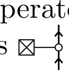
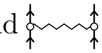
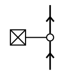
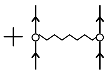
1. Expand the electronic Hamiltonian H in terms of Φ-normal-ordered operators using Wick's theorem for graphs, writing the core Hamiltonian and electron repulsion operators as  $\equiv h_p^q a_q^p$ and  $\equiv \frac{1}{4}\overline{g}_{pq}^{rs} a_{rs}^{pq}$.

$H =$  $+$  $= ?$

2. Evaluate the following using Wick's theorem for graphs. Fully simplify your answer assuming the indices refer to a basis of canonical Hartree-Fock spin-orbitals.

$$\langle \Phi_{ijk}^{abc} | F_{\mathrm{c}}\, C_3 | \Phi \rangle = \,?$$

$$F_{\mathrm{c}} \equiv f_p^q \tilde{a}_q^p$$

$$C_3 \equiv (\tfrac{1}{3!})^2 c_{def}^{lmn} \tilde{a}_{lmn}^{def}$$

3. (a) Explain how to get from the projected CCD Schrödinger equation

$$E_\mathrm{c}\, t_{ab}^{ij} = \langle \Phi_{ij}^{ab} | H_\mathrm{c} \exp(T_2) | \Phi \rangle \qquad H_\mathrm{c} = F_\mathrm{c} + V_\mathrm{c} \qquad \begin{array}{l} F_\mathrm{c} \equiv f_p^q \tilde{a}_q^p \\ V_\mathrm{c} \equiv \tfrac{1}{4} \overline{g}_{pq}^{rs} \tilde{a}_{rs}^{pq} \end{array} \tag{1}$$

to the working equation for CCD amplitudes

$$t_{ab}^{ij} = (\mathcal{E}_{ab}^{ij})^{-1} \langle \Phi_{ij}^{ab} | V_\mathrm{c} \exp(T_2) | \Phi \rangle_\mathrm{L} \qquad \mathcal{E}_{ab}^{ij} \equiv \epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b \tag{2}$$

assuming a canonical Hartree-Fock reference.[1]

(b) Write out an algorithm to numerically solve equation 2.

[1]Hint: You only need to evaluate three diagrams to answer this question.

Extra Credit: Derive the following interpretation rule in your own words:

> Each open cycle in a graph contributes $(-)^{h_i} a^p_q$ to the normal-ordered product of operators, where p and q label the free ends and h_i is the number of hole contractions in the cycle. A closed cycle (loop) contributes $(-)^{h_i+1}$.