On the closed form of Wigner rotation matrix elements*

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The closed forms of some rotation matrix elements $d^j_{m'm}(\pi/2)$ are presented. The closed forms of summation involved two binomials and some special hypergeometric functions are also obtained. The MAPLE V program which calculates $d^j_{m'm}(\beta)$, $d^j_{m'm}(\pi/2)$ and the help file are given in appendix.

1. Introduction

An arbitrary rotation of a coordinate frame about its origin in the three-dimensional space can be completely specified by three real parameters. The most useful description of rotation in the literature and in textbooks is that in terms of the Euler angles α, β, γ. The matrix representations to the finite rotations in terms of Euler angles were first derived by Wigner [1,2] (therefore, they are often named Wigner rotation matrix elements), and subsequently their many properties and different derivations have been investigated by many authors [3–8]. Because the rotation matrix elements involve the sum of a product of two binomial coefficients and sines and cosines of a half-angles, any calculation involving them is tedious. Although the properties of the rotation matrix elements have been well investigated, the calculation of functional expressions is still not satisfactory to us. Even the results of numerical calculations are correct only to five significant figures as the angular momentum quantum number increases to $j = 13$ [9]. The reason for the inaccuracy may be lies in the operations dealing with large numbers (such as factorials). These cannot be handled by FORTRAN or BASIC programs, for example, unless they have good arithmetic methods [10]. Fortunately, symbolic calculation

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systems, such as, MAPLE V, MATHEMATICA, REDUCE, MacSyma and DERIVE, etc., can overcome the problem of operations involving large numbers to obtain both exact functional expressions and correct numerical numbers with the desired significant figures.

In section 2 of this paper, we simply summarize the notation and properties of the rotation matrix elements for convenient reference. In section 3, we mainly discuss the special properties of the rotation matrix elements with $\beta = \pi/2$. The similarity transformation for any rotation angle β around the Y axis can be converted to a combination of a rotation of $\pi/2$ around the Y axis and a rotation with respect to the Z axis. This similarity transformation will convert the powers of sines and cosines of half-angles to sines and cosines of multiples of β. A method has been proposed to find closed forms of rotation matrix elements with $\beta = \pi/2$. These closed forms allow calculations up to j greater than 200 (which are still very fast!). Many closed forms of summations involving two binomials are also obtained. Since the rotation matrix elements are related to the Jacobi polynomials and hypergeometrical functions, many closed forms of hypergeometrical functions and Jacobi polynomials can be obtained (we leave the Jacobi polynomial evaluation to the interested reader). The rotation matrix elements play an important role in atomic and molecular physics, chemical physics, molecular spectroscopy, angular momentum theory, group theoretical applications and nuclear physics.

2. Expressions for Wigner rotation matrix elements

A $2j+1$-dimensional irreducible vector space, $V(j)$, of the group of proper rotations in the 3-dimensional space $O^+(3)$ is spanned by a set of $2j+1$ basis functions $\{\psi_{jm}, m = -j \text{ to } j\}$. Since an irreducible vector space of a group is an invariant space with respect to any operator of the group, we may then express an Eulerian rotation upon one of the basis functions of $V(j)$ as

$$R\Psi_{jm} = \sum_{m'} D^j_{m'm}(\alpha\beta\gamma)\Psi_{jm'}\,, \tag{1}$$

where the rotation matrix elements are defined as

$$D^j_{m'm}(\alpha\beta\gamma) = \langle jm' \mid e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} \mid jm\rangle\,. \tag{2}$$

Since the matrix representative of J_z is diagonal in this base, eq. (2) becomes

$$\begin{aligned} D^j_{m'm}(\alpha\beta\gamma) &= e^{-im'\alpha}\langle jm' \mid e^{-i\beta J_y} \mid jm\rangle e^{-im\gamma} \\ &= e^{-im'\alpha} d^j_{m'm}(\beta) e^{-im\gamma}\,. \end{aligned} \tag{3}$$

