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Analytical and numerical treatment of auxiliary function $B^{j}_{m'm}(\beta)$ for finite rotation matrix elements

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Abstract In this study, a new method evaluate the auxiliary function $B^{j}_{m'm}(\beta)$ which the function appears in the matrix elements $d^{j}_{m',m}(\beta)$ are formulated. Also, the generating functions, Rodrigues' formula, and orthogonality relationships for the $B^{j}_{m'm}(\beta)$ function are presented. To analyze their formal mathematical structure, $B^{j}_{m'm}(\beta)$ functions are expressed in terms of the Jacobi, Gegenbauer, Legendre, and Chebyshev polynomials. $B^{j}_{m'm}(\beta)$ functions and their linear combinations are calculated numerically for large values of the indices j, m', m quantum numbers and β angles by using generating function. Finally, evaluating numerical values for them are checked with obtained control expressions and results of Öztekin and Özcan (J Math Chem 44:28, 2008).

Keywords Rotation matrix elements · Auxiliary functions · Generating functions

1 Introduction

The matrix representations of finite rotations appear occasionally in physical problems such as of angular momentum. In quantum chemistry and physics, they occur for instances as factor of applications of these molecular spectroscopy. Their many properties and derivations have been investigated by Edmonds [1], Fano and Racah [2], Rose [3], Zare [4], Ivanic and Ruedenberg [5], Altmann and Bradley [6], and recently Choi et al. [7].

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The Wigner D functions denotes an element of the rotation matrix, the rotation being describing by a set of three Euler angles, which we shall called α, β, and γ. Their properties can be easily found in the literature. The dependence on α and γ of the matrix representation of the rotation operator R can be determined very simply. We shall follow the notation of Ref. [3]. The elements of the finite rotation matrix can be make dependent of them through

$$\begin{aligned} D^{j}_{m',m}(\alpha\beta\gamma) &= e^{-im'\alpha}\left\langle jm' \left| e^{-i\beta J_y} \right| jm \right\rangle e^{-im\gamma} \\ &= e^{-im'\alpha} d^{j}_{m',m}(\beta)\, e^{-im\gamma} \end{aligned} \tag{1}$$

Since $d^{j}_{m',m}(\beta)$ is unitary and real, the following symmetry relations are satisfied

$$\begin{aligned} d^{j}_{m',m}(\beta) &= d^{j}_{m,m'}(-\beta) \\ &= (-1)^{m-m'} d^{j}_{m,m'}(\beta) \\ &= (-1)^{m-m'} \left(d^{j}_{m',m}(\beta) \right)^{*} \\ &= d^{j}_{-m,-m'}(\beta) \\ &= (-1)^{m-m'} d^{j}_{-m',-m}(\beta) \end{aligned} \tag{2}$$

Once we obtain the matrix elements $d^{j}_{m',m}(\beta)$, the construction of the full rotation matrix elements $D^{j}_{m',m}$ is simple because of Eq. 1. Using the group theory, a general expressions $D^{j}_{m',m}$ has been obtained Wigner and also given by Rose [3]

$$\begin{aligned} d^{j}_{m',m}(\beta) = &\left\{ \frac{F_m(j+m)\, F_{m'}(j+m')}{F_m(j)\, F_{m'}(j)} \right\}^{1/2} \left(\cos\frac{\beta}{2} \right)^{2j} \\ &\sum_i (-1)^{i+m'-m} \frac{F_m(m'+i)\, F_{i-m}(j)\, F_{m'+i}(j)}{F_m(i)} \left(\tan\frac{\beta}{2} \right)^{m'-m+2i} \end{aligned} \tag{3}$$

where $F_m(n)$ are binomial coefficients and the sum over i runs through all integer values for which the factorials involved exists.

