Problem Set 7
Physics 480 / Fall 1999
Professor Klaus Schulten

Problem 1: Angular Momentum Operators

Do Exercise 5.4.1 of the notes handed out in class.

Problem 2: $Y_{3m}(\theta, \phi)$

Construct all spherical harmonics $Y_{3m}(\theta, \phi)$ following the path $Y_{33} \rightarrow Y_{32} \rightarrow \ldots \rightarrow Y_{3-3}$ as suggested in the class notes.

Problem 3: Triplet Molecule

A molecule in a so-called triplet state is described by spin states $|1, m\rangle$, $m = 1, 0, -1$ and spin operators $\vec{S} = (S_1, S_2, S_3)$. The spin states $|1, m\rangle$ behave like angular momentum states with $\ell = 1$ and the spin operators correspond to the angular momentum oprators $\mathcal{J}_k$, i.e., it holds

$$\begin{aligned} S_3 \,|1,\, m\rangle &= \hbar m \,|1,\, m\rangle \\ S^2 \,|1,\, m\rangle &= 2\,\hbar^2 \,|1,\, m\rangle \\ (S_1 \,-\, i\,S_2)\,|1,\, m\rangle &= \hbar\sqrt{(1+m)(1-m+1)}\,|1,\, m-1\rangle \end{aligned}$$

etc. The latter relationships allow one to determine the matrix representation of the spin operators $\vec{S} = (S_1, S_2, S_3)$.

(a) Determine the matrix representation of $\vec{S} = (S_1, S_2, S_3)$ and S^2 in the basis $\{|1, m\rangle,\, m = 1, 0, -1\}$.

(b) The Hamiltonian for a triplet molecule, accounting also for the presence of an external magnetic field $\vec{B} = (B_1, B_2, B_3)$, is (in convenient units, not specified further)

$$H \;=\; D\,S_3^2 \;-\; E\,(S_1^2 \;-\; S_2^2) \;+\; \vec{B}\cdot\vec{S}\,. \qquad (1)$$

Determine the 3×3 Hamiltonian matrix in the basis $\{|1,\, m\rangle\,,\; m = 1, 0, -1\}$.

(c) Determine the stationary states of this system for a magnetic field $\vec{B} = (B_1, 0, 0)$. Employ for this purpose the `Mathematica` commands `h = {{H11, H12, H13}, {H21, H22, H23}, {H31, H32, H33}}` and `Eigenvalues[N[h]]` where H_{jk} are the respective matrix elements of the Hamiltonian. Plot the energies of the stationary states as a function of $B_1 \geq 0$ for $D = 3\,,\; E = 1$.

The problem set needs to be handed in by Tuesday,November 9.
The web page of Physics 480 is at
`http://www.ks.uiuc.edu/Services/Class/PHYS480/`