Wigner [1,2] first derived the expression for the rotation matrix element $d^j_{m'm}(\beta)$ and Rose [5] modified it as follows:

$$d^j_{m'm}(\beta) = \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}\right]^{1/2} \sum_s (-1)^{m'-m+s} \binom{j+m}{s} \binom{j-m}{j-m'-s} \times \left(\cos\frac{\beta}{2}\right)^{2j+m-m'-2s} \left(\sin\frac{\beta}{2}\right)^{m'-m+2s}, \tag{4}$$

where (:)'s are binomial coefficients. The summation over s is restricted to the argument of any factorial which is non-negative. Let $s = j - m' - \sigma$, then $d^j_{m'm}(\beta)$ is related to other definitions [12] by

$$\begin{aligned} d^j_{m'm}(\beta) \quad &(\text{Rose [5]}) = d^j_{m'm}(\beta) \quad (\text{Brink \& Satchler [6], Zare [8]}) \\ &= (-1)^{m'-m} d^j_{m'm}(\beta) \quad (\text{Edmonds [4], Wigner [1,2], Fano \& Racah [3]}) . \end{aligned} \tag{5}$$

From eq. (4) we can obtain the symmetry properties of $d^j_{m'm}(\beta)$, where j, m' and m may be either integral or half-integral:

$$d^j_{m'm}(\beta) = (-1)^{m'-m} d^j_{mm'}(\beta) = (-1)^{m'-m} d^j_{-m'-m}(\beta) = (-1)^{m'-m} d^j_{m'm}(-\beta) , \tag{6a}$$

$$d^j_{m'm}(\pi + \beta) = (-1)^{j-m'} d^j_{-m'm}(\beta) , \tag{6b}$$

$$d^j_{m'm}(\pi - \beta) = (-1)^{j-m'} d^j_{m,-m'}(\beta) , \tag{6c}$$

$$d^j_{m'm}(\pi) = (-1)^{j+m} \delta_{m+m',0} , \tag{6d}$$

$$d^j_{m'm}(-\pi) = (-1)^{j-m} \delta_{m+m',0} , \tag{6e}$$

$$d^j_{m'm}(0) = \delta_{m',m} . \tag{6f}$$

The $d^j_{m'm}(\beta)$ satisfy the following differential equations:

$$\left\{\frac{d^2}{d\beta^2} + \cot\beta \frac{d}{d\beta} - \frac{m^2 + m'^2 - 2mm'\cos\beta}{\sin^2\beta} + j(j+1)\right\} d^j_{m'm}(\beta) = 0 \tag{7}$$

and [13]

$$\begin{aligned} &\left\{j^2 \cos\beta - m'm - j\sin\beta \frac{d}{d\beta}\right\} d^j_{m'm}(\beta) \\ &\quad = [(j+m)(j-m)(j+m')(j-m')]^{1/2} d^{j-1}_{m'm}(\beta) \end{aligned} \tag{8a}$$

and

$$\begin{aligned} &\left\{(j+1)^2 \cos\beta - m'm + (j+1)\sin\beta \frac{d}{d\beta}\right\} d^j_{m'm}(\beta) \\ &\quad = [(j+m+1)(j-m+1)(j+m'+1)(j-m'+1)]^{1/2} d^{j+1}_{m'm}(\beta) . \end{aligned} \tag{8b}$$

The detailed descriptions of eqs. (8a) and (8b) can be found in [13]. Eqs. (5) to (8b) can also be translated to the rotational wave functions $D^j_{m'm}(\alpha\beta\gamma)$ (not normalized).

3. On the rotation matrix elements of $\beta = \pi/2$

3.1. THE CALCULATION OF $d^j_{m'm}(\beta)$

The disadvantage of eq. (4) is that it expresses the rotation matrix elements in terms of powers of $\cos(\beta/2)$ and $\sin(\beta/2)$. Wigner [14] has shown the matrix representatives for an arbitrary β can be obtained by the following similarity transformation:

$$R(0,\beta,0) = R\left(\frac{\pi}{2},0,0\right)R\left(0,\frac{\pi}{2},0\right)R(\beta,0,0)R\left(0,-\frac{\pi}{2},0\right)R\left(-\frac{\pi}{2},0,0\right). \qquad (9)$$

