1. Perturbation theory and the linked diagram theorem

Definition 1.1. ***Model problem.*** In perturbation theory, the *model Hamiltonian* is an operator $H_0 \approx H_e$ which approximates the full Hamiltonian and has eigenfunctions spanning the complete n-particle Fock space. An obvious choice in electronic structure is the diagonal one-particle component of H_e, which is diagonal in the determinant basis.

$$H_0 \Phi_{i_1\cdots i_k}^{a_1\cdots a_k} = \mathcal{E}_{i_1\cdots i_k}^{a_1\cdots a_k} \Phi_{i_1\cdots i_k}^{a_1\cdots a_k} \qquad H_c = H_0 + V_c \qquad H_0 \equiv f_p^p \tilde{a}_p^p \qquad \mathcal{E}_{i_1\cdots i_k}^{a_1\cdots a_k} \equiv \left(f_{a_1}^{a_1} + \cdots + f_{a_k}^{a_k} - f_{i_1}^{i_1} - \cdots - f_{i_k}^{i_k}\right)$$

where the perurbation is $V_c \equiv f_p^q (1-\delta_p^q)\tilde{a}_q^p + \frac{1}{4}\overline{g}_{pq}^{rs}\tilde{a}_{rs}^{pq}$. In this context, the reference determinant Φ is termed the *model function*. Note that we are playing fast and loose with Einstein summation here: the i and a indices are not summed over, but the p index in H_0 is. The eigenvalue can be determined by noting that $a_p^p \Phi_k = n_p^k \Phi_k$ where n_p^k is the occupation number of ψ_p in Φ_k. Therefore $\tilde{a}_p^p = a_p^p - \tilde{a}_{p^\circ}^{p^\circ} = a_p^p - n_p$ which implies that $\tilde{a}_p^p \Phi_k = (n_p^k - n_p)\Phi_k$. It then follows that $\sum_p f_p^p \tilde{a}_p^p \Phi_k = (\sum_{p\in\Phi_k} f_p^p - \sum_{p\in\Phi} f_p^p)\Phi_k$, which leads to the expression above for $\mathcal{E}_{i_1\cdots i_k}^{a_1\cdots a_k}$.

Definition 1.2. ***Model space projection operators.*** The projection $P = |\Phi\rangle\langle\Phi|$ onto the model function is termed the *model space projection operator*, and its orthogonal complement $Q = 1 - P = \sum_k (\frac{1}{k!})^2 \sum_{\substack{a_1\cdots a_k \\ i_1\cdots i_k}} |\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}\rangle\langle\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}|$ is the *orthogonal space projection operator*. Note that $P^2 = Q^2 = 1$ and $PQ = QP = 0$ are necessary consequences of the fact that P and Q are projection operators for orthogonal subspaces, and note that $P + Q = 1$. Assuming *intermediate normalization*, where we normalize the wavefunction to satisfy $\langle\Phi|\Psi\rangle = 1$ rather than $\langle\Psi|\Psi\rangle = 1$, the model space projection operator takes the wavefunction into our model function, $P\Psi = \Phi\langle\Phi|\Psi\rangle = \Phi$.

Definition 1.3. ***Resolvent.*** Let R_0 be minus[1] the inverse of H_0 in the orthogonal space, so that $-R_0 H_0 = Q$. The operator R_0 is termed the *resolvent*. Explicitly, we can apply resolution of the identity in the orthogonal space to get

$$R_0 = (-H_0)^{-1} Q = \sum_k \left(\tfrac{1}{k!}\right)^2 \sum_{\substack{a_1\cdots a_k \\ i_1\cdots i_k}} (-H_0)^{-1} |\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}\rangle\langle\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}| = \sum_k \left(\tfrac{1}{k!}\right)^2 \sum_{\substack{a_1\cdots a_k \\ i_1\cdots i_k}} \frac{|\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}\rangle\langle\Phi_{i_1\cdots i_k}^{a_1\cdots a_k}|}{\mathcal{D}_{i_1\cdots i_k}^{a_1\cdots a_k}} \qquad \mathcal{D}_{i_1\cdots i_k}^{a_1\cdots a_k} \equiv -\mathcal{E}_{i_1\cdots i_k}^{a_1\cdots a_k}$$

where we recognize that H_0^{-1} does not exist outside of the model space because $H_0\Phi = 0 \implies H_0 P = 0$. Note that R_0 simply acts as the null operator outside of the orthogonal space, so that $R_0 Q = R_0$ and $R_0 P = 0$.

Definition 1.4. ***Rayleigh-Schrödinger perturbation theory.*** Projecting the Schrödinger equation by R_0, recognizing that $R_0 H_0 = -Q \implies R_0 H_0 \Psi = -Q\Psi = (P-1)\Psi = \Phi - \Psi$, we obtain the following recursive equation for Ψ.

$$R_0(H_0 + V_c)\Psi = \Phi - \Psi + R_0 V_c \Psi = E_c R_0 \Psi \implies \Psi = \Phi + R_0(V_c - E_c)\Psi$$

Straightforward induction leads to $\Psi = \sum_{k=0}^n (R_0(V_c - E_c))^k \Phi + (R_0(V_c - E_c))^{n+1}\Psi$. Noting that $H_0\Phi = 0$ and $\langle\Phi|\Psi\rangle = 1$, projecting the Schrödinger equation by Φ gives an expression for the correlation energy: $E_c = \langle\Phi|V_c|\Psi\rangle$. Assuming the series converges, this leads to the following expressions for the wavefunction and the correlation energy.

$$\Psi = \sum_{k=0}^{\infty} (R_0(V_c - E_c))^k \Phi \qquad\qquad E_c = \sum_{k=0}^{\infty} \langle\Phi|V_c(R_0(V_c - E_c))^k|\Phi\rangle \tag{1.1}$$

Introducing a perturbation parameter $V_c \mapsto \lambda V_c$ and expanding the wavefunction and energy in a Taylor series

$$\Psi(\lambda) = \sum_k \frac{1}{k!}\lambda^k \left(\frac{\partial^k \Psi}{\partial \lambda^k}\right)_{\lambda=0} \equiv \sum_k \lambda^k \Psi^{(k)} \qquad\qquad E_c(\lambda) = \sum_k \frac{1}{k!}\lambda^k \left(\frac{\partial^k E_c}{\partial \lambda^k}\right)_{\lambda=0} \equiv \sum_k \lambda^k E_c^{(k)}$$

allows us to separate eq (1.1) in orders of λ. The first-order energy contribution vanishes $\lambda E_c^{(1)} = \lambda\langle\Phi|V_c|\Phi\rangle = 0$ since V_c is composed of Φ-normal operators. The first order wavefunction contribution is $\lambda\Psi^{(1)} = \lambda R_0(V_c - E_c^{(1)})\Phi = \lambda R_0 V_c \Phi$,

[1] The annoying sign factor is required for consistency with the standard definition $R_0 \equiv (E_0 - H_0)^{-1} Q$. Since we have already subtracted off E_0, we have $R_0 = (-H_0)^{-1} Q$. This also results in a more convenient sign rule for the bracketing theorem.

