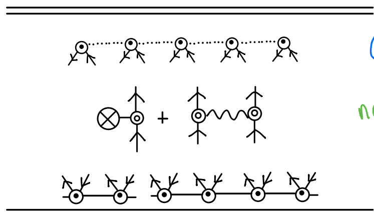
Question 1 (6 points)

a)



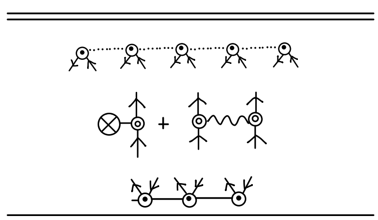
(-5)

need (-1)

(+6)

Yes, this term contributes to pentuples amplitudes in CCSDTQP, since the excitation levels balance and one can form connected diagrams.

b)



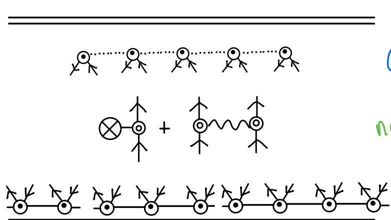
(-5)

need (+2)

(+3)

No, this does not contribute to pentuples amplitudes in CCSDTQP. Though the excitation levels balance out, one cannot form connected diagrams.

c)



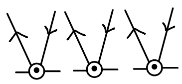
(-5)

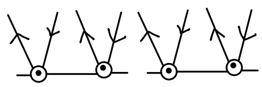
need (-4)

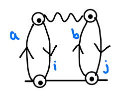
(+9)

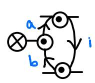
No, this term does not contribute to pentuples amplitudes in CCSDTQP. The excitation levels do not balance to 0.

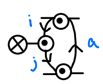
Question 2 (12 points)

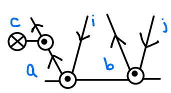
a)  $\frac{1}{3!}\left(t_a^i \tilde{a}_i^a\right)^3 = \frac{1}{3!}T_1^3$

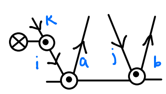
b)  $\frac{1}{2!}\left(\left(\frac{1}{2!}\right)^2 t_{ab}^{ij} \tilde{a}_{ij}^{ab}\right)^2 = \frac{1}{2}T_2^2$

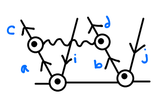
c)  $\left(\frac{1}{2}\right)^2 \bar{g}_{ij}^{ab} t_{ab}^{ij}$

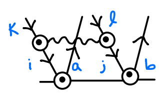
d)  $c_i^a f_a^b c_b^i$

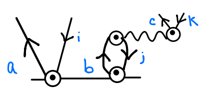
e)  $-c_i^a f_j^i c_a^j$

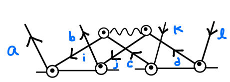
f)  $(-1)^0(-1)^0\frac{1}{2!} f_c^a t_{ab}^{ij} \tilde{a}_{ij}^{cb} = \frac{1}{2} f_c^a t_{ab}^{ij} \tilde{a}_{ij}^{cb}$

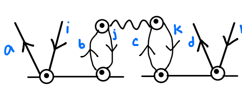
g)  $(-1)^1(-1)^0\frac{1}{2!} f_i^k t_{ab}^{ij} \tilde{a}_{kj}^{ab} = -\frac{1}{2} f_i^k t_{ab}^{ij} \tilde{a}_{kj}^{ab}$

h)  $(-1)^0(-1)^0\left(\frac{1}{2!}\right)^3 \bar{g}_{cd}^{ab} t_{ab}^{ij} \tilde{a}_{ij}^{cd} = \left(\frac{1}{2}\right)^3 \bar{g}_{cd}^{ab} t_{ab}^{ij} \tilde{a}_{ij}^{cd}$

