Problem Set 3
Physics 481 / Spring 2000
Professor Klaus Schulten

Problem 1: Construct Clebsch-Gordan coefficients

Complete exercise 6.2.1 of the class notes.

Problem 2: Classical and non-classicalClebsch-Gordan coefficients[1]

(a) Plot the function

$$f_k(m) \; = \; (120, 20|60, m, 60 + k, 20 - m) \tag{1}$$

for $k = 0, 10, 20$ using the mathematica command
ListPlot[N[Table[{m, ClebschGordan[{60, m}, {60+k, 20-m}, {120,20}]}, {m, -40 ,60,1}]], PlotJoined → True, PlotRange → All]

(b) Show that the length of a quantum mechanical angular momentum state $j, m\rangle$ can be expanded

$$J\hbar \; = \; \left[\hbar^2 \, j(j+1)\right]^{\frac{1}{2}} \; = \; \hbar \left(j + \frac{1}{2}\right) \; + \; \mathrm{O}\left(\frac{1}{j}\right) \; . \tag{2}$$

(c) One can associate with a Clebsch-Gordan coefficient $(j_1, m_1|j_2, m_2, j_3, m_3)$ a triangle with edges $J_1 = j_1 + \frac{1}{2}$, $J_2 = j_2 + \frac{1}{2}$, and $J_3 = j_3 + \frac{1}{2}$. Specifing the vertices through their two associated edges, i.e., vertex (1,2) being the vertex joining edge 1 and 3, the vertices of the triangle associated with $(j_1, m_1|j_2, m_2, j_3, m_3)$ can be given z-coordidinates $z_{(1,3)} = 0$, $z_{(3,2)} = m_3$, and $z_{(1,2)} = m_1$. The projection of this triangle onto the x, y-plane has area

[1] **Semiclassical approximations to 3j- and 6j-coefficients for quantum-mechanical coupling of angular momenta**, K. Schulten and R.G. Gordon, *J. Math. Phys.* **16**: 1971–1988 (1975)

A that can be evaluated according to the formula

$$A^2 = -\frac{1}{16}\begin{vmatrix} 0 & J_1^2 - m_1^2 & J_2^2 - m_2^2 & 1 \\ J_1^2 - m_1^2 & 0 & J_3^2 - m_3^2 & 1 \\ J_2^2 - m_2^2 & J_3^2 - m_3^2 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{vmatrix} \tag{3}$$

Plot A^2 for the series of Clebsch-Gordan coefficients $f_k(m)$ defined in (a), adopting the mathematica command suggested above, and relate the A^2-values to the magnitude of the associated Clebsch-Gordan coefficients. Use the result to distinguish for each case, i.e., k = 0, 10, 20, non-classical regions $[m_{-60}, m_{\rm left}]$ and $[m_{\rm right}, m_{60}]$ as well as the classical region $[m_{\rm left}, m_{\rm right}]$

Problem 3: Spin Coupling

Consider a system of four spin-$\frac{1}{2}$ particles described in the basis

$$\mathfrak{B}_1 = \{|\frac{1}{2},\sigma_1\rangle_1 \, |\frac{1}{2},\sigma_2\,\rangle_2|\frac{1}{2},\sigma_3\,\rangle_3|\frac{1}{2},\sigma_4\rangle_4, \sigma_j = \pm\frac{1}{2}, j = 1,2,3,4\} \tag{4}$$

which, obviously, is of dimension sixteen.

(a) Determine sixteen states in which the four spins are coupled to total spin states. Employ the the `mathematica` command `ClebschGordan`$[\{j_1, m_1\}$, $\{j_2, m_2\}$, $\{J, M\}]$ to determine the needed Clebsch-Gordan coefficients if you do not know them already. One such state is, for example,
$|1, -1(1,0)(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})\rangle$ where the notation adopted here means that the first and second spins, i.e., $|\frac{1}{2},\sigma_1\rangle_1 \, |\frac{1}{2},\sigma_2\rangle_2$ have been coupled to a an $\ell = 1$ state, the third and the fourth spins, i.e., $|\frac{1}{2},\sigma_3\rangle_3 \, |\frac{1}{2},\sigma_4\rangle_4$ have been coupled to an $\ell = 0$ state, and the states $\ell = 1$ and $\ell = 2$ states have been coupled to a total $\ell = 1$ state. Express the sixteen states in terms of the elements of the basis $\mathfrak{B}_1$ defined above.

(b) Show that the sixteen states determined in (a) define a new basis $\mathfrak{B}_2$ of orthonormal states. Employ `mathematica` to evaluate the necessary scalar products.

