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, and energy of -7.8362021822923005, when correct energy should be -7.8399080148963369. in my new implementation, I am splitting it into the following cases.

1 r.e. cases 1 and 3

why did you treat: *alpha, alpha -¿ alpha alpha* and *beta, beta -¿ beta, beta* as seperate cases? even though you later said that: *1 and 3 are similar cases without any special mathematics, and we both agree that 2 may be something different.* are 1 and 3 just *similar* cases, or the *same*, which is my current thinking? my current implementation for both of these cases, treating both cases on equal footing, is:

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

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

2 r.e. case 2

I think now I know how to navigate this without referencing an kind of superposition or mean values. I am always going to have $\delta_{[m][p]}\delta_{[n][q]} = 0/1$ with $\delta_{[m][q]}\delta_{[n][p]}$ being the exact opposite. therefore in my new implementation I have that only one of the associated integrals survive.

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

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

$$= (-1)^{\varepsilon(\kappa)}((mp|nq)) \tag{6}$$

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

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

$$= (-1)^{\varepsilon(\kappa)}(-(mq|np)) \tag{8}$$

however, with this I am getting the same faulty energy as in my old implementation where I didn't seperate into cases at all, and when I think about it more, it seems like the same thing theoretically. this makes me wonder whether I made any theoretical progress here separating into cases, or if it is the same thing? that is, when I think about it some more, these cases just seem like the same thing as

$$= (-1)^{\varepsilon(\kappa)}((mp|nq)\delta_{[m][p]}\delta_{[n][q]} - (mq|np)\delta_{[m][q]}\delta_{[n][p]}) \tag{9}$$

with the only difference being that I have separated the problem into the multiple possible cases.
for reference, with with my new case specific implementation, I am getting -7.8362021822923005, which is the same as for my old unspecific implementation.