which can be directly evaluated using Wick's theorem and Φ normal ordering

$$\begin{aligned}
\Psi^{(1)} = R_0 V_c \Phi &= \sum_k \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1\cdots a_k \\ i_1\cdots i_k}} |\Phi^{a_1\cdots a_k}_{i_1\cdots i_k}\rangle \frac{\langle\Phi|\tilde{a}^{i_1\cdots i_k}_{a_1\cdots a_k} V_c|\Phi\rangle}{\mathcal{D}^{a_1\cdots a_k}_{i_1\cdots i_k}} \\
&= \sum_{ia} |\Phi^a_i\rangle \frac{\sum_{pq} f^q_p (1-\delta^q_p)\langle\Phi|\vdots\tilde{a}^{i^\circ}_{a^\bullet}\tilde{a}^{p^\bullet}_{q^\circ}\vdots|\Phi\rangle}{f^i_i - f^a_a} + \frac{1}{4}\sum_{ijab}|\Phi^{ab}_{ij}\rangle \frac{\frac{1}{4}\sum_{pqrs}\overline{g}^{rs}_{pq} P^{(p/q)}_{(r/s)}\langle\Phi|\vdots\tilde{a}^{i^\circ j^{\circ\circ}}_{a^\bullet b^{\bullet\bullet}}\tilde{a}^{p^\bullet q^{\bullet\bullet}}_{r^\circ s^{\circ\circ}}\vdots|\Phi\rangle}{f^i_i + f^j_j - f^a_a - f^b_b} \\
&= \sum_{ia} |\Phi^a_i\rangle \frac{f^i_a}{f^i_i - f^a_a} + \frac{1}{4}\sum_{ijab}|\Phi^{ab}_{ij}\rangle \frac{\overline{g}^{ij}_{ab}}{f^i_i + f^j_j - f^a_a - f^b_b}
\end{aligned}$$

where we have recognized that only singly and doubly excited determinants can fully contract V_c. The second-order energy contribution, $\lambda^2 E^{(2)}_c = \lambda^2\langle\Phi|V_c|\Psi^{(1)}\rangle$, can be evaluated from our expression for $\Psi^{(1)}$.

$$E^{(2)} = \sum_{ia}\langle\Phi|V_c\tilde{a}^a_i|\Phi\rangle\frac{f^i_a}{f^i_i - f^a_a} + \frac{1}{4}\sum_{ijab}\langle\Phi|V_c\tilde{a}^{ab}_{ij}|\Phi\rangle\frac{\overline{g}^{ij}_{ab}}{f^i_i + f^j_j - f^a_a - f^b_b} = \sum_{ia}\frac{f^a_i f^i_a}{f^i_i - f^a_a} + \frac{1}{4}\sum_{ijab}\frac{\overline{g}^{ab}_{ij}\overline{g}^{ij}_{ab}}{f^i_i + f^j_j - f^a_a - f^b_b}$$

The one-particle contributions involving f^a_i are present only for ROHF references, since $f^a_i = 0$ for canonical Hartree-Fock orbitals. The second order wavefunction contribution is $\lambda^2\Psi^{(2)} = -\lambda^2 E^{(2)}_c R_0\Phi + \lambda^2 R_0(V_c - E^{(1)}_c)R_0(V_c - E^{(1)}_c)\Phi = \lambda^2 R_0 V_c R_0 V_c \Phi$ since $R_0\Phi = 0$ and $E^{(1)}_c = 0$. The third order energy can be then obtained from $\Psi^{(2)}$ as $\lambda^3 E^{(3)}_c = \lambda^3\langle\Phi|V_c|\Psi^{(2)}\rangle$. In this manner, one can (in principle) solve the Schrödinger equation recursively by alternately evaluating the wavefunction and energy contributions at increasing orders in the perturbation parameter.

Derivation 1.1. Writing the RSPT wavefunction equation as $\Psi = \sum_{k=0}^{\infty}(R_0V_c - R_0E_c)^k\Phi$, note that, if R_0 and V_c were to commute, we could apply the binomial theorem to write the right-hand side as $\sum_{p=0}^{k}\binom{k}{p}(-)^p(R_0V_c)^{k-p}(R_0E_c)^p$. Since they don't commute, we have to follow for the following generalization of the binomial expansion

$$(R_0E_c - R_0V_c)^k = \sum_{p=0}^{k}(-)^p\{R_0E_c\}^p\text{insert}\{R_0V_c\}^{k-p}$$

where $\{B_1,\ldots,B_p\}\text{insert}\{A\}^{k-p}$ denotes the sum over all $\binom{k}{p}$ possible ways of inserting $k-p$ copies of A into the product $B_1\cdots B_p$. For example, $\{B_1,B_2\}\text{insert}\{A\}^2$ evaluates to $AAB_1B_2 + AB_1AB_2 + AB_1B_2A + B_1AAB_2 + B_1AB_2A + B_1B_2AA$. This allows the wavefunction expansion to be easily grouped by orders

$$\begin{aligned}
\Psi &= \sum_{k=0}^{\infty}\sum_{p=0}^{k}(-)^p\{R_0E_c\}^p\text{insert}\{R_0V_c\}^{k-p}\Phi \\
&= \sum_{n=0}^{\infty}\sum_{(n_1,n_2)}^{\mathcal{C}_2(n)\cup\{(0,n)\}}\sum_{(r_1,\ldots,r_m)}^{\mathcal{C}(n_1)}(-)^m\{R_0E^{(r_1)}_c,\ldots,R_0E^{(r_m)}_c\}\text{insert}\{R_0V_c\}^{n_2}\Phi = \sum_{n=0}^{\infty}\Psi^{(n)}
\end{aligned}$$

where $\mathcal{C}(n)$ denotes the set of integer compositions of n, i.e. all ordered tuples $(r_1,\ldots,r_m)$ of strictly positive integers that add up to n. $\mathcal{C}_k(n) \subset \mathcal{C}(n)$ is the set of k-tuple integer compositions of n, i.e. all $(r_1,\ldots,r_k)$ of fixed length k such that $r_1 + \cdots + r_k = n$. The rearrangement follows from the fact that all possible terms of the form $(-)^k\{R_0E^{(n_1)}_c,\ldots,R_0E^{(n_k)}_c\}\text{insert}\{R_0V_c\}^{n_{k+1}}\Phi$ contribute to the sum, and the composition sums group these into all possible terms of this form that are of a given order n in the perturbation parameter λ. Note that we have appended the tuple $(0,n)$ to our sum over $\mathcal{C}_2(n)$ but not $(n,0)$ since R_0 acting directly on Φ gives 0. These results are summarized in lem 1.1.