Therefore,

$$\begin{aligned}&\langle jm' \mid R(0,\beta,0) \mid jm\rangle \\ &\quad= \langle jm' \mid R\left(\frac{\pi}{2},0,0\right)R\left(0,\frac{\pi}{2},0\right)R(\beta,0,0)R\left(0,-\frac{\pi}{2},0\right)R\left(-\frac{\pi}{2},0,0\right) \mid jm\rangle \\ &\quad= (-1)^{-m}e^{i(m-m')\pi/2}\sum_{m_2}(-1)^{m_2}\Delta^j_{m'm_2}e^{-im_2\beta}\Delta^j_{m_2m'}, \end{aligned} \qquad (10)$$

where $\Delta^j_{m'm} \equiv d^j_{m'm}(\pi/2)$, and this equation can be simplified to

$$d^j_{m'm}(\beta) = \Delta^j_{m'0}\Delta^j_{m0}\kappa(0) + 2\sum_{m''>0}\Delta^j_{m'm''}\Delta^j_{mm''}\kappa(m''\beta) \qquad (11a)$$

for integral j, m', m, and

$$d^j_{m'm}(\beta) = 2\sum_{m''\geqslant 1/2}\Delta^j_{m'm''}\Delta^j_{mm''}\kappa(m''\beta) \qquad (11b)$$

for half-integral j, m', m, where

$$\kappa(x) = \begin{cases} \cos x & \text{if } m'-m = 0 \pmod 4, \\ -\sin x & \text{if } m'-m = 1 \pmod 4, \\ -\cos x & \text{if } m'-m = 2 \pmod 4, \\ \sin x & \text{if } m'-m = 3 \pmod 4. \end{cases} \qquad (12)$$

Therefore, in principle, to calculate $d^j_{m'm}(\beta)$ one only needs to know $\Delta^j_{m'm}$. Both the exact and numerical values of $\Delta^j_{m'm}$, have been calculated for $0 \leqslant m', m, j \leqslant 20$ in the present work. Note that Behkami [9] has tabulated $\Delta^j_{m'm}$, $j \leqslant 13$, numerically and Bradley [15] used a desk machine to construct the tables of $\Delta^j_{m'm}$ from $j = 0$ up to $j = 20$, numerically. The tables of $\Delta^j_{m'm}$ have been deposited with the Royal Society and the Library of Congress. The general forms for different $m' = j - k'$,

$m = j - k$, k', $k = 0, 1, \ldots, 20$, have also been calculated by a MAPLE program and the program is given in the appendix. Both procedures for calculating eqs. (4) and (11) have been written and run under the MAPLE V system. The results agree with each other. In terms of eqs. (6a) and (6c) (three properties), it is easy to show that the number of different matrix elements to be tabulated from $(2j^2+1)^2$ reduce to $(j+1)(j+2)/2$ for integer j, and to $(2j+1)(2j+3)/8$ when j is a half-integer. Previously Buckmaster [16] used two properties of $d^j_{m'm}(\beta)$ and reduced the tabulated numbers from $(2j^2+1)^2$ to $(j+1)^2$ for integer j and $(2j+1)(2j+3)/4$ for the half-integer j.

3.2. THE CLOSED FORMS OF SOME SPECIAL $\Delta^j_{m'm}$

When $\beta = \pi/2$, eq. (4) reduces to

$$\Delta^j_{m'm} = \left(\frac{1}{2}\right)^j \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}\right]^{1/2} \sum_s (-1)^{m'-m+s} \binom{j+m}{s} \binom{j-m}{j-m'-s} \tag{13}$$

and eq. (6c) becomes

$$\Delta^j_{m'm} = (-1)^{j+m} \Delta^j_{-m'm} \,. \tag{14}$$

It is easy to show that

$$\Delta^j_{00} = 0 \tag{15}$$

if j = odd, and

$$\Delta^j_{0m} = (-1)^{j+m} \Delta^j_{0m} \neq 0 \tag{16}$$

only if $j+m$ = even. It can also be shown that

$$\Delta^{2j}_{11} = \Delta^{2j}_{00} = \frac{(-1)^j \Gamma(j+1/2)}{j!\sqrt{\pi}} \,. \tag{17}$$

Here Γ's are the gamma functions, $j = 1, 2, 3, \ldots$, and from eq. (13) we have

$$\Delta^j_{jj} = \left(\frac{1}{2}\right)^j \,. \tag{18}$$

By using our previous results [17] and combining them with eq. (17) we obtain the following closed forms:

$$\Delta^{2k+1}_{11} = \frac{(-1)^k \Gamma(k+1/2)}{2(k+1)!\sqrt{\pi}} \,, \tag{19}$$

$$\Delta_{\frac{1}{2}\frac{1}{2}}^{2k+\frac{3}{2}} = \frac{(-1)^{k+1}\Gamma(k+\frac{3}{2})}{2(k+1)!\sqrt{2\pi}} , \tag{20}$$

$$\Delta_{\frac{1}{2}\frac{1}{2}}^{2k+\frac{1}{2}} = \frac{(-1)^{k}\Gamma(k+\frac{1}{2})}{k!\sqrt{2\pi}} . \tag{21}$$

