- Roughly speaking, in Davidson algorithm, one needs to implement the function which maps an input FCI vector $|\Psi\rangle$ into $\hat{H}|\Psi\rangle$.

- We need to first think about how to represent & store the FCI vectors $|\Psi\rangle$ numerically. One can think of a basis consisting of determinants $|\Phi\rangle$, and we can store the coefficients $\langle\Phi|\Psi\rangle$. Let's take H_6 as an example. You have suggested to enumerate all the α and β determinants (C_6^3 each), which is reasonable. We need to further notice that suitable $|\Phi\rangle$ should be a product of the α and β determinants, $|\Phi_{IJ}\rangle = |\Phi_I^\alpha\rangle \otimes |\Phi_J^\beta\rangle$. So if there are C_6^3 each, the total number of possible FCI vectors spanning the variational space should be $(C_6^3)^2 = 400$. Numerically this can be a 400×1 `np.array`.

- We then think of how to perform matrix-vector multiplications. Previously we just build the 400×400 Hamiltonian matrix $\langle\Phi|\hat{H}|\Phi'\rangle$ and store it. However, when system size becomes large, this is no longer feasible. An observation is that Hamiltonian matrix in FCI space is in fact very sparse – we are told by Slater-Condon rules that if the determinants differ by more than 2 excitations, then the matrix element between them is zero, so storing everything is not efficient.

- An approach is to get rid of the FCI matrix representation of the Hamiltonian and do everything directly under second-quantization. We expand

$$\hat{H}|\Psi\rangle = \sum_I \langle\Phi_I|\Psi\rangle\hat{H}|\Phi_I\rangle = \sum_I C_I\hat{H}|\Phi_I\rangle \tag{1}$$

We can then think of applying $\hat{H}$ to each $|\Phi_I\rangle$ determinant. For example for 1-body $\hat{H} = \sum_{\mu\nu} h_{\mu\nu}c_\mu^\dagger c_\nu$, we have

$$\hat{H}|\Phi_I\rangle = \sum_{\mu\nu} h_{\mu\nu}c_\mu^\dagger c_\nu|\Phi_I\rangle = \sum_{\mu\nu}(-1)^{\sigma(I,\mu,\nu)}h_{\mu\nu}|\Phi_{f(I,\mu,\nu)}\rangle \tag{2}$$

A key observation is that when we apply $c_\mu^\dagger c_\nu$ to a determinant $|\Phi_I\rangle$, it gives us some other determinant $|\Phi_{f(I,\mu,\nu)}\rangle$ with a phase factor $(-1)^{\sigma(I,\mu,\nu)}$. Here f is a function that takes numbers I, μ, ν and outputs a number $J = f(I, \mu, \nu)$ to indicate that we have reached the J-th determinant. An intuitive thinking is that for H_6, we can start from the zeroth ($I = 0$) determinant $|000111\rangle_\alpha \otimes |000111\rangle_\beta$, remove the electron in the zeroth α orbital ($\nu = 0$) and add it to the third orbital ($\mu = 3$), this actually gives us this determinant $|001110\rangle \otimes |000111\rangle$,

which is the first $(J = 1)$. So $f(0, 3, 0) = 1$. You may notice that when we talk about the "first", "second" or the "zeroth" determinants, we are actually referring to the "addresses" of the determinants, i.e. address is something one use to "label" the determinants.

- If we know the functions $f(I, \mu, \nu)$ and $\sigma(I, \mu, \nu)$, it is then simple to compute

$$\hat{H}|\Psi\rangle = \sum_I C_I \hat{H}|\Phi_I\rangle = \sum_I C_I \sum_{\mu\nu} (-1)^{\sigma(I,\mu,\nu)} h_{\mu\nu} |\Phi_{f(I,\mu,\nu)}\rangle \tag{3}$$

as a summation. Note that here only the molecular integrals appear (not the FCI Hamiltonian matrices!). We need to be able to compute $f(I, \mu, \nu)$ and $\sigma(I, \mu, \nu)$, and this can be done by some binary operations. I would like to recommend Chapter 11.8 of the book *Molecular Electronic-Structure Theory* for detailed explanations. Also, maybe you can look at the `fci.cistring.gen_linkstr_index` function in PySCF for more hints.