Lemma 1.1. ***The Energy Substitution Lemma.*** *The nth-order contribution to the wavefunction is given by*

$$\Psi^{(n)} = (R_0V_c)^n\Phi + \sum_{(n_1,n_2)}^{\mathcal{C}_2(n)}\sum_{(r_1,\ldots,r_m)}^{\mathcal{C}(n_1)}(-)^m\{R_0E^{(r_1)}_c,\ldots,R_0E^{(r_m)}_c\}\text{insert}\{R_0V_c\}^{n_2}\Phi$$

which can be evaluated as the sum of a principal term, $(R_0V_c)^n\Phi$, *plus all possible m-tuple substitutions of adjacent factors $(R_0V_c)^{r_k}$ in the principal term by $R_0E^{(r_k)}_c$ times a sign factor $(-)^m$.*

Example 1.1. Using the energy substitution lemma, we can directly write down the first few wavefunction contributions

$$\begin{aligned}
\Psi^{(1)} &= R_0 V_c \Phi \\
\Psi^{(2)} &= R_0 V_c R_0 V_c \Phi - R_0 E_c^{(1)} R_0 V_c \Phi - R_0 V_c R_0 E_c^{(1)} \Phi \\
\Psi^{(3)} &= R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 E_c^{(2)} R_0 V_c \Phi - R_0 V_c R_0 E_c^{(2)} \Phi + R_0 E_c^{(1)} R_0 E_c^{(1)} R_0 V_c \Phi + R_0 E_c^{(1)} R_0 V_c R_0 E_c^{(1)} \Phi \\
&\quad + R_0 V_c R_0 E_c^{(1)} R_0 E_c^{(1)} \Phi - R_0 E_c^{(1)} R_0 V_c R_0 V_c \Phi - R_0 V_c R_0 E_c^{(1)} R_0 V_c \Phi - R_0 V_c R_0 V_c R_0 E_c^{(1)} \Phi
\end{aligned}$$

where we have directly evaluated the formula of lem 1.1 without simplifying. These expressions can be simplified by recognizing that $E_c^{(1)} = 0$ and that any term with an energy factor next to Φ vanishes since $R_0 \Phi = 0$. Omitting these terms, the wavefunction contributions can be simplified as follows.

$$\begin{aligned}
\Psi^{(1)} &= R_0 V_c \Phi \\
\Psi^{(2)} &= R_0 V_c R_0 V_c \Phi \\
\Psi^{(3)} &= R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 E_c^{(2)} R_0 V_c \Phi \\
\Psi^{(4)} &= R_0 V_c R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 E_c^{(3)} R_0 V_c \Phi - R_0 E_c^{(2)} R_0 V_c R_0 V_c \Phi - R_0 V_c R_0 E_c^{(2)} R_0 V_c \Phi \\
\Psi^{(5)} &= R_0 V_c R_0 V_c R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 E_c^{(4)} R_0 V_c \Phi + R_0 E_c^{(2)} R_0 E_c^{(2)} R_0 V_c \Phi - R_0 E_c^{(3)} R_0 V_c R_0 V_c \Phi \\
&\quad - R_0 V_c R_0 E_c^{(3)} R_0 V_c \Phi - R_0 E_c^{(2)} R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 V_c R_0 E_c^{(2)} R_0 V_c R_0 V_c \Phi - R_0 V_c R_0 V_c R_0 E_c^{(2)} R_0 V_c \Phi
\end{aligned}$$

Projecting these equations by $\langle \Phi | V_c$ then yields $E_c^{(2)}$, $E_c^{(3)}$, $E_c^{(4)}$, $E_c^{(5)}$, and $E_c^{(6)}$.

Theorem 1.1. ***The Bracketing Theorem.*** *The nth-order contribution to the wavefunction consists of a principal term $(R_0 V_c)^n \Phi = R_0 V_c \cdots R_0 V_c \Phi$ plus the sum over all possible ways of inserting one or more pairs of brackets $\langle \cdots \rangle \equiv \langle \Phi | \cdots | \Phi \rangle$ into the principal term, $R_0 V_c \cdots R_0 \langle V_c \cdots R_0 V_c \rangle \cdots R_0 V_c \Phi$, allowing nested brackets. Each of these terms gets a phase factor $(-)^k$ where k is the total number of brackets.*

Proof: This obviously holds for $\Psi^{(1)}$ since $\Psi^{(1)} = R_0 V_c \Phi$ and there are no possible bracketings. Assume it holds up to $n-1$ and consider n. By the substitution lemma, $\Psi^{(n)}$ equals a principal term $R_0 V_c \cdots R_0 V_c \Phi$ plus all unique substitutions of factors $(R_0 V_c)^{r_1}, \ldots, (R_0 V_c)^{r_m}$ in the principal term with energy factors $R_0 E_c^{(r_1)}, \ldots, R_0 E_c^{(r_m)}$, weighted by a sign $(-)^m$. But, by our inductive assumption, the substituted energies $E_c^{(r_k)} = \langle \Phi | V_c | \Psi^{(r_k)} \rangle$ are sums of a principal term $\langle V_c R_0 V_c \cdots R_0 V_c \rangle$ plus all possible bracketings, with the appropriate sign factor, which shows that $\Psi^{(n)}$ is the sum over all nested bracketings and completes the proof.

Example 1.2. Noting that bracketings of the form $R_0 \langle V_c \rangle$ vanish because $\langle V \rangle_c = E_c^{(1)} = 0$, and that any bracketing including the last factor vanishes because $R_0 \langle V_c \cdots R_0 V_c \rangle \Phi = \langle V_c \cdots R_0 V_c \rangle R_0 \Phi = 0$, we can write down the bracketing theorem expansion for the first few contributions to the wavefunction as follows.

$$\begin{aligned}
\Psi^{(1)} &= R_0 V_c \Phi \\
\Psi^{(2)} &= R_0 V_c R_0 V_c \Phi \\
\Psi^{(3)} &= R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 \langle V_c R_0 V_c \rangle R_0 V_c \Phi \\
\Psi^{(4)} &= R_0 V_c R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 \langle V_c R_0 V_c \rangle R_0 V_c R_0 V_c \Phi - R_0 V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \Phi - R_0 \langle V_c R_0 V_c R_0 V_c \rangle R_0 V_c \Phi \\
\Psi^{(5)} &= R_0 V_c R_0 V_c R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 \langle V_c R_0 V_c \rangle R_0 V_c R_0 V_c R_0 V_c \Phi - R_0 V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c R_0 V_c \Phi \\
&\quad - R_0 V_c R_0 V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \Phi + R_0 \langle V_c R_0 V_c \rangle R_0 \langle V_c R_0 V_c \rangle R_0 V_c \Phi - R_0 \langle V_c R_0 V_c R_0 V_c \rangle R_0 V_c R_0 V_c \Phi \\
&\quad - R_0 V_c R_0 \langle V_c R_0 V_c R_0 V_c \rangle R_0 V_c \Phi - R_0 \langle V_c R_0 V_c R_0 V_c R_0 V_c \rangle R_0 V_c \Phi + R_0 \langle V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \rangle R_0 V_c \Phi
\end{aligned}$$

The bracketing expansions for the corresponding energies are as follows.

