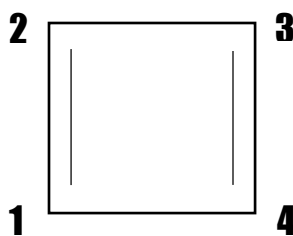


HW #6 Chem 2430

1. Consider an H atom in its 2s level in the presence of electric field in the z direction of strength. The electron couples to the field via the $e\mathcal{E}z$ operator. This hybridizes the 2s orbital. Assume that the hybridization is caused by mixing with the $2p_z$ orbital. How does the energy and the wavefunction depend on \mathcal{E} ?

2. The Huckel matrix for cyclobutadiene is

$$\begin{pmatrix} \alpha & \beta & 0 & \beta \\ \beta & \alpha & \beta & 0 \\ 0 & \beta & \alpha & \beta \\ \beta & 0 & \beta & \alpha \end{pmatrix}$$



Use symmetry to block diagonalize the matrix and use the block-diagonalized matrix to compute the eigenvalues.

3. Given $A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$, and D is the diagonal matrix with the eigenvalues of A on its diagonal,

Find the matrix U that transforms A to D via $U^T A U$.

If $B = e^A$, derive B.

4. Work through problems 7.55 and 7.56 of the text.