CHEM2504 HW 1

Due: Mar 12, 3:00 pm, 2024

For Hermitian matrix $H = \begin{bmatrix} E_1 & V \\ V & E_2 \end{bmatrix}$, $E_1 < E_2$ and V is a real number

1. Write out its analytical expression for the eigenvalues and eigenvectors (remember to normalize!).

   Hint: you can set a parameter θ (for which $\tan\theta = \frac{2|V|}{E_1 - E_2}$) to simplify your expression of eigenvectors.

2. Now, let's treat V as a perturbation, write down the analytical expression of perturbed eigen values E_+ and E_- by V up to the second order.

3. Increase V from 0 to 0.02 eV, set $E_1 = -0.1$ eV, $E_2 = 0.1$ eV, plot E_+, E_- as a function of V computed by the perturbation theory (based on question 2) and the exact solution (by question 1).