$$\begin{aligned}
E_c^{(2)} &= \langle V_c R_0 V_c \rangle \\
E_c^{(3)} &= \langle V_c R_0 V_c R_0 V_c \rangle \\
E_c^{(3)} &= \langle V_c R_0 V_c R_0 V_c R_0 V_c \rangle - \langle V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \rangle \\
E_c^{(4)} &= \langle V_c R_0 V_c R_0 V_c R_0 V_c R_0 V_c \rangle - \langle V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c R_0 V_c \rangle - \langle V_c R_0 V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \rangle - \langle V_c R_0 \langle V_c R_0 V_c R_0 V_c \rangle R_0 V_c \rangle \\
E_c^{(5)} &= \langle V_c R_0 V_c R_0 V_c R_0 V_c R_0 V_c R_0 V_c \rangle - \langle V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c R_0 V_c R_0 V_c \rangle - \langle V_c R_0 V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c R_0 V_c \rangle \\
&\quad - \langle V_c R_0 V_c R_0 V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \rangle + \langle V_c R_0 \langle V_c R_0 V_c \rangle R_0 \langle V_c R_0 V_c \rangle R_0 V_c \rangle - \langle V_c R_0 \langle V_c R_0 V_c R_0 V_c \rangle R_0 V_c R_0 V_c \rangle \\
&\quad - \langle V_c R_0 V_c R_0 \langle V_c R_0 V_c R_0 V_c \rangle R_0 V_c \rangle - \langle V_c R_0 \langle V_c R_0 V_c R_0 V_c R_0 V_c \rangle R_0 V_c \rangle + \langle V_c R_0 \langle V_c R_0 \langle V_c R_0 V_c \rangle R_0 V_c \rangle R_0 V_c \rangle
\end{aligned}$$

Remark 1.1. Individual terms in the perturbation expansion are readily evaluated using Wick's theorem and Φ-normal ordering. Using resolution of the identity in the orthogonal space, the general structure of a principal term is as follows.

$$(R_0V_c)^n|\Phi\rangle = Q(R_0V_c)^n|\Phi\rangle = \sum_k |\Phi_k\rangle\langle\Phi_k|(R_0V_c)^n|\Phi\rangle = \sum_k |\Phi_k\rangle \sum_{k_1\cdots k_n} \frac{\langle\Phi_k|V_c|\Phi_{k_1}\rangle\langle\Phi_{k_1}|V_c|\Phi_{k_2}\rangle\langle\Phi_{k_2}|\cdots|\Phi_{k_n}\rangle\langle\Phi_{k_n}|V_c|\Phi\rangle}{\mathcal{D}_{k_1}\mathcal{D}_{k_2}\cdots\mathcal{D}_{k_n}}$$

Terms with bracketing insertions differ from the principal term by a scalar $\langle\cdots\rangle$ which can be factored out, leaving a squared resolvent at the point of insertion. By orthonormality of the determinant basis, the squared resolvent equals

$$R_0^2 = \sum_{k_1k_2} \frac{|\Phi_{k_1}\rangle\langle\Phi_{k_1}|\Phi_{k_2}\rangle\langle\Phi_{k_2}|}{\mathcal{D}_{k_1}\mathcal{D}_{k_2}} = \sum_{k_1k_2} \frac{|\Phi_{k_1}\rangle\delta_{k_1k_2}\langle\Phi_{k_2}|}{\mathcal{D}_{k_1}\mathcal{D}_{k_2}} = \sum_k \frac{|\Phi_k\rangle\langle\Phi_k|}{\mathcal{D}_k^2}$$

which is of course equal to $(H_0^2)^{-1}$ restricted to the orthogonal space, $R_0^2H_0^2 = Q$. Consequently, every wavefunction contribution is proportional to a term of the following generic form

$$R_0^{p_1}V_cR_0^{p_2}V_c\cdots R_0^{p_n}V_c|\Phi\rangle = \sum_k |\Phi_k\rangle\langle\Phi|\tilde{a}_k^\dagger R_0^{p_1}V_cR_0^{p_2}V_c\cdots R_0^{p_n}V_c|\Phi\rangle \qquad R_0^p = \sum_k \frac{|\Phi_k\rangle\langle\Phi_k|}{\mathcal{D}_k^p}$$

which can be evaluated by determining all complete Φ-normal contractions of $\tilde{a}_k^\dagger R_0^{p_1}V_cR_0^{p_2}V_c\cdots R_0^{p_n}V_c$, where $\tilde{a}_k^\dagger$ is a de-excitation operator $\tilde{a}_k^\dagger \in \{\tilde{a}_{a_1\cdots a_n}^{i_1\cdots i_n} \mid {}^{i_1<\cdots<i_n,}_{a_1<\cdots<a_n}\}$.

Remark 1.2. Note that, when an operator of the form $M_\mathrm{o} = \sum_i a_i|\Phi\rangle m_i\langle\Phi|a^i$ or $M_\mathrm{v} = \sum_a a^a|\Phi\rangle m_a\langle\Phi|a_a$ is contracted on the left and on the right, we can make the following rearrangement

$$\sum_i \overbracket{a^p a_i}|\Phi\rangle m_i\langle\Phi|\overbracket{a^i a_s} = |\Phi\rangle\langle\Phi|m_p\,\overbracket{a^p a_s} \qquad \sum_a \overbracket{a_q a^a}|\Phi\rangle m_a\langle\Phi|\overbracket{a_a a^r} = |\Phi\rangle\langle\Phi|m_q\,\overbracket{a_q a^r}$$

where the requirement that m_p have a hole index and m_q have a particle index is taken care of by the contractions. In words, contracting one operator to the left side of M_o and another operator to the right side is equivalent to contracting these operators to each other and freezing out the term from M_o that matches the left (or, equivalently, the right) index. This generalizes directly to operators of the form $\sum_{\substack{i_1<\cdots<i_k\\a_1<\cdots<a_k}} \tilde{a}_{i_1\cdots i_k}^{a_1\cdots a_k}|\Phi\rangle M_{i_1\cdots i_k}^{a_1\cdots a_k}\langle\Phi|\tilde{a}_{a_1\cdots a_k}^{i_1\cdots i_k}$ and can be used to simplify the contractions of an operator product with an intervening resolvent, QR_0^nQ':

$$\vdots\overline{\overline{QR_0^nQ'}}\vdots = \sum_k \frac{\vdots\overline{\overline{Q\tilde{a}_k}}\vdots|\Phi\rangle\langle\Phi|\vdots\overline{\overline{\tilde{a}_k^\dagger Q'}}\vdots}{\mathcal{D}_k^n} = |\Phi\rangle\langle\Phi|\sum_k \frac{\vdots\overline{\overline{Q\tilde{a}_k}}\vdots\vdots\overline{\overline{\tilde{a}_k^\dagger Q'}}\vdots}{\mathcal{D}_k^n} = |\Phi\rangle\langle\Phi|\vdots\overline{\overline{Q\overset{R_0^n}{\vdots}Q'}}\vdots\,.$$

