

# FCI Questions

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two differences

$$\langle \Psi | V | \Psi(k \rightarrow k', l \rightarrow l') \rangle = [mp|nq] - [mq|np] \quad (1)$$

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

there are 2, I think, cases to go from here. let's consider that the shared orbs are  $\{a,b,c,d\}$  with the differences orbs an determinant 1 being  $\{m,n\}$  and in determinant 2 being  $\{p,q\}$ .  $m,n$ , and  $p,q$  can all have the same spin, or the unique herbs in each determinant can be of different spin, like  $m$  and  $n$  being in a combination of alpha and beater. I read the part where you said that second quantization already takes into account the indistinguishability of fermions, but I don't understand how that could manifest itself here. we can't just label  $m$  and  $n$  by indices and setting  $m$  being alpha and  $n$  being beta, because they are in indistinguishable particles. thought is that the same should go for  $p$  and  $q$ . apart from indistinguishability matters of fermions, my understanding is that because  $h_6$  is not an ionic species, the number of alpha herbs needs to equal the number of beta herbs. this means, that we can't have  $m$  and  $n$  with same spin, and  $p$  and  $q$  with the same, but opposite spin, as this would violate the fact that the spin of a total valid determinant has to be 0 and we cannot choose the common orbs  $\{a,b,c,d\}$  to have a spin that would offset the spins of the BOTH sets of unique herbs, which could be 1 or negative one. in other words, for for a generic determined  $\{a,b,c,d,e,f\}$  need,  $N_\alpha = N_\beta$ , so  $\{m,n\}$  and  $\{p,q\}$  cannot BOTH be of different spin, so  $m,n$  and  $p,q$  must BOTH be spin alpha/beater, OR  $m$  and  $n$  and  $p$  and  $q$  BOTH having different spins so that the combined spin of the pair is 0. once again, I will bring up indistinguishability here: if  $m$  and  $n$  have diff spin, we cannot just assign specific spin indices to each them, because they

are indistinguishable particles. how does second quantization automatically take this into account?

## 1 Case 1

All 2x2=4 (m,n,p,q)unique orbs can be of the same spin.

$$(mp|nq)\delta_{[m][p]}\delta_{[n][q]} - (mq|np)\delta_{[m][q]}\delta_{[n][p]} \quad (3)$$

$$= (mp|nq) - (mq|np) \quad (4)$$

## 2 case 2

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

this boils down to find out the manifestation of something like  $\delta_{[m][p]}\delta_{[n][q]}$ . this is where I reference the superposition principle, because I don't see how the deltas can be evaluated otherwise, since m,n,p,q have indefinite spin, so my thought Was that  $\delta_{[m][p]}$  is sometimes equal to 0 and sometimes equal to 1, so we give it a value of 1/2.

$$[mp|nq] - [mq|np] \quad (5)$$

$$= (1/2) * (1/2) * (mp|nq) - (1/2) * (1/2) * (mq|np) \quad (6)$$

although I do understand that we are dealing with matrix elements, I don't see how I can evaluate the delta functions without invoking something like the superposition principle.