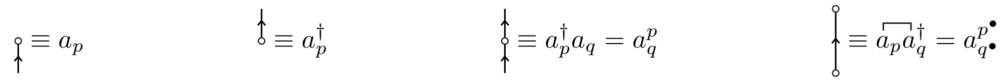
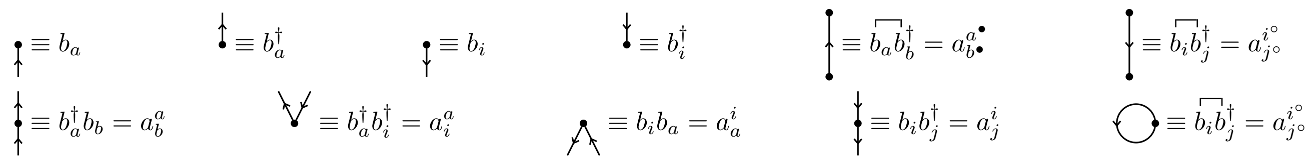
1. Diagram notation

Notation 1.1. *Diagram notation.* In diagram notation, particle-hole operators are written as oriented lines extending from a vertex. Particle annihilation operators enter the vertex from below, particle creation operators leave the vertex at the top, and single-excitation operators have both creation and annihilation lines. Contractions are represented by joining particle-hole lines with compatible position and orientation.



$\equiv a_p$ $\quad \equiv a_p^\dagger$ $\quad \equiv a_p^\dagger a_q = a^p_q$ $\quad \equiv \overline{a_p a_q^\dagger} = a^{p\bullet}_{q\bullet}$

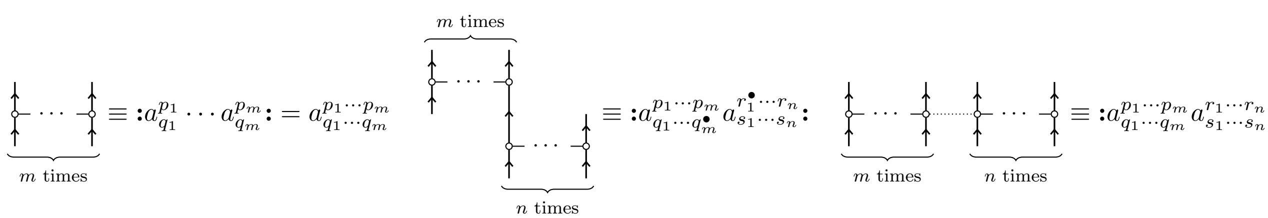
Quasiparticle operators with respect to Φ are distinguished by the use of closed-circle vertices, with particle lines pointing upward and with hole lines pointing downward. Single-excitation operators split into four cases (vv, vo, ov, and oo) representing the virtual and occupied blocks of a^p_q. Internal contractions of single-excitation operators (*bubble contractions*) are implicitly taken to be hole contractions with respect to Φ.



$\equiv b_a$ $\quad \equiv b_a^\dagger$ $\quad \equiv b_i$ $\quad \equiv b_i^\dagger$ $\quad \equiv \overline{b_a b_b^\dagger} = a^{a\bullet}_{b\bullet}$ $\quad \equiv \overline{b_i b_j^\dagger} = a^{i\circ}_{j\circ}$

$\equiv b_a^\dagger b_b = a^a_b$ $\quad \equiv b_a^\dagger b_i^\dagger = a^a_i$ $\quad \equiv b_i b_a = a^i_a$ $\quad \equiv b_i b_j^\dagger = a^i_j$ $\quad \equiv \overline{b_i b_j^\dagger} = a^{i\circ}_{j\circ}$