(c) Let $\vec{S}_1$, $\vec{S}_2$, $\vec{S}_3$ and $\vec{S}_4$ denote the spin operators which measure the properties of the states $|\frac{1}{2},\sigma_1\rangle_1$, $|\frac{1}{2},\sigma_2\rangle_2$, $|\frac{1}{2},\sigma_3\rangle_3$ and $|\frac{1}{2},\sigma_4\rangle_4$, respectively.

Demonstrate that the elements of the basis $\mathfrak{B}_2$ are eigenstates of the following operators

$$[\vec{S}_1]^2, [\vec{S}_2]^2, [\vec{S}_3]^2, [\vec{S}_4]^2, [\vec{S}_1+\vec{S}_2]^2, [\vec{S}_3+\vec{S}_4]^2, [\vec{S}_1+\vec{S}_2+\vec{S}_3+\vec{S}_4]^2, [\vec{S}_1+\vec{S}_2+\vec{S}_3+\vec{S}_4]_3 \tag{5}$$

where we employed a, hopefully, obvious notation.

Problem 4: Reaction Between Triplet Molecules

Two triplet molecules collide in a state

$$|1, m_1\rangle_1 \, |1, m_2\rangle_2 \;=\; |1, m_1; 1, m_2\rangle \; . \tag{6}$$

The interaction is

$$V \;=\; A\vec{S}_1 \cdot \vec{S}_2 \tag{7}$$

where A is an interaction constant, the value of which is immaterial for the following. The molecules can either react to form overall singlet ($J = 0$), triplet ($J = 1$), or quintet ($J = 2$) products, the reaction probability, for an $|1, m_1; 1, m_2\rangle$ initial state, being

$$p(m_1, m_2 \to J) \;=\; \sum_M |\langle 1, m_1; 1, m_2|V|J, M(1,1)\rangle|^2 \; . \tag{8}$$

Determine the reaction ratios

$$p(m_1, m_2 \to 0) \;:\; p(m_1, m_2 \to 1) \;:\; p(m_1, m_2 \to 2) \tag{9}$$

for all m_1, m_2 combinations. Employ the Clebsch-Gordan coefficients provided in Table 6.1 of the class notes as well as (as a check) the `mathematica` command `ClebschGordan`$[\{j_1, m_1\}, \;\; \{j_2, m_2\}, \; \{J, M\}]$.

Problem 5: Spin-Orbit Coupling for Hydrogen-Like Atoms

Relativistic effects lead to the effective Hamiltonian for an electron in a hydrogen-like atom

$$H \;=\; H_o \;+\; V \tag{10}$$

where

$$H_o \;=\; -\frac{\hbar^2}{2m_e}\nabla^2 \;-\; \frac{Ze^2}{r} \tag{11}$$

is the non-relativistic Hamiltonian and

$$V = \frac{Ze^3\hbar}{4m_e^2c^2r^3}\,\vec{S}\cdot\vec{J} \tag{12}$$

is the so-called spin-orbit coupling. Here $\vec{S}$ is the spin operator of the electron and $\vec{J}$ the orbital angular momentum operator. Describe the states of the electron in terms of wave functions

$$\Psi(\vec{r}) = g(r)\,\mathfrak{Y}_{JM}(\ell,\frac{1}{2}|\theta,\phi) \tag{13}$$

where $\mathfrak{Y}_{JM}(\ell,\frac{1}{2})$ describes the total angular momentum–spin state, i.e.,

$$\mathfrak{Y}_{JM}(\ell,\frac{1}{2}|\theta,\phi) = \sum_m \langle J,M|\ell,m,\frac{1}{2},M-m\rangle\,Y_{\ell m}(\theta,\phi)\chi_{\frac{1}{2}M-m}\,. \tag{14}$$

(a) Using the `mathematica` command

```
In[1]:=     ClebschGordan[{J-1/2, m}, {1/2, M-m}, {J, M}]
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determine the analytical expressions for the Clebsch-Gordan coefficents $\langle J,M|\ell,m,\frac{1}{2},M-m\rangle$ where $\ell = J \pm \frac{1}{2}$

(b) Derive the radial equation obeyed by $g(r)$ as defined in (13).

(c) The solutions (13) are eigenstates of H_o if one chooses for $g(r)$ the radial wave functions for the non-relativistic hydrogen-type atoms. Assuming the corresponding states as zero order states describe their shifts due to spin-orbit coupling for the states with main quantum numbers $n = 1,2,3$, i.e., for the so-called s,p,d states, in 1st order perturbation theory

$$E_{\text{state}} = \langle\text{state}|H_o|\text{state}\rangle + \langle\text{state}|V|\text{state}\rangle\,. \tag{15}$$

Due Tuesday, February 29 in mail box of Gheorghe-Sorin Paraoan.