylm*,l,m,theta,phi,*Sin*) or (*trig*,*Ylm*,l,m,theta,phi,*Cos*) or (*trig*,*Ylm*,l,m,theta,phi,*halftheta*)	To expand the spherical harmonic $Y_{lm}(\vartheta,\varphi)$ in terms of a power series in $\sin\vartheta$, $\cos\vartheta$, $\sin\frac{\vartheta}{2}$ or $\cos\frac{\vartheta}{2}$, respectively.
(*trig*,*dmatrix*,j,p,q,beta)	Expands the rotation matrix $d^j_{pq}(\beta)$ in terms of a power series in $\sin\frac{\beta}{2}$ and $\cos\frac{\beta}{2}$.
(*Ylm*,*dmatrix*,j,p,q,beta) or (*Ylm*,*Dmatrix*,j,p,q,alpha,beta,gamma)	Expands the rotation matrix $d^j_{pq}(\beta)$ or the Wigner D-function $D^j_{pq}(\alpha,\beta,\gamma)$ in terms of the spherical harmonics.
(*Ylm*,wexpr)	Expands all rotation matrices in wexpr in terms of the spherical harmonics; wexpr can be either of type Racahexpr or Racahsum.

A more detailed description for the procedures can be found in Appendix A and in the file `Racah-commands.ps` which is distributed together with the program.

Integrals involving products of the rotation matrices. There are known various integrals over the full range of β (i.e. $0 \leqslant \beta \leqslant \pi$) which are often used in the evaluation of expressions

$$\int_0^\pi \mathrm{d}\beta \, \sin\beta d^j_{00}(\beta) = 2\delta_{j0}, \tag{21}$$

$$\int_0^\pi \mathrm{d}\beta \, \sin\beta d^j_{pq}(\beta) d^{j'}_{pq}(\beta) = \frac{2}{2j+1}\delta_{jj'}, \tag{22}$$

$$\int_0^\pi \mathrm{d}\beta \, \sin\beta d^{j_1}_{p_1q_1}(\beta) d^{j_2}_{p_2q_2}(\beta) d^{j_3}_{p_3q_3}(\beta)\delta_{p_1+p_2,p_3}\delta_{q_1+q_2,q_3} = \frac{2}{2j_3+1}\langle j_1p_1, j_2p_2|j_3p_3\rangle\langle j_1q_1, j_2q_2|j_3q_3\rangle. \tag{23}$$

Similar relations can be found also for products of more than three rotation matrices; in such cases, however, it might be simpler to first carry out a Clebsch–Gordan expansion on some part of the integrand before the integral is evaluated in detail. In the literature, moreover, there are often displayed so-called *invariant summations of integrals* involving the Wigner D-functions. In the RACAH program, we need not to deal with such invariant rules explicitly as they are included indirectly by cycling through the orthogonality and integral rules from above.

3. Extension and distribution of the RACAH program

During recent years, the RACAH package has grown considerably in its capabilities to deal with expressions from the theory of angular momentum. While originally the main attention in developing the program was paid

(i) to the algebraic manipulation [3] and in particular to the simplification of sums (over products) of the Wigner $n-j$ symbols [4,6], more recently we also followed two other lines:
(ii) to improve the numerical support of an enlarged number of symbols and functions from the theory of angular momentum [5], and
(iii) to incorporate the basic quantities from the atomic shell model as they are closely related to the concept of angular momentum [14,15].

In the latter case, we now provide access not only to the coefficients of fractional parentage (of various types) and the matrix elements of the unit tensors but also to the angular integrals for one- and two-particle operators, taken within a basis of symmetry-adapted subshell states. The implementation of this third line now builds up the JUCYS module and, owing to its particular range of applications, this might become separated from the future development of the RACAH program. With the present extension to the program, we *turn back* again our emphasis to the symbolic simplification of so-called Racah expressions which, apart from the Wigner $n-j$ symbols, Clebsch–Gordan coefficients as well as (various) integrals over the spherical harmonics, may now also include the Wigner rotation matrices and integrals hereover. Fig. 1 shows the *updated* general structure of Racah expressions which are currently supported by the program.

There is no need here to recall all the strategies which we follow internally within the RACAH program in order to achieve a symbolic evaluation of Racah expressions such as displayed in Fig. 1. As before, the program attempts to simplify a given expression by reducing successively the number of summation indices and/or the number of symbols and functions. However, while such a stepwise reduction of the complexity of an expression does not always ensure to obtain finally the *most simple form*, it typically results in a considerable simplification, in particular, when compared with the complexity of the original expressions as found by the straightforward coupling of all the angular momenta involved.