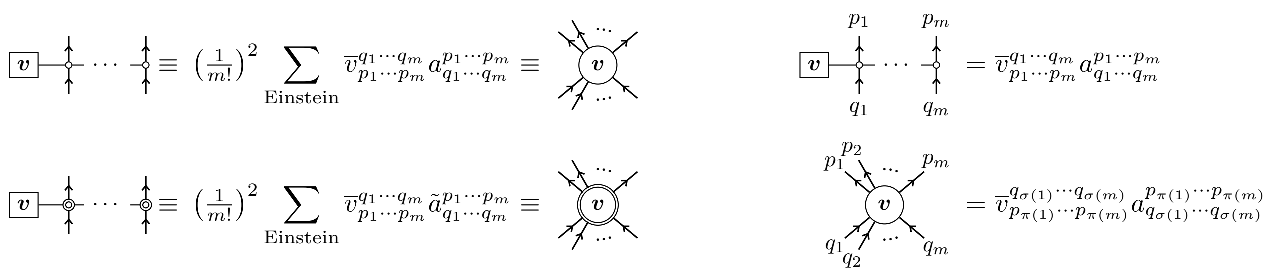
Higher excitation operators are depicted by joining single-excitation operators with a solid line. Contracted operators are implicitly normal ordered together. Normal-ordered products of uncontracted operators are joined with a dotted line.



$\equiv :a^{p_1}_{q_1}\cdots a^{p_m}_{q_m}: = a^{p_1\cdots p_m}_{q_1\cdots q_m}$ $\quad \equiv :a^{p_1\cdots p_m}_{q_1\cdots q_m^\bullet}\, a^{r_1^\bullet\cdots r_n}_{s_1\cdots s_n}:$ $\quad \equiv :a^{p_1\cdots p_m}_{q_1\cdots q_m}\, a^{r_1\cdots r_n}_{s_1\cdots s_n}:$

Φ-normal-ordering is indicated by the use of double-circle vertices, ⊚ and ◉ instead of ∘ and •.

Definition 1.1. *m-electron operators in Diagram notation.* The primary building blocks of a graph are m-electron operators, which can be represented in two equivalent ways. The *Goldstone representation* depicts an operator as a label attached to the corresponding excitation operator, whereas the *Hugenholtz representation* depicts the operator as a single vertex with m outgoing and incoming lines. Note that $\left(\frac{1}{m!}\right)^2 \sum_{\text{Einstein}}$ is baked into the definition (see def 1.2 and ax 1.1).



$$\equiv \left(\frac{1}{m!}\right)^2 \sum_{\text{Einstein}} \overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m} a^{p_1\cdots p_m}_{q_1\cdots q_m} \equiv \qquad = \overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m} a^{p_1\cdots p_m}_{q_1\cdots q_m}$$

$$\equiv \left(\frac{1}{m!}\right)^2 \sum_{\text{Einstein}} \overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m} \tilde{a}^{p_1\cdots p_m}_{q_1\cdots q_m} \equiv \qquad = \overline{v}^{q_{\sigma(1)}\cdots q_{\sigma(m)}}_{p_{\pi(1)}\cdots p_{\pi(m)}} a^{p_{\pi(1)}\cdots p_{\pi(m)}}_{q_{\sigma(1)}\cdots q_{\sigma(m)}}$$

The labeled diagrams on the right represent just the summand of the operator, which highlights the difference between representations. Both summands correspond to an excitation operator weighted by its antisymmetrized interaction tensor,[1] but whereas the Goldstone summand specifies an ordering for the indices of its corresponding algebraic term, the Hugenholtz summand does not. Since the phases of $\overline{v}^{q_1\cdots q_m}_{p_1\cdots p_m}$ and $a^{p_1\cdots p_m}_{q_1\cdots q_m}$ cancel under index permutation, the two labeled diagrams are actually equal – a Hugenholtz summand can be expanded into a Goldstone summand by simply choosing an arbitrary ordering for the indices. In practice, the symmetry of the Hugenholtz operator simplifies the enumeration of Wick expansions whereas the Goldstone operator makes it easier to evaluate a graph's overall phase.

