Efficient Computation of Clebsch-Gordan Coefficients

William O. Straub
Pasadena, California 91104
March 14, 2014

Abstract

The problem of angular momentum addition requires the calculation of Clebsch-Gordan coefficients. While systems involving small values of momenta and spin present no special problem, larger systems require extensive computational effort. This paper describes a straightforward method for computing the coefficients for any two-particle problem exactly by means of a simplified form of the recursion formula in a notation that is particularly accessible to the third- or fourth-year student. The method is summarized in a brief BASIC program.

1. Problem Overview

Consider the addition of orbital and spin angular momenta for two particles (or two unconnected systems) that reside in uncoupled eigenstates designed as $|\,j_1 m_1\rangle$ and $|\,j_1 m_1\rangle$. A product state $|\,j\,m\rangle$ is to be constructed that is composed of combinations of these individual state eigenkets. The spin terms m_k may take on any integer or half-integer values between $-j_k \leqslant m_k \leqslant j_k$. Although there can be a total of $(2j_1+1)\cdot(2j_2+1)$ possible spin pairs m_1, m_2, each pair must satisfy $m_1 + m_2 = m$ if the corresponding CG coefficient is to be non-zero. Similarly, the product-space orbital momentum j must satisfy the triangle rule $|\,j_1 - j_2| \leqslant j \leqslant j_1 + j_2$, while the product spin m must satisfy $-j \leqslant m \leqslant j$. The CG coefficients, which we denote here as $\langle j_2 m_2|\langle j_1 m_1|jm\rangle$, effectively superpose all state products via the closure relation

$$|jm\rangle = \sum_{m_1,m_2} |j_1 m_1\rangle|j_2 m_2\rangle\langle j_2 m_2|\langle j_1 m_1|jm\rangle \tag{1.1}$$

A particular CG coefficient therefore represents the (real) probability amplitude for the corresponding product ket $|j_1 m_1\rangle|j_2 m_2\rangle$ (a more proper expression would be $|j_1 m_1\rangle \otimes |j_2\, m_2\rangle$, since the systems must be unconnected). The summation over spins introduces many disallowed states, so that the number of non-zero CG coefficients is comparatively small. If we restrict the spins in (1.1) so that only allowed state products appear in the summation, then the problem can be restated more succinctly as

$$|jm\rangle = \sum_{k=1}^{n} |j_1 m_{1,k}\rangle|j_2 m_{2,k}\rangle\langle j_2 m_{2,k}|\langle j_1 m_{1,k}|jm\rangle$$

where k represents an allowed spin pair index and n is the total number of such pairs (this is also the number of non-zero CG coefficients). In the following, we shall assume that all valid spin pairs for a particular problem have been identified (this will be demonstrated shortly). We can then drop the somewhat imposing notation for the CG coefficient by expressing it instead as

$$C_k = \langle\, j_2 m_{2,k}|\langle\, j_1 m_{1,k}|\, jm\rangle$$

We can now write

$$|jm\rangle = \sum_{k=1}^{n} C_k\, |j_1 m_{1,k}\rangle|j_2\, m_{2,k}\rangle \tag{1.2}$$

By assigning $m_{1,1}$ as the lowest allowed spin for particle 1 (and $m_{1,n}$ as the highest value), we can develop a convenient method for relabelling all of the spin indices that will greatly simplify the determination of the C_k.

2. Approach

In order to solve (1.2) for the CG coefficients, we must first know how many non-zero coefficients exist for a given problem and what the allowed spin pairs are. Both of these questions can be answered by plotting the

condition $m_2 = m - m_1$ on the $m_1 m_2$ plane and observing the locations of the quantities $m_{1,1}$ and $m_{1,n}$. It is easy to verify that if $j_2 - j_1 \geqslant m$, then the lowest possible spin for particle 1 must be $m_{1,1} = -j_1$; otherwise, $m_{1,1} = m - j_2$. Similarly, it can be shown that the highest possible spin for particle 1 is $m_{1,n} = m + j_2$ when $j_1 - j_2 \geqslant m$; otherwise, $m_{1,n} = j_1$. The number of states n spanning the lowest and highest spins can then be determined by $n = m_{1,n} - m_{1,1} + 1$. However, for computational purposes it is easier to dispense with the inequality conditions altogether and just use the equivalent identities

