1. Derive the recursive equation for the wavefunction, starting from the λ-dependent Schrödinger equation.

$$\Psi(\lambda) = \Phi + R_0(\lambda V_\mathrm{c} - E(\lambda))\Psi(\lambda) \tag{1}$$

Assume intermediate normalization and note that $R_0 H_0 = -Q$ follows** from the definition of R_0.

Answer: Operating R_0 on both sides of $0 = (H(\lambda) - E(\lambda))\,\Psi(\lambda) = (H_0 + \lambda V_\mathrm{c} - E(\lambda))\,\Psi(\lambda)$ gives

$$\begin{aligned} 0 &= R_0 H_0 \Psi(\lambda) + R_0(\lambda V_\mathrm{c} - E(\lambda))\Psi(\lambda) \\ &= -Q\Psi(\lambda) + R_0(\lambda V_\mathrm{c} - E(\lambda))\Psi(\lambda) \\ &= -\Psi(\lambda) + \Phi + R_0(\lambda V_\mathrm{c} - E(\lambda))\Psi(\lambda) \end{aligned}$$

where the last step follows from $Q = 1_n - P$ and intermediate normalization: $\langle \Phi | \Psi(\lambda) \rangle = 1 \implies P\Psi(\lambda) = \Phi$. Adding $\Psi(\lambda)$ to both sides gives equation 1.

****Extra Credit**: Define "resolvent" and explain why this follows from your definition.

Answer: The resolvent is the negative inverse of H_0 in the orthogonal space, $R_0 = -\,H_0^{-1}\big|_\mathrm{o}$, which implies that $R_0 H_0 = -\,1\big|_\mathrm{o}$. Resolution of the identity in the orthogonal space gives Q.

$$1\big|_\mathrm{o} = \sum_{k=1}^{n} (\tfrac{1}{k!})^2 \sum_{\substack{a_1\cdots a_k \\ i_1\cdots i_k}} |\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}\rangle\langle\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}| = Q$$

2. Determine the first- and second-order components of Ψ by differentiating equation 1. You do not need to fully evaluate and simplify your answer,[1] but you should eliminate all terms that vanish and explain why each one evaluates to zero.[2]

Answer: The λ-dependent first and second derivatives are as follows

$$\begin{aligned}\frac{\partial\Psi(\lambda)}{\partial\lambda} &= R_0\left(V_\mathrm{c} - \frac{\partial E(\lambda)}{\partial\lambda}\right)\Psi(\lambda) + R_0(\lambda V_\mathrm{c} - E(\lambda))\frac{\partial\Psi(\lambda)}{\partial\lambda}\\ \frac{\partial^2\Psi(\lambda)}{\partial\lambda^2} &= -R_0\frac{\partial^2 E(\lambda)}{\partial\lambda^2}\Psi(\lambda) + 2R_0\left(V_\mathrm{c} - \frac{\partial E(\lambda)}{\partial\lambda}\right)\frac{\partial\Psi(\lambda)}{\partial\lambda} + R_0(\lambda V_\mathrm{c} - E(\lambda))\frac{\partial^2\Psi(\lambda)}{\partial\lambda^2}\end{aligned}$$

where we have used the product rule: if $f = gh$, then $f' = g'h + gh'$ and $f'' = g''h + 2g'h' + gh''$. Evaluating these derivatives at $\lambda = 0$ after dividing the second equation by 2 gives the following

$$\begin{aligned}\Psi^{(1)} &= R_0 V_\mathrm{c}\Phi - E^{(1)}R_0\Phi - R_0 E^{(0)}\Psi^{(1)}\\ \Psi^{(2)} &= -E_\mathrm{c}^{(2)}R_0\Phi + R_0 V_\mathrm{c}\Psi^{(1)} - E_\mathrm{c}^{(1)}R_0\Psi^{(1)} - R_0 E_\mathrm{c}^{(0)}\Psi^{(2)}\end{aligned}$$

since $\Psi^{(0)}$ is the ground-state eigenvector of H_0, which is Φ. It follows that $E_\mathrm{c}^{(0)} = \langle\Phi|H_0|\Phi\rangle = 0$. Furthermore, using the relation in footnote 2 we have that $E_\mathrm{c}^{(1)} = \langle\Phi|V_\mathrm{c}|\Phi\rangle = 0$. Since R_0 is only acts on the orthogonal space we have $R_0 = R_0 Q$, which implies $R_0\Phi = R_0 Q\Phi = 0$. Therefore,

$$\begin{aligned}\Psi^{(1)} &= R_0 V_\mathrm{c}\Phi\\ \Psi^{(2)} &= R_0 V_\mathrm{c}\Psi^{(1)}\end{aligned}$$

are the non-vanishing contributions to $\Psi^{(1)}$ and $\Psi^{(2)}$.

[1]That is, your final answer may contain R_0's and V_c's.

