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

2.1 the unique spin orbs in each determinant are of different spins.

The fermions we are dealing with are indistinguishable, so I need to find out the manifestation of something like $\delta_{[m][p]}\delta_{[n][q]}$ where I have the differences between the determinants stored in the tuple like ([m,n], [p,q]). I've recognized that since the particles are indistinguishable the differences should actually be stored inset like ({m,n}, {p,q}) but if I'm understanding correctly this difference just makes my program slower because I'm not taking advantage of the inherent symmetry and shouldn't really affect the energetics, so I don't have to worry about changing it for now. So, $\delta_{[m][p]}$ is in the super position of being unity or 0, if the spins might be the same or different, so in this case I would set $\delta_{[m][p]} = 1/2$. so with this modification, my derivation should look like

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

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

however, theoretically this isn't giving me a correct energy when I implemented it into my program so I am very confused like garnet (lol). I hope this makes sense this time. what do I need to think about to get the theoretics correct here?