$$\begin{aligned} m_{1,1} &= \frac{m - j_1 - j_2 + |\, j_1 - j_2 + m|}{2} \\ m_{1,n} &= \frac{m + j_1 + j_2 - |\, j_1 - j_2 - m|}{2} \end{aligned} \tag{2.1}$$

(We omit the proof for brevity.) Once $m_{1,1}$ and $m_{1,n}$ have been determined, we can calculate all of the other values $m_{1,k}$ by addition: $m_{1,k+1} = m_{1,k} + 1$, etc., up to $m_{1,n}$. The allowed spins for particle 2 may then be determined using $m_{2,k} = m - m_{1,k}$.

We begin the solution of (1.2) by imposing the condition that the eigenvalues of the total angular momentum operator $\hat{J}^2$ acting on $|\, jm\rangle$ must be the same as those obtained by action of $\hat{J}^2$ on $|\, j_1 m_{1,k}\rangle |\, j_2 m_{2,k}\rangle$. That is, we demand that

$$\hat{J}^{\,2} |jm\rangle = j(j+1)\hbar^2 |jm\rangle$$

be expandable in terms of the operator $\hat{J} = \hat{J}_1 + \hat{J}_2$, where $\hat{J}_k = \hat{J}_{kx}\,\hat{e}_x + \hat{J}_{ky}\,\hat{e}_y + \hat{J}_{kz}\,\hat{e}_z$ $(k = 1, 2)$. However, things are made difficult by the fact that the operators $\hat{J}_{kx}$ and $\hat{J}_{ky}$ acting on $|\, j_1 m_{1,k}\rangle |\, j_2 m_{2,k}\rangle$ lead to extremely complicated expressions. Fortunately, the total angular momentum operator $\hat{J}^{\,2}$ is expressible in terms of the quantities $\hat{J}_k$ via the familiar identity

$$\hat{J}^2 = \hat{J}_1^2 + \hat{J}_2^2 + 2\hat{J}_{1z}\hat{J}_{2z} + \hat{J}_{1+}\hat{J}_{2-} + \hat{J}_{1-}\hat{J}_{2+} \tag{2.2}$$

where the quantities $\hat{J}_{k\pm} = \hat{J}_{kx} \pm i\hat{J}_{ky}$ are the raising $(+)$ and lowering $(-)$ operators (or "ladder" operators) for particle k, which increase or decrease the spin component by one unit (the normalization constant for the lth spin pair is $\sqrt{j_k(j_k+1) - m_{k,l}(m_{k,l} \pm 1)}\hbar$). The operators in (2.2) provide convenient "access" to the eigenvalues we need to pull out of $|\, j_1 m_{1,k}\rangle |\, j_2 m_{2,k}\rangle$ because they involve only the commuting operators $\hat{J}_k^2$ and $\hat{J}_{kz}$ and the ladder operators. Therefore, we have

$$\hat{J}^{\,2} |jm\rangle = \sum_{k=1}^{n} C_k \left[\hat{J}_1^2 + \hat{J}_2^2 + 2\hat{J}_{1z}\hat{J}_{2z} + \hat{J}_{1+}\hat{J}_{2-} + \hat{J}_{1-}\hat{J}_{2+}\right] |jm_{1,k}\rangle |jm_{2,k}\rangle$$

