UCLWig3j Theory

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1 Introduction

We seek an efficient calculation of the Wigner 3j symbol for a restricted range of inputs.

2 Definition and Properties

The Wigner 3j symbol is defined to be

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{(a-b-\gamma)} \sqrt{\Delta(a,b,c)}$$
$$\times \sqrt{(a+\alpha)!(a-\alpha)!(b+\beta)!(b-\beta)!(c+\gamma)!(c-\gamma)!} \times \sum_t \frac{(-1)^t}{x(t)}. \quad (1)$$

Here the sum is over all values of t for which all the arguments to the factorials in

$$x(t) = t!(c-b+t+\alpha)!(c-a+t-\beta)!(a+b-c-t)!(b-t+\beta)!(a-t-\alpha)! \quad (2)$$

are non-negative, while

$$\Delta(a,b,c) = \frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!} \quad (3)$$

is the *triangle coefficient*.

The Wigner 3j symbol is unchanged under an even permutation of the columns, e.g.

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = \begin{pmatrix} c & a & b \\ \gamma & \alpha & \beta \end{pmatrix}; \quad (4)$$

while an odd permutation of the columns introduces a phase factor, e.g.

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{(a+b+c)} \begin{pmatrix} b & a & c \\ \beta & \alpha & \gamma \end{pmatrix}. \quad (5)$$

There are several other symmetries as well, but we will not need these.

We seek to calculate the restricted version

$$\mathrm{w}(j) \equiv \begin{pmatrix} j_1 & j_2 & j \\ m & -m & 0 \end{pmatrix} \quad (6)$$

where j_1 and j_2 are non-negative integers, m is 0 or 2, and j steps through the range of values $|j_1 - j_2| \leq j \leq j_1 + j_2$. When writing $\mathrm{w}(j)$ the dependence on j_1, j_2 and m is to be understood.

Let $g = \max(j_1, j_2)$ and $h = \min(j_1, j_2)$. Expressions that are symmetric in j_1 and j_2 may then be written in terms of g and h; for example, $j_1 + j_2 = g + h$, while the constraint on j becomes $g - h \leq j \leq g + h$. We will make such substitutions without further comment.

Our goal is to calculate $\mathrm{w}(j)$ for the full range of j values $g - h \leq j \leq g + h$; we are helped here by the recursion relation that links three successive values of w:

$$(j-1)A(j)\,\mathrm{w}(j) + B(j-1)\,\mathrm{w}(j-1) + jA(j-1)\,\mathrm{w}(j-2) = 0 \tag{7}$$

where

$$\begin{aligned} A(k) &= k\sqrt{k^2 - (j_1 - j_2)^2}\sqrt{(j_1 + j_2 + 1)^2 - k^2} \\ &= k\sqrt{k^2 - (g-h)^2}\sqrt{(g+h+1)^2 - k^2} \end{aligned} \tag{8}$$

and

$$B(k) = -2mk(2k+1)(k+1). \tag{9}$$

For this result see for example equations 1(b), 1(c) and 1(d) in Schulten and Gordon (Computer Physics Communications 11 (1976) 269-278). The notation in that paper and in this note may be equated by using Eq 4.

Our strategy is to calculate the 3j symbol first for the lowest and second-lowest values of j, and then to apply the recursion relation to calculate the 3j symbol for higher values of j.

3 $j = g - h$

Assume that j has its lowest value i.e. $j = g - h$. We see

$$x(t) = t!(-h+t+m)!(g-2h+t+m)!(2h-t)!(g-t-m)!(h-t-m)! \tag{10}$$

Recall that all factorial arguments must be non-negative. The second and last factors together then force $t = h - m$; if this quantity is non-negative then we see that all the factorial arguments will be non-negative and so this will be the unique value of t; if this quantity is negative then no t values are allowed and $\mathrm{w}(j)$ will be zero.

3.1 $h - m \geq 0$

Assuming then that $t = h - m \geq 0$, we calculate

$$x(t) = (h-m)!(g-h)!(h+m)!(g-h)! \tag{11}$$

The triangle coefficient becomes:

$$\begin{aligned} \Delta(j_1, j_2, j) &= \frac{(j_1 + j_2 - j)!(j_1 - j_2 + j)!(-j_1 + j_2 + j)!}{(j_1 + j_2 + j + 1)!} \\ &= \frac{(2h)!(2g-2h)!}{(2g+1)!}. \end{aligned} \tag{12}$$

