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

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

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

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

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

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

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

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

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

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

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

$$\langle K|\mathscr{O}_2|K\rangle = \frac{1}{2}\sum_{m}^{N}\sum_{n}^{N} [mm|nn] - [mn|nm] = \frac{1}{2}\sum_{m}^{N}\sum_{n}^{N} \langle mn||mn\rangle$$

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

$$\langle K|\mathscr{O}_2|L\rangle = \sum_{n}^{N} [mp|nn] - [mn|np] = \sum_{n}^{N} \langle mn||pn\rangle$$

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

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

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