Two State Systems (Perturbation Theory)

a.

$\hat{H} = \begin{pmatrix} a_0 & a_1 \\ a_1 & a_0 \end{pmatrix}$

Diagonalization is straightforward giving:

Eigenstate $|\eta_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ has energy $E_1^{(0)} = a_0 + a_1$.

Eigenstate $|\eta_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ has energy $E_2^{(0)} = a_0 - a_1$.

b.

$\hat{H}' = \begin{pmatrix} a_3 & 0 \\ 0 & -a_3 \end{pmatrix}$,

whence $H'_{1,1} = 0$ and $H'_{2,2} = 0$. Thus the leading correction is second order. Now $H'_{1,2} = H'_{2,1} = a_3$ so

Shift in E_1 is $\displaystyle\sum_{m \neq 1} \frac{H'_{1,m} H'_{m,1}}{E_1^{(0)} - E_m^{(0)}} = \frac{H'_{1,2} H'_{2,1}}{E_1^{(0)} - E_2^{(0)}} = \frac{a_3^2}{2a_1}$.

Shift in E_2 is $\displaystyle\sum_{m \neq 2} \frac{H'_{2,m} H'_{m,2}}{E_2^{(0)} - E_m^{(0)}} = \frac{H'_{2,1} H'_{1,2}}{E_2^{(0)} - E_1^{(0)}} = -\frac{a_3^2}{2a_1}$.

Similarly, to first order

$$|\eta_1\rangle \approx |\eta_1^{(0)}\rangle + |\eta_2^{(0)}\rangle \left[\frac{H'_{2,1}}{E_1^{(0)} - E_2^{(0)}} \right] = |\eta_1^{(0)}\rangle + |\eta_2^{(0)}\rangle \left[\frac{a_3}{2a_1} \right] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 + a_3/(2a_1) \\ 1 - a_3/(2a_1) \end{pmatrix}$$

$$|\eta_2\rangle \approx |\eta_2^{(0)}\rangle + |\eta_1^{(0)}\rangle \left[\frac{H'_{1,2}}{E_2^{(0)} - E_1^{(0)}} \right] = |\eta_2^{(0)}\rangle + |\eta_1^{(0)}\rangle \left[-\frac{a_3}{2a_1} \right] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 - a_3/(2a_1) \\ -1 + a_3/(2a_1) \end{pmatrix}$$

c.

The exact eigenvalues of $\hat{H} = \begin{pmatrix} a_0 + a_3 & a_1 \\ a_1 & a_0 - a_3 \end{pmatrix}$ are

$$\begin{aligned} E_{1,2} &= a_0 \pm \sqrt{a_1^2 + a_3^2} \\ &= a_0 \pm a_1 \left[1 + \left(\frac{a_3}{a_1} \right)^2 \right]^{1/2} \\ &\approx a_0 \pm a_1 \pm \frac{a_3^2}{2a_1}. \end{aligned}$$

⟦*Grading:* 3 points for part **a**, 4 points for part **b**, 3 points for part **c**.⟧