5.73

Quiz 18 ANSWERS

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.

$$0 = \begin{vmatrix} 2-E & 4 \\ 4 & 8-E \end{vmatrix}$$

$$16 - 10E + E^2 - 16 = 0$$

$$E = 0, +10$$

$$E_{\text{lowest}} \leq 0$$

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?

$$\begin{pmatrix} 2 & 4 \\ 4 & 8 \end{pmatrix} 5^{-1/2} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = 5^{-1/2} \begin{pmatrix} 2+8 \\ 4+16 \end{pmatrix} = (10)5^{-1/2} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

The eigenvector belongs to $E = 10$.

(over)

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

$$E_{\text{lower}} = 2 - \frac{16}{6} = -\frac{2}{3}$$

$$E_{\text{upper}} = 8 + \frac{16}{6} = 10\frac{2}{3}$$

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

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

$$\tilde{S}^{-1/2} = \begin{pmatrix} 2^{-1/2} & 0 \\ 0 & 1.6^{-1/2} \end{pmatrix}$$

$$\tilde{\tilde{H}} = \tilde{S}^{-1/2}\begin{pmatrix} 18 & 6 \\ 6 & 2 \end{pmatrix}\tilde{S}^{-1/2} = \tilde{S}^{-1/2}\begin{pmatrix} 18\cdot 2^{-1/2} & 6\cdot 1.6^{-1/2} \\ 6\cdot 2^{-1/2} & 2\cdot 1.6^{-1/2} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{18}{2} & 6\cdot(3.2)^{-1/2} \\ \text{sym} & \frac{2}{1.6} \end{pmatrix} = \begin{pmatrix} 9 & 3.354 \\ \text{sym} & 1.25 \end{pmatrix}$$

E. The trace of a Hermitian matrix is the sum of the eigenvalues.

What is the sum of the eigenvalues of $\tilde{\tilde{\mathbf{H}}}$?

9 + 1.25 = 10.25

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