# Fock Routine

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This is probably a simple question, but I am not understanding why my Fock construction doesn't seem to match that of PySCF. My test case for the $G_0W_0$ energy matches that of PySCF when I use the dTDA for my TDDFT and a Fock matrix @HF density, which I assume means the density matrix here. Are their instances where this means something different? One you say to evaluate something at the HF/DFT density, is that synonymous with saying to use the density matrix for that mean field object? What I am doing seems correct, but when I compare it to

```
mf_hf.get_fock(dm=mf_dft.make_rdm1())
```

I get different results. I assume this is why I am getting different results for the $G_0W_0$ energy. I am using the following code to construct my Fock matrix:

```
def fock_dft(mf):
    '''Calculates the HF fock matrix using the DFT electron
    density in AO basis for a given set of molecular orbitals
    and occupations.

    Parameters:
    mf (object): The object representing the mean-field
    calculation.

    Returns:
    mo_fock (ndarray): The Fock matrix in the molecular
    orbital basis.
    '''
    # make the common variables
    n_orbitals = mf.mol.nao_nr()

```

```
13    # initialize the ao_fock matrix in the atomic orbital
      basis
14    ao_fock = np.zeros((n_orbitals, n_orbitals))
15
16    # get the core hamiltonian
17    h_core = mf.get_hcore()
18
19    # get the coulumb term
20    coulumb_matrix = np.zeros((n_orbitals, n_orbitals))
21    coulumb_matrix += np.einsum('rs,pqrs->pq', mf.make_rdm1()
      , mf.mol.intor('int2e').reshape((n_orbitals, n_orbitals,
      n_orbitals, n_orbitals)))
22
23    # get the exchange term
24    exchange_matrix = np.zeros((n_orbitals, n_orbitals))
25    exchange_matrix += np.einsum('rs,prqs->pq', mf.make_rdm1
      (), mf.mol.intor('int2e').reshape((n_orbitals, n_orbitals,
       n_orbitals, n_orbitals)))
26
27    # add the terms
28    ao_fock += (h_core + coulumb_matrix - 0.5*exchange_matrix
      )
29
30    # convert the fock matrix to the molecular orbital basis
31    mo_fock = np.einsum('ia,ij,jb->ab', mf.mo_coeff, ao_fock,
      mf.mo_coeff)
32
33    return mo_fock
```

Maybe this is a simple question, but when you say that the HF Fock matrix is diagonal in the energies in the canonical representation, what does this mean? I am familiar with what the term canonical means in second quantization, that is, the appropriate ordering of orbitals. I don't know how to think about this in first quantization?