$D^{j}_{m',m}$ matrix elements have been expressed by product of two auxiliary functions as following forms [8];

$$D^{j}_{m'm}(\alpha, \beta, \gamma) = e^{-im'\alpha} A^{j}_{m',m}(\beta)\, B^{j}_{m',m}(\beta)\, e^{-im\gamma} \tag{4}$$

The representations of the auxiliary functions $A^{j}_{m',m}(\beta)$ and $B^{j}_{m',m}(\beta)$ are defined by Eqs. 12 and 13 in Ref. [8]:

$$A^{j}_{m',m}(\beta) = \left[\frac{(j+m)!\,(j+m')!}{(j-m)!\,(j-m')!}\right]^{1/2} \left(\cos\frac{\beta}{2}\right)^{m+m'} \left(\sin\frac{\beta}{2}\right)^{m'-m}$$
$$B^{k}_{i,l}(\beta) = \frac{1}{\Gamma(k)}\left(\frac{2}{\cos\beta - 1}\right)^{i} {}_2F_1\left(i, l; k; \frac{\cos\beta + 1}{\cos\beta - 1}\right) \tag{5}$$

In Ref. [8], it was demonstrated that the auxiliary functions for $d^{j}_{m',m}(\beta)$ coefficients are a fairly complicated mathematical objects. Therefore, in this paper I prefer to use a completely different approach, namely, that of generating functions. These functions have a relatively easy mathematical structure to obtain recurrence relations, orthogonality relationships, special values, and analytical expressions for $B^{j}_{m',m}(\beta)$ functions. Consequently, these functions may be considered to find some fundamental entities for $B^{j}_{m',m}(\beta)$ and so far $d^{j}_{m',m}(\beta)$. Because of the simplicity of the generating functions it is an obvious idea to evaluate new analytical expressions for $B^{j}_{m',m}(\beta)$ and consequently $d^{j}_{m',m}(\beta)$ matrix elements.

In Sect. 3 of this paper, I shall discuss the relevant properties of generating functions for $B^{j}_{m',m}(\beta)$ functions. As can be seen from Eqs. 1 and 4 of this study and Eq. 11 of Ref. [8], $d^{j}_{m',m}(\beta)$ matrix elements are written as multiplied of two auxiliary functions such as $A^{j}_{m',m}(\beta)$ and $B^{j}_{m',m}(\beta)$ given by Eq. 5. Because of the auxiliary function $A^{j}_{m',m}(\beta)$ involve the product of two trigonometric functions the numerical calculations involving them is simplest. It is more interesting to obtain $B^{j}_{m',m}(\beta)$ functions by numerically and analytically as happened with many polynomials. To accomplish this task, I shall present the $B^{j}_{m',m}(\beta)$ functions in terms of other special functions of mathematics and mathematical physics such as beta functions, Gegenbauer, Legendre, Jacobi, and Chebyshew polynomials and functions. The required background mathematics is assembled in Sect. 3. Finally, we would like to emphasize that this paper is devoted to derivation of analytical expressions for $B^{j}_{m',m}(\beta)$ functions.

The final section in this paper provides information about the computational implementation and the documentation of the advantages of the new approach as regards speed and accuracy for numerical calculations of $B^{j}_{m',m}(\beta)$ auxiliary function. Obtained numerical results for $B^{j}_{m',m}(\beta)$ functions compared with results of Ref. [8]. In this comparison a perfect matching is obtained.

2 Definitions and basic properties

The Jacobi polynomials $P^{(\alpha,\beta)}_{n}(x)$ may be expressed in terms of hypergeometric functions as follows [9];

$$P^{(\alpha,\beta)}_{n}(x) = \frac{(-1)^n\,\Gamma(n+1+\beta)}{n!\,\Gamma(1+\beta)} F\left(n+\alpha+\beta+1, -n; 1+\beta; \frac{1+x}{2}\right)$$
$$= \frac{\Gamma(n+1+\alpha)}{n!\,\Gamma(1+\alpha)}\left(\frac{1+x}{2}\right)^{n} F\left(-n, -n-\beta; \alpha+1; \frac{x-1}{x+1}\right) \tag{6}$$