Here $k = 0, 1, 2, \ldots$. Also we have

$$\Delta_{20}^{2k} = (-1)^{k+1}\left[\frac{k(2k+1)}{(k+1)(2k-1)}\right]^{1/2} \frac{\Gamma(k+1/2)}{k!\sqrt{\pi}} , \tag{22}$$

$$\Delta_{21}^{2k+1} = \frac{(-1)^{k+1}[k(2k+3)]^{1/2}\Gamma(k+\frac{1}{2})}{(k+1)!\sqrt{2\pi}} , \tag{23}$$

$$\Delta_{21}^{2k} = (-1)^{k}\sqrt{\frac{2}{\pi}}\, \frac{\Gamma(k+\frac{1}{2})}{k![(2k+1)(k+1)]^{1/2}} , \tag{24}$$

$$\Delta_{22}^{2k} = (-1)^{k}\, \frac{(2k^2+k-4)\Gamma(k+\frac{1}{2})}{(k+1)!(2k-1)\sqrt{\pi}} , \tag{25}$$

$$\Delta_{22}^{2k+1} = (-1)^{k}\, \frac{4\Gamma(k+3/2)}{(k+1)!(2k+1)\sqrt{\pi}} , \tag{26}$$

where $k = 1, 2, 3, \ldots$. Moreover,

$$\Delta_{10}^{2k+1} = (-1)^{k+1}\left[\frac{2k+1}{2(k+1)}\right]^{1/2} \frac{\Gamma(k+1/2)}{k!\sqrt{\pi}} , \tag{27}$$

where $k = 0, 1, 2, 3, \ldots$, and

$$\Delta_{30}^{2k+1} = (-1)^{k}\left[\frac{k(2k+1)(2k+3)}{(k+1)(k+2)(2k-1)}\right]^{1/2} \frac{\Gamma(k+1/2)}{k!\sqrt{2\pi}} , \tag{28}$$

where $k = 1, 2, 3, \ldots$, and

$$\Delta_{33}^{2k} = (-1)^{k}\, \frac{(2k^2+k-19)\Gamma(k+\frac{1}{2})}{(k+1)!(2k-1)\sqrt{\pi}} , \tag{29}$$

where $k = 2, 3, 4, \ldots$, and

$$\Delta_{33}^{2k+1} = (-1)^{k}\, \frac{3(6k^2+9k-16)\Gamma(k+\frac{1}{2})}{2(k+2)!(2k-1)\sqrt{\pi}} , \tag{30}$$

where $k = 1, 2, 3, \ldots$, and

$$\Delta_{40}^{2k} = (-1)^k \left[\frac{k(2k+1)(2k+3)(k-1)}{(k+1)(k+2)(2k-1)(2k-3)}\right]^{1/2} \frac{\Gamma(k+1/2)}{k!\sqrt{\pi}}\,, \tag{31}$$

$$\Delta_{44}^{2k} = (-1)^k \,\frac{(576-67k-133k^2+4k^3+4k^4)\Gamma(k+\frac{1}{2})}{(2k-3)(k+2)!(2k-1)\sqrt{\pi}}\,, \tag{32}$$

$$\Delta_{44}^{2k+1} = (-1)^{k+1}\,\frac{16(17-3k-2k^2)\Gamma(k+\frac{3}{2})}{(2k+1)(k+2)!(2k-1)\sqrt{\pi}}\,, \tag{33}$$

where $k = 2, 3, 4, \ldots$. Somewhat more general forms are

$$\Delta_{m0}^{j} = \frac{(-1)^m\sqrt{\pi}}{2^m\Gamma(1+(j+m)/2)\Gamma(1/2-(j-m)/2)}\left[\frac{(j+m)!}{(j-m)!}\right]^{1/2} \tag{34}$$