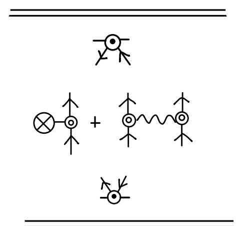
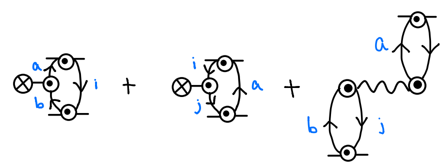
i)  $(-1)^1(-1)^1\left(\frac{1}{2!}\right)^3 \bar{g}_{ij}^{kl} t_{ab}^{ij} \tilde{a}_{kl}^{ab}$

j)  $(-1)^0(-1)^{1+1}(-1)^0 \bar{g}_{jc}^{bk} t_{ab}^{ij} \tilde{a}_{ik}^{ac} = \bar{g}_{jc}^{bk} t_{ab}^{ij} \tilde{a}_{ik}^{ac}$

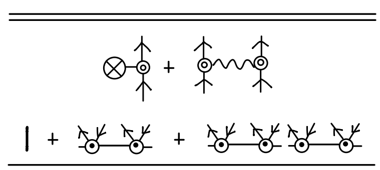
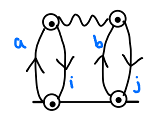
k)  $(-1)^1(-1)^1\left(\frac{1}{2!}\right)^4 \bar{g}_{ij}^{cd} t_{ab}^{ij} t_{cd}^{kl} \tilde{a}_{kl}^{ab} = \left(\frac{1}{2}\right)^4 \bar{g}_{ij}^{cd} t_{ab}^{ij} t_{cd}^{kl} \tilde{a}_{kl}^{ab}$

l)  $(-1)^0(-1)^0(-1)^{1+1}(-1)^{1+1}\frac{1}{2!} \bar{g}_{jk}^{bc} t_{ab}^{ij} t_{cd}^{kl} \tilde{a}_{il}^{ad} = \frac{1}{2} \bar{g}_{jk}^{bc} t_{ab}^{ij} t_{cd}^{kl} \tilde{a}_{il}^{ad}$

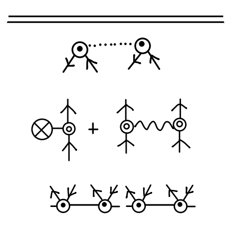
Question 3 (9 points)

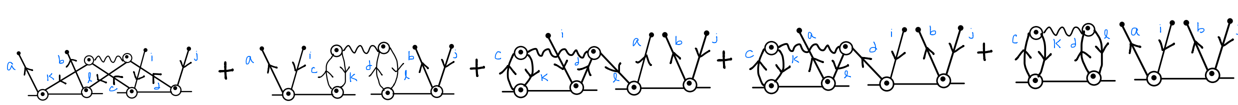
$\langle \Phi | C_1^{\dagger} H_c C_1 | \Phi \rangle \equiv$  $=$ 

$c^a_i f^b_a c^i_b \quad - \; c^a_i f^i_j c^j_a \quad + \; \bar{g}^{bi}_{ja} c^a_i c^j_b$

$\langle \Phi | H_c (1 + T_2 + \frac{1}{2} T_2^2) | \Phi \rangle \equiv$  $=$ 

$\left(\frac{1}{2}\right)^2 \bar{g}^{ab}_{ij} t^{ij}_{ab}$

$\langle \Phi^{ab}_{ij} | H_c (\frac{1}{2} T_2^2) | \Phi \rangle \equiv$  $=$



$\left(\frac{1}{2}\right)^2 \bar{g}^{cd}_{kl} t^{kl}_{ab} t^{ij}_{cd} \qquad \frac{1}{2} \hat{P}^{(i/j)}_{(a/b)} \bar{g}^{cd}_{kl} t^{ik}_{ac} t^{lj}_{db} \qquad -\frac{1}{2} \hat{P}^{(i/j)} \bar{g}^{cd}_{kl} t^{ki}_{cd} t^{lj}_{ab} \qquad -\frac{1}{2} \hat{P}_{(a/b)} \bar{g}^{cd}_{kl} t^{kl}_{ca} t^{ij}_{db} \qquad \left(\frac{1}{2}\right)^2 \bar{g}^{cd}_{kl} t^{kl}_{cd} t^{ij}_{ab}$