A generalized hypergeometric series is given by

$$ {}_pF_q\left(a_1, a_2, \ldots a_p; b_1, b_2, \ldots b_q; z\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k \ldots \left(a_p\right)_k z^k}{(b_1)_k (b_2)_k \ldots \left(b_q\right)_k k!} \tag{7} $$

where $(a)_k$ is denoted the Pochhammer symbols and Pochhammer symbols are defined following form with the help of the Gamma functions by;

$$ (a)_k = \frac{\Gamma(a+k)}{\Gamma(a)} = a(a+1)\ldots(a+k-1) $$

The generating function of Jacobi polynomials are defined as [9]

$$ \sum_{n=0}^{\infty} P_n^{(\alpha,\beta)}(x)\, t^n = 2^{\alpha+\beta} \frac{(1-t+R)^{-\alpha}}{R(1+t+R)^{\beta}} \tag{8} $$

where

$$ R = \sqrt{1-2xt+t^2} $$

We define Gegenbauer polynomials which are related to hypergeometric functions and Jacobi polynomials. These relationships are defined as following form [9]

$$ \begin{aligned} C_n^m(x) &= \frac{\Gamma(n+2m)}{\Gamma(n+1)\Gamma(2m)} F\left(2m+n, -n; m+1/2; \frac{1-x}{2}\right) \\ &= \frac{\Gamma(n+2m)\Gamma(m+1/2)}{\Gamma(n+m+1/2)\Gamma(2m)} P_n^{(m-1/2,m-1/2)}(x) \end{aligned} \tag{9} $$

The product of two Gegenbauer polynomials can be written as following form [10]

$$ \begin{aligned} C_a^b(x)\, C_c^d(x) &= \sum_{m=0}^{N} (-1)^m a_m(b, a; d, c)(2x)^{a+c-2m} \\ &= \sum_{m=0}^{N} (-1)^m a_m(d, c; b, a)(2x)^{a+c-2m} \end{aligned} \tag{10} $$

where

$$ N = \left[\frac{b+c}{2}\right] - \frac{1-(-1)^{bc}}{2} $$

The orthogonality integral for the Gegenbauer polynomials are given by following form [9]

$$\int_{-1}^{1} C_n^{\lambda}(\beta)\, C_m^{\lambda}(\beta) \left(1-\beta^2\right)^{\lambda-1/2} d\beta = \begin{cases} 0, & n \neq m \\ \pi \frac{2^{1-2\lambda}\Gamma(n+2\lambda)}{n!(\lambda+n)[\Gamma(\lambda)]^2}, & n = m \end{cases} \tag{11}$$

3 Properties and special values of auxiliary function $B^{j}_{m'm}(\beta)$

Now, let us introduce a generating function of two variables;

$$f_{m'm}(\beta, t) = \frac{(1-t+R)^{m-m'}}{R(1+t+R)^{m+m'}} = \sum_{j=m'}^{\infty} \frac{(j+m)! B^{j}_{m'm}(\beta)}{2^{2m'}(j-m')!} t^{j-m'} \tag{12}$$

where

$$R = \sqrt{1 - 2t\cos\beta + t^2} \tag{13}$$

For the first few $B^{j}_{m'm}(\beta)$ functions we need the coefficients t^0, t^1 and t^2. These powers of t appear only in the terms $j = m'$, $m'+1$, and $m'+2$ and hence we may limit our attention to the first three terms of the infinite series. The coefficient of t^j, $B^{j}_{m'm}(\beta)$, is defined to be an auxiliary function order of j. Expanding the Maclaurin series, we have

$$\begin{aligned} B^{m'}_{m'm}(\beta) &= \frac{1}{(m+m')!} \\ B^{m'+1}_{m'm}(\beta) &= \frac{1}{(m+m'+1)!}\left\{\left(m'+1\right)\cos\beta - m\right\} \\ B^{m'+2}_{m'm}(\beta) &= \frac{2m^2 - m' - 2\sin^2\beta - 2m\left(3+2m'\right)\cos\beta + \left(2m'^2 + 7m' + 1\right)\cos^2\beta}{2(m+m'+2)!} \end{aligned} \tag{14}$$

In employing general treatment, we find that the Rodrigues' formula for the $B^{j}_{m'm}(\beta)$ auxiliary function.

