FCI Questions

Patryk Kozlowski

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1 r.e. point 2

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

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

I think my misunderstanding stems from a failure to understand how the simplification from equation 1 to equation 2 occurs. Previously, I thought that something like $[mp|nq]$ simplified to $(mp|nq)\delta_{[m][p]}\delta_{[n][q]}$ where in my code I would just implement a delta fn and evaluate it for m and p and then n and q, which I would just pop from the set of differences so as to make sure that I am preserving indistinguishability (I know that I am referencing indistinguishability allot even though you have repeatedly told me that it doesn't matter in second quantization, but I just don't know how to think about these things differently :( ), but now I'm not sure because $\delta_{[m][p]}$ in my thinking is pretty close to what you said was wrong when you said: *"electron a with spin upward excited from orbital m to n and electron b with spin ..." blabla* instead of the proper form, which is: *we should be saying "we are calculating matrix element between two states, between which there is only two-electron difference of the occupation, which is m-alpha spin orbital and blabla".* How ells can think about simplifying from spin 2 electron integrals to special 2 electron integrals?

2 r.e. point 3

you said *you performed a (1 alpha + 1 beta) excitation, and I don't think this is something prohibited.* I'm not quite understanding this; were you under the impression that I said this in my previous questions? so, if 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} the only thing that I meant is that m and n cannot BOTH be alpha, while p and q are BOTH beta. however, I think we can have m being alpha and n being beta (it could very well be the opposite because they are indistinguishable Fermions in a set) and the same going for p and q, so that the total spin of determinants 1 and 2 are the same and 0 for neutral h6.

in my previous question set, I referenced that I thought there would be a number of different cases. this would be the case if some of these delta forms mattered ($\delta_{[m][p]}$) to distinguish between different cases but now, I'm not so sure whether they "deserve" an implementation in my code.