Matrix elements between Slater determinants for one-electron operators

$$\hat{O}_1 = \sum_{i=1}^{N} \hat{o}(\mathbf{x}_i) \tag{1}$$

Case 1, identical determinants:

$$\psi_K = |...\varphi_m\varphi_n...\rangle \tag{2}$$

$$\langle\psi_K|\hat{O}_1|\psi_K\rangle = \sum_{m}^{N} \int \varphi_m^*(\mathbf{x}_1)\hat{o}(\mathbf{x}_1)\varphi_m(\mathbf{x}_1)d\mathbf{x}_1 \tag{3}$$

Case 2, one spin orbital different:

$$\begin{aligned} \psi_K &= |...\varphi_m\varphi_n...\rangle \\ \psi_L &= |...\varphi_p\varphi_n...\rangle \end{aligned} \tag{4}$$

$$\langle\psi_K|\hat{O}_1|\psi_L\rangle = \int \varphi_m^*(\mathbf{x}_1)\hat{o}(\mathbf{x}_1)\varphi_p(\mathbf{x}_1)d\mathbf{x}_1 \tag{5}$$

Case 3, two spin orbitals different:

$$\begin{aligned} \psi_K &= |...\varphi_m\varphi_n...\rangle \\ \psi_L &= |...\varphi_p\varphi_q...\rangle \end{aligned} \tag{6}$$

$$\langle\psi_K|\hat{O}_1|\psi_L\rangle = 0 \tag{7}$$

Matrix elements between Slater determinants for two electron operators

$$\hat{O}_2 = \sum_{i=1}^{N}\sum_{j>i}^{N} \hat{o}(\mathbf{x}_i, \mathbf{x}_j) \tag{8}$$

Case 1, identical determinants:

$$\psi_K = |...\varphi_m\varphi_n...\rangle \tag{9}$$

$$\begin{aligned} \langle\psi_K|\hat{O}_2|\psi_K\rangle &= \tfrac{1}{2}\textstyle\sum_m^N\sum_n^N [\int\int \varphi_m^*(\mathbf{x}_1)\varphi_n^*(\mathbf{x}_2)\hat{o}(\mathbf{x}_1,\mathbf{x}_2)\varphi_m(\mathbf{x}_1)\varphi_n(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 \\ &\quad - \textstyle\int\int \varphi_m^*(\mathbf{x}_1)\varphi_n^*(\mathbf{x}_2)\hat{o}(\mathbf{x}_1,\mathbf{x}_2)\varphi_n(\mathbf{x}_1)\varphi_m(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2] \end{aligned} \tag{10}$$

Case 2, one spin orbital different:

$$\begin{aligned} \psi_K &= |...\varphi_m\varphi_n...\rangle \\ \psi_L &= |...\varphi_p\varphi_n...\rangle \end{aligned} \tag{11}$$

$$\begin{aligned} \langle\psi_K|\hat{O}_2|\psi_L\rangle &= \textstyle\sum_n^N [\int\int \varphi_m^*(\mathbf{x}_1)\varphi_n^*(\mathbf{x}_2)\hat{o}(\mathbf{x}_1,\mathbf{x}_2)\varphi_p(\mathbf{x}_1)\varphi_n(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 \\ &\quad - \textstyle\int\int \varphi_m^*(\mathbf{x}_1)\varphi_n^*(\mathbf{x}_2)\hat{o}(\mathbf{x}_1,\mathbf{x}_2)\varphi_n(\mathbf{x}_1)\varphi_p(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2] \end{aligned} \tag{12}$$

Case 3, two spin orbitals different:

$$\begin{aligned} \psi_K &= |...\varphi_m\varphi_n...\rangle \\ \psi_L &= |...\varphi_p\varphi_q...\rangle \end{aligned} \tag{13}$$

$$\begin{aligned} \langle\psi_K|\hat{O}_2|\psi_L\rangle &= \int\int \varphi_m^*(\mathbf{x}_1)\varphi_n^*(\mathbf{x}_2)\hat{o}(\mathbf{x}_1,\mathbf{x}_2)\varphi_p(\mathbf{x}_1)\varphi_q(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 \\ &\quad - \int\int \varphi_m^*(\mathbf{x}_1)\varphi_n^*(\mathbf{x}_2)\hat{o}(\mathbf{x}_1,\mathbf{x}_2)\varphi_q(\mathbf{x}_1)\varphi_p(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 \end{aligned} \tag{14}$$