

$$\int dx_1 \int dx_2 \frac{\rho(x_1) \rho(x_2)}{r_{12}} \quad \rho(x) = \|\psi(x)\|^2 = \psi^* \psi$$

$$= \int dx_1 dx_2 \psi^*(x_1) \psi(x_1) \frac{1}{r_{12}} \psi^*(x_2) \psi(x_2)$$

$$\hat{x}_1 \quad \hat{x}_2 \quad \hat{x}_3$$

$$g(x_1) = (g_1 \hat{x}_1 + g_2 \hat{x}_2 + g_3 \hat{x}_3)$$

$$g(x_1) x_i(x_1) = \epsilon_i x_i(x_1)$$

$$x_i(x_1) = (c_{1,i} \hat{x}_1 + c_{2,i} \hat{x}_2 + c_{3,i} \hat{x}_3)$$

$$(g_1 \hat{x}_1 + g_2 \hat{x}_2 + g_3 \hat{x}_3)(c_{1,i} \hat{x}_1 + c_{2,i} \hat{x}_2 + c_{3,i} \hat{x}_3) = \epsilon_i x_i$$

$$\begin{pmatrix} g_1 c_{1,i} & g_1 c_{2,i} & g_1 c_{3,i} \\ g_2 c_{1,i} & g_2 c_{2,i} & g_2 c_{3,i} \\ g_3 c_{1,i} & g_3 c_{2,i} & g_3 c_{3,i} \end{pmatrix} \odot \begin{pmatrix} \hat{x}_1 \hat{x}_1 & \hat{x}_2 \hat{x}_1 & \hat{x}_3 \hat{x}_1 \\ \hat{x}_1 \hat{x}_2 & \hat{x}_2 \hat{x}_2 & \hat{x}_3 \hat{x}_2 \\ \hat{x}_1 \hat{x}_3 & \hat{x}_2 \hat{x}_3 & \hat{x}_3 \hat{x}_3 \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} 1 & 1 & 1 & | & 0 & 0 & 0 & 0 \end{pmatrix}$$

3 occ 4 unocc

$$\begin{pmatrix} 1 & 1 & 0 & | & 0 & 0 & 0 & 1 \\ & & & & 0 & 0 & 1 & 0 \\ & & & & 0 & 1 & 0 & 0 \\ & & & & 1 & 0 & 0 & 0 \end{pmatrix}$$

single

$$\# = \begin{pmatrix} N_{\text{bos}} \\ N_e \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & | & 1 & 0 & 0 & 1 \\ & & & & 1 & 0 & 1 & 0 \\ & & & & 1 & 1 & 0 & 0 \\ & & & & 0 & 1 & 0 & 1 \\ & & & & 0 & 1 & 1 & 0 \\ & & & & 0 & 0 & 1 & 1 \end{pmatrix}$$

double

$$\begin{pmatrix} 0 & 0 & 0 & | & 1 & 1 & 1 & 0 \\ & & & & 1 & 1 & 0 & 1 \\ & & & & 1 & 0 & 1 & 1 \\ & & & & 0 & 1 & 1 & 1 \end{pmatrix}$$

triple

$$S: a \rightarrow r$$

$$\hat{a}_r^\dagger \hat{a}_a$$

$$S: b \rightarrow s$$

$$\hat{a}_s^\dagger \hat{a}_b$$

$$D: a \rightarrow r$$

$$\hat{a}_r^\dagger \hat{a}_a$$

$$b \rightarrow s$$

$$\cdot \hat{a}_s^\dagger \hat{a}_b$$