Q3: $$E_{trial} = \frac{\langle \psi_{trial} | \hat{H} | \psi_{trial} \rangle}{\langle \psi_{trial} | \psi_{trial} \rangle} \quad (1)$$

$$\langle \psi_{trial} | H | \psi_{trial} \rangle = \sum_i^N \sum_j^N c_i^* c_j \langle \phi_i | H | \phi_j \rangle \quad (2)$$

$$= \sum_{i,j}^N c_i^* c_j \langle \phi_i | H | \phi_j \rangle \quad (3)$$

$$H_{ij} = \langle \phi_i | H | \phi_j \rangle \quad (4)$$

$$\langle \psi_{trial} | H | \psi_{trial} \rangle = \sum_{i,j}^{N,N} c_i^* c_j \cdot H_{ij} \quad (5)$$

$$\langle \psi_{trial} | \psi_{trial} \rangle = \sum_{i,j}^{N,N} c_i^* c_j \langle \phi_i | \phi_j \rangle \quad (6)$$

$$S_{ij} = \langle \phi_i | \phi_j \rangle \quad (7)$$

S_{ij} are overlap integrals between the different $\{\phi_j\}$ functions. So Equation (6) become

$$\langle \psi_{trial} | \psi_{trial} \rangle = \sum_{i,j}^{N,N} c_i^* c_j \cdot S_{ij} \quad (8)$$

Substituting Equations (5) and (8) into variational energy formula results ~~in~~

$$E_{trial} = \frac{\sum_{i,j}^{N,N} c_i^* c_j H_{ij}}{\sum_{i,j}^{N,N} c_i^* c_j S_{ij}} \quad (9)$$

The expression for variational energy (9) can be rearranged

$$E_{trial} \sum_{i,j}^{N,N} c_i^* c_j S_{ij} = \sum_{i,j}^{N,N} c_i^* c_j \cdot H_{ij} \quad (10)$$

Differentiating both sides of equation (10) for the k^{th} coefficent gives

$$\frac{\partial E_{trial}}{\partial c_k} \sum_{i,j}^{N,N} c_i^* c_j \cdot S_{ij} + E_{trial} \sum_i^N \sum_j^N \left[\frac{\partial c_i^*}{\partial c_k} c_j + \frac{\partial c_j}{\partial c_k} \cdot c_i^* \right] S_{ij} \quad (11)$$

$$= \sum_{i,j}^{N,N} \left[\frac{\partial c_i^*}{\partial c_k} c_j + \frac{\partial c_j}{\partial c_k} c_i^* \right] H_{ij}$$

$$\underbrace{\frac{\partial E_{trial}}{\partial c_k}\sum_{i,j}^{N,N} c_i^* c_j . S_{ij} + E_{trial}\sum_i\sum_j\left[\frac{\partial c_i^*}{\partial c_k}c_j + \frac{\partial c_j}{\partial c_k}.c_i^*\right]S_{ij}}_{\text{product rule}} = \sum_{i,j}^{N,N}\left[\frac{\partial c_i^*}{\partial c_k}c_j + \frac{\partial c_j}{\partial c_k}c_i^*\right]H_{ij}$$

Since the coefficent are linearly independent

$$\frac{\partial c_i^*}{\partial c_k} = \delta_{ik}$$

and

$$S_{ij}^* = S_{ji}$$

and also since the Hamiltonian is a Hermitian Operator

$$H_{ij}^* = H_{ji}$$

$$\frac{\partial E_{trial}}{\partial c_k}\sum_i^N\sum_j^N c_i^* c_j . S_{ij} + 2E_{trial}\sum_i S_{ik} = 2\sum_i c_i . H_{ik} \quad ... 12$$

At the minimum variational energy,

$$\frac{\partial E_{trial}}{\partial c_k} = 0 \quad \text{------} \quad 13$$

$$\sum_i^N c_i\left(H_{ik} - E_{trial}.S_{ik}\right) = 0 \quad \text{------} \quad 14$$

$$c_i.H_{ik} = c_i.E_{trial}\, S_{ik} \quad \text{------} \quad 15$$

$S_{ik} = S_{ij}$ Orthonormal PIB $S_{ij} = 1$ if $i=j$ ------ 16

k is arbitory choice. $k=j$ $S_{ij} = 0$ if $i \neq j$

$$c_i.H_{ij} = c_i.E_{trial} \quad \text{------} \quad 17$$

or

$$C.H = C.E_{trial} \quad \text{------} \quad 18$$