[1] In the original paper [J. Goldstone, *P. Roy. Soc. A* **239**, (1957)], Goldstone's diagrams were actually defined in terms of non-antisymmetrized integrals. The *antisymmetrized Goldstone diagrams* used here are sometimes called *Brandow diagrams*.

Definition 1.2. ***Graph.*** A *graph*[2] is a 4-tuple $G = (O, L, h, t)$ where O is a set of electron operators, L is a set of lines, and h and t are maps from L to O that return the *head* $h(l) \in O$ and *tail end* $t(l) \in O$ of every line $l \in L$. Here, we allow for *external lines* in which either $h(l)$ or $t(l)$ equals e, the *free end*, which is formally considered a member of O. Lines no free end are termed *internal*. If l and l' share the same tail and the same head, they are termed *equivalent lines* and we write $l \sim l'$. If o and o' can be exchanged, attaching the ends of one to the other and vice versa, without altering G then they are termed *interchangeable operators*. Repeated copies of the same operator are formally distinguished as elements of O and termed *identical operators*, denoted $o \simeq o'$. If identical operators are interchangeable, they are termed *equivalent*, denoted $o \sim o'$. See ex A.2. The *rules of interpretation* for translating G into an algebraic expression are given in ax 1.1.

Definition 1.3. ***Summand graph.*** A *summand graph*[3] $\Sigma(G)$ of G is a 3-tuple $\Sigma(G) = (G, S, s)$ where S is a set of symbols and $s : L \to S$ is a *label map* assigning one symbol $s(l) \in S$ to each line $l \in L$. Pictorially, this corresponds to labeling each line in G with an index, p, q, r, s, etc. $\Sigma(G)$ translates directly into an algebraic summand according to def 1.1 and nt 1.1, with top-to-bottom ordering in the graph corresponding to left-to-right ordering in the expression.

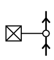
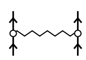
Definition 1.4. ***Degeneracy.*** The *line degeneracy* or simply *degeneracy* of G is the number of permutational symmetries in $\Sigma(G)$, a positive integer denoted $\mathrm{dg}(G)$. Formally, if $S = \{s_1, \dots, s_n\}$ with $s(l_i) = s_i$, then $\mathrm{dg}(G)$ is the number of label permutations $\Sigma_\pi(G) = (G, S, s_\pi)$, where $\pi \in \mathrm{S}_n$ and $s_\pi(l_i) = s_{\pi(i)}$, that don't change the summand graph, $\Sigma_\pi(G) = \Sigma(G)$. If G has no identical operators, then $\mathrm{dg}(G) = |L_1|! \cdots |L_m|!$ where $L = L_1 \cup \cdots \cup L_m$ partitions L into equivalent lines and $|L_i|$ denotes the number of elements in the set L_i.

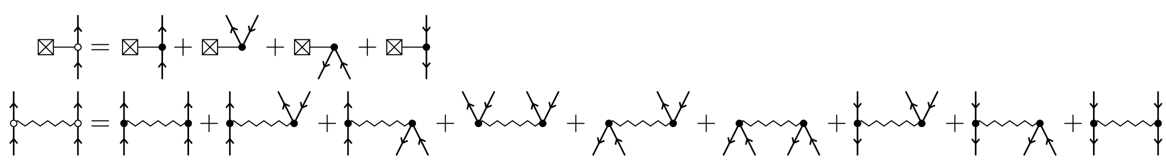
Axiom 1.1. ***Rules of interpretation.*** The algebraic intepretation of G is obtained from $\Sigma(G)$ as follows. See ex A.1.

1. Multiply $\Sigma(G)$ by $\mathrm{dg}(G)^{-1}$, termed the *degeneracy factor*.
2. Sum each index in $\Sigma(G)$ over its range.

