want to write out an algorithm by which i would generate and simplify fci matrix

1. **determine size of fci matrix.** i believe this would be done by supposing i have N electrons and 2m orbitals and determining how many excitations it is possible to make from a "ground state" configuration, thereby determining the dimension of the fci matrix. **not sure how to make this calculation.**

2. **for each excitation level, construct all determinants possible in an occupation number rep and store them as sets.** For example, consider our h6 system of 6 e- in the minimal basis of 6 orbs (each spatial orb fits two spin orbs), so for example, a singly excited state would be (1,2,3,4,5,12) or (-1,1,-2,2,-3,6) with the - sign denoting spin down e-. a doubly excited state could be (1,2,3,4,11,12) or (-1,1,-2,2,-6,6). the mel of these two would be denoted as $\left\langle \Psi_6^{12} \left| O_1 + O_2 \right| \Psi_{5,6}^{11,12} \right\rangle$. **i have reviewed the fock space in second quantization and that has helped a lot. but still struggling to understand how both $\left\langle \Psi_6^{12} \left| O_1 + O_2 \right| \Psi_{5,6}^{11,12} \right\rangle$ and $\left\langle \Psi_5^{11} \left| O_1 + O_2 \right| \Psi_{5,6}^{11,12} \right\rangle$ and many other possible mels of this form with presumably different values would all fit into the individual fci mel $\left\langle \Psi_i^r \left| O_1 + O_2 \right| \Psi_{i,j}^{r,s} \right\rangle$.**

3. the actual evaluation of such mels in second quantization will be simple, implementing, for example, $a_{12}^\dagger$ as (12,1) and a_6 as (6,0) with the tuple denoting (orb to be acted on, 1 for creation and 0 for annhilation) and then **i have the 1e- and 2e- operators already given to me in presumably a det basis, which i don't compeletely understand how to use these given arrays based off my bolded confusion in 2**; my review of the fock space in second quantization was helpful in figuring this out along with the how i will compute the associated phase factor. **i think i will implement the condon rules to reduce and simplify the individual fci elements that i need to compute, before i do the computationally intensive portion of computing the mels in second quantization?**

4. use numpy to diagonalize the fci matrix and then proceed to the next step of the project, which is figuring out a more efficient diagonalization method.

i am beginning to figure out using dictation to visualize physics in latex, as you can see above. i think this will be a very helpful conceptual tool for me and also a helpful way for you to better understand my questions. i am just mentioning this to emphasize that there should no longer be any barriers for me with visualizing physics in latex; so if you feel that something needs more visualization to make what dam asking make mar sense, that should be es for me to do.

i dictated the final portion of the last sentence, so actually let me know if there is any trouble for you with understanding it. for example, i'm was recognized as dam, so sounding my dictation excerpt out is helpful. if the dictation of sentences is incomprehesible, i will go back to typing which is a bit slower for me; but leaving you confused about what i mean when i'm dictating is a waste of time and it not that much of a burden to type out sentences; dictating them is just a bit faster, so i wanted to try it out and see if you can understand it. **your feedback on your ability to comprehend my dictation would**

be appreciated,