

$$\hat{Q}_1$$

Case 1:  $|k\rangle = | \dots m m \dots \rangle$   $\{ \dots m, m \dots \} \equiv \{ occ \}$

$$\langle k | \hat{Q}_1 | k \rangle = \sum_i^{occ} \langle i | h | i \rangle$$

Case 2  $|k\rangle = | \dots m m \dots \rangle$

$$|l\rangle = | \dots p m \dots \rangle$$

$$\langle k | \hat{Q}_1 | l \rangle = \langle m | h | p \rangle$$

Case 3  $|k\rangle = | \dots m m \dots \rangle$

$$|l\rangle = | \dots p \bar{p} \dots \rangle$$

$$\langle k | \hat{Q}_1 | l \rangle = 0$$

$\hat{\Theta}_2$

Case 1:  $|k\rangle = |\dots m m \dots\rangle$

$$\langle k | \hat{\Theta}_2 | k \rangle = \frac{1}{2} \sum_i^{occ} \sum_j^{occ} \langle ij | | ij \rangle$$

Example: base  $\{a, b, c, d\}$

$$|k\rangle = |abc\rangle \Rightarrow occ \equiv \{a, b, c\}$$

Case 2:  $|k\rangle = |\dots m m \dots\rangle$

$$|l\rangle = |\dots p m \dots\rangle$$

$$\langle k | \hat{\Theta}_2 | l \rangle = \sum_i^{occ} \langle m i | | p i \rangle$$

Case 3:  $|k\rangle = |\dots m m \dots\rangle$

$$|l\rangle = |\dots p f \dots\rangle$$

$$\langle k | \hat{\Theta}_2 | l \rangle = \langle m m | | p f \rangle$$