$S^2 = S_1^2 + S_2^2 + 2 S_1 \cdot S_2$

5-7 ?

Problem 2: Perturbation with 2 spins (10 points):

Let $\vec{S_1}$ and $\vec{S_2}$ be the spin operators of two spin-1/2 particles. Then $\vec{S} = \vec{S_1} + \vec{S_2}$ is the spin operator for this two-particle system.

a) (2 pts) Consider the Hamiltonian

$$\hat{H}_0 = \alpha(\hat{S}_x^2 + \hat{S}_y^2 - \hat{S}_z^2)/\hbar^2 \quad \alpha: \text{ real constant greater than } 0$$

Determine the Energy eigenvalues and degeneracies for this Hamiltonian.

b) (4 pts) Consider a perturbation to the above Hamiltonian:

$$\hat{H}_1 = \lambda(\hat{S_{1x}} - \hat{S_{2x}}) \quad \lambda: \text{ real constant greater than } 0.$$

Calculate the new energies and degeneracies to first-order in perturbation theory.

? c) (3 pts) Now consider an unperturbed Hamiltonian

$$\hat{H}_0 = -A(\hat{S}_{1z} + \hat{S}_{2z}) \quad A: \text{ real constant greater than } 0$$

with a perturbing Hamiltonian of the form

$$\hat{H}_1 = B(\hat{S}_{1x}\hat{S}_{2x} - \hat{S}_{1y}\hat{S}_{2y}) \quad B: \text{ real constant greater than } 0$$

by means of perturbation theory, calculate the ground state energy of $\hat{H}_0$ and calculate the first and second order shifts of the ground state energy of $\hat{H}_0$ as a consequence of the perturbation $\hat{H}_1$.

? d) (1 pt) The exact ground state energy for $\hat{H}_0 + \hat{H}_1$ found in part c) is

$$E_{ground} = -\frac{\hbar}{2}\sqrt{4A^2 + B^2\hbar^2}$$

Compare your results from c) to the exact energy. What conditions on A and B are required so that your results from c) and d) agree?

$S_1^2 = S_{1x}^2 + S_{1y}^2 + S_{1z}^2$

$S_2^2 = S_{2x}^2 + S_{2y}^2 + S_{2z}^2$

$S^2 = S_x^2 + S_y^2 + S_z^2 - 2 S_1 \cdot S_2$

$S_x^2 + S_y^2 = S^2 - S_z^2 + 2S_1 \cdot S_2$

Jan 2018

Quantum #2

a) $H_0 = \frac{\alpha}{\hbar^2}\left(S_x^2 + S_y^2 - S_z^2\right)$

$= \frac{\alpha}{\hbar^2}\left(S^2 - 2S_z^2\right)$

$S^2 |j,m\rangle = j(j+1)\hbar^2 |j,m\rangle$

$S_z^2 |j,m\rangle = m^2\hbar^2 |j,m\rangle$

* We write our states in the $|s_1, s_2; j, m\rangle$ basis

$|s_1 - s_2| \leq j \leq s_1 + s_2$

$0 \leq j \leq 1$

Possible $|j,m\rangle$ states: $|0,0\rangle$, $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$

$H_0 |0,0\rangle = \frac{\alpha}{\hbar^2}(S^2 - 2S_z^2)|0,0\rangle$

$= \frac{\alpha^2}{\hbar^2}(0(0+1) - 2(0^2)\hbar^2$

$= 0$

$H_0 |1,1\rangle = \frac{\alpha}{\hbar^2}(S^2 - 2S_z^2 |1,1\rangle$

$= \frac{\alpha}{\hbar^2}(1(1+1) - 2(1)^2)\hbar^2$

$= 0$

$H_0 |1,0\rangle = \frac{\alpha}{\hbar^2}(S^2 - 2S_z^2)|1,0\rangle$

$= \frac{\alpha}{\hbar^2}(1(1+1) - 2(0)^2)\hbar^2$

$= 2\alpha$

$H_0 |1,-1\rangle = \frac{\alpha}{\hbar^2}(S^2 - 2S_z^2)|1,-1\rangle$

$= \frac{\alpha}{\hbar^2}(1(1+1) - 2(-1)^2)\hbar^2$

$= 0$

$\Rightarrow$ Triplet state at $E = 0$, $|0,0\rangle, |1,1\rangle, |1,-1\rangle$

Singlet state at $E = 2\alpha$; $|1,0\rangle$

#2 (cont.)