$$B^{m'+r}_{m'm}(\beta) = \frac{2^{2m'}}{(m+m'+r)!}\left\{ \frac{\partial^r}{\partial t^r} f_{m'm}(\beta, t)\bigg|_{t=0} \right\} \tag{15}$$

where $r = 0, 1, 2, \ldots$

Our generating function provides still more information about the $B^{j}_{m'm}(\beta)$ auxiliary function. If we take $m' = m = 0$ in Eq. 12, we can be rewritten [9]

$$\begin{aligned} B^{j}_{0,0}(\beta) &= P_j^{(0,0)}(\cos\beta) \\ &= P_j(\cos\beta) \end{aligned} \tag{16}$$

The other special values can be found in case $\beta = 0, \pi$;

$$\begin{aligned} B^{j}_{m',m}(0) &= (-1)^{j-m'} \frac{B\left(j-m+1, m+m'+1\right)}{B\left(j+m+1, m'-m+1\right)} B^{j}_{m',m}(\pi) \\ &= \frac{B\left(j-m+1, m+m'+1\right)}{(m'+m)!B\left(j+m+1, m'-m+1\right)} \end{aligned} \tag{17}$$

where $B(a, b)$ is the beta function.

If we set $m = 0, m' = n - 1/2$ in Eq. 12, the function of $B^{j}_{m'm}(\beta)$ can be rewritten in terms of Gegenbauer polynomials by using Eqs. 6 and 9;

$$B^{j}_{n-1/2,0}(\beta) = \frac{2^{2(3n-1)}}{\sqrt{\pi}} \frac{\Gamma\left(2\left(j-n+1\right)\right)\Gamma(n)\Gamma(j+n+1)}{\Gamma(2j+2n+1)\Gamma(j-n+1)} C^{n}_{j-n+1/2}(\cos\beta) \tag{18}$$

If we set $n = 0$ in Eq. 18, we have

$$B^{j}_{-1/2,0}(\beta) = \frac{T_{j+1/2}(\cos\beta)}{\sqrt{\pi}} \tag{19}$$

where T is the Chebyshev functions [9].

By using the product of two auxiliary functions with same arguments, the following symmetry relationships may easily be obtained from in terms of the Gegenbauer polynomials;

$$B^{j}_{n-1/2,0}(\beta)\, B^{l}_{m-1/2,0}(\beta) = A^{jl}_{nm} G^{lm}_{jn}(\cos\beta) \tag{20}$$

$$= A^{lj}_{mn} G^{lm}_{jn}(\cos\beta) \tag{21}$$

$$= A^{lj}_{mn} G^{jn}_{lm}(\cos\beta) \tag{22}$$

$$= A^{jl}_{nm} G^{jn}_{lm}(\cos\beta) \tag{23}$$

Where we use following definitions

$$G^{lm}_{jn}(x) = C^{n}_{j-n+1/2}(x)\, C^{m}_{l-m+1/2}(x) \tag{24}$$

and

$$A_{mn}^{lj} = 2^{2(3(n+m)-2)} \frac{\Gamma(n)\Gamma(m)\Gamma(j+n+1)\Gamma(l+m+1)}{\pi\Gamma(j-n+1)\Gamma(l-m+1)} \frac{\Gamma(2(j-n+1))\Gamma(2(l-m+1))}{\Gamma(2j+2n+1)\Gamma(2l+2m+1)} \tag{25}$$

In this special case, the orthogonality relationship for $B_{m'm}^{j}(\beta)$ auxiliary functions is obtained following integral equality by using Eqs. 11 and 20–24;

$$(j+1/2)\int_0^\pi B_{n-1/2,0}^{j}(\beta)\, B_{n-1/2,0}^{l}(\beta)\,(\sin\beta)^{2n}\, d\beta = \pi\frac{A_{nn}^{jl}\Gamma(j+n+1/2)}{2^{2n-1}\Gamma(j-n-1/2)\,[\Gamma(n)]^2}\delta_{j,l} \tag{26}$$