Of course, the incorporation of the Wigner D-functions and rotation matrices into the framework of RACAH has caused a number of modifications in the code which we shall briefly summarize here. Since, in RACAH, all parts of a typical expression from Racah's algebra are treated as logical objects in course of the symbolic manipulation, a new data type dmatrix has been defined with respect to which any variable or expression may be tested. For this additional type, a call `type(a,dmatrix)` returns a boolean value of either *true* or *false* similar as for all other types of MAPLE. Internally, the data type dmatrix has the list structure

dmatrix := [*dmatrix*‡, j, p, q, ang]

which, in a general Racah expression, now occurs as an additional substructure of the Rproduct list, aside of other substructures such as wnj to represent a Wigner $n-j$ symbol or Ylm for a spherical harmonic, respectively. As before, all these substructures are allowed to occur in any arbitrary number and order in the Rproduct list. Obviously there is no need to introduce also a data structure for the D-functions in addition, as these functions are internally treated in terms of the reduced rotation matrices owing to the relation $D^j_{pq}(\alpha,\beta,\gamma) = e^{-i(\alpha p+\gamma q)} d^j_{pq}(\beta)$, cf. Eq. (3), and by incorporating the first exponential factor $e^{-i(\alpha p+\gamma q)}$ into the expression of Rfactor. Apparently, this internal treatment of the Wigner D-functions does not restrict the application of the RACAH program but helps reduce the number of algebraic rules that need to be incorporated and recognized by the program.

At the user level, the main modifications of the present extension mainly concerns the procedures Racah_evaluate(), Racah_expand(), and the new command Racah_asymptotics(). Similar as for the Wigner $n-j$ symbols and spherical harmonics, Racah_evaluate() tests for the occurrence of one or several rotation matrices in a given expression. If found, it attempts a simplification of the overall expression by calling the proper sum and integration rules. In order that an integral can be evaluated explicitly, however, it is usually necessary that a factor $\sin\beta$ has been added before Racah_evaluate() is invoked. The integrals over α and γ (if one starts from expressions which include the Wigner D-functions), in contrast, can be carried out by calling MAPLE's integration procedures if the dependence of the overall expressions on these variables is properly analyzed before. Note that for these angles, the upper and lower bounds of the integrals must be given explicitly since otherwise MAPLE might not be able to determine the integral. By defining the boundaries, the user may wish to control the volume of the integration, for instance, if Wigner functions with integer or half-integer j values occur simultaneously (cf. Ref. [1], Section 4.10 for a more detailed discussion). In using the Euler angles α, β, and γ in the set-up of some Racah expression, the user has to be aware that `gamma` is a protected name in MAPLE (to represent Euler's constant) which should be avoided in this form. Although the use of this 'variable' does often not cause a termination of the program immediately, it may result in rather surprising ERRORs later in course of the algebraic manipulation. Therefore, we often use the variable `gamma1` instead, cf. Table 1. There is another word of caution here which the reader should keep in mind: Although the RACAH program allows for a fast symbolic manipulation of expressions, it appears internally often difficult to recognize the proper definition of the substructures of an expression. Therefore, the user must ensure that all angular momenta must finally evaluate (if given explicitly) to integer and half-integer values and that they satisfy proper coupling conditions.

Apart from the symmetries and the frequently occurring sum and integration rules, we now also support the transformation between the various types of special functions. To this end, Racah_expand() has been entirely reworked to incorporate a much larger set of special functions into which an expression can be transformed; cf. Table 1 for the various argument options of this procedure. In addition to the mutual transformation between the spherical harmonics and the rotation matrices, these functions may now be expressed also in terms of the hypergeometric functions or the Jacobi, Gegenbauer, or (associated) Legendre polynomials. Moreover, products of the spherical harmonics or Wigner rotation matrices may be re-expressed in terms of a corresponding Clebsch–Gordan expansion. With regard to the asymptotic behavior of the rotation matrices and spherical harmonics, the command Racah_asymptotics() has been added to the code to provide the user also with the asymptotic expressions in the limit of quite different parameters. Table 2 summarizes the main features of this procedure.

As previously, the RACAH package as a whole is distributed by the tar file `Racah2004.tar` from which the `Racah2004` root directory is (re-)generated by the command `tar -xvf Racah2004.tar`. For WINDOWS, moreover, we also provide the *zipped* file `Racah2004-windows.zip` which comprises the same root directory. This directory contains the source code libraries (for MAPLE 7 and 8), a `Read.me` for the installation of the program as well as the document `Racah-commands.ps`. In fact, this document may serve as a short manual which provides the definition of all the *data structures* of the RACAH program as well as an alphabetic list of all user relevant (and exported) commands. Although emphasis was placed to preserve the compatibility of the program with respect to earlier releases of MAPLE, this cannot always be ensured due to changes in the MAPLE syntax. However, care has been taken to modify the *visible part* of the procedures as little as possible. The `Racah2004` root also contains an example of a `.mapleinit` file which can easily be modified and incorporated into the user's `home`. Making use of such a `.mapleinit` file, then, the module Racah should be available like any other module of MAPLE.