Combining yields

$$\begin{aligned} \mathrm{w}(j) = (-1)^{(j_1 - j_2)} \times \sqrt{\frac{(2h)!(2g-2h)!}{(2g+1)!}} \times \\ \sqrt{(g+m)!(g-m)!(h+m)!(h-m)!(g-h)!(g-h)!} \times \\ \frac{(-1)^{(h-m)}}{(h-m)!(g-h)!(h+m)!(g-h)!} \end{aligned} \tag{13}$$

Now m is even, so the sign on the right hand side may be simplified by noting that $j_1 - j_2 + h - m \equiv |j_1 - j_2| + h \equiv g - h + h \equiv g \mod 2$. Thus

$$\begin{aligned} w(j) &= (-1)^g \sqrt{\frac{(2h)!(2g-2h)!}{(2g+1)!} \frac{(g-m)!}{(h-m)!(g-h)!} \frac{(g+m)!}{(h+m)!(g-h)!}} \\ &= \frac{(-1)^g}{\sqrt{2g+1}} \prod_{i=1}^{g-h} \sqrt{\left(\frac{2i-1}{2h+2i-1}\right)\left(\frac{2i}{2h+2i}\right)\left(\frac{h-m+i}{i}\right)\left(\frac{h+m+i}{i}\right)} \\ &= \frac{(-1)^g}{\sqrt{2g+1}} \prod_{i=1}^{g-h} \sqrt{\left(\frac{2i-1}{i}\right)\left(\frac{2i}{i}\right)\left(\frac{h-m+i}{2h+2i-1}\right)\left(\frac{h+m+i}{2h+2i}\right)}. \end{aligned} \tag{14}$$

3.2 $h - m < 0$

Alternatively if $h - m < 0$ then in this case there are no valid t values and so

$$\begin{pmatrix} j_1 & j_2 & j \\ m & -m & 0 \end{pmatrix} = 0. \tag{15}$$

4 $j = g - h + 1$

Assume that j has its second-lowest value i.e. $j = g - h + 1$. Here the third item $\mathrm{w}(j-2)$ in the recursion equation is not defined (as $(j-2) < g - h$ in this case); however the recursion relation still holds provided that we set $\mathrm{w}(j-2) = 0$. Hence we can solve for $\mathrm{w}(j)$ in terms of $\mathrm{w}(j-1)$, but only providing that the prefactor $(j-1)A(j)$ for $\mathrm{w}(j)$ does not vanish. Actually we need only consider $j - 1 = 0$, as $A(j)$ never vanishes in this case (to see this, note that $A(j) = j\sqrt{j^2 - (g-h)^2}\sqrt{(g+h+1)^2 - j^2}$ and for this to vanish we must have $j = 0$, or $j = g - h$, or $j = g + h + 1$, none of which are possible given that $j = g - h + 1$ and $j \leq g + h$). Thus the only case that needs special handling is $j - 1 = 0$ i.e. $j = 1$; all other cases may be handled using the recursion formula.

4.1 $j = 1$

Now $j = 1$ and $j = g - h + 1$ together imply $g = h$ and hence $j_1 = j_2$; we will use J to denote the common value of j_1 and j_2 and note that $j \leq g + h$ implies $J \geq 1$. We seek to calculate

$$\mathrm{w}(j) = \mathrm{w}(1) = \begin{pmatrix} J & J & 1 \\ m & -m & 0 \end{pmatrix} = \begin{pmatrix} 1 & J & J \\ 0 & m & -m \end{pmatrix} \tag{16}$$

where the final equality follows from Eq. 4. We apply Eq. 1 to the right-hand symbol. In this case

$$x(t) = t!t!(J - 1 + t - m)!(1-t)!(J + m - t)!(1-t)! \tag{17}$$

To have non-negative factorial arguments we must have $t = 0$ or $t = 1$ (others are ruled out by the first or final factorial). We calculate:

$$x(0) = (J - 1 - m)!(J + m)! \qquad x(1) = (J - m)!(J + m - 1)! \tag{18}$$

and from this we see that there will be both solutions if $m = 0$ or if $m = 2$ and $J \geq 3$, one solution ($t = 1$) if $m = 2$ and $J = 2$, and no solutions if $m = 2$ and $J \leq 1$.