If one can use Eq. 6 and orthogonality relationships for the Jacobi polynomials, we immediately find generalized orthogonality integrals for $B_{m'm}^{j}(\beta)$ functions:

$$\left(2j+2m'+1\right)\int_0^\pi \left(\sin\frac{\beta}{2}\right)^{2(m'-m)+1}\left(\cos\frac{\beta}{2}\right)^{2(m'+m)+1} B_{m'm}^{j}(\beta)\, B_{m'm}^{k}(\beta)\, d\beta = \left[\frac{(j-m')!}{(j+m)!}\right]^2 \frac{\left(j+m'-m\right)!\left(j+m'+m\right)!}{j!\,(j+2m')!}\delta_{k,j} \tag{27}$$

4 Results and discussions

In this paper, various mathematical properties of $B_{m'm}^{j}(\beta)$ functions were analyzed and the relevance of some special functions of mathematics and mathematical physics were presented. In Sect. 3, $B_{m'm}^{j}(\beta)$ functions have expressed by using of generating function with two variables. It seems that generating functions have the simplest mathematical structure compared of other mathematical objects. It seems that $B_{m'm}^{j}(\beta)$ functions are convenient in which analytical manipulations of $B_{m'm}^{j}(\beta)$ coefficients are of crucial importance.

As can be seen Eq. 12, we have the relations through the auxiliary function $B_{m'm}^{j}(\beta)$ in the form of infinite series. A large number of computer calculations of such as these functions carried out by us show that the infinite series with respect to N converges rapidly. For a given pair of m', m all possible β values were screened and maximum value of the error was determined following expression. With the help of

Eqs. 7, 11, we obtain control expression for the linear combinations of $B^{j}_{m'm}(\beta)$ auxiliary functions

$$\varepsilon_{m'm}(\beta) = \left| \lim_{N\to\infty} \sum_{j=0}^{N} a^{j+m'}_{m'm} B^{j+m'}_{m'm}(\beta) - f_{m'm}(\beta) \right| \tag{28}$$

$$f_{m'm}(\beta) = \sum_{j=m'}^{\infty} a^{j}_{m'm} B^{j}_{m'm}(\beta) = 2^{2m'} \frac{(R+1/2)^{m-m'}}{R\,(R+3/2)^{m+m'}} \tag{29}$$

Where

$$a^{j}_{m'm} = \frac{(j+m)!}{2^{j-m'}(j-m')!}$$
$$R = \frac{1}{2}\sqrt{5-4\cos\beta} \tag{30}$$

As an example, let us study the case of $-\log\varepsilon_{m',m}$ having the form shown in Figs. 1 and 2. The convergence in the infinite series has been examined in numerous calculations, for which Fig. 1 shows only results for the $-\log\varepsilon_{m',m}$ for $m'=3$, $m=2$, and $\beta=\pi/6$. As upper limit of summation in Eq. 28 increases, $-\log\varepsilon_{m',m}$ increases and attains a constant value at $\beta=\pi/6$ (see Fig. 1). For a given m', m pair it was observed that the maximum error occur when $\beta\approx\pi$. Figure 2 shows plot of $-\log\varepsilon_{3,2}$ versus β angles when the values of upper limits for summation $N=25$. Note that $-\log\varepsilon_{m',m}$ is equivalent to numbers of correct decimal places.

The $B^{j}_{m'm}(\beta)$ function calculated from Eq. 15. The results are given in Table 1. It is seen Table 1 that the special values given by Eq. 17 is satisfied. Obtained numerical results in this paper are agreement with the results of Ref. [8].

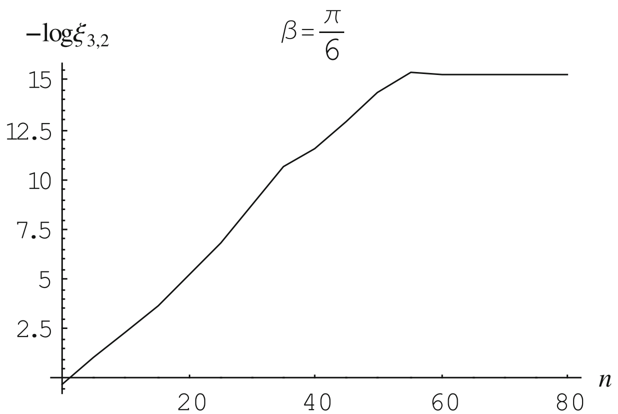

Fig. 1 The convergence of series as a function of the upper limits of summation in Eq. 28 when $\beta = 30°$