Here, we have introduced the notion of a *resolvent line* $\overset{R_0^n}{\vdots}$. Complete contractions through a resolvent line are defined as

$$\vdots\overbracket{a^{p_1}\cdots\overbracket{a^{p_k}\overbracket{a_{q_1}\cdots\overbracket{a_{q_k}\overset{R_0^n}{\vdots}a^{r_1}}\cdots a^{r_k}}a_{s_1}}\cdots a_{s_k}}\vdots \equiv \frac{\vdots\overbracket{a^{p_1}\cdots\overbracket{a^{p_k}\overbracket{a_{q_1}\cdots\overbracket{a_{q_k}a^{r_1}}\cdots a^{r_k}}a_{s_1}}\cdots a_{s_k}}\vdots}{(\mathcal{D}_{p_1\cdots p_k}^{q_1\cdots q_k})^n}\,.$$

That is, each hole contraction $\overbracket{a^p a_s}$ that passes through the resolvent line fixes a hole index in the denominator $(\mathcal{D}_{\cdots p\cdots})^n$, and each particle contraction $\overbracket{a_q a^r}$ fixes a particle index $(\mathcal{D}^{\cdots q\cdots})^n$. This result further generalizes to completely contracted products with multiple resolvents, and is codified in the next proposition.

Proposition 1.1. ***Reduced Wick theorem for RSPT.*** *For Φ-normal excitation operators Q, Q_1, $\cdots$, Q_n, we have*

$$\langle\Phi|QR_0^{p_1}Q_1R_0^{p_2}Q_2\cdots R_0^{p_n}Q_n|\Phi\rangle = \vdots\overline{\overline{Q\overset{R_0^{p_1}}{\vdots}Q_1\overset{R_0^{p_2}}{\vdots}Q_2\cdots\overset{R_0^{p_n}}{\vdots}Q_n}}\vdots\,.$$

That is, inserting a resolvent between the operators in $\langle\Phi|QQ_1\cdots Q_n|\Phi\rangle$ scales the weight of each contraction in the Wick expansion $\vdots\overline{\overline{QQ_1\cdots Q_n}}\vdots$ by a denominator factor $\mathcal{D}_{p_1\cdots p_k}^{q_1\cdots q_k}$ where $q_1,\ldots,q_k$ label the particle contractions and $p_1,\ldots,p_k$ label the hole contractions passing over the point of insertion.

Example 1.3. The reduced Wick theorem of prop 1.1 can be used to evaluate the following

$$\vdots\overline{\overline{\tilde{a}_{r_1s_1}^{p_1q_1}\overset{R_0}{\vdots}\tilde{a}_{r_2s_2}^{p_2q_2}}}\vdots = P_{(r_2/s_2)}^{(p_2/q_2)}\vdots\tilde{a}_{r_1^\bullet s_1^{\bullet\bullet}}^{p_1^\circ q_1^{\circ\circ}}\overset{R_0}{\vdots}\tilde{a}_{r_2^\circ s_2^{\circ\circ}}^{p_2^\bullet q_2^{\bullet\bullet}}\vdots$$

$$\vdots\overline{\overline{\tilde{a}_{r_1s_1}^{p_1q_1}\overset{R_0}{\vdots}\tilde{a}_{r_2s_2}^{p_2q_2}\overset{R_0}{\vdots}\tilde{a}_{r_3s_3}^{p_3q_3}}}\vdots = P_{(r_1/s_1|r_3/s_3)}^{(p_1/q_1|p_3/q_3)}\vdots\tilde{a}_{r_1^\bullet s_1^{\circ 2}}^{p_1^\circ q_1^{\circ 2}}\overset{R_0}{\vdots}\tilde{a}_{r_2^{\bullet 3}s_2^{\bullet 4}}^{p_2^{\bullet 1}q_2^{\bullet 2}}\overset{R_0}{\vdots}\tilde{a}_{r_3^{\circ 1}s_3^{\circ 2}}^{p_3^{\bullet 3}q_3^{\bullet 4}}\vdots + P_{(r_1/s_1|r_2/s_2|r_3/s_3)}^{(p_1/q_1|p_2/q_2|p_3/q_3)}\vdots\tilde{a}_{r_1^{\bullet 3}s_1^{\bullet 1}}^{p_1^{\circ 3}q_1^{\circ 1}}\overset{R_0}{\vdots}\tilde{a}_{r_2^{\circ 1}s_2^{\bullet 2}}^{p_2^{\bullet 1}q_2^{\circ 2}}\overset{R_0}{\vdots}\tilde{a}_{r_3^{\circ 2}s_3^{\circ 3}}^{p_3^{\bullet 2}q_3^{\bullet 3}}\vdots$$

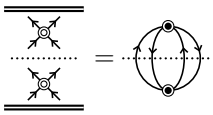
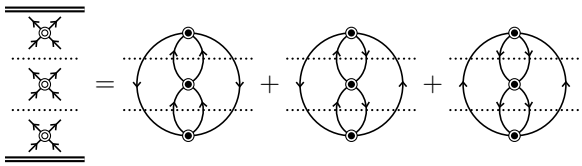
$$+ P_{(r_1/s_1|r_3/s_3)}^{(p_1/q_1|p_3/q_3)}\vdots\tilde{a}_{r_1^{\bullet 1}s_1^{\bullet 2}}^{p_1^{\circ 3}q_1^{\circ 4}}\overset{R_0}{\vdots}\tilde{a}_{r_2^{\circ 3}s_2^{\circ 4}}^{p_2^{\circ 1}q_2^{\circ 2}}\overset{R_0}{\vdots}\tilde{a}_{r_3^{\circ 1}s_3^{\circ 2}}^{p_3^{\bullet 1}q_3^{\bullet 2}}\vdots$$

in order to derive the second- and third-order energy contributions

$$E_c^{(2)} = \langle V_c R_0 V_c \rangle = \vdots \overline{\overline{V_c \overset{R_0}{\vdots} V_c}} \vdots = \left(\tfrac{1}{4}\right)^2 \overline{g}^{r_1 s_1}_{p_1 q_1} \overline{g}^{r_2 s_2}_{p_2 q_2} \vdots \overline{\overline{\tilde{a}^{p_1 q_1}_{r_1 s_1} \overset{R_0}{\vdots} \tilde{a}^{p_2 q_2}_{r_2 s_2}}} \vdots = \frac{1}{4} \frac{\overline{g}^{ab}_{ij} \overline{g}^{ij}_{ab}}{\mathcal{D}^{ab}_{ij}}$$