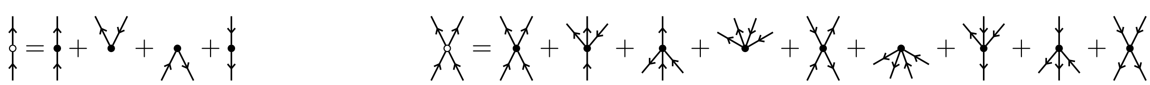
Example 1.1. The one- and two-electron components of H_e expand into occupied/virtual blocks as follows.

$$\begin{aligned} h_p^q a_q^p &= h_a^b a_b^a + h_a^i a_i^a + h_i^a a_a^i + h_i^j a_j^i \\ \tfrac{1}{4}\overline{g}_{pq}^{rs} a_{rs}^{pq} &= \tfrac{1}{4}\overline{g}_{ab}^{cd} a_{cd}^{ab} + \tfrac{1}{2}\overline{g}_{ab}^{ci} a_{ci}^{ab} + \tfrac{1}{2}\overline{g}_{ai}^{bc} a_{bc}^{ai} + \tfrac{1}{4}\overline{g}_{ab}^{ij} a_{ij}^{ab} + \overline{g}_{ia}^{bj} a_{bj}^{ia} + \tfrac{1}{4}\overline{g}_{ij}^{ab} a_{ab}^{ij} + \tfrac{1}{2}\overline{g}_{ia}^{jk} a_{jk}^{ia} + \tfrac{1}{2}\overline{g}_{ij}^{ka} a_{ka}^{ij} + \tfrac{1}{4}\overline{g}_{ij}^{kl} a_{kl}^{ij} \end{aligned}$$

Defining  $\equiv h_p^q a_q^p$ and  $\equiv \frac{1}{4}\overline{g}_{pq}^{rs} a_{rs}^{pq}$, these equations are expressed in terms of Goldstone diagrams as follows.



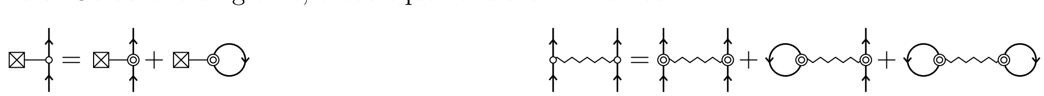
The degeneracy factors fall into three cases: $\{l_1, l_2\} \cup \{l_3, l_4\} \implies \mathrm{dg}(G)^{-1} = \frac{1}{2\cdot 2}$; $\{l_1, l_2\} \cup \{l_3\} \cup \{l_4\} \implies \mathrm{dg}(G)^{-1} = \frac{1}{2\cdot 1\cdot 1}$; and $\{l_1\} \cup \{l_2\} \cup \{l_3\} \cup \{l_4\} \implies \mathrm{dg}(G)^{-1} = \frac{1}{1\cdot 1\cdot 1\cdot 1}$. In terms of Hugenholtz diagrams, these are written as follows.



Example 1.2. The Φ-normal Wick expansion of the one- and two-electron components of H_e are as follows.

$$\begin{aligned} h_p^q a_q^p &= h_p^q \left(\tilde{a}_q^p + \tilde{a}_{q^\circ}^{p^\circ} \right) = h_p^q \tilde{a}_q^p + h_p^q \gamma_q^p \\ \tfrac{1}{4}\overline{g}_{pq}^{rs} a_{rs}^{pq} &= \tfrac{1}{4}\overline{g}_{pq}^{rs} \left(\tilde{a}_{rs}^{pq} + \hat{P}_{(r/s)}^{(p/q)} \tilde{a}_{r^\circ s}^{p^\circ q} + \hat{P}_{(r/s)} \tilde{a}_{r^\circ s^{\circ\circ}}^{p^\circ q^{\circ\circ}} \right) = \tfrac{1}{4}\overline{g}_{pq}^{rs} \tilde{a}_{rs}^{pq} + \overline{g}_{pq}^{rs} \gamma_r^p \tilde{a}_s^q + \tfrac{1}{2}\overline{g}_{pq}^{rs} \gamma_r^p \gamma_s^q \end{aligned}$$

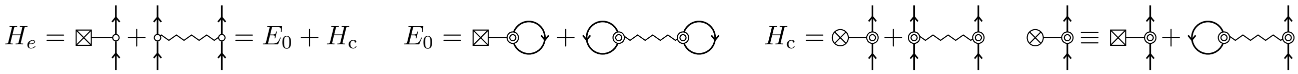
In terms of Goldstone diagrams, these equations are written as

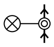


and, in terms of Hugenholtz diagrams, they are written as follows.