Carrying out the indicated operations, we obtain a set of n homogeneous linear equations in the CG coefficients:

$$\begin{aligned} &C_k \left\{ j_1(j_1+1) + j_2(j_2+1) + 2m_{1,k}m_{2,k} - j(j+1) \right\} |j_1 m_{1,k}\rangle |j_2 m_{2,k}\rangle + \\ &C_k \sqrt{j_1(j_1+1) - m_{1,k}(m_{1,k}+1)}\sqrt{j_2(j_2+1) - m_{2,k}(m_{2,k}-1)}\,|\, j_1 m_{1,k}+1\rangle |j_2 m_{2,k}-1\rangle + \\ &C_k \sqrt{j_1(j_1-1) - m_{1,k}(m_{1,k}-1)}\sqrt{j_2(j_2+1) - m_{2,k}(m_{2,k}+1)}\,|\, j_1 m_{1,k}-1\rangle |j_2 m_{2,k}+1\rangle = 0 \end{aligned} \tag{2.3}$$

The various product kets in (2.3) serve only to keep track of the indices for C_k and their coefficients; as we really have no need for them (our goal, after all, is to find the C_k), it would considerably simplify matters if we could dispense with them altogether. One way of doing this is to relabel the second and third terms in the above expression so that the corresponding product kets are the same as that in the first term, $|\, j_1 m_{1,k}\rangle |\, j_2 m_{2,k}\rangle$. We can then divide this product ket out since it is arbitrary for any k.

To accomplish this, consider the factor $m_{1,k} + 1$ in the second term above. It follows that if $m_{1,1}$ is the lowest allowable spin for particle 1, a step up to the next spin must require that $m_{1,k} + 1 = m_{1,k+1}$. Likewise, since $m_{2,k} = m - m_{1,k}$, we must have $m_{2,k} + 1 = m_{1,k-1}$. Similarly, in the third term we have $m_{1,k} - 1 = m_{1,k-1}$ and $m_{2,k} + 1 = m_{2,k-1}$. In view of this, we set $k' = k + 1$ in the second term, which changes C_k to C_{k-1} and converts

the product ket from $|\,j_1 m_{1,k}\ +1\rangle|\,j_2 m_{2,k}\ -1\rangle$ to $|\,j_1 m_{1,k}\rangle|\,j_2 m_{2,k}\rangle$. Similarly, revising the index from k to $k-1$ in the third term changes C_k to C_{k+1} with a similar change in the product ket. We then arrive at

$$\begin{aligned} &C_k\left\{\,j_1(j_1+1)+j_2(j_2+1)+2m_{1,k}m_{2,k}-j(j+1)\right\}\,|\,j_1 m_{1,k}\rangle|j_2 m_{2,k}\rangle\,+\\ &C_{k-1}\sqrt{j_1(j_1+1)-m_{1,k}\,m_{1,k-1}}\sqrt{j_2(j_2+1)-m_{2,k}\,m_{2,k-1}}\,|\,j_1 m_{1,k}\rangle|j_2 m_{2,k}\,\rangle\,+\\ &C_{k+1}\sqrt{j_1(j_1+1)-m_{1,k}\,m_{1,k+1}}\sqrt{j_2(j_2+1)-m_{2,k}\,m_{2,k+1}}\,|j_1 m_{1,k}\rangle|j_2 m_{2,k}\,\rangle\,=0 \end{aligned} \tag{2.4}$$

Again, because the product ket is arbitrary, we can drop it altogether and write

$$\begin{aligned} &C_k\left\{j_1(j_1+1)+j_2(j_2+1)+2m_{1,k}m_{2,k}-j(j+1)\right\}\,+\\ &C_{k-1}\sqrt{j_1(j_1+1)-m_{1,k}\,m_{1,k-1}}\sqrt{j_2(j_2+1)-m_{2,k}\,m_{2,k-1}}\,+\\ &C_{k+1}\sqrt{j_1(j_1+1)-m_{1,k}\,m_{1,k+1}}\sqrt{j_2(j_2+1)-m_{2,k}\,m_{2,k+1}}\,=0 \end{aligned} \tag{2.5}$$