and

$$\begin{aligned}\Delta_{m1}^{j} = {} & \frac{(-1)^{m+1}\sqrt{\pi}}{2^m}\left[\frac{(j+m)!}{j(j+1)(j-m)!}\right]^{1/2} \\ & \times\left\{\frac{m}{\Gamma(1+(j+m)/2)\Gamma(1/2-(j-m)/2)}\right. \\ & \left. + \frac{j+m+1}{\Gamma(3/2+(j+m)/2)\Gamma(-(j-m)/2)}\right\}\end{aligned} \tag{35}$$

and

$$\begin{aligned}\Delta_{m2}^{j} = {} & \frac{(-1)^{m}\sqrt{\pi}}{2^m}\left[\frac{(j+m)!}{j(j+1)(j^2+j-2)(j-m)!}\right]^{1/2} \\ & \times\left\{\frac{2m^2-j(j+1)}{\Gamma(1+(j+m)/2)\Gamma(1/2-(j-m)/2)}\right. \\ & \left. + \frac{2m(j+m+1)}{\Gamma(3/2+(j+m)/2)\Gamma(-(j-m)/2)}\right\}.\end{aligned} \tag{36}$$

To obtain eq. (34) we have used the following reactions [1,2,5]:

$$\begin{aligned}& {}_2F_1\left(m'-j, -m-j; m'-m+1; -\tan^2\frac{\beta}{2}\right) \\ & = \left[\frac{(j+m)!(j-m')!}{(j-m)!(j+m')!}\right]^{1/2} \frac{(-1)^{m'-m}(m'-m)!}{(\cos\frac{\beta}{2})^{2j+m-m'}(\sin\frac{\beta}{2})^{m'-m}}\, d_{m'm}^{j}(\beta)\,.\end{aligned} \tag{37}$$

Here $m' \geqslant m$, and [18]

$${}_2F_1 = (a, b; 1+a-b; -1) = 2^{-a}\frac{\Gamma(1+a-b)\Gamma(1/2)}{\Gamma(1-b+a/2)\Gamma(1+a)}\,, \tag{38}$$

in which $1 + a - b \neq 0, -1, -2, \ldots$, and the hypergeometric function is defined

$$ {}_2F_1(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n z^n}{(c)_n n!} \tag{39} $$

and the Pochhammer symbol is

$$ (a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}, $$

i.e.

$$ (a)_0 = 1, \quad (a)_n = a(a+1)\dots(a+n-1), \quad n = 1,2,3,\dots . $$

In principle, we can use the same method to find closed forms for Δ^j_{m3}, Δ^j_{m4}, $\Delta^j_{m5}, \dots$, etc.

3.3. THE CLOSED FORMS FOR SUMMATIONS OF TWO BINOMIAL COEFFICIENTS

Summations involving two binomial coefficients are often used in angular momentum theory and combination theory. We can rewrite eq. (13) as follows:

$$ \sum_s (-1)^s \binom{j+m}{s} \binom{j-m}{j-m'-s} = 2^j \left[\frac{(j-m)!(j+m)!}{(j-m')!(j+m')!}\right]^{1/2} (-1)^{m'-m} \Delta^j_{m'm} . \tag{40} $$

By comparing the results of the previous section with eq. (40), we then obtain the following expressions:

$$ \begin{aligned} \sum_s (-1)^s \binom{2j}{s}\binom{2j}{s} &= \sum_s (-1)^s \binom{2j+1}{s}\binom{2j-1}{s} \\ &= 2^{2j}(-1)^j \frac{\Gamma(j+1/2)}{j!\sqrt{\pi}}, \end{aligned} \tag{41} $$

$$ \sum_s (-1)^s \binom{2k}{s}\binom{2k}{2+s} = \frac{(-1)^{k+1} 2^{2k} k}{(k+1)!\sqrt{\pi}} \Gamma(k+1/2) . \tag{42} $$

