

**Table 2.3 Matrix elements between determinants for one-electron operators in terms of spin orbitals**

$$\mathcal{O}_1 = \sum_{i=1}^N h(i)$$

Case 1:  $|K\rangle = |\cdots mn \cdots\rangle$

$$\langle K|\mathcal{O}_1|K\rangle = \sum_m^N [m|h|m] = \sum_m^N \langle m|h|m\rangle$$

Case 2:  $|K\rangle = |\cdots mn \cdots\rangle$   
 $|L\rangle = |\cdots pn \cdots\rangle$

$$\langle K|\mathcal{O}_1|L\rangle = [m|h|p] = \langle m|h|p\rangle$$

Case 3:  $|K\rangle = |\cdots mn \cdots\rangle$   
 $|L\rangle = |\cdots pq \cdots\rangle$

$$\langle K|\mathcal{O}_1|L\rangle = 0$$

**Table 2.4 Matrix elements between determinants for two-electron operators in terms of spin orbitals**

$$\mathcal{O}_2 = \sum_{i=1}^N \sum_{j>i}^N r_{ij}^{-1}$$

Case 1:  $|K\rangle = |\cdots mn \cdots\rangle$

$$\langle K|\mathcal{O}_2|K\rangle = \frac{1}{2} \sum_m^N \sum_n^N [mm|nn] - [mn|nm] = \frac{1}{2} \sum_m^N \sum_n^N \langle mn||mn\rangle$$

Case 2:  $|K\rangle = |\cdots mn \cdots\rangle$   
 $|L\rangle = |\cdots pn \cdots\rangle$

$$\langle K|\mathcal{O}_2|L\rangle = \sum_n^N [mp|nm] - [mn|np] = \sum_n^N \langle mn||pn\rangle$$

Case 3:  $|K\rangle = |\cdots mn \cdots\rangle$   
 $|L\rangle = |\cdots pq \cdots\rangle$

$$\langle K|\mathcal{O}_2|L\rangle = [mp|nq] - [mq|np] = \langle mn||pq\rangle$$

where

$$|\Psi_1\rangle = |abcd\rangle$$

$$|\Psi_2\rangle = |crds\rangle$$

At first glance, it might appear that the two determinants differ in all four columns; however, by interchanging columns of  $|\Psi_2\rangle$  and keeping track of