Exercise 1: 2x2 Hamiltonian

Eigenstates and functions of a 2 by 2 matrix.

(a) Given the Hamiltonian (1):

$$H_1 = \begin{pmatrix} 0 & t \\ t & \Delta \end{pmatrix},\tag{1}$$

and the Hamiltonian (2):

$$H_2 = \begin{pmatrix} \epsilon_1 & t \\ t & \epsilon_2 \end{pmatrix}, \tag{2}$$

Show that for $\Delta = \epsilon_2 - \epsilon_1$ the Hamiltonians H_1 and H_2 have the same eigenfunctions and that the eigen energies between the two Hamiltonians are shifted by ϵ_1 .

- (b) Show that the sum of the eigenenergies of H_2 is independent of t and equal to $\epsilon_1 + \epsilon_2$
- (c) Show that if $\psi_{-} = \{\alpha, \beta\}$ is an eigenfunction of H_2 then the other eigenfunction is given as $\psi_{+} = \{\beta, -\alpha\}$
- (d) Given that $\psi_{-} = \{\alpha, \beta\}$ and $\psi_{+} = \{\beta, -\alpha\}$ are the eigenfunctions of H_2 at an eigenenergy of E_{-} and E_{+} respectively. Show that: $\alpha^2 \times E_{-} + \beta^2 \times E^{+} = \epsilon_1$ and that $\beta^2 \times E_{-} + \alpha^2 \times E^{+} = \epsilon_2$. In other words, show that the center of gravity of the Partial Density of States (PDOS) is the on-site energy.