4. Examples

To illustrate how the present extension of the RACAH program facilitates the algebraic simplification of those expressions, which include the rotation matrices, here we display a number of examples from the literature. While the first two examples can be considered as *standard problems*, referring to the use of the symmetry and orthogonality of the Wigner D-functions, the third one demonstrates how the program may help in deriving the selection rules for the absorption or emission of photons in the interaction of diatomic molecules with the radiation field.

Example 1 *(Unitary relation).* Let us start by analyzing the simple expression

$$\sum_m (-1)^{2p-q-m} D^j_{-p,-m}(\gamma,-\beta,\alpha) D^{j*}_{mq}(\alpha,\beta,\gamma) e^{-2im\alpha-2iq\gamma} \tag{24}$$

for its *orthogonality properties* with respect to products of the Wigner D-functions. Although we may expect to find a simplification due to the unitary relations (9) or (10), it cannot be *read off* immediately without using further symmetries of the rotation matrices. By using the RACAH program (in the text mode)

Table 2
Asymptotic expansions for the rotation matrices and spherical harmonics as obtained from the command Racah_asymptotics(). A second argument is used to specify the particular expansion by means of a proper *keyword* string

Argument options	Brief description of execution
(dmatrix,`"j»1"`)	Returns the asymptotic expansion of a Wigner rotation matrix d^j_{pq} [as given by dmatrix] for a large angular momentum, i.e. $j \gg 1$ (cf. Ref. [1], Eq. (4.18.1)).
(dmatrix,`"finite j*beta"`)	To return the asymptotic expansion of a rotation matrix d^j_{pq} in terms of a Bessel function in the limits of $j \to \infty$ and $\beta \to 0$ but if $j\beta < \infty$ still remains finite (cf. Ref. [1], Eq. (4.18.2)).
(dmatrix,`"beta->0"`) or (dmatrix,`"beta->Pi"`)	To return the asymptotic expression for a rotation matrix for $\beta \to 0$ or $\beta \to \pi$, respectively.
(Ylm,`"l»1"`)	Returns the asymptotic expansion of a spherical harmonic for large angular momentum, i.e. $l \gg 1$ and $l \gg m > 0$. This expansion is valid for all angles ϑ, φ with $\epsilon \leqslant \vartheta \leqslant \pi - \epsilon$, $(0 < \epsilon \ll 1/l)$ and for $0 \leqslant \varphi < 2\pi$ in zero order in l, neglecting terms of $\mathrm{O}(1/l)$ and higher.
(Ylm,`"l»1 O(1/l)"`)	To return the same as above but by including terms of the order $\mathrm{O}(1/l)$ and by neglecting only higher terms.
(Ylm,`"theta->0"`)	To return the asymptotic expansion of a spherical harmonic for $\vartheta \to 0$.
(Ylm,`"theta->Pi/2"`)	To return the same for $\vartheta \to \pi/2$, i.e. in the range $\pi/2 - \epsilon \leqslant \vartheta \leqslant \pi/2 + \epsilon$.
(Ylm,`"theta->Pi"`)	To return the same for $\vartheta \to \pi$.
(Ylm,`"McDonald"`)	Returns the asymptotic expansion of a spherical harmonic for small ϑ in terms of Bessel functions (up to $\sin(\frac{\vartheta}{2})^2$) due to the McDonald formula.
(Ylm,`"Bessel"`)	To return the asymptotic expansion of a spherical harmonic for $m, l \to \infty$, $\vartheta \to 0$ but if $l\vartheta < \infty$ still remains finite.

```
> with(Racah);
                                 Welcome to Racah!

[Racah_ClebschGordan, Racah_CondonShortley, Racah_Dmatrix, Racah_Gaunt,Racah_Umatrix,
   Racah_Wcoefficient, Racah_Ylm, Racah_add, Racah_animate3d, Racah_bipolarY,
   Racah_compute, Racah_delete, Racah_delta, Racah_diff, Racah_dmatrix,
   ...
   Racah_w3j_range, Racah_w6j, Racah_w6j_range, Racah_w9j]
```

however, we may enter this expression and test it for possible simplifications by typing

```
> wa := Racah_set(sum,m,phase,2*p-q-m,factor,exp(-I*2*m*alpha-I*2*q*gamma1),
                  Dmatrix(j,-p,-m,gamma1,-beta,alpha),
                  Dmatrixcc(j,m,q,alpha,beta,gamma1)):
> Racah_print(wa);

--->
                               SUM{m}
                               (2 p - q - m)
                            (-1)
    exp(m alpha I + q gamma1 I) exp(p gamma1 I + m alpha I)
        exp(-2 I m alpha - 2 I q gamma1)
                              d^{j}_{m,q} (beta)
                            d^{j}_{-p,-m} (-beta)
> Racah_evaluate(wa):
> Racah_print(%);
--->
                                delta(p,q)
```

