Solution to Problem Set 7
Physics 480 / Fall 1999
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Problem 1: Angular Momentum Operators

Excerise 5.4.1

Since,

$$r = \sqrt{x_1^2 + x_2^2 + x_3^2}$$

$$tg\theta = \frac{\sqrt{x_1^2 + x_2^2}}{x_3}$$

$$tg\psi = \frac{x_2}{x_1}$$

Thus we have

$$\partial_{x_1} = \frac{\partial}{\partial r}\frac{\partial r}{\partial x_1} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial x_1} + \frac{\partial}{\partial \psi}\frac{\partial \psi}{\partial x_1}$$

$$\partial_{x_1} = \frac{\partial}{\partial r}\frac{x_1}{r} + \frac{\partial}{\partial \theta}\cos^2\theta \frac{x_1}{x_3\sqrt{x_1^2 + x_2^2}} + \frac{\partial}{\partial \psi}\cos^2\psi(-\frac{x_2}{x_1^2})$$

$$\partial_{x_1} = \sin\theta\cos\psi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\psi\frac{\partial}{\partial \theta} - \frac{1}{r\sin\theta}\sin\psi\frac{\partial}{\partial \psi}$$

$$\partial_{x_2} = \frac{\partial}{\partial r}\frac{\partial r}{\partial x_2} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial x_2} + \frac{\partial}{\partial \psi}\frac{\partial \psi}{\partial x_2}$$

$$\partial_{x_2} = \frac{\partial}{\partial r}\frac{x_2}{r} + \frac{\partial}{\partial \theta}\cos^2\theta \frac{x_2}{x_3\sqrt{x_1^2 + x_2^2}} + \frac{\partial}{\partial \psi}\cos^2\psi\frac{1}{x_1}$$

$$\partial_{x_2} = \sin\theta\sin\psi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\psi\frac{\partial}{\partial \theta} + \frac{1}{r\sin\theta}\cos\psi\frac{\partial}{\partial \psi}$$

$$\partial_{x_3} = \frac{\partial}{\partial r}\frac{\partial r}{\partial x_3} + \frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial x_3} + \frac{\partial}{\partial \psi}\frac{\partial \psi}{\partial x_3}$$

$$\partial_{x_3} = \frac{\partial}{\partial r}\frac{x_3}{r} - \frac{\partial}{\partial \theta}\cos^2\theta\frac{\sqrt{x_1^2 + x_2^2}}{x_3^2}$$

$$\partial_{x_3} = \cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial \theta}$$

and,

$$L_2 = -\frac{i}{\hbar}J_2 = -x_3\partial_{x_1} + x_1\partial_{x_3}$$

$$L_2 = -r\cos\theta(\sin\theta\cos\psi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\cos\psi\frac{\partial}{\partial\theta}-\frac{1}{r\sin\theta}\sin\psi\frac{\partial}{\partial\psi})+r\sin\theta\cos\psi(\cos\theta\frac{\partial}{\partial r}-\frac{1}{r}\sin\theta\frac{\partial}{\partial\theta})$$

$$L_2 = -\cos\psi\frac{\partial}{\partial\theta} + \cot\theta\sin\psi\frac{\partial}{\partial\psi}$$

$$L_3 = -\frac{i}{\hbar}J_3 = x_2\partial_{x_1} - x_1\partial_{x_2}$$

$$\begin{aligned} L_3 &= r\sin\theta\sin\psi(\sin\theta\cos\psi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\psi\frac{\partial}{\partial\theta} - \frac{1}{r\sin\theta}\sin\psi\frac{\partial}{\partial\psi}) \\ &\quad -r\sin\theta cos\psi(\sin\theta\sin\psi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\psi\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\cos\psi\frac{\partial}{\partial\psi}) \end{aligned}$$

$$L_3 = -\frac{\partial}{\partial\psi}$$

Problem 2: Spherical Harmonics

$$L_+ = -ie^{i\varphi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi})$$

$$L_- = ie^{-i\varphi}(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\varphi})$$

$$L_3 = -\frac{\partial}{\partial\varphi}$$

$$L_3Y_{33}(\theta,\varphi) = -3iY_{33}(\theta,\varphi) \Rightarrow Y_{33}(\theta,\varphi) = P_{33}(\theta)e^{3i\varphi}$$

$$L_+Y_{33}(\theta,\varphi) = 0 \Rightarrow (\frac{\partial}{\partial\theta}-3\cot\theta)P_{33}(\theta) = 0 \Rightarrow P_{33}(\theta) = -\sqrt{\frac{7}{4\pi}\frac{1}{6!}\frac{6!}{2^3 3!}}\sin^3\theta$$

