

I am confused about the structure of the h1e.npy and h2e.npy files, which I am using to implement the Condon rule. I thought the arrays would be symmetrical, but I printed h1e.npy and I found that it isn't. For example, I know that when there is no difference in determinants, and I am dealing with a two-electron integral, the expression is something like $\frac{1}{2} \sum_m^N \sum_n^N \langle mn || mn \rangle$. However, I know that I would want to convert this to a second quantization form, but if I do not know how to access the relevant integrals, this is tricky. Like, I am not sure which entry of h2e.npy I would use to implement something like this. Perhaps I need to do some more reading on this point, but could you point me in the right direction, if so?