[2]In group theory jargon this is essentially a *directed multigraph*, except that the vertical ordering of operators matters.
[3]In group theory jargon this is an *edge-labeled directed multigraph*.

Example 1.3. The Φ-normal Wick expansion of H_e in terms of Goldstone diagrams is



where  represents the Φ-normal-ordered Fock operator, $f^q_p \tilde{a}^p_q$.

Definition 1.5. ***Contraction.*** A *graph contraction* is a map $G \mapsto c(G)$ joining one or more compatible external lines in G. For example, c might replace l_1 and l_2, which have ends $(t(l_1), h(l_1)) = (o_1, e)$ and $(t(l_2), h(l_2)) = (e, o_2)$, with l_{12}, which has ends $(t(l_{12}), h(l_{12})) = (o_1, o_2)$. Contractions c and c' of G are *equivalent* if $c(G) = c'(G)$. The number of c' equivalent to c is called the *pattern degeneracy* of c, denoted $\mathrm{pat}(c)$. The complete set of inequivalent graph contractions of G is here denoted $\mathrm{Ctr}(G)$.

Definition 1.6. ***Connected graph.*** A *path* is a sequence of lines $(l_1, \cdots, l_n)$ such that l_i is adjacent to l_{i+1} and all of the

G forms a *connected graph* if there is a path between any two of its operators.

Definition 1.7. ***Equivalent subgraph.*** If O' and L' are subsets of O and L then $G' = (O', L', h, t)$ is a *subgraph* of G, denoted $G' \subseteq G$. Given an operator subset $O' \subseteq O$, the *subgraph induced by* O' is the subgraph (O', L', h, t) where L' contains all lines in L except for those incident on operators not in O'. Suppose O_1 and O_2 are disjoint subsets of O such that $G[O_1]$ is connected and $G[O_2]$ is connected. If $G[O_1]$ and $G[O_2]$ can be exchanged in G without altering the graph then we say that they are *interchangeable subgraphs*. See ex A.3. If in addition $G[O_1]$ and $G[O_2]$ are interchangeable subgraphs that are identical, we call them *equivalent subgraphs* and write $G[O_1] \sim G[O_2]$. See ex A.4. If $O_1 = \{o_1\}$ and $O_2 = \{o_2\}$, then this is the same as saying that o_1 and o_2 are equivalent operators.

Lemma 1.1. *The pattern degeneracy of a contraction c of the graph G is given by* $\mathrm{pat}(c) = \dfrac{\mathrm{dg}(G)}{\mathrm{dg}(c(G))}$.

Proof: First, consider c' and G' which equal c and G except that identical operators are treated as distinct. If $L = L_1 \cup \cdots \cup L_m$ partitions L into equivalent lines, let $L_{i,j}$ denote the subset of lines in L_i contracted with lines from L_j under c. Let $L_{i,\mathrm{ext}}$ denote the (possibly empty) subset of L_i which is external in $c(G)$. The number of equivalent ways of partitioning L_i for contraction is then "$|L_i|$ choose $|L_{i,\mathrm{ext}}|, |L_{i,1}|, \cdots, |L_{i,m}|$". The number of equivalent ways of contracting $L_{i,j}$ with $L_{j,i}$ is $|L_{i,j}|! = |L_{j,i}|!$. Therefore, the total pattern degeneracy of c' is

$$\mathrm{pat}(c') = \prod_{i=1}^{m} \binom{|L_i|}{|L_{i,\mathrm{ext}}|, |L_{i,1}|, \ldots, |L_{i,m}|} \prod_{i=1}^{m} \prod_{j=i+1}^{m} |L_{i,j}|! = \frac{|L_1|! \cdots |L_m|!}{\prod_{i=1}^{m} |L_{i,\mathrm{ext}}|! |L_{i,1}|! \cdots |L_{i,i-1}|!} = \frac{\mathrm{dg}(G')}{\mathrm{dg}(c'(G'))}.$$