Thus:

$$Y_{33}(\theta,\varphi) = -\sqrt{\frac{7}{4\pi}\frac{1}{6!}\frac{6!}{2^3 3!}}\sin^3\theta e^{3i\varphi}$$

$$\begin{aligned} Y_{32}(\theta,\varphi) &= iL_-Y_{33}(\theta,\varphi)/\sqrt{(3+2+1)(3-2)} \\ &= \sqrt{\frac{7}{4\pi}\frac{1}{6!}\frac{6!}{2^3 3!}}e^{-i\varphi}(\frac{\partial}{\partial\theta} + 3\cot\theta)\sin^3\theta e^{3i\varphi}\frac{1}{\sqrt{6}} \\ &= \sqrt{\frac{7}{4\pi}\frac{1}{6!}\frac{6!}{2^3 3!}}\cos\theta\sin^2\theta e^{2i\varphi} \end{aligned}$$

$$
\begin{aligned}
Y_{31}(\theta,\varphi) &= iL_- Y_{32}(\theta,\varphi)/\sqrt{(3+1+1)(3-1)} \\
&= -\sqrt{\frac{7}{4\pi}\frac{1}{5!}}\frac{6!}{2^3 3!}(\frac{\partial}{\partial\theta}+2\cot\theta)\sin^2\theta\cos\theta e^{i\varphi}\frac{1}{\sqrt{10}} \\
&= -\sqrt{\frac{7}{4\pi}\frac{3!}{4!}}\frac{6!}{2^3 3!}\frac{1}{10}\sin\theta(5\cos^2\theta-1)e^{i\varphi}
\end{aligned}
$$

$$
\begin{aligned}
Y_{30}(\theta,\varphi) &= iL_- Y_{31}(\theta,\varphi)/\sqrt{(3+0+1)(3-0)} \\
&= \sqrt{\frac{7}{4\pi}\frac{3!}{4!}}\frac{6!}{2^3 3!}\frac{1}{10}(\frac{\partial}{\partial\theta}+\cot\theta)\sin\theta(5\cos^2\theta-1)\frac{1}{\sqrt{12}} \\
&= \sqrt{\frac{7}{4\pi}\frac{3!}{3!}}\frac{6!}{2^3 3!}\frac{1}{30}\cos\theta(5\cos^2\theta-3)
\end{aligned}
$$

$$
\begin{aligned}
Y_{3-1}(\theta,\varphi) &= iL_- Y_{30}(\theta,\varphi)/\sqrt{(3-1+1)(3+1)} \\
&= -\sqrt{\frac{7}{4\pi}\frac{3!}{3!}}\frac{6!}{2^3 3!}\frac{1}{30}\frac{\partial}{\partial\theta}(5\cos^3\theta-3\cos\theta)e^{-i\varphi}\frac{1}{\sqrt{12}} \\
&= \sqrt{\frac{7}{4\pi}\frac{4!}{2!}}\frac{6!}{2^3 3!}\frac{1}{120}\sin\theta(5\cos^2\theta-1)e^{-i\varphi}
\end{aligned}
$$

$$
\begin{aligned}
Y_{3-2}(\theta,\varphi) &= iL_- Y_{3-1}(\theta,\varphi)/\sqrt{(3-2+1)(3+2)} \\
&= -\sqrt{\frac{7}{4\pi}\frac{4!}{2!}}\frac{6!}{2^3 3!}\frac{1}{120}(\frac{\partial}{\partial\theta}-\cot\theta)\sin\theta(5\cos^2\theta-1)e^{-2i\varphi}\frac{1}{\sqrt{10}} \\
&= \sqrt{\frac{7}{4\pi}\frac{5!}{1!}}\frac{6!}{2^3 3!}\frac{1}{120}\sin^2\theta\cos\theta e^{-2i\varphi}
\end{aligned}
$$

$$
Y_{3-3}(\theta,\varphi) = iL_- Y_{3-2}(\theta,\varphi)/\sqrt{(3-3+1)(3+3)}
$$

$$= \quad -\sqrt{\frac{7}{4\pi}\frac{5!}{1!}}\frac{6!}{2^3 3!}\frac{1}{120}(\frac{\partial}{\partial\theta} - 2\cot\theta)\sin^2\theta\cos^2\theta e^{-3i\varphi}\frac{1}{\sqrt{6}}$$

$$= \quad \sqrt{\frac{7}{4\pi}\frac{1}{6!}}\frac{6!}{2^3 3!}\sin^3\theta e^{-3i\varphi}$$