$$E_c^{(3)} = \langle V_c R_0 V_c R_0 V_c \rangle = \vdots \overline{\overline{V_c \overset{R_0}{\vdots} V_c \overset{R_0}{\vdots} V_c}} \vdots = \left(\tfrac{1}{4}\right)^3 \overline{g}^{r_1 s_1}_{p_1 q_1} \overline{g}^{r_2 s_2}_{p_2 q_2} \overline{g}^{r_3 s_3}_{p_3 q_3} \vdots \overline{\overline{\tilde{a}^{p_1 q_1}_{r_1 s_1} \overset{R_0}{\vdots} \tilde{a}^{p_2 q_2}_{r_2 s_2} \overset{R_0}{\vdots} \tilde{a}^{p_3 q_3}_{r_3 s_3}}} \vdots = \frac{1}{4} \frac{\overline{g}^{ab}_{ij} \overline{g}^{cd}_{ab} \overline{g}^{ij}_{cd}}{\mathcal{D}^{ab}_{ij} \mathcal{D}^{cd}_{ij}} + \frac{\overline{g}^{ab}_{ij} \overline{g}^{jc}_{bk} \overline{g}^{ki}_{ca}}{\mathcal{D}^{ab}_{ij} \mathcal{D}^{ca}_{ki}} + \frac{1}{4} \frac{\overline{g}^{ab}_{ij} \overline{g}^{ij}_{kl} \overline{g}^{kl}_{ab}}{\mathcal{D}^{ab}_{ij} \mathcal{D}^{ab}_{kl}}$$

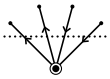
where we have used implicit summation (over all indices) to keep the expressions relatively compact. Here, we have assumed a canonical Hartree-Fock (RHF or UHF) reference so that the one-particle perturbation vanishes $f^q_p(1-\delta^q_p) = 0$ and $V_c = \frac{1}{4}\overline{g}^{rs}_{pq}\tilde{a}^{pq}_{rs}$. Non-canonical Hartree-Fock (such as ROHF) has the same second-order contribution, but introduces two additional terms at third order. In Hugenholtz diagram notation, this looks as follows.

$E_c^{(2)} =$  $E_c^{(3)} =$ 

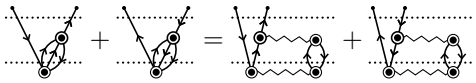
Example 1.4. Contributions to the wavefunction can be separated into singles, doubles, triples, etc. contributions by a resolution of the identity in the orthogonal space

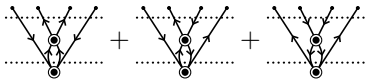
$$\Psi^{(n)} = Q\Psi^{(n)} = \sum_k \left(\tfrac{1}{k!}\right)^2 \sum_{\substack{a_1\cdots a_k \\ i_1\cdots i_k}} \Phi^{a_1\cdots a_k}_{i_1\cdots i_k} \, {}^{(n)}c^{i_1\cdots i_k}_{a_1\cdots a_k} \qquad {}^{(n)}c^{i_1\cdots i_k}_{a_1\cdots a_k} \equiv \langle \Phi | a^{i_1\cdots i_k}_{a_1\cdots a_k} | \Psi^{(n)} \rangle$$

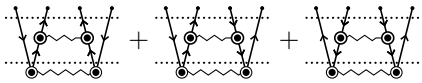
which turns the problem into one of identitfying contributions to the CI coefficients. At first order in the wavefunction, only doubles contributions are non-vanishing.

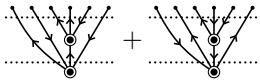
$${}^{(1)}c^i_a = \langle \tilde{a}^i_a R_0 V_c \rangle = \vdots \overline{\overline{\tilde{a}^i_a \overset{R_0}{\vdots} V_c}} \vdots = 0 \qquad {}^{(1)}c^{ij}_{ab} = \langle \tilde{a}^{ij}_{ab} R_0 V_c \rangle = \vdots \overline{\overline{\tilde{a}^{ij}_{ab} \overset{R_0}{\vdots} V_c}} \vdots =$$  $$= \frac{\overline{g}^{ij}_{ab}}{\mathcal{D}^{ab}_{ij}}$$

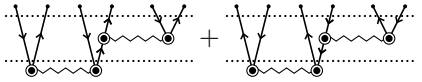
At second order in the wavefunction, singles, triples, and disconnected quadruples are introduced.

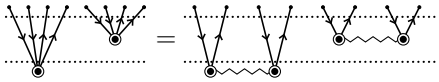
$${}^{(2)}c^i_a = \vdots \overline{\overline{\tilde{a}^i_a \overset{R_0}{\vdots} V_c \overset{R_0}{\vdots} V_c}} \vdots =$$  $$= \frac{1}{2} \frac{\overline{g}^{ef}_{am} \overline{g}^{im}_{ef}}{\mathcal{D}^a_i \mathcal{D}^{ef}_{im}} - \frac{1}{2} \frac{\overline{g}^{ie}_{mn} \overline{g}^{mn}_{ae}}{\mathcal{D}^a_i \mathcal{D}^{ae}_{mn}}$$

$${}^{(2)}c^{ij}_{ab} = \vdots \overline{\overline{\tilde{a}^{ij}_{ab} \overset{R_0}{\vdots} V_c \overset{R_0}{\vdots} V_c}} \vdots =$$ 

$=$  $$= \frac{1}{2} \frac{\overline{g}^{ef}_{ab} \overline{g}^{ij}_{ef}}{\mathcal{D}^{ab}_{ij} \mathcal{D}^{ef}_{ij}} - P^{(i/j)}_{(a/b)} \frac{\overline{g}^{ej}_{am} \overline{g}^{im}_{eb}}{\mathcal{D}^{ab}_{ij} \mathcal{D}^{eb}_{im}} + \frac{1}{2} \frac{\overline{g}^{ij}_{mn} \overline{g}^{mn}_{ab}}{\mathcal{D}^{ab}_{ij} \mathcal{D}^{ab}_{mn}}$$

$${}^{(2)}c^{ijk}_{abc} = \vdots \overline{\overline{\tilde{a}^{ijk}_{abc} \overset{R_0}{\vdots} V_c \overset{R_0}{\vdots} V_c}} \vdots =$$ 

$=$  $$= P^{(ij/k)}_{(a/bc)} \frac{\overline{g}^{ek}_{bc} \overline{g}^{ij}_{ae}}{\mathcal{D}^{abc}_{ijk} \mathcal{D}^{ae}_{ij}} - P^{(i/jk)}_{(ab/c)} \frac{\overline{g}^{jk}_{mc} \overline{g}^{im}_{ab}}{\mathcal{D}^{abc}_{ijk} \mathcal{D}^{ab}_{im}}$$

$${}^{(2)}c^{ijkl}_{abcd} = \vdots \overline{\overline{\tilde{a}^{ijkl}_{abcd} \overset{R_0}{\vdots} V_c \overset{R_0}{\vdots} V_c}} \vdots =$$  $$= P^{(ij/kl)}_{(ab/cd)} \frac{\overline{g}^{kl}_{cd} \overline{g}^{ij}_{ab}}{\mathcal{D}^{abcd}_{ijkl} \mathcal{D}^{ab}_{ij}}$$

