Homework # 5. Assigned Feb. 12; due Feb 21

1. Suppose that in a Huckel treatment of pi electron systems $\alpha(N) = 1.1\alpha(C)$, where N and C denote nitrogen and carbon atoms, respectively. Solve for the Huckel eigenvalues of benzene, pyridine, 1,4-pyrimidine, and 1,3,5-triazine. Summarize and discuss the trends in the eigenvalues. Sketch the filled pi orbitals for each molecules.

2. Using the unitary transformation discussed in class, Evaluate $\quad A := \begin{pmatrix} 2 & 2 \\ 2 & 4 \end{pmatrix} \quad$ the square root of the matrix

3. Fit the following data to a [2,2] rational function. $(x, y) = (0, 1.0000), (0.1, 1.39028), (0.2, 2.09168), (0.3, 3.60372), (0.4, 8.46774)$. Plot the input data and your rational function fit to the data. What values does your rational function fit give for the poles?

4. Consider a hypothetical atomic system which has energy levels at -5 and -4 in the absence of an electric field. Further assume that the off-diagonal matrix element coupling the two states in the presence of an electric field is $0.1*\varepsilon$, where ε is the electric field strength. What is the expression for the lower energy eigenvalue? At what values of the field are there branch points? What is the radius of convergence of a Taylor series representation of the energy of the lower energy state?