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.

$$\stackrel{\uparrow}{\Diamond} \equiv a_p^{\dagger} \qquad \qquad \stackrel{\downarrow}{\Diamond} \equiv a_p^{\dagger} a_q = a_q^p \qquad \qquad \stackrel{\Diamond}{\Diamond} \equiv \overline{a_p} \overline{a_q} = a_q^{p^{\bullet}}$$

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_q^p . Internal contractions of single-excitation operators (bubble contractions) are implicitly taken to be hole contractions with respect to Φ .

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.

$$\underbrace{\underbrace{-\cdots }_{m \text{ times}}}_{\text{m times}} \equiv :a_{q_1}^{p_1} \cdots a_{q_m}^{p_m} := a_{q_1 \cdots q_m}^{p_1 \cdots p_m} \underbrace{= :a_{q_1 \cdots q_m}^{p_1 \cdots p_m} a_{s_1 \cdots s_n}^{r_1^{\bullet} \cdots r_n} :}_{n \text{ times}} \underbrace{-\cdots }_{m \text{ times}} \underbrace{-\cdots }_{n \text{ times}} \equiv :a_{q_1 \cdots q_m}^{p_1 \cdots p_m} a_{s_1 \cdots s_n}^{r_1 \cdots r_n} :$$

 Φ -normal-ordering is indicated by the use of double-circle vertices, \otimes and \otimes instead of \circ and \bullet .

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).

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, 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 $\overline{v}_{p_1...p_m}^{q_1...q_m}$ and $a_{q_1...q_m}^{p_1...p_m}$ 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.

¹In 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 graph² 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 $l \in L$. The notation $l \sim l'$ is used to indicate that l and l' are equivalent lines, which means that they have the same head and tail. 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 with no free end are termed internal. A graph is termed closed if it contains no external lines, in which case it represents a scalar-valued algebraic term. Otherwise, the graph is open and represents an operator-valued algebraic term. The rules of interpretation for translating G into an algebraic expression are given in ax 1.1.

Definition 1.3. Connected and linked graphs. Two lines are adjacent if they share a non-free end. In a Goldstone diagram, two lines are termed Goldstone adjacent if they end on the same single-excitation vertex of an operator. The broader sense of the adjacency is then called Hugenholtz adjacency. A path is a sequence of lines (l_1, \ldots, l_n) such that l_i is adjacent to l_{i+1} and no line is repeated. In a Goldstone diagram, a Goldstone path is a path whose lines are Goldstone adjacent. Following the same nomenclature, paths in the broader sense can also be called Hugenholtz paths. A Goldstone cycle is a Goldstone path whose ends are either Goldstone adjacent or free. In the first case we call the Goldstone cycle a loop and, in the second case, we call it an open cycle. A graph is considered connected if there is a Hugenholtz path connecting any two of its operators. A disconnected component of a graph that is closed unto itself is termed unlinked. That is, provided none if its disconnected parts are closed, a disconnected graph may still be classified as linked.

Definition 1.4. Summand graph. A summand graph³ $\Sigma(G)$ 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.

Derivation 1.1. Phase rule for simplifying summand graphs with contractions. The summand graph of a pair of m-electron operators with a single particle or hole contraction has the following form in Goldstone representation

where d is a virtual index, k is an occupied index, and we are not using implicit summation. Notice that $a_{q_1\cdots q_n}^{p_1\cdots p_n}=a_{q_1}^{p_1}\cdots a_{q_n}^{p_n}$: and that moving the single-excitation operators around in the string always involves an even number of transpositions. This allows us to bring together the contracted pair of single-excitation operators without changing the sign of the expression. The contracted pair of operators can then be eliminated via

$$:a_{d^{\bullet}}^{p_{i}}a_{s_{j}}^{d^{\bullet}}:=-:a_{d^{\bullet}s_{j}}^{d^{\bullet}p_{i}}:=-(-\eta_{d}^{d})a_{s_{j}}^{p_{i}}=a_{s_{j}}^{p_{i}} \qquad \text{or} \qquad :a_{q_{i}}^{k^{\circ}}a_{k^{\circ}}^{r_{j}}:=-:a_{k^{\circ}q_{i}}^{k^{\circ}r_{j}}:=-(+\gamma_{k}^{k})a_{q_{i}}^{r_{j}}=-a_{q_{i}}^{r_{j}}$$

in the case of a particle or hole contraction, respectively. In words, a contracted pair of operators in a summand graph can be eliminated by joining their uncontracted partners into a new single-excitation operator and multiplying by -1 in the case of a hole contraction. Applying this rule to each internal line of a Goldstone cycle, one finds that

- 1. eliminating all contracted operators of an open cycle leaves $(-)^h a_q^p$, where p and q are the indices of the free ends
- 2. eliminating all contracted operators of a loop leaves $(-)^h a_d^{\bullet} = (-)^h (-\eta_d^d) = (-)^{h+1}$

where h is the total number of hole lines in the Goldstone cycle. Since the lines of any Goldstone graph uniquely partition into Goldstone cycles, these rules provide a quick way to resolve the operator component of any diagram into a normal-ordered product of uncontracted operators times a phase factor.