Here, the indices m, n, e, f are implicitly summed over, and the Hugenholtz diagrams have been translated into Goldstone diagrams in order to evaluate the phase of each term. The disconnected quadruples term can be factored as follows

$$P^{(ij/kl)}_{(ab/cd)} \frac{\overline{g}^{kl}_{cd} \overline{g}^{ij}_{ab}}{\mathcal{D}^{abcd}_{ijkl} \mathcal{D}^{ab}_{ij}} = \frac{1}{2} P^{(ij/kl)}_{(ab/cd)} \left(\frac{\overline{g}^{kl}_{cd} \overline{g}^{ij}_{ab}}{\mathcal{D}^{abcd}_{ijkl} \mathcal{D}^{ab}_{ij}} + \frac{\overline{g}^{ij}_{ab} \overline{g}^{kl}_{cd}}{\mathcal{D}^{abcd}_{ijkl} \mathcal{D}^{cd}_{kl}} \right) = \frac{1}{2} P^{(ij/kl)}_{(ab/cd)} \left(\frac{\overline{g}^{kl}_{cd} \overline{g}^{ij}_{ab} \left(\mathcal{D}^{cd}_{kl} + \mathcal{D}^{ab}_{ij} \right)}{\mathcal{D}^{abcd}_{ijkl} \mathcal{D}^{ab}_{ij} \mathcal{D}^{cd}_{kl}} \right) = \frac{1}{2} P^{(ij/kl)}_{(ab/cd)} \, {}^{(1)}c^{ij}_{ab} \, {}^{(1)}c^{kl}_{cd}$$

where we have combined fractions and used $\mathcal{D}^{abcd}_{ijkl} = \mathcal{D}^{ab}_{ij} + \mathcal{D}^{cd}_{kl}$. Plugging this result into the CI wave operator, we find that the lowest-order contribution to the quadruple excitation operator is a product of two double excitation operators.

$${}^{(2)}\hat{C}_4 = \left(\tfrac{1}{4!}\right)^2 {}^{(2)}c^{ijkl}_{abcd} \tilde{a}^{abcd}_{ijkl} = \tfrac{1}{2} \left(\tfrac{1}{4!}\right)^2 \left(P^{(ij/kl)}_{(ab/cd)} \, {}^{(1)}c^{ij}_{ab} \, {}^{(1)}c^{kl}_{cd} \right) \tilde{a}^{abcd}_{ijkl} = \tfrac{1}{2} \left(\tfrac{1}{4} \, {}^{(1)}c^{ij}_{ab} \tilde{a}^{ab}_{ij} \right) \left(\tfrac{1}{4} \, {}^{(1)}c^{kl}_{cd} \tilde{a}^{cd}_{kl} \right) = \tfrac{1}{2} \, {}^{(1)}\hat{C}_2^2$$

Definition 1.5. Diagrams with external lines are termed *open*, whereas those with only internal lines are *closed*. A diagram in which there is a path between any two operators is termed *connected*. Otherwise, the diagram is *disconnected* and comprises one or more parts without cross-contractions. A disconnected diagram is considered *linked* if none of its parts is closed. A disconnected diagram with a closed part is *unlinked*.

Definition 1.6. In perturbation theory, there is one more distinction to be made, owing to the presence of resolvent lines. The parts of a disconnected diagram are termed *separate* if they each have their own set of resolvent lines. On the other hand, if some disconnected parts of a diagram share one or more resolvent lines, we consider the parts to make up one *combined* diagram. The unliked diagrams arising from bracketed terms form a subcategory of separated diagrams which are termed *insertion diagrams*. Insertion diagrams have the form

$$\underbrace{\cdots R_0\langle V_c\cdots R_0V_c\rangle R_0V_c\cdots}_{\text{insertion diagram}} = \underbrace{(\cdots R_0R_0V_c\cdots)}_{\textit{remainder diagram}}\ \underbrace{\langle V_c\cdots R_0V_c\rangle}_{\textit{inserted diagram}}$$

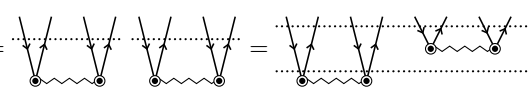
where the *inserted diagram* is closed and the *remainder diagram* may be closed or open, with a squared resolvent at the point of insertion.

Theorem 1.2. ***The Frantz-Mills Factorization Theorem.*** *A diagram with separate parts that are open at the top and closed at the bottom equals the sum over all relative orderings in the corresponding combined diagram.*

Proof: Apart from the resolvent lines, the separate and combined diagrams are identical and share a common numerator, so we need only consider the denominators. Let $\mathcal{D}_1,\ldots,\mathcal{D}_n$ be the denominator factors for one diagram with operators $O_1,\ldots,O_n$, ordered from bottom to top, and let $\mathcal{D}'_1,\ldots,\mathcal{D}'_{n'}$ and $O'_1,\ldots,O'_{n'}$ be the denominators and operators of another diagram. We proceed by induction on $n+n'=m$, starting with $m=2$ as a base case. The only non-trivial possibility for $m=2$ is $n=n'=1$, in which there are two possible orderings for the combined diagram: O_1 above O'_1 or vice versa. Either way the upper resolvent line generates a denominator factor $\mathcal{D}_1+\mathcal{D}'_1$, but in the first case the factor from the lower resolvent is $\mathcal{D}'_1$ and in the second case it is $\mathcal{D}_1$. The sum of the denominators for these two orderings is $\frac{1}{\mathcal{D}_1(\mathcal{D}_1+\mathcal{D}'_1)}+\frac{1}{\mathcal{D}'_1(\mathcal{D}_1+\mathcal{D}'_1)}=\frac{\mathcal{D}_1+\mathcal{D}'_1}{\mathcal{D}_1(\mathcal{D}_1+\mathcal{D}'_1)\mathcal{D}'_1}=\frac{1}{\mathcal{D}_1\mathcal{D}'_1}$, confirming the proposition for $m=2$. Now, assume the proposition for $m-1$ and consider m. The topmost resolvent generates the same denominator factor $\mathcal{D}_n+\mathcal{D}'_{n'}$ for all orderings of the combined diagram. Factoring this out, we have one set of orderings with O_n as the topmost operator factor which, by our inductive assumption, add up to $\frac{1}{\mathcal{D}_1\cdots\mathcal{D}_{n-1}\mathcal{D}'_1\cdots\mathcal{D}'_{n'}}$, while the remaining orderings all have $O'_{n'}$ as the topmost operator and add up to $\frac{1}{\mathcal{D}_1\cdots\mathcal{D}_n\mathcal{D}'_1\cdots\mathcal{D}'_{n'-1}}$. The total sum is therefore $\frac{1}{\mathcal{D}_n+\mathcal{D}'_{n'}}\left(\frac{1}{\mathcal{D}_1\cdots\mathcal{D}_{n-1}\mathcal{D}'_1\cdots\mathcal{D}'_{n'}}+\frac{1}{\mathcal{D}_1\cdots\mathcal{D}_n\mathcal{D}'_1\cdots\mathcal{D}'_{n'-1}}\right)=\frac{1}{\mathcal{D}_1\cdots\mathcal{D}_n\mathcal{D}'_1\cdots\mathcal{D}'_{n'}}$, which proves the proposition for all m. For multiple separate parts, the proposition still follows by combining one pair at a time, since the set of final orderings is the cartesian product of the pairwise orderings.

