FCI Questions

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two differences

$$\langle \Psi | V | \Psi(k \to k', l \to l') \rangle = [mp|nq] - [mq|np] \tag{1}$$

$$= (mp|nq)\delta_{[m][p]}\delta_{[n][q]} - (mq|np)\delta_{[m][q]}\delta_{[n][p]} \tag{2}$$

there are a few cases to go from from here.

1 Case 1

All 2x2=4 (m,n,p,q)so not unique orbs can be of the same spin.

$$= (mp|nq) - (mq|np) \tag{3}$$

2 case 2

the unique spin orbs in each determinant are of different spins. My thought is that because we're working in quantum mechanics we will be dealing with expectation values. So, $|\delta_{[m][p]}\delta_{[n][q]}| = 0.5$ and $|\delta_{[m][q]}\delta_{[n][p]}| = 0.5$. So,

$$[mp|nq] - [mq|np] \tag{4}$$

$$= (1/2) * (mp|nq) - (1/2) * (mq|np) \tag{5}$$

previously I wasn't thinking about the too electron different case in terms of different cases, like I do here.however my energy went from aomething like -7.83, so close to correct, to -7.75, so not so close.I am confused because initially I was not treating the two electron difference case correctly in terms of theoretics(or so I think), but now I am, and my energy is getting further away. can you give any hints, or should I just spend some more time thinking about this?