

I'm beginning to learn how to conceptualize for myself and for a mentor without handwriting. Let me know if you need more visualization and I would be happy to make changes in the way I present material. Also, it will be ideal if you can look at my code through GitHub. I'm trying to set that up, but I first need to overcome my struggles with understanding git to do that lol

i've started implementing fci and i have some questions. I realize that in order to use the Condon rules to simplify the fci matrix elements, I first need to generate them. So I need to implement each matrix element (an example of one is given below). I don't know how I would do this, but thinking of putting both determinants in maximum coincidence and just recording an array of tuples that describe how they differ. For example, for the below matrix element I would record [(i,r), (j,s)]. Thoughts?

Then, I assume there would be a lot of different doubles, so in reality the below matrix element would be an array (in this case shape = (1,sum of how many doubles are possible)). Is this correct?

How large would the above sum of how many doubles are possible be? Is this just how many ways there are to arrange N electrons into 2m orbitals (times 2 bc each orbital can have 2 electrons) such that it is a doubly excited configuration? Is this the right way to calculate that (not just for doubles, but for all excitations possible)? $\langle \Psi_0 | O_1 + O_2 | \Psi_{ij}^{rs} \rangle$