b) $H_1 = \lambda(S_{1x} - S_{2x})$

* Given $S_\pm = S_x \pm i S_y$, we can rewrite our perturbation as:

$$S_{1x} = (S_{1+} - S_{1-}) \cdot \frac{1}{2}$$

$$S_{2x} = (S_{2+} - S_{2-}) \cdot \frac{1}{2}$$

↳ $H_1 = \frac{\lambda}{2}(S_{1+} - S_{1-} - S_{2+} + S_{2-})$

* Note: Using this form of the operator requires rewriting our states in the $|s_1, s_2; s_{1z}, s_{2z}\rangle$ basis.

* The equation that governs first order perturbation theory is:

$$\Delta E^{(1)} = \langle n^{(0)} | H_1 | n^{(0)} \rangle$$

* For the $|1,1\rangle$ state:

$$|1,1\rangle = |1/2, 1/2\rangle$$

$$\Delta E^{(1)} = \langle 1/2, 1/2 | \left(\frac{\lambda}{2}[S_{1+} - S_{1-} - S_{2+} + S_{2-}]\right) | 1/2, 1/2 \rangle$$

$$= 0$$

↳ S_{i+} operators go to unallowed states

S_{i-} operators push state to an orthogonal state, resulting in inner product of 0

* For the $|1,-1\rangle$ state:

$$|1,-1\rangle = |-1/2, -1/2\rangle$$

$$\Delta E^{(1)} = \langle -1/2, -1/2 | \frac{\lambda}{2}(S_{1+} - S_{1-} - S_{2+} + S_{2-}) | -1/2, -1/2 \rangle$$

$$= 0$$

↳ S_{i-} operators go to unallowed state

S_{i+} operators push state to an orthogonal state, resulting in inner product of 0

#2 (cont.)

b) * For the $|1,0\rangle$ state:

$$|1,0\rangle = \frac{1}{\sqrt{2}}|{-\tfrac{1}{2}},\tfrac{1}{2}\rangle + \frac{1}{\sqrt{2}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle$$

$$\Delta E^{(1)} = \frac{1}{\sqrt{2}}\left(\langle\tfrac{1}{2},-\tfrac{1}{2}| + \langle-\tfrac{1}{2},\tfrac{1}{2}|\right)\left(\frac{\lambda}{2}\left[S_{1+} - S_{1-} - S_{2+} + S_{2-}\right]\right)\left(|\tfrac{1}{2},-\tfrac{1}{2}\rangle + |-\tfrac{1}{2},\tfrac{1}{2}\rangle\right)$$

$$= \frac{\lambda}{4}\Big[\langle\tfrac{1}{2},-\tfrac{1}{2}|\overset{0}{\cancel{S_{1+}}} - \overset{0}{\cancel{S_{1-}}} - \overset{0}{\cancel{S_{2+}}} + \overset{0}{\cancel{S_{2-}}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle + \langle\tfrac{1}{2},-\tfrac{1}{2}|\overset{0}{\cancel{S_{1+}}} - \overset{0}{\cancel{S_{1-}}} - \overset{0}{\cancel{S_{2+}}} + \overset{0}{\cancel{S_{2-}}}|-\tfrac{1}{2},\tfrac{1}{2}\rangle$$

$$+ \langle-\tfrac{1}{2},\tfrac{1}{2}|\overset{0}{\cancel{S_{1+}}} - \overset{0}{\cancel{S_{1-}}} - \overset{0}{\cancel{S_{2+}}} + \overset{0}{\cancel{S_{2-}}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle + \langle-\tfrac{1}{2},\tfrac{1}{2}|\overset{0}{\cancel{S_{1+}}} - \overset{0}{\cancel{S_{1-}}} - \overset{0}{\cancel{S_{2+}}} + \overset{0}{\cancel{S_{2-}}}|-\tfrac{1}{2},\tfrac{1}{2}\rangle\Big]$$

$$= 0$$

↳ All operators either push states to unallowed values of $S_{iz} = \pm\tfrac{3}{2}$ or to $|\pm\tfrac{1}{2},\pm\tfrac{1}{2}\rangle$ states which are orthogonal to our known state.