Example 1.5. The equation ${}^{(2)}\hat{C}_4=\frac{1}{2}{}^{(1)}\hat{C}_2^2$ derived in ex 1.4 is an example of the Frantz-Mills factorization theorem

$$\tfrac{1}{2}{}^{(1)}\hat{C}_2^2=\tfrac{1}{2}\left(\tfrac{1}{4}\frac{\overline{g}^{ij}_{ab}}{\mathcal{D}^{ab}_{ij}}\tilde{a}^{ab}_{ij}\right)\left(\tfrac{1}{4}\frac{\overline{g}^{kl}_{cd}}{\mathcal{D}^{cd}_{kl}}\tilde{a}^{cd}_{kl}\right)=$$



$$=\left(\tfrac{1}{2}\right)^4\frac{\overline{g}^{kl}_{cd}\overline{g}^{ij}_{ab}}{\mathcal{D}^{abcd}_{ijkl}\mathcal{D}^{ab}_{ij}}\tilde{a}^{abcd}_{ijkl}={}^{(2)}\hat{C}_4$$

where we have only one diagrammatically unique ordering for the combined diagram. If instead we had two different operators $\hat{V}$ and $\hat{W}$, this equation would instead read as follows.

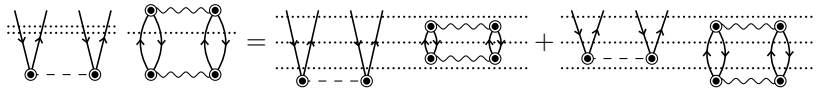
$$\updownarrow$$

$$\left(\tfrac{1}{4}\frac{v^{ij}_{ab}}{\mathcal{D}^{ab}_{ij}}\tilde{a}^{ab}_{ij}\right)\left(\tfrac{1}{4}\frac{w^{kl}_{cd}}{\mathcal{D}^{cd}_{kl}}\tilde{a}^{cd}_{kl}\right)=\left(\tfrac{1}{2}\right)^4\frac{w^{kl}_{cd}v^{ij}_{ab}}{\mathcal{D}^{abcd}_{ijkl}}\left(\frac{1}{\mathcal{D}^{ab}_{ij}}+\frac{1}{\mathcal{D}^{cd}_{kl}}\right)\tilde{a}^{abcd}_{ijkl}$$

Corollary 1.1. ***The Frantz-Mills Factorization Theorem for Insertion Diagrams.*** *An insertion diagram equals the sum over all relative orderings in the corresponding combined diagram that keep the top operator of the inserted diagram below the upper resolvent at the point of insertion in the remainder diagram.*

Proof: Consider the Frantz-Mills Factorization Theorem for open diagrams as an equation, with the separated diagram on the left and the sum over combined diagrams on the right. Notice that the equation still holds true if we attach a feature to the top of any one of the parts, provided we apply this manipulation to each term on both sides of the equation. Therefore, we can "cap" one of the parts with an operator, add a resolvent line above that, and attach whatever features we want to the top of the other operator. This turns the left-hand side into an insertion diagram, and proves the proposition.

Example 1.6. Closing one of the diagrams in ex 1.5 and adding a resolvent line, we get the following.



Remark 1.3. Recall that an unlinked diagram is a diagram with a disconnected part that is closed. For the following proof, the term *unlinked part* will be used exclusively to refer to the *closed parts* of a *combined* diagram. The remaining parts of the combined diagram will be referred to as the *remainder diagram*.

Theorem 1.3. ***The Linked Diagram Theorem.*** *The nth RSPT order wavefunction and energy contributions are given by the linked component of the principal term in the bracketing expansion.*

$$\Psi^{(n)} = ((R_0 V_c)^n \Phi)_{\mathrm{L}} \qquad\qquad E^{(n+1)} = \langle V_c (R_0 V_c)^n \rangle_{\mathrm{L}}$$

That is, the bracketed terms exactly cancel with the unlinked component of the principal term.

Proof: If $\Psi^{(n)}$ is linked then every unlinked contribution to $V_c \Psi^{(n)}$ has an open part and vanishes in the energy expression $E^{(n+1)} = \langle \Phi | V_c | \Psi^{(n)} \rangle = \langle \Phi | V_c | \Psi^{(n)} \rangle_{\mathrm{L}}$. Therefore, we restrict our attention to the wavefunction. We proceed by induction on the maximum allowed nesting depth k in the bracketing expansion. If $k = 0$ we have only the principal component. Assume it gives rise to at least one diagram with an unlinked part. By the nature of the expansion, all other orderings of the parts in this diagram also contribute, and at least one of those orderings places all vertices of the unlinked part adjacent to each other. This implies that we could place brackets around those vertices without killing the term, which is a contradiction. Therefore, the proposition holds for $k = 0$. Now, suppose the proposition holds up to $k - 1$ and consider k. By the energy substitution lemma, we have a sum over all possible m-tuple substitutions of adjacent factors $(R_0 V_c)^r$ in the principale term by $R_0 E_c^{(r)}$ times a sign factor $(-)^m$ for the number of substitutions. By our inductive assumption, each substituted energy $E_c^{(r)}$ equals $\langle V_c (R_0 V_c)^{(r-1)} \rangle_{\mathrm{L}}$. Then the following lemma proves that these linked bracketings cancel with the unlinked contributions to the principal term, proving the result to all orders.

Lemma 1.2. *Restricting the bracketing expansion of $\Psi^{(n)}$ to non-nested insertions and keeping only the linked contributions to each bracket $\langle \cdots \rangle \mapsto \langle \cdots \rangle_{\mathrm{L}}$ gives the linked component of the principal term, $((R_0 V_c)^n \Phi)_{\mathrm{L}}$.*

Proof: Suppose the expansion allows at most k brackets. Consider one of the terms with $k - 1$ brackets, together with the term (if it exists) that shares the same $k - 1$ insertions but has an additional insertion below them. If there is more than one, pick the term with the lowest insertion. Since the two terms differ by one bracket, they are opposite in sign. Therefore, by cor 1.1, the k-bracket term cancels all of the unlinked contributions to the $(k - 1)$-bracket term for which the top of the unlinked part is at the level of the insertion. Proceeding to the next lowest k-bracket term, we successively cancel all unlinked contributions to the $(k-1)$-bracket term below the lowest point of insertion. Continuing this procedure, we cancel all k-bracket terms against all unlinked contributions below the lowest insertions of the $(k - 1)$-bracket terms. Note that all unlinked contributions *above* the lowest insertions are still present, which allows us to now cancel against each $(k - 2)$-bracket term. Applying this procedure iteratively to the terms with the most brackets, we can eliminate each current set of maximally bracketed terms, until we end up with just the principal term.