Corollary 1.1. Phase rule for closed graphs. After eliminating all contracted operator pairs, the sign of a closed summand graph is $(-)^{h+l}$, where h is the total number of holes in the graph and l is the number of loops.

Proof: By definition, every Goldstone cycle in a closed graph is a loop. Let h_i be the number of holes in the i^{th} loop. Then, by der 1.1, the fully contracted operator product evaluates to $\prod_{i=1}^{l} (-)^{h_i+1} = (-)^{\sum_i h_i+l} = (-)^{h+l}$.

²In group theory jargon this is essentially a *directed multigraph*, except that the vertical ordering of operators matters.

³In group theory jargon this is an *edge-labeled directed multigraph*.

Definition 1.5. Degeneracy. The line degeneracy or simply degeneracy of G is the number of permutational symmetries in $\Sigma(G)$, a positive integer here denoted $\mathrm{dg}(G)$. Formally, this can be defined as follows. If $S = \{s_1, \ldots, s_n\}$ is the label set of $\Sigma(G)$ and $s(l_i) = s_i$ is its label map, we can define a new summand graph $\Sigma_{\pi}(G) = (G, S, s_{\pi})$ with a permuted label map s_{π} given by $s_{\pi}(l_i) = s_{\pi(i)}$, where π is a permutation in S_n . Then $\mathrm{dg}(G)$ is the number of $\Sigma_{\pi}(G)$ that are equal to $\Sigma(G)$. If $L_1 \cup \cdots \cup L_m$ partitions the line set of G into equivalent lines and $|L_i|$ denotes the number of elements in the set L_i , then $\mathrm{dg}(G) = |L_1|! \cdots |L_m|!$. The degeneracy factor becomes slightly more complicated for graphs with repeated operators, which will be considered below in section 1.1.

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

- 1. Multiply $\Sigma(G)$ by $dg(G)^{-1}$, 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.

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

which, defining $\boxtimes - \stackrel{\downarrow}{\downarrow} \equiv h_p^q a_q^p$ and $\stackrel{\downarrow}{\downarrow} \sim \sim \stackrel{\downarrow}{\downarrow} \equiv \frac{1}{4} \overline{g}_{pq}^{rs} a_{rs}^{pq}$, can be expressed in terms of Goldstone diagrams as

The degeneracy factors fall into three cases: $\{l_1, l_2\} \cup \{l_3, l_4\} \implies \operatorname{dg}(G)^{-1} = \frac{1}{2 \cdot 2}; \{l_1, l_2\} \cup \{l_3\} \cup \{l_4\} \implies \operatorname{dg}(G)^{-1} = \frac{1}{2 \cdot 1 \cdot 1};$ and $\{l_1\} \cup \{l_2\} \cup \{l_3\} \cup \{l_4\} \implies \operatorname{dg}(G)^{-1} = \frac{1}{1 \cdot 1 \cdot 1 \cdot 1}.$ 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.

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

In terms of Goldstone diagrams and Hugenholtz diagrams, these equations are written as follows.

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

$$H_e = \boxtimes \longrightarrow + \longrightarrow \longrightarrow = \underbrace{\boxtimes \longrightarrow + \bigodot \longrightarrow}_{E_0} + \underbrace{\boxtimes \longrightarrow}_{H_-} \longrightarrow + \underbrace{\boxtimes}_{H_-} \longrightarrow + \underbrace{\coprod}_{H_-} \longrightarrow + \underbrace{\boxtimes}_{H_-} \longrightarrow + \underbrace{\boxtimes}$$

where \otimes \Rightarrow \equiv \boxtimes \Rightarrow \Rightarrow \Rightarrow is the Φ -normal-ordered Fock operator, $f_p^q \tilde{a}_q^p = h_p^q \tilde{a}_q^p + \overline{g}_{pr}^{qs} \gamma_s^r \tilde{a}_q^p$.

Definition 1.6. 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 pat(c). The complete set of inequivalent graph contractions of G is here denoted Ctr(G).

