M98Q.3—Variational Principle

Problem

a) Let $|\lambda\rangle$ be the ground state and $E(\lambda)$ the ground state energy of a Hamiltonian $H(\lambda) = H_1 + \lambda H_2$ that depends linearly on a real parameter λ. Use the variational principle based on the trial wave function $|\tilde{\lambda}\rangle$ with $\tilde{\lambda}$ fixed to show that $E(\lambda)$ is a concave function ($E''(\lambda) \leq 0$) in λ.

[Hint: It is enough to show that $E(\lambda) - E(\tilde{\lambda}) \leq (\lambda - \tilde{\lambda})\langle\tilde{\lambda}|H_2|\tilde{\lambda}\rangle = (\lambda - \tilde{\lambda})E'(\tilde{\lambda})$.]

b) Consider the Hamilton operator given by the following matrix,

$$H(a,b) = \begin{pmatrix} 1 & a & ab \\ a & 1 & b \\ ab & b & 1 \end{pmatrix}, \qquad b \neq 0,$$

depending on real parameters a and b. Let $E(a,b)$ be the corresponding ground state energy. Show that the function $E(a,b)$ is concave in each of the parameters.

c) Show that $E(a,b)$ in part b) is monotone decreasing in a for $a \geq 0$ and fixed $b \neq 0$.

[Hint: Start by showing that $\left.\frac{\partial E(a,b)}{\partial a}\right|_{a=0} = 0$.]