As seen from the first (input) line, the expression can be entered rather similar to its mathematical form including a proper notation for the complex-conjugate of the D-functions. The whole expression (24) finally simplifies to a Kronecker δ_{pq} by taking the symmetries and orthogonality of the Wigner D-functions into account. For such a simple example, of course, the main advantage is that the final result is sorted out properly without that the user need to remember to all the detailed symmetries of the Wigner rotation matrices and related functions.

Example 2 *(Rotational invariance of scalar quantities).* Since the spherical harmonics $\{Y_{LM}(\theta,\phi), M=-L,-L+1,\ldots,L\}$ are known to form a spherical tensor of rank L, the expression

$$Q=\frac{4\pi}{2L+1}\sum_M Y^*_{LM}(\theta_i,\phi_i)Y_{LM}(\theta_j,\phi_j) \tag{25}$$

is invariant under rotation even if the polar angles (θ_i,ϕ_i) and (θ_j,ϕ_j) refer to two different sets of coordinates [16,17]. We may prove this explicitly by carrying out a rotation $\mathbf{R}Y_{LM}(\theta_i,\phi_i)=\sum_{M'}D^L_{M'M}(\phi,\theta,\chi)Y_{LM'}(\theta_i,\phi_i)$ on both spherical harmonics in Eq. (25)

$$Q'=\frac{4\pi}{2L+1}\sum_M\sum_{M_1}\sum_{M_2}D^{L*}_{M_1M}(\phi,\theta,\chi)D^L_{M_2M}(\phi,\theta,\chi)Y^*_{LM_1}(\theta_i,\phi_i)Y_{LM_2}(\theta_j,\phi_j), \tag{26}$$

and by *evaluating* this expression by means of the RACAH program

```
> Qprime:=Racah_set(sum,M,M1,M2,factor,4*Pi/(2*L+1),
                    Dmatrixcc(L,M1,M,phi,theta,chi),Dmatrix(L,M2,M,phi,theta,chi),
                    Ylmcc(L,M1,thetai,phii),Ylm(L,M2,thetaj,phij)):
> Racah_print(Qprime);

--->
                       SUM{M,M1,M2}
                               M1
                            (-1)
```

```
    4 exp(-M2 phi I - M chi I) exp(M1 phi I + M chi I) Pi
    -----------------------------------------------------
                           2 L + 1
                  Y_{L,-M1} (thetai,phii)
                    d^{L}_{M2,M} (theta)
                    d^{L}_{M1,M} (theta)
                   Y_{L,M2} (thetaj,phij)
> Racah_evaluate(Qprime):
> Racah_print(%);

--->
           SUM{M1}
                 M1
             (-1)
             4 Pi
             -------
             2 L + 1
    Y_{L,-M1} (thetai,phii)
    Y_{L,M1} (thetaj,phij)
```

which, indeed, shows that $Q' = Q$ is invariant under a rotation of the coordinates if the symmetry of the spherical harmonics $Y^*_{L,M}(\vartheta,\varphi) = (-1)^M Y_{L,-M}(\vartheta,\varphi)$ is taken into account. Note that in typing the expression (26), we did not specify the range of the summation indices in detail, say for $M = -L,\dots,L$. In general, these ranges of summation need not to be given explicitly as the RACAH program analyzes the overall Racah expression for its dependence on the summation indices. Then, if a summation index is recognized to be a *magnetic*-type quantum number, the *full* range is adopted as default, such as $M = -L, -L+1,\dots,L$. Internally, moreover, the Wigner D-functions, $D^j_{pq}(\alpha,\beta,\gamma)$, are always treated in terms of its factorized form (3) as described above.