Here $k = 1,2,3,\dots$, and

$$ \sum_s (-1)^s \binom{2k+1}{s}\binom{2k}{s} = \frac{(-1)^k 2^{2k} \Gamma(k+1/2)}{k!\sqrt{\pi}}, \tag{43} $$

$$ \sum_s (-1)^s \binom{2k+2}{s}\binom{2k+1}{s} = \frac{(-1)^{k+1} 2^{2k+1} \Gamma(k+3/2)}{(k+1)!\sqrt{\pi}}, \tag{44} $$

$$\sum_s (-1)^s \binom{2k+2}{s}\binom{2k-2}{s} = \frac{(-1)^k 2^{2k}(2k^2+k-4)\Gamma(k+1/2)}{(2k-1)(k+1)!\sqrt{\pi}}\,, \tag{45}$$

$$\sum_s (-1)^s \binom{2k+3}{s}\binom{2k-1}{s} = \frac{(-1)^k 2^{2k+3}\Gamma(k+3/2)}{(2k+1)(k+1)!\sqrt{\pi}}\,, \tag{46}$$

$$\sum_s (-1)^s \binom{2k+3}{s}\binom{2k-3}{s} = \frac{(-1)^k 2^{2k}(2k^2+k-19)\Gamma(k+1/2)}{(2k-1)(k+1)!\sqrt{\pi}}\,, \tag{47}$$

where $k = 2, 3, 4, \ldots$, and

$$\sum_s (-1)^s \binom{2k+4}{s}\binom{2k-2}{s} = \frac{(-1)^k 3 \times 2^{2k}(6k^2+9k-16)\Gamma(k+1/2)}{(k+2)!(2k-1)\sqrt{\pi}}\,, \tag{48}$$

where $k = 1, 2, 3, \ldots$, and

$$\sum_s (-1)^s \binom{2k+1}{s}\binom{2k+1}{1+s} = \frac{(-1)^k 2^{2k}(2k+1)\Gamma(k+1/2)}{(k+1)!\sqrt{\pi}}\,, \tag{49}$$

where $k = 0, 1, 2, \ldots$, and

$$\sum_s (-1)^s \binom{2k+1}{s}\binom{2k+1}{3+s} = \frac{(-1)^{k+1} 2^{2k} k(2k+1)\Gamma(k+1/2)}{(k+2)!\sqrt{\pi}}\,, \tag{50}$$

where $k = 0, 1, 2, \ldots$, and

$$\sum_s (-1)^s \binom{k}{s}\binom{k}{m+s} = \frac{2^{k-m} k!\sqrt{\pi}}{(k-m)!\Gamma(1+(k+m)/2)\Gamma(1/2-(k-m)/2)}\,, \tag{51}$$

$$\sum_s (-1)^s \binom{k+m}{s}\binom{k-m}{s-m} = \frac{(-1)^m 2^{k-m}(k+m)!\sqrt{\pi}}{(k)!\Gamma(1+(k+m)/2)\Gamma(1/2-(k-m)/2)}\,, \tag{52}$$

where $m = 0, \pm 1, \pm 2, \ldots$, and

$$\sum_s (-1)^s \binom{2k+5}{s}\binom{2k-3}{s} = \frac{(-1)^{k+1} 2^{2k+5}(17-3k-2k^2)\Gamma(k+3/2)}{(2k+1)(2k-1)(k+2)!\sqrt{\pi}}\,, \tag{53}$$

where $k = 2, 3, \ldots$, and

$$\sum_s (-1)^s \binom{2k+4}{s}\binom{2k-4}{s} = \frac{(-1)^k 2^{2k}(576-67k-133k^2+4k^3+4k^4)\Gamma(k+\frac{1}{2})}{(2k-3)(2k-1)(k+2)!\sqrt{\pi}}, \tag{54}$$

$$\sum_s (-1)^s \binom{k+m}{s}\binom{k-m}{k-1-s} = \frac{(-1)^{m+1}2^{k-m}(k+m)!\sqrt{\pi}}{(k+1)!} \times \left\{ \frac{m}{\Gamma(1+(k+m)/2)\Gamma(1/2-(k-m)/2)} + \frac{k+m+1}{\Gamma(3/2+(k+m)/2)\Gamma(-(k-m)/2)} \right\}, \tag{55}$$

where $\Gamma(0) = \infty$, and

$$\sum_s (-1)^s \binom{k+m}{s}\binom{k-m}{k-2-s} = \frac{(-1)^m 2^{k-m}\sqrt{\pi}(k+m)!}{(k+2)!} \times \left\{ \frac{2m^2-k(k+1)}{\Gamma(1+(k+m)/2)\Gamma(1/2-(k-m)/2)} + \frac{2m(k+m+1)}{\Gamma(3/2+(k+m)/2)\Gamma(-(k-m)/2)} \right\}, \tag{56}$$

$$\sum_s (-1)^s \binom{2k+1}{s}\binom{2k-1}{1+s} = \frac{(-1)^{k+1}2^{2k}\Gamma(k+1/2)}{(k+1)!\sqrt{\pi}}, \tag{57}$$

$$\sum_s (-1)^s \binom{2k+2}{s}\binom{2k}{1+s} = \frac{(-1)^k 2^{2k+1}\Gamma(k+1/2)}{(k+1)!\sqrt{\pi}}. \tag{58}$$