Problem 3: Triplet Molecule

a)The spin states are

$$|1,1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|1,0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|1,-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The action of the spin operators are given by

$$S_3|1,m\rangle = \hbar m|1,m\rangle$$

$$S^2|1,m\rangle = 2\hbar^2|1,m\rangle$$

$$S^-|1,m\rangle = \hbar\sqrt{(1+m)(2-m)}|1,m-1\rangle$$

$$S^+|1,m\rangle = \hbar\sqrt{(2+m)(1-m)}|1,m+1\rangle$$

S_3 : By inspection,

$$S_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

S^- : Since $S^-|1,1\rangle = \sqrt{2}\hbar|1,0\rangle \qquad S^-|1,0\rangle = \sqrt{2}\hbar|1,-1\rangle$ it follows

$$S^- = \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2}\hbar & 0 & 0 \\ 0 & \sqrt{2}\hbar & -1 \end{pmatrix}$$

$$S^+ = (S^-)^\dagger = \begin{pmatrix} 0 & \sqrt{2}\hbar & 0 \\ 0 & 0 & \sqrt{2}\hbar \\ 0 & 0 & 0 \end{pmatrix}$$

Since $S^\pm = S_1 \pm iS_2$

$$S_1 = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$S_2 = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

It follows from inspection

$$S^2 = \hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

b.

$$H = DS_3^2 - E(S_1^2 - S_2^2) + \vec{B}.\vec{S}$$

Using the matrix representation we just derived for $\vec{S}$

$$S_1^2 = \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

$$S_2^2 = \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

Therefore,

$$H = \begin{pmatrix} D\hbar^2 + B_3\hbar & \frac{\hbar}{\sqrt{2}}(B_1 - iB_2) & -E\hbar^2 \\ \frac{\hbar}{\sqrt{2}}(B_1 + iB_2) & 0 & \frac{\hbar}{\sqrt{2}}(B_1 - iB_2) \\ -E\hbar^2 & \frac{\hbar}{\sqrt{2}}(B_1 + iB_2) & D\hbar^2 - B_3\hbar \end{pmatrix}$$

c. For $B = (B_1, o, o), D = 3, E = 1, \hbar = 1$

$$H = \begin{pmatrix} 3 & \frac{B_1}{\sqrt{2}} & -1 \\ \frac{B_1}{\sqrt{2}} & 0 & \frac{B_1}{\sqrt{2}} \\ -1 & \frac{B_1}{\sqrt{2}} & 3 \end{pmatrix}$$

The eigenvalues are $4, 1 \pm \sqrt{1 + B_1^2}$

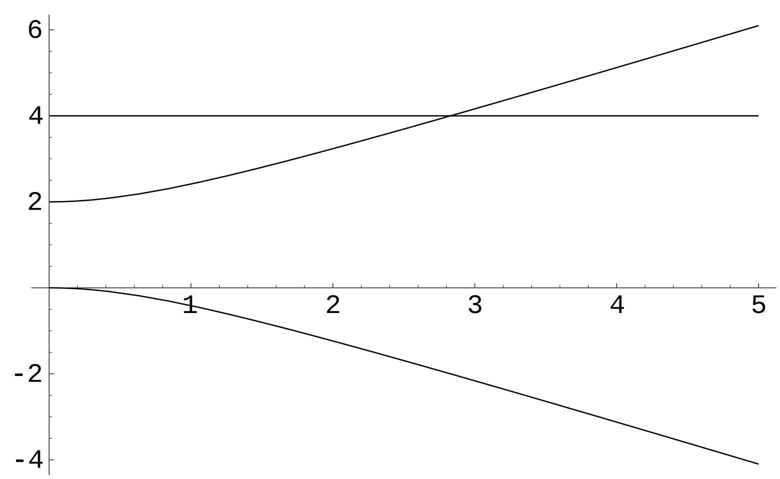

Figure 1: Energies of the stationary states as a fn. of B1