CEM 993 **Spring 2023**

Assignment No. 3 (20 pts.) **Due Date: March 1, 2023**

1. (6 pts.) Let
$$H = \sum_{p,q} \langle p|z|q\rangle X_p^\dagger X_q + \tfrac{1}{2} \sum_{p,q,r,s} \langle pq|v|rs\rangle X_p^\dagger X_q^\dagger X_s X_r \tag{1}$$
be the Hamiltonian containing up to two-body terms. Use the anti-commutation relations for the creation and annihilation operators to show that if the domain of operator H is restricted to an N-electron Hilbert space with a fixed number of particles N, we can write
$$H = \tfrac{1}{2} \sum_{p,q,r,s} \langle pq|w|rs\rangle X_p^\dagger X_q^\dagger X_s X_r, \tag{2}$$
where
$$\langle pq|w|rs\rangle = \langle pq|v|rs\rangle + \frac{1}{N-1}\left(\delta_{pr}\langle q|z|s\rangle + \delta_{qs}\langle p|z|r\rangle\right). \tag{3}$$

2. (8 pts.) Let Z_N be a generic one-body operator in the normal-product form,
$$Z_N = \sum_{p,q} \langle p|z|q\rangle N[X_p^\dagger X_q], \tag{4}$$
and let T_1 be a one-body particle-hole excitation operator,
$$T_1 = \sum_{i,a} \langle a|t_1|i\rangle N[X_a^\dagger X_i]. \tag{5}$$
Use the hole-particle variant of Wick's theorem to prove that
$$[Z_N, T_1]\,|\Phi\rangle = \sum_{a,i}\left(\sum_b \langle a|z|b\rangle\langle b|t_1|i\rangle - \sum_j \langle a|t_1|j\rangle\langle j|z|i\rangle\right)|\Phi_i^a\rangle + \left(\sum_{a,i}\langle a|t_1|i\rangle\langle i|z|a\rangle\right)|\Phi\rangle, \tag{6}$$
where [,] is the commutator, $|\Phi\rangle$ is the Fermi vacuum state, and $|\Phi_i^a\rangle$ are the singly excited determinants relative to $|\Phi\rangle$. You will have a chance to prove the same identity using diagrams later. The above equation is a demonstration of the fact (used, for example, in coupled-cluster theory) that commutators of many-body operators produce *connected* quantities (diagrams) only.

3. (6 pts.) Use the results obtained in Problem 2, particularly Eq. (6), to derive the formulas for
$$\langle\Phi|\,[Z_N, T_1]\,|\Phi\rangle, \tag{7}$$
$$\langle\Phi_i^a|\,[Z_N, T_1]\,|\Phi\rangle, \tag{8}$$
and
$$\langle\Phi_{ij}^{ab}|\,[Z_N, T_1]\,|\Phi\rangle \tag{9}$$
in terms of matrix elements $\langle p|z|q\rangle$ and $\langle b|t_1|j\rangle$. As in Problem 2, [,] is the commutator, $|\Phi\rangle$ is the Fermi vacuum state, and $|\Phi_i^a\rangle$ is the singly excited determinant relative to

$|\Phi\rangle$. $|\Phi_{ij}^{ab}\rangle$ is the doubly excited determinant relative to $|\Phi\rangle$. The remaining definitions are the same as in Problem 2. In general, what are the values of n in the expression

$$\langle\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}|\,[Z_N,T_1]\,|\Phi\rangle, \tag{10}$$

where $|\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle$ is the n-tuply excited determinant relative to $|\Phi\rangle$, that produce non-zero results? Justify your answer. How would your answer change if we considered

$$\langle\Phi_{i_1\ldots i_n}^{a_1\ldots a_n}|Z_N T_1|\Phi\rangle \tag{11}$$

instead (i.e., if we replaced the commutator of Z_N and T_1 by their product)?