Lemma 1.1. The pattern degeneracy of a contraction c is $pat(c) = \frac{dg(G)}{dg(c(G))}$.

Proof: Let L be the line set of G and let L_c be the line set of c(G). If $L = L_1 \cup \cdots \cup L_m$ partitions L into equivalent lines, let $L_{i,j} = L_{j,i}$ denote the subset of lines in L_c that result from contracting lines from L_i with lines from L_j . Let $L_{i,0}$ denote the subset of lines from L_i which is unchanged by c. Then $L_c = \bigcup_{i=1}^m (L_{i,0} \cup L_{i,1} \cup \cdots \cup L_{i,i-1})$ partitions L_c into equivalent lines. By standard counting techniques, the number of equivalent ways of partitioning L_i for contraction is $|L_i|$ choose $|L_{i,0}|, |L_{i,1}|, \cdots, |L_{i,m}|$, and the number of ways of forming $L_{i,j}$ for a given partition of L_i and L_j is $|L_{i,j}|! = |L_{j,i}|!$. Therefore, the total pattern degeneracy of c is

$$\operatorname{pat}(c) = \prod_{i=1}^{m} {|L_{i}| \choose |L_{i,0}|, |L_{i,1}|, \dots, |L_{i,m}|} \prod_{i=1}^{m} \prod_{j=i+1}^{m} |L_{i,j}|! = \frac{|L_{1}|! \cdots |L_{m}|!}{\prod_{i=1}^{m} |L_{i,0}|! |L_{i,1}|! \cdots |L_{i,i-1}|!} = \frac{\operatorname{dg}(G)}{\operatorname{dg}(c(G))}.$$

Theorem 1.1. Wick's theorem for diagrams. $G = :G: + \sum_{c \in Ctr(G)} :c(G):$

Proof: This follows by expanding G as $\frac{1}{\operatorname{dg}(G)} \sum_{\text{Einstein}} \Sigma(G)$, applying the standard algebraic Wick's theorem to the summand graph, $\Sigma(G) = :\Sigma(G): + \sum_{c \in \operatorname{Ctr}(G)} \operatorname{pat}(c) : \Sigma(c(G)):$, and writing $\operatorname{pat}(c)$ as $\frac{\operatorname{dg}(G)}{\operatorname{dg}(c(G))}$.

$$G = \frac{1}{\operatorname{dg}(G)} \sum_{\text{Einstein}} \Sigma(G) = \frac{1}{\operatorname{dg}(G)} \sum_{\text{Einstein}} : \Sigma(G) : + \sum_{c \in \operatorname{Ctr}(G)} \frac{1}{\operatorname{dg}(c(G))} \sum_{\text{Einstein}} : \Sigma(c(G)) : = :G : + \sum_{c \in \operatorname{Ctr}(G)} : c(G) : = :G : + \sum_{c \in \operatorname{Ctr}(G$$

In words, any graph is equal to its normal-ordered form plus the sum over all unique graph contractions.

Remark 1.1. The practical advantage of the graphical form of Wick's theorem is that there are far fewer unique graph contractions than there are algebraic contractions. Effectively, graphical notation makes the permutational symmetries of m-electron operators obvious, which tends to make them easier to manipulate.

1.1 Generalization for repeated operators

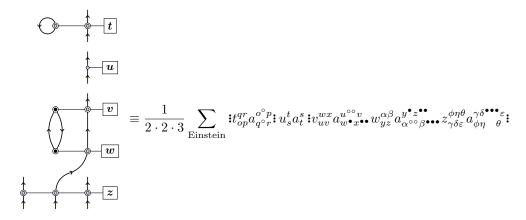
Definition 1.7. Repeated copies of the same operator are formally distinguished as elements of O and are referred to as *identical operators*. Operators whose interaction vertices can be interchanged without altering the graph are termed *interchangeable operators*. If two identical operators are interchangeable, they are termed *equivalent*.

Definition 1.8. 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*. If identical operators are interchangeable, they are termed *equivalent*, denoted $o \sim o'$. See ex A.2.

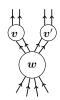
Definition 1.9. Equivalent subgraph. If O' and L' are subsets of O and L then G' = (O', L', h, t) is a subgraph of G, denoted $G' \subseteq G$. Given an operator subset $O' \subseteq O$, the subgraph induced by O' is the subgraph (O', L', h, t) where L' contains all lines in L except for those incident 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.

A. Examples

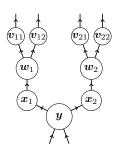
Example A.1. Graph.



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.

