

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

$$\Psi(\lambda) = \Phi + R_0(\lambda V_c - E(\lambda))\Psi(\lambda) \quad (1)$$

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

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

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

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

²You may take $E_c^{(m+1)} = \langle \Phi | V_c | \Psi^{(m)} \rangle$ as given.

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

$${}^{(1)}c_{ab}^{ij} = \langle \Phi_{ij}^{ab} | R_0 V_c | \Phi \rangle \qquad {}^{(2)}c_{abcd}^{ijkl} = \langle \Phi_{ijkl}^{abcd} | R_0 V_c R_0 V_c | \Phi \rangle \qquad (2)$$

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