Example 3 *(Selection rules for the rotational transitions of diatomic molecules).* Microwave spectroscopy is known to provide an invaluable tool for determining the geometrical structure and the dipole moments of gas–phase molecules. To analyze the observed spectra, then, the Born–Oppenheimer approximation is often utilized in the theoretical description, by which the electrons are assumed to move very rapidly around the nuclei (and where the translational motion of the molecule as a whole is also separated). Generally, in fact, it can be shown that this approximation is very well satisfied in order to generate the molecular wavefunctions. An additional separation of the Hamiltonian into a rotational and vibrational part further implies a *rovibrational* wave function of the form

$$\psi_{\nu JKM} = \chi_\nu(q) D^J_{KM}(\Omega)$$

where $q = R - R_e$ denotes the displacement of the atom from its equilibrium distance (bond length) and $D^J_{KM}(\Omega) \equiv D^J_{KM}(\varphi,\vartheta,\xi)$ a Wigner D-function. In this form, the (Euler) angles ϑ, φ, and ξ describe the rotation of the body-fixed coordinates (with $\mathbf{e}_z$ parallel to the internuclear axis) with respect to the coordinates in the laboratory.

In understanding the microwave spectrum, one is mainly interested in the electric-dipole allowed E1 transitions among the rovibrational levels of the electronic ground state, $\nu_i J_i K_i M_i \to \nu_f J_f K_f M_f$. Although the dipole moment $\vec{\mu} = \vec{\mu}(q)$ depend in general, of course, on the internuclear distance, its modulus $|\vec{\mu}(q)| = |\vec{\mu}_o| + \frac{\partial\vec{\mu}}{\partial q}|_{q=0} \cdot \mathbf{q} + \cdots \approx \mu_o$ is taken to be constant in lowest-order approximation and is often called the *permanent* dipole moment. In the laboratory (space-fixed) coordinates, nevertheless, the dipole moment

$$\vec{\mu}_o = \mu_x \mathbf{e}_x + \mu_y \mathbf{e}_y + \mu_z \mathbf{e}_z = \mu_o(\sin\vartheta\cos\varphi\,\mathbf{e}_x + \sin\vartheta\sin\varphi\,\mathbf{e}_y + \cos\vartheta\,\mathbf{e}_z) \tag{27}$$

still depends on the orientation of the molecules. While, in this low-order approximation, the dipole operator $\vec{\mu}_o$ cannot cause transitions between different vibrational states of the molecule, it may lead to transitions between the rotational levels of the same vibrational state ($\nu = \text{const.}$). In the following, we further investigate these rotational transitions and leave other transitions aside concerning the vibrational, translational, or even the electronic state of the molecule [18].

In the absence of an electric or magnetic field, all directions are equivalent in the laboratory frame. Therefore, the three components of the dipole moment $\vec{\mu}_o$ are given by

$$\mu^{fi} = \mu_0 \int \mathrm{d}\Omega\, D^{J_f *}_{M_f K_f}(\Omega) \begin{Bmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{Bmatrix} D^{J_i}_{M_i K_i}(\Omega) \neq 0, \tag{28}$$

where $\int \mathrm{d}\Omega \ldots = \int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \sin\theta\,\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\xi \ldots$ and where the entries in the curly brackets refer to the x-, y-, and z-components of the dipole moment. We may evaluate these integrals by means of RACAH program in order to determine the selection rules for the

E1 allowed transitions, i.e. the conditions on the $J_i K_i M_i$ and $J_f K_f M_f$ quantum numbers for which a non-zero value may arise for any of the three integrals in Eq. (28).

Obviously, the r.h.s. of Eq. (28) fulfills our notion of being a Racah expression as shown in Fig. 1. Therefore, we can enter these three integrals directly into MAPLE and evaluate them by means of the RACAH program. For instance, if μ_z^{fi} is taken, we arrive after the integration over φ and ξ at

```
> mu_z := Racah_set(int,varphi,0,2*Pi,int,xi,0,2*Pi,int,vartheta,
                    factor,sin(vartheta),factor,cos(vartheta),
                    Dmatrixcc(Jf,Mf,Kf,varphi,vartheta,xi),
                    Dmatrix(Ji,Mi,Ki,varphi,vartheta,xi)):
> mu_z1:=Racah_integrate(mu_z):
> Racah_print(%);

--->
            /
           |
           | dvartheta
           |
          /

        2
     4 Pi  sin(vartheta) cos(vartheta)
        delta(Mi,Mf) delta(Ki,Kf)
        d^{Ji}_{Mi,Ki} (vartheta)
        d^{Jf}_{Mf,Kf} (vartheta)
```

