Problem M98Q.3

(a) As suggested in the problem, it is sufficient to show that $E(\lambda)$ lies below its tangent line at $\tilde{\lambda}$; i.e. that

$$E(\lambda) \le E(\tilde{\lambda}) + (\lambda - \tilde{\lambda})\, E'(\tilde{\lambda}).$$

By the variational principle applied to the Hamiltonian $H_1 + \lambda H_2$, we must have

$$\left\langle \tilde{\lambda} \middle| (H_1 + \lambda H_2) \middle| \tilde{\lambda} \right\rangle \ge E(\lambda).$$

Subtracting from this the identity

$$\left\langle \tilde{\lambda} \middle| (H_1 + \tilde{\lambda} H_2) \middle| \tilde{\lambda} \right\rangle = E(\tilde{\lambda})$$

gives the desired inequality

$$(\lambda - \tilde{\lambda}) \left\langle \tilde{\lambda} \middle| H_2 \middle| \tilde{\lambda} \right\rangle \ge E(\lambda) - E(\tilde{\lambda}).$$

(b) We may write

$$H(a,b) = \begin{bmatrix} 1 & a & 0 \\ a & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + b \begin{bmatrix} 0 & 0 & a \\ 0 & 0 & 1 \\ a & 1 & 0 \end{bmatrix},$$

so by part (a) the ground-state energy $E(a,b)$ must be concave in b. Similarly, writing

$$H(a,b) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & b \\ 0 & b & 1 \end{bmatrix} + a \begin{bmatrix} 0 & 1 & b \\ 1 & 0 & 0 \\ b & 0 & 0 \end{bmatrix},$$

shows that $E(a,b)$ is concave in b.

(c) As in part (b), write

$$H(a,b) = H_0(b) + aH'(b) \quad \text{where} \quad H_0(b) := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & b \\ 0 & b & 1 \end{bmatrix} \quad \text{and} \quad H'(b) := \begin{bmatrix} 0 & 1 & b \\ 1 & 0 & 0 \\ b & 0 & 0 \end{bmatrix},$$

with $b \neq 0$ fixed. The eigenstates of H_0 are given by

$$|\psi_0\rangle := \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \text{and} \quad |\psi_\pm\rangle := \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ \pm 1 \end{bmatrix},$$

with corresponding eigenvalues $E_0 := 1$ and $E_\pm := 1 \pm b$. If $b > 0$, the state $|\psi_-\rangle$ is the ground state, and if $b < 0$ then the state $|\psi_+\rangle$ is the ground state.

For simplicity assume that $b > 0$ (the derivation for $b < 0$ is similar). By first-order perturbation theory, we obtain we obtain

$$[\partial_a E(a,b)|_{a=0} = \langle \psi_- | H'(b) | \psi_- \rangle = 0$$

as desired. Then by concavity $\partial_a E(a,b) \le 0$ for all $a \ge 0$.[1] By the mean value theorem, for any $a_2 > a_1 \ge 0$ it follows that

$$E(a_2, b) - E(a_1, b) = (a_2 - a_1)\, \partial_a E(a^*, b) \le 0$$

as desired, for some $a^* \in (a_1, a_2)$.

[1] Except on a measure-zero set of non-differentiable points.