3.4. SPECIAL VALUES OF HYPERGEOMETRIC FUNCTIONS

When $\beta = \pi/2$, eq. (37) becomes

$$ {}_2F_1(m'-j, -m-j; m'-m+1; -1) = \left[\frac{(j+m)!(j-m')!}{(j-m)!(j+m')!}\right]^{1/2} (-1)^{m'-m}(m'-m)!\Delta^j_{m'm}, \tag{59}$$

where $m' \geqslant m$, and, using eqs. (17), (19), (35), (36) and (59), we obtain some special values of the hypergeometric functions:

$$ {}_2F_1(-2j,-2j;1;-1) = {}_2F_1(1-2j,-1-2j;1;-1) = \frac{(-1)^j 2^{2j}\Gamma(j+1/2)}{j!\sqrt{\pi}}, \quad (60) $$

$$ {}_2F_1(-2j,-2-2j;1;-1) = \frac{(-1)^j 2^{2j}\Gamma(j+1/2)}{(j+1)!\sqrt{\pi}}, \quad (61) $$

where $m = 1, 2, 3, \ldots$, and

$$ {}_2F_1(m-j,-1-j;m;-1) = 2^{j-m}(m-1)!\sqrt{\pi} \times \left\{ \frac{m}{\Gamma(1+(j+m)/2)\Gamma(1/2-(j-m)/2)} + \frac{j+m+1}{\Gamma(3/2+(j+m)/2)\Gamma(-(j-m)/2)} \right\}, \quad (62) $$

$$ {}_2F_1(m-j,-2-j;m-1;-1) = 2^{j-m}\sqrt{\pi}(m-2)! \times \left\{ \frac{2m^2-j(j+1)}{\Gamma(1+(j+m)/2)\Gamma(1/2-(j-m)/2)} + \frac{2m(j+m+1)}{\Gamma(3/2+(j+m)/2)\Gamma(-(j-m)/2)} \right\}, \quad (63) $$

where $m = 2, 3, 4, \ldots$. The interested reader can use the same technique to obtain many other special values of the hypergeometric functions. Therefore, it is noteworthy that the relation between the sum over binomial coefficients and hypergeometric function are also obtainable:

$$ \sum_s (-1)^s \binom{j+m}{s} \binom{j-m}{j-m'-s} = \frac{(j-m)!}{(m'-m)!(j-m')!}\, {}_2F_1(m'-j,-m-j;m'-m+1;-1), \quad (64) $$

where $m' \geqslant m$.

4. Conclusions

In this work we have presented many relations between $\Delta^j_{m'm}$ and gamma functions, and summations involving two binomial coefficients, and hypergeometric functions. Even though a general closed form for $\Delta^j_{m'm}$ has not been found yet, a useful way to determine closed forms of $\Delta^j_{m'm}$, with special values of m' or m has been explored. Since $d^j_{m'm}(\beta)$ is related to the Jacobi polynomials [17], many relations between the Jacobi polynomials and summations involving two binomial coefficients, and hypergeometric functions can be deduced. Some of the applications of $\Delta^{j}_{m'm}$ can be found in refs. [11,15,18,19].