including now two Kronecker δ-factors and a summation over a product of two Wigner rotation matrices. For the further simplification of this integral, there are two steps necessary to evaluate the integral over ϑ because the additional $\cos\vartheta$ factor must be first 're-written' in terms of proper rotation matrices. Therefore, in order to obtain the final expression, we must call twice Racah_evaluate(), but where we print also the intermediate results for the guidance of the reader

```
> mu_z2:=Racah_evaluate(mu_z1): Racah_print(%);
  mu_z3:=Racah_evaluate(mu_z2): Racah_print(%);

--->

         /
        |
        | dvartheta
        |
       /

         2
      4 Pi  sin(vartheta)
 delta(Kf,Ki) delta(Mf,Mi)
  d^{1}_{0,0} (vartheta)
 d^{Ji}_{Mf,Kf} (vartheta)
 d^{Jf}_{Mf,Kf} (vartheta)

Setting boundaries of vartheta to 0 and Pi...

--->
            (2 Ji - Mf - Kf)
         (-1)

                    2
                8 Pi

     delta(Kf,Ki) delta(Mf,Mi)
     w3j(Ji,1,Jf,Mf,0,-Mf)
     w3j(Ji,1,Jf,Kf,0,-Kf)
```

For the z-component of the transition moment, therefore, we finally obtain

$$\mu_z^{fi} \sim \delta_{K_f,K_i}\delta_{M_f,M_i}\begin{pmatrix} J_i & 1 & J_f \\ M_f & 0 & -M_f \end{pmatrix}\begin{pmatrix} J_i & 1 & J_f \\ K_f & 0 & -K_f \end{pmatrix}$$

and with a rather similar result also for the two other components μ_x^{if} and μ_y^{if}, respectively.

Here, we leave these computations to the reader. A more straightforward derivation of the selection rules for the E1 transitions among the rovibrational levels is obtained if the dipole moment $\vec{\mu} = \mu_{-1}\mathbf{e}_{-1} + \mu_0\mathbf{e}_0 + \mu_{+1}\mathbf{e}_{+1}$ is taken within spherical rather than cartesian coordinates. In such coordinates, of course, the three components $\mu_q \sim Y_{1q}(\vartheta,\varphi) \sim D^1_{q0}(\ldots)$, $q = 0, \pm 1$ (ξ arbitrary) are known to transform like the Wigner functions of rank 1 and with one of the magnetic quantum number being *zero*. By omitting further phase considerations, we may therefore evaluate

```
> u_q: = Racah_set(int,varphi,0,2*Pi,int,xi,0,2*Pi,int,vartheta,
                    factor,sin(vartheta),
                    Dmatrixcc(Jf,Mf,Kf,varphi,vartheta,xi),
                    Dmatrix(1,q,0,varphi,vartheta,xi),
                    Dmatrix(Ji,Mi,Ki,varphi,vartheta,xi)):
> u_q1 := Racah_integrate(u_q):
> Racah_print(u_q1);

--->

       /
      |
      | dvartheta
      |
     /

        2
    4 Pi sin(vartheta)
    delta(Mi+q,Mf) delta(Ki,Kf)
    d^{Ji}_{Mi,Ki} (vartheta)
    d^{1}_{q,0} (vartheta)
    d^{Jf}_{Mf,Kf} (vartheta)
```

and, again, evaluate this expression by a call to Racah_evaluate(),

```
> u_q2:=Racah_evaluate(u_q1):
> Racah_print(u_q2);

Setting boundaries of vartheta to 0 and Pi...

--->
         (2 Ji - Mi - q - Kf)
     (-1)

                    2
            8 Pi

    delta(Kf,Ki) delta(Mf,Mi+q)
       w3j(1,Ji,Jf,q,Mi,-Mi-q)
        w3j(1,Ji,Jf,0,Kf,-Kf)
```

from which the selection rules can be easily read off. Taking the Kronecker symbols into account and by making use of the triangular rules for the Wigner $3-j$ symbols we see that, for a nonvanishing permanent dipole moment μ_o, the selection rules become

$$\Delta J = J_i - J_f = 0, \pm 1, \qquad M_i - M_f = 0, \pm 1, \qquad K_i - K_f = 0 \tag{29}$$

since $q = 0, \pm 1$. For this reason, microwave spectroscopy may connect within lowest order only rotational states that differ in the total angular momentum by $\Delta J \leqslant 1$ [18].

In summary, a new and extended version of the RACAH program has been presented which enlarges its range of application considerably. As seen from the last example, this concerns especially the description of all those quantum processes where, within a first step of the derivation, different axes in space are used for quantization. With the present implementation of the algebraic properties and rules of the Wigner rotation matrices, we therefore hope to provide a useful tool for quite different fields in physics. But despite of all recent advances, there is still room for further improvements of the RACAH program concerning, for instance, various concepts from the theory of spherical tensor operators or the use of the (hyper-)spherical harmonics in spaces $\mathcal{R}^n$ with a dimension $n > 3$. Since, eventually, the success of such a development depends on the acceptance at the user's side, comments on the RACAH program and the report of bugs are always appreciated.

