

FCI Questions

Patryk Kozlowski

May 27, 2023

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 a generic determined $\{a,b,c,d,e,f\}$ need, $N_\alpha = N_\beta$, so $\{m,n\}$ and $\{p,q\}$ cannot be of different spin, so m,n and p,q has both 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.