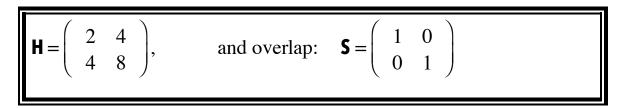
5.73 Quiz 18

1.



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 $\begin{pmatrix} 5^{-1/2} \\ 2 \cdot 5^{-1/2} \end{pmatrix}$ 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 $\tilde{\mathbf{H}}$ via $\tilde{\mathbf{H}} = \tilde{\mathbf{S}}^{-1/2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \mathbf{H} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \tilde{\mathbf{S}}^{-1/2}$ 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 $\tilde{\tilde{H}}$? MIT OpenCourseWare <u>https://ocw.mit.edu/</u>

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