

Degenerate Perturbation Theory

Suppose we have two spin-1/2 particles. The states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ start out degenerate. We then add a perturbation that takes the form $\hat{H}' = V_0 \left(\frac{4}{\hbar^2} \hat{S}^2 + \frac{6}{\hbar} \hat{S}_z^{(1)} - 6 \right)$ where $\hat{S}^2$ refers to the total spin. (This perturbation could plausibly describe a hydrogen atom in a $l = 0$ state placed in a weak magnetic field.)

(a) Treat $|\psi_a^0\rangle = |\uparrow\downarrow\rangle$ and $|\psi_b^0\rangle = |\downarrow\uparrow\rangle$. Construct the W matrix.

Reminder: $\hat{S}^2|\uparrow\downarrow\rangle = \hat{S}^2|\downarrow\uparrow\rangle = \hbar^2(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$.

(b) Find the eigenvalues and eigenvectors of this matrix.

(c) Also determine the energy shift for the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$.

$$(a) \hat{H}'|\uparrow\downarrow\rangle = V_0 \left(\frac{4}{\hbar^2} \hbar^2 (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) + \frac{6+\hbar}{\hbar} |\uparrow\downarrow\rangle - 6|\uparrow\downarrow\rangle \right) = V_0(1|\uparrow\downarrow\rangle + 4|\downarrow\uparrow\rangle)$$

$$\hat{H}'|\downarrow\uparrow\rangle = V_0 \left(\frac{4}{\hbar^2} \hbar^2 (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) + \frac{6-\hbar}{\hbar} |\downarrow\uparrow\rangle - 6|\downarrow\uparrow\rangle \right) = V_0(4|\uparrow\downarrow\rangle - 5|\downarrow\uparrow\rangle)$$

$$W_{aa} = \langle\uparrow\downarrow|\hat{H}'|\uparrow\downarrow\rangle = 1V_0$$

$$W_{bb} = \langle\downarrow\uparrow|\hat{H}'|\downarrow\uparrow\rangle = -5V_0$$

$$W_{ab} = W_{ba}^* = \langle\uparrow\downarrow|\hat{H}'|\downarrow\uparrow\rangle = 4V_0$$

Therefore
$$W = V_0 \begin{pmatrix} 1 & 4 \\ 4 & -5 \end{pmatrix}$$

(b) Remember, $E_{\pm}^1 = \frac{1}{2}[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}]$

$$E_{\pm}^1 = \frac{V_0}{2}[1 - 5 \pm \sqrt{(1+5)^2 + 4|4|^2}] = \frac{V_0}{2}[-4 \pm 10]$$

$$E_+^1 = 3V_0 \quad \text{and} \quad E_-^1 = -7V_0$$

We'll do $|\psi_+^1\rangle$ (with eigenvalue $3V_0$) first.

$$\begin{pmatrix} 1 & 4 \\ 4 & -5 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha + 4\beta \\ 4\alpha - 5\beta \end{pmatrix} = 3 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$\alpha + 4\beta = 3\alpha$ which implies that $\alpha = 2\beta$. This gives $\begin{pmatrix} 2 \\ 1 \end{pmatrix}$ which normalizes to

$$|\psi_+^1\rangle = \sqrt{\frac{1}{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

Now we'll do $|\psi_-^1\rangle$ (with eigenvalue $-7V_0$).

$$\begin{pmatrix} 1 & 4 \\ 4 & -5 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha + 4\beta \\ 4\alpha - 5\beta \end{pmatrix} = -7 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$\alpha + 4\beta = -7\alpha$ which implies that $2\alpha = -\beta$. This gives $\begin{pmatrix} 1 \\ -2 \end{pmatrix}$ which normalizes

to
$$|\psi_-^1\rangle = \sqrt{\frac{1}{5}} \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

(c) $|\uparrow\uparrow\rangle = |1\ 1\rangle$ (i.e. an eigenstate of $\hat{S}^2$ with eigenvalue $2\hbar^2$). This means that $\hat{H}'|\uparrow\uparrow\rangle = V_0 \left(\frac{4}{\hbar^2} 2\hbar^2 + \frac{6+\hbar}{\hbar} \frac{1}{2} - 6 \right) |\uparrow\uparrow\rangle = 5V_0 |\uparrow\uparrow\rangle$.

$$\hat{H}'|\downarrow\downarrow\rangle = V_0 \left(\frac{4}{\hbar^2} 2\hbar^2 + \frac{6-\hbar}{\hbar} \frac{1}{2} - 6 \right) |\downarrow\downarrow\rangle = -1V_0 |\downarrow\downarrow\rangle.$$