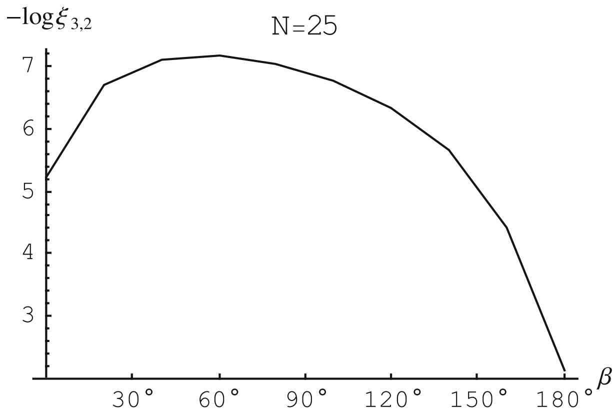

Fig. 2 Plot of $-\log \varepsilon_{3,2}$ versus β angles when $N = 25$

Table 1 The values of $B^{j}_{m'm}(\beta)$ functions for selected quantum numbers and β angles

j	m'	m	β	$B^{j}_{m',m}(\beta)$
2	0	0	$\pi/3$	-0.125
2	2	1	$\pi/4$	0.166666666667
3	2	1	$\pi/6$	0.066586508806
5	3	2	$\pi/3$	-0.00037202381
5	4	-2	0	1.166666666667
5	4	-2	π	-0.5
6	2	3	π	0.008333333333
10	8	2	$\pi/6$	$7.795597062 \times 10^{-8}$
15	14	10	$\pi/2$	$-6.446950284 \times 10^{-25}$
18	18	-5	$\pi/3$	$1.605904384 \times 10^{-10}$
25	20	-8	0	$8.007120227 \times 10^{-8}$
25	20	-8	π	$-2.087675699 \times 10^{-9}$
30	10	10	π	$4.110317623 \times 10^{-19}$
40	36	15	$\pi/6$	$8.065414833 \times 10^{-69}$

For some selected parameters, numerical values of the product two $B^{j}_{m'm}(\beta)$ functions are presented in Table 2. Products of two $B^{j}_{m'm}(\beta)$ functions calculated from Eq. 18 are checked for their accuracy by the symmetry relationships given in Eqs. 20–23. In this comparison a perfect matching is obtained. It should be noted that these equations presented in this paper can be used to calculate any $B^{j}_{m'm}(\beta)$ function and their product for the arbitrary values β angles and quantum numbers. All numerical calculations are performed on a P. IV 2.8 GHz computer using MATHEMATICA 5.0 [11].

Table 2 The values of the product of two $B^{j}_{m'm}(\beta)$ functions in some values of parameters

j	l	n	m	β	$B^{j}_{n-1/2,0}(\beta)\, B^{l}_{m-1/2,0}(\beta)$	Eq. 20	Eq. 21	Eq. 22	Eq. 23
2	2	1/2	1/2	$\pi/3$	0.015625	0.015625	0.015625	0.015625	0.015625
3	2	3/2	1/2	$\pi/3$	−0.0078125	−0.0078125	−0.0078125	−0.0078125	−0.0078125
5	4	3/2	1/2	$\pi/6$	0.00677490234	0.00677490234	0.00677490234	0.00677490234	0.00677490234
5	5	5/2	3/2	$\pi/6$	0.07822983384	0.07822983384	0.07822983384	0.07822983384	0.07822983384
10	7	5/2	3/2	$\pi/2$	−0.00071207682	−0.00071207682	−0.00071207682	−0.00071207682	−0.00071207682

We believe that presented new approach in this paper for the calculation of the $d^{j}_{m'm}(\beta)$ coefficient is important. Following studies related to this work will include calculation of $d^{j}_{m'm}(\beta)$ coefficient.

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