Equation (2.5) is a particularly simple form of the recursion relations for the CG coefficients. It can be viewed as the homogeneous matrix expression $AC=0$, where the square matrix A (of rank n) has diagonal elements corresponding to the coefficients of C_k, while the two off-diagonal elements correspond to the coefficients of C_{k-1} and C_{k+1}. The coefficient matrix is therefore tridiagonal with a bandwidth of two. Note also that off-diagonal terms like $m_{1,k}\cdot m_{1,k+1}$ are invariant with respect to interchange of the indices k and $k+1$; thus, $A_{k\,k+1}=A_{k+1\,k}$, so the coefficient matrix A is symmetric. Tridiagonal, symmetric matrices are very easy to manipulate and, although the matrix is singular, we can solve for the C_k using the fact that the CG coefficients are the components of a unit vector (that is, the sum of the squares of the CG coefficients is unity). This condition uniquely (up to a sign) determines the coefficients. The CG coefficients are therefore simply the components of the n-dimensional nullspace vector associated with the coefficient matrix A.

3. Computational Procedure

To find the C_k, we must solve the homogenous set of equations given by

$$\begin{pmatrix} a_{11} & a_{12} & 0 & 0 & 0 & \cdots & 0\\ a_{12} & a_{22} & a_{23} & 0 & 0 & \cdots & 0\\ 0 & a_{23} & a_{33} & a_{34} & 0 & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & 0 & 0 & a_{n-1\,n} & a_{nn} \end{pmatrix} \begin{pmatrix} C_1\\ C_2\\ C_3\\ \vdots\\ C_n \end{pmatrix} = \begin{pmatrix} 0\\ 0\\ 0\\ \vdots\\ 0 \end{pmatrix},$$

subject to $|C|=1$, where

$$a_{k\,k}=j_1(j_1+1)+j_2(j_2+1)+2m_{1,k}m_{2,k}-j(j+1) \tag{3.1}$$

and

$$a_{k\,k+1}=\sqrt{j_1(j_1+1)-m_{1,k}m_{1,k+1}}\sqrt{j_2(j_2+1)-m_{2,k}m_{2,k+1}} \tag{3.2}$$

Any backward-substitution procedure can be used to solve for the coefficients. It is conventional to fix the sign of the coefficients by taking C_n to be a positive number.

4. Example

Suppose we are given two particles with $j_1=3$ and $j_2=6$, which we wish to combine into a product state in which $j=5$, $m=3$. Our definition for n tells us that there will be a total of 7 CG coefficients; that is, in order

for $m_{1,k} + m_{2,k} = 3$, the particle spins can combine only in the seven ordered pairs

$$\begin{aligned}
m_{1,1},\, m_{2,1} &= -3, 6 \\
m_{1,2},\, m_{2,2} &= -2, 5 \\
m_{1,3},\, m_{2,3} &= -1, 4 \\
m_{1,4},\, m_{2,4} &= \ 0, 3 \\
m_{1,5},\, m_{2,5} &= \ 1, 2 \\
m_{1,6},\, m_{2,6} &= \ 2, 1 \\
m_{1,7},\, m_{2,7} &= \ 3, 0
\end{aligned}$$

as is easily confirmed by the formulas given earlier. The matrix elements may be computed from (3.1) and (3.2); they are

$$\begin{aligned}
a_{11} &= -12 & a_{12} &= a_{21} = 6\sqrt{2} \\
a_{22} &= 4 & a_{23} &= a_{32} = 2\sqrt{55} \\
a_{33} &= 16 & a_{34} &= a_{43} = 6\sqrt{10} \\
a_{44} &= 24 & a_{45} &= a_{54} = 12\sqrt{3} \\
a_{55} &= 28 & a_{56} &= a_{65} = 20 \\
a_{66} &= 28 & a_{67} &= a_{76} = 6\sqrt{7} \\
a_{77} &= 24
\end{aligned}$$

with all the other matrix elements being zero. We therefore have to solve the system

