Anharmonic Coupling

a)

$$\hat{U}' = k\hat{Q}_1\hat{Q}_2^2$$

Use $\hat{a}$ and $\hat{a}^+$

$$\hat{a}_i^+ = \frac{1}{\sqrt{2\mu_i}}\left(\hat{p}_i + i\mu\omega\hat{Q}_i\right)$$

$$\hat{a}_i = \frac{1}{\sqrt{2\mu_i}}\left(\hat{p}_i - i\mu\omega\hat{Q}_i\right)$$

so

$$\hat{Q}_i = \frac{\sqrt{2\mu_i}}{2i\mu\omega}\left(\hat{a}_i^+ - \hat{a}_i\right)$$

so

$$\hat{U}' = k\hat{Q}_1\hat{Q}_2^2 \overset{\text{prop. to}}{\propto} \left(\hat{a}_1^+ - \hat{a}_1\right)\left(\hat{a}_2^+ - \hat{a}_2\right)^2$$

$$= \left(a_1^+ - a_1\right)\left(\hat{a}_2^+\hat{a}_2^+ - \hat{a}_2^+\hat{a}_2 - \hat{a}_2\hat{a}_2^+ + \hat{a}_2\hat{a}_2\right)$$

so this part says

$\Delta v_1 = \pm 1$

b/c $a_1^+|v_1, v_2, \ldots\rangle \propto |v_1+1, v_2, \ldots\rangle$

and $a_1|v_1, v_2, \ldots\rangle \propto |v_1-1, \ldots\rangle$

And this part says

$\Delta v_2 = +2, 0, 0, \text{ or } -2$

by similar arguments

selection rules

b) The influence of the anharmonic coupling is by far the largest on the states that are closest in energy because of the energy denominators that appear in perturbation theory

$$|\psi_n^{(1)}\rangle = \sum_m \frac{\langle \psi_m^{(0)} | \hat{U} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle$$

When $E_n - E_m$ is close to zero, this term dominates the sum, so we don't need to consider other terms.

c) The thing to do is diagonalize the Hamiltonian in the (nearly) degenerate subspace

$$\hat{H} = \hat{H}_0 + \hat{U}'$$

$$\langle 100 | \hat{H} | 100 \rangle = E_{100}^{(0)} \quad \text{b/c} \quad \langle 100 | \hat{U}' | 100 \rangle$$

$$\langle 020 | \hat{H} | 020 \rangle = E_{020}^{(0)}$$

$$\langle 100 | \hat{H}_0 | 020 \rangle = \langle 020 | \hat{H}_0 | 100 \rangle = 0$$

$$V \equiv \langle 100 | \hat{U}' | 020 \rangle$$

So in the nearly degenerate subspace

$$\boldsymbol{H} = \begin{bmatrix} E_{100}^{(0)} & V \\ V & E_{020}^{(0)} \end{bmatrix}$$

Finding the new energy eigenvalues

$$\det(H - EI) = \begin{vmatrix} E_{100}^{(0)} - E & V \\ V & E_{020}^{(0)} - E \end{vmatrix} = 0$$

$$(E_{100}^{(0)} - E)(E_{020}^{(0)} - E) - V^2 = 0$$

Now write

$$E_{100}^{(0)} = \bar{E}_0 + \Delta \qquad \bar{E} = \frac{E_{100}^{(0)} + E_{020}^{(0)}}{2}$$

$$E_{020}^{(0)} = \bar{E}_0 - \Delta \qquad \Delta = \frac{E_{100}^{(2)} - E_{020}^{(2)}}{2}$$

$$(\bar{E}_0 + \Delta - E)(\bar{E}_0 - \Delta - E) - V^2 = 0$$

$$(E_0^2 - \Delta^2) - E(\bar{E}_0 - \cancel{\Delta}) - E(\bar{E}_0 + \cancel{\Delta}) + E^2 - V^2 = 0$$

$$\bar{E}_0^2 - \Delta^2 - V^2 - 2E\bar{E}_0 + E^2 = 0$$

$$E^2 - 2E\bar{E}_0 - (\Delta^2 + V^2) + \bar{E}_0^2 = 0$$

$$E = +\frac{2\bar{E}_0}{2} \pm \frac{\sqrt{\cancel{4}(\cancel{\bar{E}_0})^2 - 4(1)(\cancel{\bar{E}_0}^2 - \Delta^2 - V^2)}}{2}$$

$$\boxed{E_{\pm} = \bar{E}_0 \pm [\Delta^2 + V^2]^{1/2}}$$

So for E_+, $E_{100} - E_+ = \cancel{E_0} + \Delta - (\cancel{E_0} + (\Delta^2 + V^2)^{1/2})$

$$= \Delta - (\Delta^2 + V^2)^{1/2}$$

$$E_{020} - E_+ = \cancel{E_0} - \Delta - (\cancel{E_0} + (\Delta^2 + V^2)^{1/2})$$

$$= -\Delta - (\Delta^2 + V^2)^{1/2}$$

$$\begin{bmatrix} \Delta - (V^2+\Delta^2)^{1/2} & V \\ V & -\Delta - (\Delta^2+V^2)^{1/2} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = 0$$

$C_1(\Delta - (V^2+\Delta^2)^{1/2}) + C_2 V = 0$ for E_+

$$\boxed{\frac{C_1}{C_2} = \frac{V}{(V^2+\Delta^2)^{1/2} - \Delta}}$$

Now if we take $C_1 = -\sin\theta$ $C_2 = \cos\theta$, then we get

$$\tan\theta = \frac{V}{(V^2+\Delta^2)^{1/2} - \Delta}$$

Using the trig identity $\tan^2(2\theta) = \dfrac{2\tan\theta}{1-\tan^2\theta}$, this can be rearranged to

$$\boxed{\tan(2\theta) = \frac{V}{\Delta}}$$

and $E_+ \rightarrow |\beta\rangle$

$E_- \rightarrow |\alpha\rangle$

See Nesbitt Paper for d)