4.1.1 $m = 0$

We see

$$\mathrm{w}(j) = \mathrm{w}(1) = \begin{pmatrix} J & J & 1 \\ 0 & 0 & 0 \end{pmatrix} = -\begin{pmatrix} J & J & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{19}$$

where in the final equality we have exchanged the first two columns and applied Eq 5. Thus

$$\mathrm{w}(j) = 0. \tag{20}$$

4.1.2 $m = 2$ and $J \geq 3$

Here we use Eq 1 with $t = 0$ and $t = 1$ to calculate:

$$\begin{aligned} \mathrm{w}(j) = \begin{pmatrix} 1 & J & J \\ 0 & 2 & -2 \end{pmatrix} &= (-1)^{(1-J+2)} \sqrt{\frac{(2J-1)!}{(2J+2)!}} \times (J+2)!(J-2)! \\ &\quad \times \left(\frac{1}{(J-3)!(J+2)!} - \frac{1}{(J-2)!(J+1)!} \right) \\ &= (-1)^{(1-J)} \sqrt{\frac{(2J-1)!}{(2J+2)!}} \times \left(\frac{(J-2)!}{(J-3)!} - \frac{(J+2)!}{(J+1)!} \right) \\ &= 4(-1)^J \sqrt{\frac{(2J-1)!}{(2J+2)!}} \\ &= 2(-1)^J \sqrt{\frac{1}{J(J+1)(2J+1)}}. \end{aligned} \tag{21}$$

4.1.3 $m = 2$ and $J = 2$

Here we use Eq 1 with $t = 1$ to calculate:

$$\begin{aligned} \mathrm{w}(j) = \begin{pmatrix} 1 & J & J \\ 0 & 2 & -2 \end{pmatrix} &= (-1)^{(1-J+2)} \sqrt{\frac{(2J-1)!}{(2J+2)!}} \times (J+2)!(J-2)! \\ &\quad \times \left(-\frac{1}{(J-2)!(J+1)!} \right) \\ &= (-1)^J \sqrt{\frac{(2J-1)!}{(2J+2)!}} \frac{(J+2)!}{(J+1)!} \\ &= 4(-1)^J \sqrt{\frac{(2J-1)!}{(2J+2)!}} \qquad \text{(as } J = 2\text{)} \\ &= 2(-1)^J \sqrt{\frac{1}{J(J+1)(2J+1)}}. \end{aligned} \tag{22}$$

Note that by coincidence this matches the formula for the $m = 2$ and $J \geq 3$ case.

4.1.4 $m = 2$ and $J \leq 1$

In this case there are no valid values of t and hence $\mathrm{w}(j) = 0$.

4.2 $j > 1$

In this case the recursion formula may be applied to calculate:

$$\begin{aligned}
\mathrm{w}(j) &= -\frac{B(j-1)}{(j-1)A(j)}\,\mathrm{w}(j-1) \\
&= \frac{2m(2(g-h+1)-1)}{\sqrt{(g-h+1)^2-(g-h)^2}\sqrt{(g+h+1)^2-(g-h+1)^2}}\,\mathrm{w}(j-1) \\
&= \frac{m(2g-2h+1))}{\sqrt{2g-2h+1}\sqrt{h(g+1)}}\,\mathrm{w}(j-1) \\
&= m\sqrt{\frac{2g-2h+1}{h(g+1)}}\,\mathrm{w}(j-1)
\end{aligned} \tag{23}$$

Note that when $m = 0$ we have $\mathrm{w}(j) = 0$.

5 $j > g - h + 1$

Here we may use the recursion to compute:

$$\mathrm{w}(j) = -\frac{1}{(j-1)A(j)}\left(B(j-1)\,\mathrm{w}(j-1) + jA(j-1)\,\mathrm{w}(j-2)\right) \tag{24}$$

with

$$\begin{aligned}
B(j-1) &= -2mj(j-1)(2j-1) \\
A(j-1) &= (j-1)\sqrt{(j-1)^2-(g-h)^2}\sqrt{(g+h+1)^2-(j-1)^2} \\
&= (j-1)\sqrt{(j-1-g+h)(j-1+g-h)(g+h+2-j)(g+h+j)} \\
A(j) &= j\sqrt{j^2-(g-h)^2}\sqrt{(g+h+1)^2-j^2} \\
&= j\sqrt{(j-g+h)(j+g-h)(g+h+1-j)(g+h+1+j)}
\end{aligned} \tag{25}$$

After cancelling common factors of j and $j-1$ we have

$$\begin{aligned}
\mathrm{w}(j) = {} & \frac{2m(2j-1)}{\sqrt{(j-g+h)(j+g-h)(g+h+1-j)(g+h+1+j)}}\,\mathrm{w}(j-1) \\
& -\sqrt{\left(\frac{j-1-g+h}{j-g+h}\right)\left(\frac{j-1+g-h}{j+g-h}\right)\left(\frac{g+h+2-j}{g+h+1-j}\right)\left(\frac{g+h+j}{g+h+1+j}\right)}\,\mathrm{w}(j-2)
\end{aligned} \tag{26}$$

When $m = 0$ we see that the first term on the right vanishes. Coupled with Eq 20 this implies that every second $\mathrm{w}(j)$ (starting with the second one) vanishes.