Notes on the numerical calculation of Clebsch-Gordan coefficients

Reference SN: Sakurai and Napolitano, *Modern Quantum Mechanics*, 2nd ed.

- I have implemented a simple Python function to demonstrate the calculation of Clebsch-Gordan coefficients:

  `http://github/jddmartin/simple_clebsch_gordan`

  The purpose of these notes is to document the usage of some of the equations in this code. Boxed equations are explicitly used in the code.

- Notation: in this discussion we will abbreviate the Clebsch-Gordan notation of SN from $\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle$ to $\langle j_1 j_2; m_1, m_2 | j, m\rangle$.

- we begin with the general recursion relations for Clebsch-Gordan coefficients:

$$C_\pm(j, m')\,\langle j_1 j_2; m_1', m_2' | j, m' \pm 1\rangle = C_\pm(j_1, m_1' \mp 1)\,\langle j_1 j_2; m_1' \mp 1, m_2' | j, m'\rangle + C_\pm(j_2, m_2' \mp 1)\,\langle j_1 j_2; m_1', m_2' \mp 1 | j, m'\rangle \quad (1)$$

  where

$$\boxed{C_\pm(j, m) = \sqrt{j(j+1) - m(m \pm 1)}.} \quad (2)$$

  For the derivation of Eq. 1, see pages 224-225 of SN culminating in SN3.8.49.

- for evaluation of the general case $\langle j_1 j_2; m_1, m_2 | j, m\rangle$, when $m \neq j$, we will use the lower sign version of Eq. 1 to determine a Clebsch-Gordan coefficient $\langle j_1 j_2; m_1, m_2 | j, m\rangle$ in terms of the coefficents:

$$\langle j_1 j_2; m_1 + 1, m_2 | j, m+1\rangle \text{ and } \langle j_1 j_2; m_1\, m_2 + 1 | j, m+1\rangle.$$

  The relevant equation is determined by substitution of $m' = m + 1$, $m_1' = m_1$ and $m_2' = m_2$ into the lower sign recursion relation of Eq. 1, to give:

$$\boxed{\langle j_1 j_2; m_1, m_2 | j, m\rangle = \frac{1}{C_-(j, m+1)}[C_-(j_1, m_1 + 1)\,\langle j_1 j_2; m_1 + 1, m_2 | j, m+1\rangle + C_-(j_2, m_2 + 1)\,\langle j_1 j_2; m_1, m_2 + 1 | j, m+1\rangle].} \quad (3)$$

- when we have to evaluate the Clebsch-Gordan coefficients $\langle j_1 j_2; m_1, j - m_1 | j, j\rangle$ we will use the upper sign recursion relation of Eq. 1 to determine this coefficient in terms of the $\langle j_1 j_2; m_1 + 1, j - m_1 - 1 | j, j\rangle$ coefficient.

- the relevant formula can be obtained from the general recursion relation by substitution of $m_1' = m_1 + 1$ and $m_2' = j - m_1$ into the upper sign version of Eq. 1 and rearrangement:

$$\boxed{\langle j_1 j_2; m_1, j - m_1 | j, j\rangle = \frac{-\,C_+(j_2, j - m_1 - 1)}{C_+(j_1, m_1)}\,\langle j_1 j_2; m_1 + 1, j - m_1 - 1 | j, j\rangle\,.} \quad (4)$$

- we must be able to calculate the special Clebsch-Gordan coefficient $\langle j_1 j_2; j_1, j - j_1 | j, j\rangle$ (the termination of the recursion relation of Eq. 4).

  This coefficient is defined by convention to be both positive and real. To determine its magnitude, we use the orthonormality constraints of the Clebsch-Gordan coefficients (see SN3.8.42):

$$\sum_{m_1, m_2} \langle j_1 j_2; m_1, m_2 | j, m\rangle \langle j_1 j_2; m_1, m_2, j', m'\rangle = \delta_{j,j'}\delta_{m,m'} \tag{5}$$

  specializing to:

$$\sum_{m_1 = j_1, j_1 - 1, \ldots} | \langle j_1 j_2; m_1, j - m_1 | j, j\rangle |^2 = 1. \tag{6}$$

  Rearranging gives:

$$\frac{1}{|\langle j_1 j_2; j_1, j - j_1 | j, j\rangle|^2} = 1 + \frac{1}{|\langle j_1 j_2; j_1, j - j_1 | j, j\rangle|^2} \sum_{m_1 = j_1 - 1, j_1 - 2, \ldots} | \langle j_1 j_2; m_1, j - m_1 | j, j\rangle |^2 \tag{7}$$

  This equation can be written in a slightly different form suitable for use of a specialized form of the general recursion relationship (Eq. 1):

$$\frac{1}{|\langle j_1 j_2; j_1, j - j_1 | j, j\rangle|^2} = 1 + f(j_1) \times [1 + f(j_1 - 1) \times [1 + f(j_1 - 2) \times [...]]] \tag{8}$$

  where

$$f(m_1) \equiv \left| \frac{\langle j_1 j_2; m_1 - 1, j - (m_1 - 1) | j, j\rangle}{\langle j_1 j_2; m_1, j - m_1 | j, j\rangle} \right|^2. \tag{9}$$

  We can obtain an expression for $f(m_1)$ from the upper-sign version of the general recursion relationship (Eq. 1). Substitution of $m_1' = m_1$ and $m_2' = j - m_1 + 1$ and rearrangment gives:

$$\boxed{f(m_1) = \left| \frac{C_+(j_2, j - m_1)}{C_+(j_1, m_1 - 1)} \right|^2.} \tag{10}$$

- note Eq. 8 may be evaluated using recursion:

$$\boxed{s(m_1) = 1 + f(m_1) \times s(m_1 - 1).} \tag{11}$$

  The recursion terminates when the Clebsch-Gordan coefficient in the numerator of Eq. 10 is known to be zero. i.e. the magnitude of either one of the uncoupled magnetic quantum numbers are larger than allowed by j_1 and j_2.

- finally, the required Clebsch-Gordan coefficient is (through rearrangment of Eq. 8):

$$\boxed{\langle j_1 j_2; j_1, j - j_1 | j, j\rangle = \frac{1}{\sqrt{s(j_1)}},} \tag{12}$$

  making use of the convention that this coefficient is real and positive.

Comments are welcome. - JDDM.