Quantum Chemistry HW5

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1)

$$\hat{C}(x,y)\{f_n(x)g_m(y)\} = \hat{A}(x)\{f_n(x)g_m(y)\} + \hat{B}(y)\{f_n(x)g_m(y)\}$$

$$= g_m(y)\hat{A}(x)\{f_n(x)\} + \hat{B}(y)\{g_m(y)f_n(x)\}$$

$$= g_m(y)(a_n f_n(x)) + f_n(x)\hat{B}(y)\{g_m(y)\}$$

$$= g_m(y)(a_n f_n(x)) + f_n(x)(b_m g_m(y))$$

$$= (a_n + b_m)(f_n(x)g_m(y)).$$

□

2)

$\rho(r) = \sum_{k\in occ} \varphi_k^*(r)\varphi_k(r)$, where $\rho(r)$ is one electron wave function or orbital.

$$\varphi_k(r) = \sum_i C_{ik} g_i(r)$$

$$\varphi_k^*(r) = \sum_j C_{jk}^* g_j^*(r)$$

$$\varphi_k^*(r)\varphi_k(r) = \sum_i \sum_j C_{ik} C_{jk}^* g_i(r) g_j^*(r)$$

$$\rho(r) = \sum_i \sum_j \left(\sum_{k\in occ} C_{ik} C_{jk}^*\right) g_i(r) g_j^*(r)$$

Now define density matrix $D_{ij} = \sum_{k\in occ} C_{ik} C_{jk}^*$ then

$$\rho(r) = \sum_i \sum_j D_{ij} g_i(r) g_j^*(r)$$

□