5.73

Quiz 18

1.

$$\mathbf{H} = \begin{pmatrix} 2 & 4 \\ 4 & 8 \end{pmatrix}, \qquad \text{and overlap:} \quad \mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

A. Use the variational method (which in this case is identical to quasidegenerate perturbation theory) to find an upper bound on the energy of the lowest energy state.

B. Show that $\begin{pmatrix} 5^{-1/2} \\ 2 \bullet 5^{-1/2} \end{pmatrix}$ is an eigenfunction of **H**. What is the eigenvalue of **H** to which this eigenfunction belongs?

C. What would you get for the energy levels and eigenfunctions using ordinary **nondegenerate** perturbation theory?

D. Use the same **H** but let the overlap matrix be $\mathbf{S} = \begin{pmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{pmatrix}$.

This corresponds to a basis set that is neither normalized nor othogonal. **S** is diagonalized by

$$\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 0.9 & 0.1 \\ 0.1 & 0.9 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 1.6 \end{pmatrix} = \tilde{\mathbf{S}}.$$

Find $\tilde{\mathbf{S}}^{-1/2}$ and derive $\tilde{\tilde{\mathbf{H}}}$ via $\tilde{\tilde{\mathbf{H}}}=\tilde{\mathbf{S}}^{-1/2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\mathbf{H}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\tilde{\mathbf{S}}^{-1/2}$ where

$$\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\mathbf{H}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 18 & 6 \\ 6 & 2 \end{pmatrix}.$$

E. The trace of a Hermitian matrix is the sum of the eigenvalues. What is the sum of the eigenvalues of $\tilde{\tilde{\mathbf{H}}}$?