• 1 i) Show $\tilde{F} = \langle \tilde{\Psi} | \hat{F} | \tilde{\Psi} \rangle = Tr(\underline{\underline{f}}\ \underline{\underline{P}})$

$$\hat{F} = \hat{f}(x) + \hat{f}(y).$$

$\tilde{\Psi}$ is our slater determinant of basis functions.

Suppose we perform a unitary transformation $U$, $\chi_a' = \sum_b \chi_b U_{ba}$.

Since our $\tilde{\Psi}$ is defined to be $\det(\underline{\underline{A}})$, $\underline{\underline{A}} = \begin{pmatrix} \chi_1(x) & \chi_2(x) \\ \chi_1(y) & \chi_2(y) \end{pmatrix}$, then $\underline{\underline{A}}' = \underline{\underline{A}}U$ will have $\tilde{\Psi}' = \det(\underline{\underline{A}}\underline{\underline{U}}) = \det(\underline{\underline{A}})\det(\underline{\underline{U}})$. $\because$ $\underline{\underline{U}}$ is unitary, the new antisymmetric wavefunction differs just by a potational factor, of which vanishes in matrix elements.

$\because$ It is always possible to find such $\underline{\underline{U}}$ that diagonalizes $\varepsilon$ (Szabo 122), then we have $\langle \chi_a' | \hat{f} | \chi_b' \rangle = \varepsilon_b \delta_{ab}$. We can just drop the prime since it's arbitrary:

$\Rightarrow$ $\langle \tilde{\Psi} | \hat{F} | \tilde{\Psi} \rangle = \sum_{ab} \langle \chi_a | \hat{f} | \chi_b \rangle$ by orthonormality, where the little $\hat{f}$ is an one electron operator $\chi_a = \sum_{v=1}^{k} c_{va}\phi_v(\tau_1)$, $\hat{f}|\chi_a\rangle = \varepsilon_a |\chi_a\rangle$.

Then we have: $\sum_a \langle \chi_a | f | \chi_a \rangle$

$$= \sum_a \int d\tau\, \chi_a^*(\tau) f(\tau) \chi_a(\tau)$$

For $\chi_a = \sum_v^K c_{va}\phi_a(\tau)$, we get:

$$\sum_a \left( \int d\tau \sum_v^k \sum_v^k c_{va} c_{va} \phi_{va}^*(\tau) \phi_{va}(\tau) \right.$$

$$= \sum_a \left( \sum_{v,v}^{k,k} c_{va} c_{va}^* \int d\tau\, \phi_{va}^*(\tau) \phi_{va}(\tau) \right)$$

$$= \sum_a \left( \sum_{v,v}^{k,k} c_{va} c_{va}^* F_{vv} \right)$$

$$= \sum_{v,v}^{k,k} F_{vv} \sum_a c_{va} c_{va}^*$$

$$= Tr(\underline{\underline{f}}\ \underline{\underline{P}}). \quad , \text{ where } \underline{\underline{f}}_{vv} = F_{vv},\ \underline{\underline{P}}_{vv} = \sum_a c_{va} c_{va}^*.$$