DRILL 5

1) show that for $\int \psi_k^* \psi_L \, dv = \delta_{K}$, $C^{-1}C = CC^{-1}(1)$ must be true.

$$\psi_i = \sum_{j=1}^{n} c_{ji} f_j$$

$$\therefore \int \psi_k^* \psi_L \, dv = \int \sum_{j=1}^{n} c_{jk}^* f_j \sum_{j=1}^{n} c_{jL} f_j$$

when $i \neq j$ then $\int f_i f_j$ goes to zero

when $i = j$, $1 = \int c_{ik}^* c_{jL} \underbrace{f_i^* f_j}_{\delta_{ij}} \, dv$

$\therefore$ $c_{ik}^* c_{jL}$ must equal 1 or δ_{KL} when $i = j$

The only way to get a matrix such that $c_{ij} = 1$ when $i = j$ is if ~~the~~ ~~two~~ one matrix is multiplied by its inverse matrix.

if C is unitary (1) then

$(c_{ij})(c_{ji}^*) = I$ because the conjugate transpose of $c_{ij} = c_{ij}^{-1}$ inverse

and $\sum c_{ik}^* c_{jL} = \delta_{KL}$

because $C^{-1}C = \underbrace{CC^{-1}}_{\text{identity matrix}} 1 \rightarrow \delta_{KL}$

$\Rightarrow$ given that $C^{-1}_{ij} = c^*_{ji}$

then $C^{-1}_{ki} c_{jL} = C_{KL} = \underline{\underline{\delta_{KL}}}$.

2. $H_{ij} = \int f_i^* \hat{H} f_j \, dV$ &

$$E_{ij} = \int \psi_i^* \hat{H} \psi_j \, dV = \sum_{k=1}^{n} \sum_{l=}^{n} C^*_{ki} C_{lj} H_{kl}$$

To show : $C^{-1} H C = E$

$HC = CE$

$$\psi_i = \sum_k C_{ki} f_k$$

$$E_{ij} = \cancel{\int \psi_i^*} \int \psi_i^* \hat{H} \psi_j \, dV$$

$$= \int \sum_k (C_{ki} f_k)^* \hat{H} \sum_l (C_{lj} f_l) \, dV$$

$$= \sum_k \sum_l \int C_{ki}^* C_{lj} f_k^* \hat{H} f_l \, dV$$

$$= \sum_k \sum_l C_{ki}^* C_{lj} \int f_k^* \hat{H} f_l \, dV$$

$$= \sum_k \sum_l C_{ki}^* C_{lj} H_{kl}$$

but $C_{ki}^* = C_{ik}^{-1}$

$$\therefore \quad E_{ij} = \sum_k \sum_l C_{ik}^{-1} H_{kl} C_{lj}$$

$E = C^{-1} \overline{HC}$

$CE = CC^{-1} HC$

but $CC^{-1} = 1$ (given)

$\therefore \quad CE = HC$

Drill 4.3

We have that

$$\mathbf{H}\,\mathbf{C} = \mathbf{C}\,\mathbf{E}$$

and we require that the matrix $\mathbf{C}$ diagonalizes $\mathbf{E}$:

$$\mathbf{C}^{\dagger}\,\mathbf{H}\,\mathbf{C} = \begin{bmatrix} E_{11} & 0 & \dots & 0 \\ 0 & E_{22} & \dots & 0 \\ \dots & & & \\ 0 & 0 & \dots & E_{nn} \end{bmatrix}$$

We have to show that n values of E_{ii} are the roots of the secular equation

$$|\mathbf{H} - E\,\mathbf{1}| = 0$$

and that the column vector $\mathbf{C}_i$ is determined by the system of homogeneous linear equations

$$\mathbf{H}\,\mathbf{C}_i = E_{ii}\,\mathbf{C}_i$$

or

$$\mathbf{C}_i\;[\mathbf{H} - E_{ii}\,\mathbf{1}] = 0$$

Drill 4.3

We can rewrite now our matrix equation in terms of n vector and matrix equations

$$\mathbf{C}_i^\dagger \, \mathbf{H}\mathbf{C}_i = E_{ii}$$

Multiplying by $\mathbf{C}_i$ on the left both the sides

$$\mathbf{C}_i \, \mathbf{C}_i^\dagger \, \mathbf{H}\mathbf{C}_i = \mathbf{H}\mathbf{C}_i = \mathbf{C}_i \, E_{ii} = E_{ii} \, \mathbf{C}_i \quad \Rightarrow \quad [\mathbf{H} - E_{ii} \, \mathbb{1}] \, \mathbf{C}_i = 0$$

We have $(n + 1)$ unknowns for n equations. However, for this system to have a non-trivial solution it is required that the secular determinant is zero.

$$|\mathbf{H} - E_{ii} \, \mathbb{1}| = 0$$

This is an equation of order n in E_{ii} and it gives n roots for E_{ii}.

Now we can substitute one of the found eigenvalues in the system

$$[\mathbf{H} - E_{ii} \, \mathbb{1}] \, \mathbf{C}_i = 0$$

and find the corresponding eigenvector, as there are n unknown for n equations now.

Matris #5

4. $f_i = \sum_i a_i \phi_i$ (ϕ_i complete. orthonormal)

$u_i = \sum_i d_i f_i = \sum_{i,j} d_j a_i \phi_i = \sum_i c_i \phi_i$

$\int u_i^* \hat{H} u_j \, dv$

$= \int \sum_i c_i^* \phi_i^* \hat{H} \sum_j c_j \phi_j \, dv$

$= \sum_i c_i^* \sum_j c_j^* \int \phi_i^* \hat{H} \phi_j \, dv$

$= \sum_i c_i^* \sum_j c_j^* \delta_{ij}$

So only when $i=j$. $E_{ii} = \int u_i^* \hat{H} u_i \, dv$

$E_{ii} \geq E_{11}$

$\therefore \int u^* \hat{H} u \geq E_{11}$