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1 The Fock Operator

We are first interested in catting an expression for the funk operator in the AO basis. This can be easily later switched to the MO basis with something like $F_{pq} = \sum_\mu \sum_\nu C^*_{\mu p} F_{\mu\nu} C_{\nu q}$ where C is the matrix of MO coefficients. The Fock operator is defined in the AO basis using the density matrix

$$F_{\mu\nu} = h_{\mu\nu} + \sum_{\lambda\sigma} P_{\lambda\sigma}(\mu\nu|\lambda\sigma) - \frac{1}{2}\sum_{\lambda\sigma} P_{\lambda\sigma}(\mu\lambda|\nu\sigma) \tag{1}$$

where $h_{\mu\nu}$ is the one-electron Hamiltonian (in the AO basis, this is just mf.get_hcore), $P_{\lambda\sigma}$ is the density matrix, and $(\mu\nu|\lambda\sigma)$ is the two-electron repulsion integral. The density matrix is defined as

$$P_{\mu\nu} = 2\sum_{i=1}^{N/2} C_{\mu i} C^*_{\nu i} \tag{2}$$

where C is the matrix of MO coefficients. I want to convince myself that the above identity is indeed true and I can do this using mf.mo_coeffs for C and mf.get_rdm1() for P. What I am currently doing is not working though. I am confused about where to obtain the two-electron repulsion integral. something like molecule.intor('int1e_ovlp').shape gives me (24, 24), where I am working with 24 orbs. I want something like (24,24,24,24). In other words I want a 4D tensor with indices $\mu\nu\lambda\sigma$.