Suppose we have a system with 4 spatial orbitals ($M = 8$ spin orbitals) and $N = 4$ electrons, the many-body ground state wavefunction of the system will be a superposition of the states shown in Figure 1. Since we have 4 electrons with 8 places for the electron, we have

$$^{8}C_4 = \frac{8!}{4!(8-4)!} = 70 \sim O(M^N)$$

possible configurations. Note that the left-most state is the Hartree-Fock/DFT state. In other words, the ground state will be of the form

$$|\Psi_{GS}\rangle = c_1 |\Psi_1\rangle + c_2 |\Psi_2\rangle + c_3 |\Psi_3\rangle + \cdots + c_{70} |\Psi_{70}\rangle , \tag{1}$$

where $|\Psi_i\rangle$ are the states listed in Figure 1.

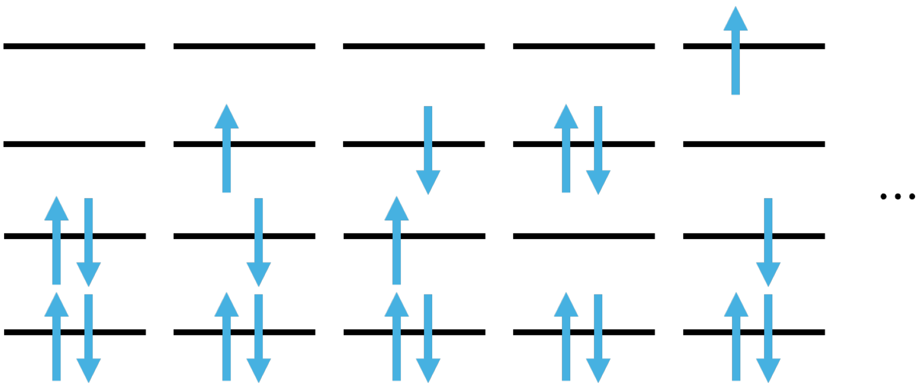

Figure 1: Configurations of 8 spin orbitals and 4 electrons. The leftmost state is the HF state.

When M and N are large (Figure 2), we will have to deal with the huge number of configurations $^{M}C_N$ when we try to solve using classical computers. On the other hand, we will also have to deal with the large number of qubits M when we try to solve using quantum computers.

To reduce the complexity of the system, notice that in the ground state, the c_i of the states (Equation 1) in Figure 3 are small. Hence, we just assume the high orbitals are always empty, and the lowest orbital are always occupied as shown in Figure 4. This leaves us with fewer number of configurations to deal with, also with fewer number of qubits to apply.

The derivation for getting the active space h_{pq} and h_{pqrs} is shown in `http://arxiv.org/abs/2009.01872`. However, the DFT active space is quite complicated and so we will try to do the HF active space first. The code to get the HF active space is shown in `active_space.py` file.

