Chem 337, Fall 2016, Problems and **auxiliary problems, given in bold face**

problem set 12

11/22/16

15. a. Using the prescription presented in class for the diagonalization of a $2\times2$ matrix, calculate $U$, $U^\dagger$, $U^\dagger H U$, when $H = \begin{pmatrix} 2 & 5 \\ 5 & 1 \end{pmatrix}$.

b. Solve for the eigenvalues of this same matrix, $H$, using the determinant method and compare solutions.

Now for the wavefunctions:

c. Using the determinant method, solve for the wavefunction coefficients $c_1$ and $c_2$ for each of the two energies. (Plug the energies, in turn, into the original “secular” equations):

$$(2 - E) c_1 + 0.5 c_2 = 0$$
$$0.5 c_1 + (1 - E) c_2 = 0$$
solve for $c_1$ in terms of $c_2$ and normalize: $c_1^2 + c_2^2 = 1$

d. Solve for the wavefunction coefficients by picking out columns in $U$ from part (a). The first column are the coefficients $c_1$ and $c_2$ for the wavefunction corresponding to the first energy and the second column are the coefficients $c_1$ and $c_2$ for the wavefunction corresponding to the second energy. These coefficients are already normalized. Compare these results from your answer to part (c).

16. Diagonalize

$$\begin{pmatrix} E_1 + \varepsilon a & c \\ c & E_1 + \varepsilon b \end{pmatrix}$$

and show that the result is identical to the diagonalization of

$$\begin{pmatrix} \varepsilon a & c \\ c & \varepsilon b \end{pmatrix}$$

with $E_1$ added to the answers.