Phys 448 HW 10

1) BD 9.1
2) Suppose that on one of the sites (#2) of a benzene molecule (BD 7.10) an "impurity" $^{14}$C atom replaces the normal $^{12}$C atom. The atoms are nearly chemically identical, but the change in mass causes the distance between the $^{14}$C and its neighbors to be slightly different. This in turn implies that the tunneling of an electron between the $^{14}$C and its neighbors is slightly different, *i.e.* the coupling changes as $A \to A + b$. We wish to calculate the effect of the change in the tunneling on the energy levels using perturbation theory. First, divide the Hamiltonian into the $H_0$ of BD 7.10 and a perturbation $H_1$. Write these matrices in the $\{|\xi_n\rangle\}$ basis. As usual, find the eigenvectors and eigenvalues of the unperturbed Hamiltonian using the CSCO of $H_0$ and $R$. In Mathematica, defining a function

   toPolar[x_] := x /. a_ -> Abs[a] Exp[I Arg[a]]

   will convert ugly complex numbers into a nicer polar form.
3) Use first order perturbation theory to find the energy shift of the lowest and highest energy level of the benzene molecule due to the impurity.
4) The first two pairs of excited states of the molecule are two-fold degenerate, so degenerate perturbation theory is required to find their energy shifts. Find the effective 2-level Hamiltonians for each degenerate pair, using the CSCO basis, and find the resulting energies.
5) Plot the energies from perturbation theory of each of the states as a function of $-1 < \frac{b}{A} < 1$. Also find the exact energies and plot them on the same plot. Comment on the range over which perturbation theory gives good results.
6) A three-level quantum system has energies $\{A, 0, -A/2\}$. A perturbation is added: $V = b(|1\rangle\langle 2| + |2\rangle\langle 3|) + \text{h.c.}$ where h.c. denotes Hermitian conjugate. Find the energy shifts to second order.