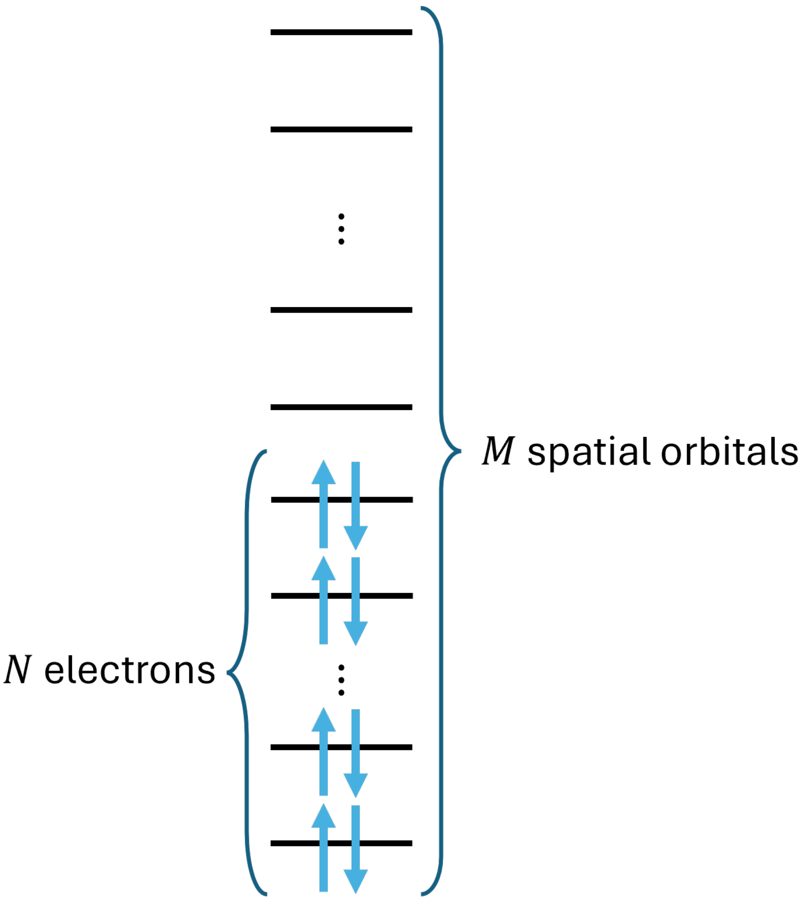

Figure 2: HF state of system with large M and N

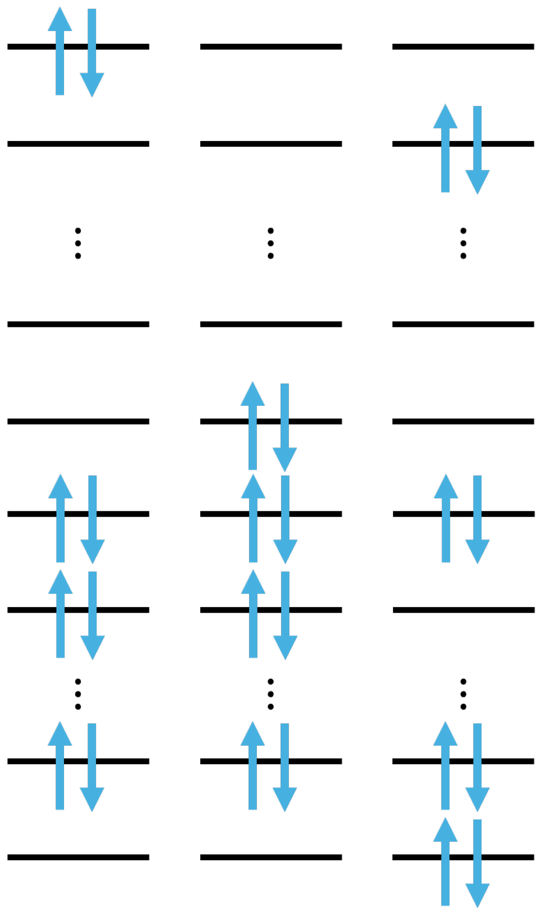

Figure 3: The states above does not contribute much towards the ground state energy

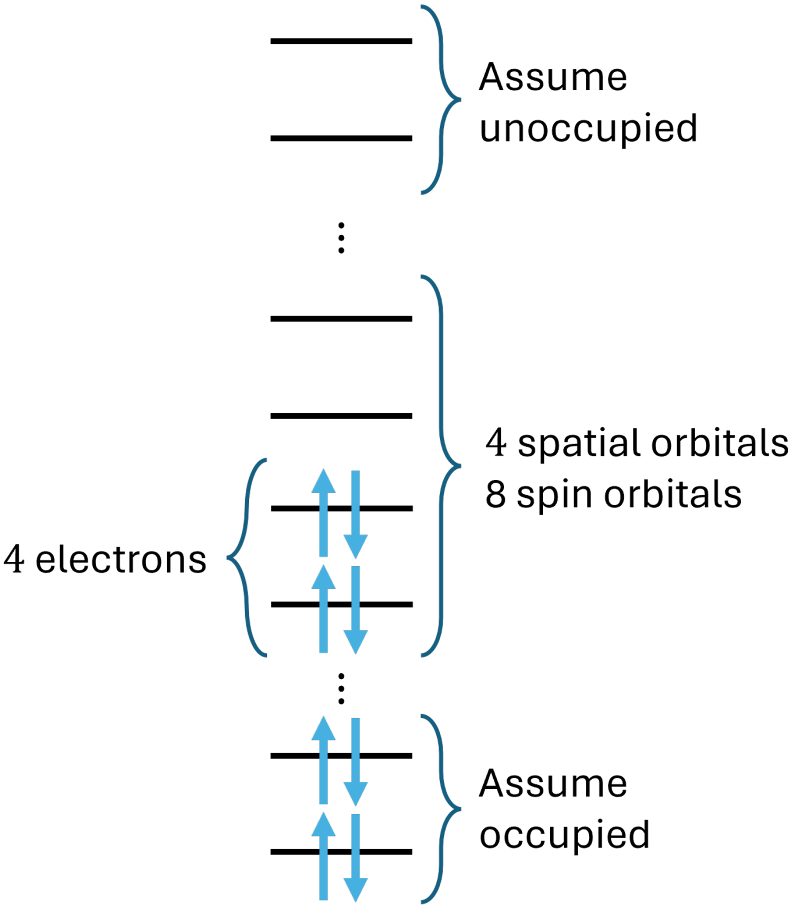

Figure 4: Here, we assume the high orbitals are always empty, and the lowest orbitals are always occupied, leaving us with ${}^8C_4 = 70$ states.