FCI Questions

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the below is referencing your previous post, by the way.

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

$$= (-1)^{\varepsilon(\kappa)}((mp|nq)\delta_{[m][p]}\delta_{[n][q]} - (mq|np)\delta_{[m][q]}\delta_{[n][p]}) \tag{2}$$

my old implementation was treating the above equation very literally; so I was actually implementing the kronecker deltas and getting an incorrect, but close, energy of -7.8362021822923005, when correct energy should be -7.8399080148963369. if my implementation of the two electron difference prior was incorrect, I am a little bit confused as to why I was getting an energy that was somewhat close. Was it a fluke or was I actually doing something right? is this something you think you can answer?

1 r.e. case 2

I understand that you were telling me that indistinguishability is already factored into second quantitation, but I think where I might be going wrong, is that I'm just not understanding how it is so? referencing this: *Maybe you treated first the orbitals and then the spins, so you have the idea of 4 sub-cases.* I know that thinking about the theory in latex is more important than thinking about the implementation in python, but I was just hoping that you could take quick look at my determinant basis generation in my code, which I think I am doing in terms of spin orbitals, but I might be wrong? for example, I am generating all possible combinations of alpha and beater strings, and then making all unique combinations of those. if I understand what you're saying correctly, then I am always going to have $\delta_{[m][p]}\delta_{[n][q]} = 1$

with $\delta_{[m][q]}\delta_{[n][p]}$ always being 0. I guess I'm just not understanding why $\delta_{[m][q]}\delta_{[n][p]}$ cannot ever equal 1. I think this boils down to how were you able to decide whether to "label" m or n by alpha/beater automatically or does second quantitation already do this for me in some way?

1.1 [m] == [p] and [n] == [q]

$$\langle\Psi|V|\Psi(k \to k', l \to l')\rangle = [mp|nq] - [mq|np] \tag{3}$$

$$= (-1)^{\varepsilon(\kappa)}((mp|nq)) \tag{4}$$

1.2 [m] == [q] and [n] == [p]

I'm just not understanding how this case could not survive?

$$\langle\Psi|V|\Psi(k \to k', l \to l')\rangle = [mp|nq] - [mq|np] \tag{5}$$

$$= (-1)^{\varepsilon(\kappa)}(-(mq|np)) \tag{6}$$

2 one of your previous comments

only [m p — n q] is contributing, [m q — n p] vanishes; only [m q — n p] is contributing, [m p — n q] vanishes; only [m p — n q] is contributing, [m q — n p] vanishes: only [m q — n p] is contributing, [m p — n q] vanishes; So I don't think there will be two terms. I think I am understanding that there will never be two terms, from:

$$\langle\Psi|V|\Psi(k \to k', l \to l')\rangle = [mp|nq] - [mq|np] \tag{7}$$

$$= (-1)^{\varepsilon(\kappa)}((mp|nq)\delta_{[m][p]}\delta_{[n][q]} - (mq|np)\delta_{[m][q]}\delta_{[n][p]}) \tag{8}$$

but I just don't see how case 1.2 won't ever be a "factor"?