Theorem 1.1. ***Wick's theorem for diagrams.***

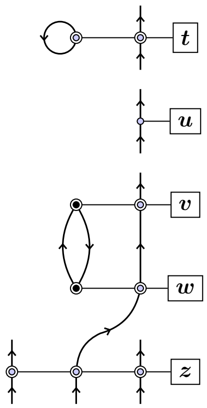
Proof:

$$\tfrac{1}{\mathrm{dg}(G)} \sum_{\text{Einstein}} \Sigma(G) = \tfrac{1}{\mathrm{dg}(G)} \sum_{\text{Einstein}} {:}\Sigma(G){:} + \sum_{c \in \mathrm{Ctr}(G)} \mathrm{pat}(c)\, \tfrac{1}{\mathrm{dg}(G)} \sum_{\text{Einstein}} {:}\Sigma(c(G)){:}$$

and since $\mathrm{pat}(c)\,\mathrm{dg}(G)^{-1} = \mathrm{dg}(c(G))^{-1}$, this is equivalent to $G = {:}G{:} + \sum_{c \in \mathrm{Ctr}(G)} {:}c(G){:}$.

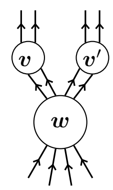
A. Parenthetical results

Example A.1. ***Graph.***

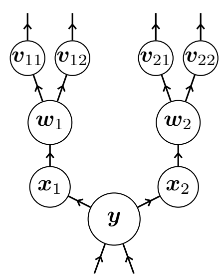


$$\equiv \frac{1}{2\cdot 2\cdot 3}\sum_{\text{Einstein}} \vdots\, t^{qr}_{op}\, a^{o^{\circ}\;p}_{q^{\circ}\;r} \,\vdots\, u^{t}_{s} a^{s}_{t} \left(\vdots\, v^{wx}_{uv}\, a^{u^{\circ\circ}\;\;v}_{\;\;w^{\bullet}\;x^{\bullet\bullet}}\, w^{\alpha\beta}_{yz}\, a^{y^{\bullet}\;z^{\bullet\bullet}}_{\;\;\alpha^{\circ\circ}\;\beta^{\bullet\bullet\bullet}}\, z^{\phi\eta\theta}_{\gamma\delta\varepsilon}\, a^{\gamma\delta^{\bullet\bullet\bullet}\;\varepsilon}_{\phi\eta\;\;\;\theta} \,\vdots \right)$$

Example A.2. ***Equivalent operators.*** If v and v' in the following graph are identical, then they are *equivalent operators*, $v \sim v'$. Otherwise, v and v' are *interchangeable* but *inequivalent operators*.



Example A.3. ***Interchangeable subgraphs.*** $G[\{x_1, w_1, v_{11}, v_{12}\}]$ and $G[\{x_2, w_2, v_{21}, v_{22}\}]$ in the following graph are interchangeable subgraphs. Also, $G[\{v_{11}\}]$ is interchangeable with $G[\{v_{12}\}]$ and $G[\{v_{21}\}]$ is interchangeable with $G[\{v_{22}\}]$.



Example A.4. ***Equivalent subgraphs.*** If $v \simeq v'$ and $x \simeq x'$ in the following graph, then $G[\{v, x\}]$ and $G[\{v', x'\}]$ are *equivalent subgraphs*, $G[\{v, x\}] \sim G[\{v', x'\}]$. Otherwise, they are *interchangeable* but *inequivalent subgraphs*.