* For the $|0,0\rangle$ state:

$$|0,0\rangle = \frac{1}{\sqrt{2}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle - \frac{1}{\sqrt{2}}|-\tfrac{1}{2},\tfrac{1}{2}\rangle$$

$\Delta E^{(1)} = 0$ by same logic as for $|1,0\rangle$ state

⇒ Second order pertubation theory needed to break this degenerecy

c) $H_0 = -A(S_{1z} + S_{2z})$

* We want our states in the $|S_{1z}, S_{2z}\rangle$ basis

$$H_0|\tfrac{1}{2},\tfrac{1}{2}\rangle = -A(S_{1z}+S_{2z})|\tfrac{1}{2},\tfrac{1}{2}\rangle = -A(\tfrac{1}{2}+\tfrac{1}{2}) = -A\hbar \leftarrow \boxed{\text{Ground State}}$$

$$H_0|-\tfrac{1}{2},-\tfrac{1}{2}\rangle = -A(S_{1z}+S_{2z})|-\tfrac{1}{2},-\tfrac{1}{2}\rangle = -A(-\tfrac{1}{2}-\tfrac{1}{2}) = A\hbar$$

$$H_0|\tfrac{1}{2},-\tfrac{1}{2}\rangle = -A(S_{1z}+S_{2z})|\tfrac{1}{2},-\tfrac{1}{2}\rangle = -A(\tfrac{1}{2}-\tfrac{1}{2}) = 0$$

$$H_0|-\tfrac{1}{2},\tfrac{1}{2}\rangle = -A(S_{1z}+S_{2z})|-\tfrac{1}{2},\tfrac{1}{2}\rangle = -A(-\tfrac{1}{2}+\tfrac{1}{2}) = 0$$

#2 (cont.)

c) $H_1 = B(S_{1x}S_{2x} - S_{1y}S_{2y})$

$= \frac{B}{2}(S_{1+}S_{2+} + S_{1-}S_{2-})$

* The equation for the first order energy correction is:

$$\Delta E^{(1)} = \langle n^{(0)} | H_1 | n^{(0)} \rangle$$

$$= \langle \tfrac{1}{2}, \tfrac{1}{2} | \tfrac{B}{2}(S_{1+}S_{2+} + S_{1-}S_{2-}) | \tfrac{1}{2}, \tfrac{1}{2} \rangle$$

$$= \frac{B}{2}\Big[\underbrace{\cancel{\langle \tfrac{1}{2}, \tfrac{1}{2} | S_{1+}S_{2+}}}_{\text{unallowed state}} \overset{0}{|} \tfrac{1}{2}, \tfrac{1}{2} \rangle + \langle \tfrac{1}{2}, \tfrac{1}{2} | \underbrace{\cancel{S_{1-}S_{2-}}}_{\text{orthogonality}} \overset{0}{|} \tfrac{1}{2}, \tfrac{1}{2} \rangle$$

$$= 0$$

* The equation governing second order perturbation energy corrections is:

$$\Delta E^{(2)} = \sum_{k \neq n} \frac{|\langle k | H_1 | n \rangle|^2}{E_n - E_k}$$

* our only non-zero component will be $|k\rangle = |-\tfrac{1}{2}, -\tfrac{1}{2}\rangle$

$$= \frac{|\langle -\tfrac{1}{2}, -\tfrac{1}{2} | \tfrac{B}{2}(S_{1+}S_{2+} + S_{1-}S_{2-}) | \tfrac{1}{2}, \tfrac{1}{2} \rangle|^2}{-A - A}$$

$$= \frac{B^2}{8A^2} \left| \left(\sqrt{(\tfrac{1}{2}+\tfrac{1}{2})(\tfrac{1}{2}-\tfrac{1}{2}+1)} \right)^2 \right|^2$$

$$= \frac{B^2}{8A} |(1)(1)|^2$$

$$= \frac{B^2 \hbar^2}{8A^2}$$

d) $A \in \mathbb{R}$, $B = 0$