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Appendix A. Additional and modified procedures for the RACAH package

In this appendix, we briefly summarize the new and modified procedures (arranged in alphabetical order) that are available for the interactive use of the RACAH package. As before, we follow the style of the former *Maple Handbook* [19] to provide a short description of each command but without showing explicit examples. The idea is to give just sufficient information that the test examples in Section 4 can be followed up by the reader. A full account of all presently available commands as seen by the user is given in the file `Racah-commands.ps` which is distributed together with the source code.

- **Racah_asymptotics(dmatrix,"j»1")**
  Returns the asymptotic expression for a rotation matrix $d^{(j)}_{pq}(\beta)$ in the limit that $j \gg 1$.
  Output: An algebraic expression is returned.
  Argument options: See Section 3, Table 2 for further optional arguments.
  Additional information: Instead of a rotation matrix (dmatrix), asymptotic expressions can be obtained also for the spherical harmonics (i.e. for the internal data type Ylm). ♣ To arrive at an asymptotic expansion, the two *magnetic* quantum numbers p and q must be given numerically. ♣ Infinitesimal rotations are not (yet) supported for the rotation matrix $d^j_{pq}(\beta)$.
  See also: Racah_expand().
- **Racah_expand(*ClebschGordan*,wexpr)**
  Carries out a Clebsch–Gordan expansion on wexpr which can be of the type Ylm, dmatrix, Racahexpr, or Racahsum (see below).
  Output: An expression is returned.
  Argument options: See Section 3, Table 1 for further optional arguments.
  Additional information: For (*ClebschGordan*,wexpr), an alternative keyword *CG* can be used. Moreover, an optional third argument can be used to declare the depth of the expansion. ♣ For expansions with keywords *hypergeom* and *Jacobi*, the magnetic quantum numbers should represent either integer and half integers. Otherwise, the program terminates with an appropriate ERROR message. ♣ Numerical arguments are checked to represent proper magnetic quantum numbers and angles. ♣ For the expansion of a rotation matrix $d^j_{pq}(\beta)$ or a Wigner D-function in terms of spherical harmonics, at least one of the magnetic quantum numbers p or q must be zero, i.e. an expansion is possible only for $d^j_{0k}(\beta)$, $d^j_{k0}(\beta)$, $D^j_{0k}(\alpha, \beta, \gamma)$, or $D^j_{k0}(\alpha, \beta, \gamma)$, respectively. If, moreover, j and k are given numerically, they must represent integers; the program terminates with a ERROR message if this is not the case.
- **Racah_recursionfordmatrix(nrule,dmatrix)**
  Applies one of the known recursion relations for the Wigner rotation matrix dmatrix as 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 either be an integer in the range $n = 1, \ldots, 21$ or one of the allowed keywords as displayed in Table 3.
  See also: Racah_recursionforw3j().
- **Racah_set(*keyword*$_1$(args$_1$),..., *keyword*$_n$(args$_n$))**
  Enters one or more Wigner $n-j$ symbols, spherical harmonics, and Wigner rotation matrices, or other substructures from Racah's algebra into the (internal MAPLE) representation of a Racahexpr. *keyword* can describe any structure of type int, Racahexpr, tdelta, wnj, Ylm, and now dmatrix.
  Argument options:(*Racahexpr*(wnj$_1$,..., wnj$_n$, Ylm$_1$,..., Ylm$_n$, dmatrix$_1$, ..., dmatrix$_n$, ...)) to enter Wigner $n-j$ symbols wnj$_i$, spherical harmonics Ylm$_i$, and Wigner rotation matrices dmatrix$_i$ into a single Racahexpr. ♣ (*dmatrix*(j,p,q,beta),...) or (*dmatrix*,j,p,q,beta) to enter a Wigner rotation matrix $d^j_{pq}(\beta)$; a type dmatrix expression is returned. ♣ (*Dmatrix*(j,p,q,alpha,beta,gamma1),...) to enter a Wigner D-function $D^j_{pq}(\alpha, \beta, \gamma)$. The additional keywords *Dmatrixcc* and *conjugateDmatrix* can be used to enter the complex conjugate of a Wigner D-function $D^j_{pq}(\alpha, \beta, \gamma)$.