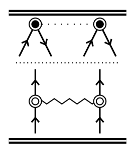
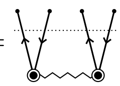
[2]You may take $E_\mathrm{c}^{(m+1)} = \langle\Phi|V_\mathrm{c}|\Psi^{(m)}\rangle$ as given.

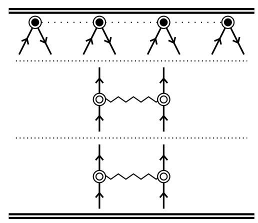
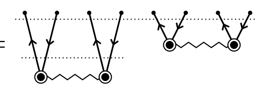
3. Evaluate the following contributions to the CI doubles and quadruples coefficients.

$$ {}^{(1)}c^{ij}_{ab} = \langle \Phi^{ab}_{ij} | R_0 V_\mathrm{c} | \Phi \rangle \qquad\qquad {}^{(2)}c^{ijkl}_{abcd} = \langle \Phi^{abcd}_{ijkl} | R_0 V_\mathrm{c} R_0 V_\mathrm{c} | \Phi \rangle \tag{2} $$

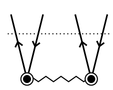
Use your answer to show that ${}^{(2)}C_4 = \frac{1}{2}{}^{(1)}C_2^2$.

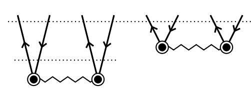
Answer: Only the +2 fluctuation potential contributions can fully contract the products, so there is only one unique graph contraction for each one. Note that the off-diagonal Fock operator has no excitation level +2 component, so the results are the same whether or not we assume Brillouin's theorem.

$${}^{(1)}c^{ij}_{ab} =$$  $$=$$  $$= \frac{\overline{g}^{ij}_{ab}}{\mathcal{E}^{ij}_{ab}}$$

$${}^{(2)}c^{ijkl}_{abcd} =$$  $$=$$  $$= P^{(ij/kl)}_{(ab/cd)} \frac{\overline{g}^{ij}_{ab}\,\overline{g}^{kl}_{cd}}{\mathcal{E}^{ijkl}_{abcd}\mathcal{E}^{ij}_{ab}}$$

The corresponding operators are

$${}^{(1)}C_2 =$$  $$= \frac{1}{2^2}\sum_{\substack{ab\\ij}} \frac{\overline{g}^{ij}_{ab}}{\mathcal{E}^{ij}_{ab}} \tilde{a}^{ab}_{ij}$$

$${}^{(2)}C_4 = =$$  $$= \frac{1}{2^4}\sum_{\substack{abcd\\ijkl}} \frac{\overline{g}^{ij}_{ab}\,\overline{g}^{kl}_{cd}}{\mathcal{E}^{ijkl}_{abcd}\mathcal{E}^{ij}_{ab}} \tilde{a}^{abcd}_{ijkl}$$

and by duplicating and reindexing the quadruples operator we get the following.

$$
\begin{aligned}
{}^{(2)}C_4 = \frac{1}{2^4}\sum_{\substack{abcd\\ijkl}} \frac{\overline{g}^{ij}_{ab}\,\overline{g}^{kl}_{cd}}{\mathcal{E}^{ijkl}_{abcd}\mathcal{E}^{ij}_{ab}} \tilde{a}^{abcd}_{ijkl} &= \frac{1}{2}\left(\frac{1}{2^4}\sum_{\substack{abcd\\ijkl}} \frac{\overline{g}^{ij}_{ab}\,\overline{g}^{kl}_{cd}}{\mathcal{E}^{ijkl}_{abcd}\mathcal{E}^{ij}_{ab}} \tilde{a}^{abcd}_{ijkl} + \frac{1}{2^4}\sum_{\substack{cdab\\klij}} \frac{\overline{g}^{kl}_{cd}\,\overline{g}^{ij}_{ab}}{\mathcal{E}^{klij}_{cdab}\mathcal{E}^{kl}_{cd}} \tilde{a}^{cdab}_{klij} \right) \\
&= \frac{1}{2}\cdot\frac{1}{2^4}\sum_{\substack{abcd\\ijkl}} \frac{\overline{g}^{ij}_{ab}\,\overline{g}^{kl}_{cd}\cancel{(\mathcal{E}^{kl}_{cd}+\mathcal{E}^{ij}_{ab})}}{\cancel{\mathcal{E}^{ijkl}_{abcd}}\mathcal{E}^{ij}_{ab}\mathcal{E}^{kl}_{cd}} \tilde{a}^{abcd}_{ijkl} \\
&= \frac{1}{2}\left(\frac{1}{2^4}\sum_{\substack{ab\\ij}} \frac{\overline{g}^{ij}_{ab}}{\mathcal{E}^{ij}_{ab}} \tilde{a}^{ab}_{ij} \right)\left(\frac{1}{2^4}\sum_{\substack{cd\\kl}} \frac{\overline{g}^{kl}_{cd}}{\mathcal{E}^{kl}_{cd}} \tilde{a}^{cd}_{kl} \right) \\
&= \frac{1}{2}\,{}^{(1)}C_2^2
\end{aligned}
$$