$$\begin{pmatrix}
-12 & 6\sqrt{2} & 0 & 0 & 0 & 0 & 0 \\
6\sqrt{2} & 4 & 2\sqrt{55} & 0 & 0 & 0 & 0 \\
0 & 2\sqrt{55} & 16 & 6\sqrt{10} & 0 & 0 & 0 \\
0 & 0 & 6\sqrt{10} & 24 & 12\sqrt{3} & 0 & 0 \\
0 & 0 & 0 & 12\sqrt{3} & 28 & 20 & 0 \\
0 & 0 & 0 & 0 & 20 & 28 & 6\sqrt{7} \\
0 & 0 & 0 & 0 & 0 & 6\sqrt{7} & 24
\end{pmatrix}
\begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

subject to $|C| = 1$. The student should have no difficulty showing that the solution is

$$\begin{pmatrix}
\langle 3,-3|\langle 6,6|5,3\rangle \\
\langle 3,-2|\langle 6,5|5,3\rangle \\
\langle 3,-1|\langle 6,4|5,3\rangle \\
\langle 3,0|\langle 6,3|5,3\rangle \\
\langle 3,1|\langle 6,2|5,3\rangle \\
\langle 3,2|\langle 6,1|5,3\rangle \\
\langle 3,3|\langle 6,0|5,3\rangle
\end{pmatrix}
=
\begin{pmatrix}
\sqrt{11/91} \\
\sqrt{22/91} \\
-\sqrt{10/91} \\
-1/\sqrt{91} \\
\sqrt{7/39} \\
-8/\sqrt{273} \\
2/\sqrt{39}
\end{pmatrix}$$

5. Computer Program

The two-particle procedure is very easy to implement on a computer. It can be used to calculate the CG coefficients of systems having extremely large momenta and spin exactly (within the limits of floating-point precision). The following BASIC program uses the formulas presented above to compute the CG coefficients in decimal format (the student might want to modify the program to output the coefficients for simple problems in terms of ratios of integers, as we have done in the example problem). Because the backward-substitution procedure needs only the last $n - 1$ rows of the $n \times n$ coefficient matrix A (which is sparse with never more than

$2n-2$ non-zero elements), the program constructs a vector B from these elements in lieu of storing the entire coefficient matrix.

For a large problem like $j=50, m=40, j_1=30, j_2=40$, the typical personal computer can compute the 31 CG coefficients in a fraction of a second. However, the decimal output is a serious limitation. For this example, the value of $\langle 30,30|\langle 40,10|50,40\rangle$ is approximately 0.1246637149976796; by comparison, Mathematica returns

$$\begin{aligned}\langle 30,30|\langle 40,10|50,40\rangle &= \frac{261}{2}\sqrt{\frac{27564505}{30205852104326}} \\ &= 0.12466371499767958758\ldots\end{aligned}$$

which is decidedly more useful.

```
CLEAR
DEFDBL A-S: DIM B(2000), C(2000)
INPUT "Enter J,M,J1,J2 ", J, M, J1, J2
M1 = (M-J1-J2+ABS(J1-J2+M))/2 :  N = (M+J1+J2-ABS(J1-J2-M))/2-M1+1
1:  FOR X = N-1 TO 1 STEP -1
IF FLAG = 1 THEN GOTO 2
B(2*X) = J1*(J1+1)+J2*(J2+1)+2*(M1+X)*(M-M1-X)-J*(J+1) :  C(N) = 1
B(2*X-1) = SQR((J1*(J1+1)-(M1+X)*(M1+X-1))*(J2*(J2+1)-(M-M1-X)*(M-M1-X+1)))
2:  C(X) = -(B(2*X)*C(X+1)+B(2*X+1)*C(X+2))/B(2*X-1)
SUM = SUM + C(X)
NEXT X
FLAG = FLAG + 1
IF FLAG = 1 THEN C(N) = SQR(1/(SUM+1)) :  GOTO 1
FOR X = 1 TO N
PRINT USING "#.###############"; C(X)
NEXT X
END
```