Table 3
Recursion relations for the Wigner rotation matrices. The *keywords* from column 2 can be used alternatively to specify the proper recursion; cf. Ref. [1], Eqs. (4.8.1)–(4.8.21)

nrule	Keyword	Short description
1	`"j->j+-"`	$d^j_{pq} \to d^{j-1}_{pq}, d^j_{pq}, d^{j+1}_{pq}$
2	`"j->j+-; p-"`	$d^j_{pq} \to d^{j-1}_{p-1q}, d^j_{p-1q}, d^{j+1}_{p-1q}$
3	`"j->j+-; p+"`	$d^j_{pq} \to d^{j-1}_{p+1q}, d^j_{p+1q}, d^{j+1}_{p+1q}$
4	`"j->j+-; q-"`	$d^j_{pq} \to d^{j-1}_{pq-1}, d^j_{pq-1}, d^{j+1}_{pq-1}$
5	`"j->j+-; q+"`	$d^j_{pq} \to d^{j-1}_{pq+1}, d^j_{pq+1}, d^{j+1}_{pq+1}$
6	`"j->j+-; pq-"`	$d^j_{pq} \to d^{j-1}_{p-1q-1}, d^j_{p-1q-1}, d^{j+1}_{p-1q-1}$
7	`"j->j+-; pq+"`	$d^j_{pq} \to d^{j-1}_{p+1q+1}, d^j_{p+1q+1}, d^{j+1}_{p+1q+1}$
8	`"j->j+-; p-; q+"`	$d^j_{pq} \to d^{j-1}_{p-1q+1}, d^j_{p-1q+1}, d^{j+1}_{p-1q+1}$
9	`"j->j+-; p+; q-"`	$d^j_{pq} \to d^{j-1}_{p+1q-1}, d^j_{p+1q-1}, d^{j+1}_{p+1q-1}$
10	`"j->j+-1/2; pq-1/2"`	$d^j_{pq} \to d^{j-1/2}_{p-1/2q-1/2}, d^{j+1/2}_{p-1/2q-1/2}$
11	`"j->j+-1/2; a"`	$d^j_{pq} \to d^{j-1/2}_{p-1/2q+1/2}, d^{j+1/2}_{p-1/2q+1/2}$
12	`"j->j+-1/2; pq+1/2"`	$d^j_{pq} \to d^{j-1/2}_{p+1/2q+1/2}, d^{j+1/2}_{p+1/2q+1/2}$
13	`"j->j+-1/2; b"`	$d^j_{pq} \to d^{j-1/2}_{p+1/2q-1/2}, d^{j+1/2}_{p+1/2q-1/2}$
14	`"j->j--1/2; c"`	$d^j_{pq} \to d^{j-1/2}_{p+1/2q+1/2}, d^{j-1/2}_{p-1/2q+1/2}$
15	`"j->j--1/2; d"`	$d^j_{pq} \to d^{j-1/2}_{p+1/2q-1/2}, d^{j-1/2}_{p-1/2q-1/2}$
16	`"q->q+-"`	$d^j_{pq} \to d^j_{pq-1}, d^j_{pq+1}$
17	`"p->p+-"`	$d^j_{pq} \to od^j_{p-1q}, d^j_{p+1q}$
18	`"pq->p-; q+-"`	$d^j_{pq} \to d^j_{p-1q-1}, d^j_{p-1q}, d^j_{p-1q+1}$
19	`"pq->p+; q+-"`	$d^j_{pq} \to d^j_{p+1q-1}, d^j_{p+1q}, d^j_{p+1q+1}$
20	`"pq->p+-; q-"`	$d^j_{pq} \to d^j_{p-1q-1}, d^j_{pq-1}, d^j_{p+1q-1}$
21	`"pq->p+-; q+"`	$d^j_{pq} \to d^j_{p-1q+1}, d^j_{pq+1}, d^j_{p+1q+1}$

Additional information: Allowed Racah objects can be of the following types: Racahexpr, wnj, Ylm, and dmatrix. See the file `Racah-commands.ps` for a full description of this command.
See also: Racah_compute(), Racah_evaluate().

- **Racah_symmetricdmatrix(n,dmatrix)**
  Returns the nth symmetric form of $d^j_{pq}(\beta)$ where n must be in the range $1 \leqslant n \leqslant 12$, cf. Eqs. (4)–(7).
  Output: A Racahexpr is returned.
  Additional information: There are 12 symmetric forms of $d^j_{pq}(\beta)$. When n is in the range $1 \leqslant n \leqslant 8$, it returns an equivalent form where only the quantum numbers are changed, while for $9 \leqslant n \leqslant 12$ both the quantum numbers as well as the angles may change. ♣ The output Racahexpr has always a Rfactor equals 1, Rsummationset = {NULL} and Rdelta = [‘Rdelta#’].
  See also: Racah_symmetricw3j(), Racah_symmetricw6j(), Racah_symmetricw9j(), Racah_symmetricYlm().

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