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Appendix

MAPLE PROGRAM FOR ROTATION MATRIX ELEMENTS

```
# The following program calculates Wigner rotation matrix elements
# which runs on MAPLE V system.
#
'help/text/rotationmatrix' :=TEXT(
'FUNCTION: d, Rot - calculate Wigner rotation matrix elements with',
'   angle x.',
'',
'CALLING SEQUENCE: ',
'd(j, n, m, x)',
'Rot(j, n, m, x)',
'd90(j, n, m);',
'',
'PARAMETERS: ',
'j - rotational angular momentum quantum number.',
'n, m - magnetic quantum number.',
'x - Euler angle.',
'',
'SYNOPSIS: - A typical call to the d and Rot functions are',
'   d(j, n, m, x), d90(j, n, m) and Rot(j, n, m, x) where j >= 0, it can be integer',
'   or half-integer. n, m = -j to j, x is an angle (radian).',
'   - Definition of rotation matrix element is the same as',
'   Rose [5], Brink & Satchler [6], Zare [8] and Lai [12].',
'   The results of d(j, n, m, x) and Rot(j, n, m, x) should be the same.',
'',
'',
'EXAMPLES: ',
'd(1, 1, 1, x);',
'd90(1, 1, 1);',
'Rot(1, 1, 1, x);',
'd(1, 0, 0, x);',
```

```
'Rot(1, 0, 0, x);',
'd(1, 0, -1, x);',
'Rot(1, 0, -1, x);',
'd(1, -1, -1, x);',
'Rot(1, -1, -1, x);',
'd(2, 0, 0, x);',
'Rot(2, 0, 0, x);',
'd(1/2, 1/2, 1/2, x);',
'Rot(1/2, 1/2, 1/2, x);',
'd(3/2, 1/2, -3/2, x);',
'd90(3/2, 1/2, -3/2);',
'Rot(3/2, 1/2, -3/2, x);',
``,
``):
#
# Based on eq. (4)
#
d := proc (j, n, m, x)
   local d1, d2, ds, s:
   if x = Pi then
   d1 := (-1)^(j + m)*Kronecker(n + m, 0);
else
   if x = -Pi then
   d1:= (-1)^(j - m)*Kronecker(n + m, 0);
else
   if x = 2*Pi then d1:= (-1)^(2*j)*Kronecker(n, m);
else
   if x = 0 then d1 := Kronecker(n, m);
else
   d1:= (j + n)!^(1/2)*(j - n)!^(1/2)/(j - m)!^(1/2)/(j + m)!^(1/2);
   ds := 0;
   for s from 0 to 2*j
   do
if j + m - s >= 0 and j - n - s >= 0 and n + s - m >= 0 then
   ds := ds +(-1)^(n - m + s)*binomial(j + m, s)*binomial(j - m, j - n - s)
   *cos(1/2*x)^(2*j + m - n - 2*s)
   *sin(1/2*x)^(n - m + 2*s):
fi; od;
   d2 := factor(simplify(ds*d1));
   fi:
   fi;fi;fi
   end;
#
```

```
d90 := proc(j, n, m)
   local d1, s;
d1 := simplify(sqrt(j + n)!*(j - n)!/(j - m)!/(j + m)!)*
   sum((-1)**(n - m + s)*binomial(j + m, s)*binomial(j - m, j - n - s)
   *(1/2)^j, s = 0..2*j));end:
k := proc(n, m, x)
   local k1;
if type((n - m) mod 4, 0) then k1 := cos(x);
else if type(n - m mod 4, 1) then k1 := -sin(x);
else if type(n - m mod 4, 2) then k1 := -cos(x);
else if type(n - m mod 4, 3) then k1 := sin(x);
fi;fi;fi;fi; end:
#
# Based on eqs. (11a) to (12).
#
Rot:=proc(j, n, m, x)
   local d2, g2;
if x = Pi then g2 := (-1)^(j + m)*Kronecker(n + m, 0);
   else if x =-Pi then g2 := (-1)^(j - m)*Kronecker(n + m, 0);
      else if x = 0 then g2 := Kronecker(n, m);
      else if x = 2*Pi then g2 :=(-1)^(2*j)*Kronecker(n, m);
   else
if type (j, fraction) then
      d2 := 0,
for m2 from 1/2 to j
   do
      d2 := d2 + 2*d90(j, n, m2)*d90(j, m, m2)*k(n, m, m2*x);
   od;
else
      d2 := d90(j, n, 0)*d90(j, m, 0)*k(n, m, 0);
for m2 from 1 to j
   do
      d2 := d2 + 2*d90(j, n, m2)*d90(j, m, m2)*k(n, m, m2*x);
   od;
fi;fi;fi;fi;fi;
factor(simplify(d2));
end:
Kronecker := proc(n, m)
   local k1;
if n = m then k1 := 1;
   else k1 := 0;
  fi;
end:
```

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