Lecture 3.3: Wick's Theorem

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1 A note on permutations

We will use the following to denote permutations on a set of indices:

$$x_{R_1} \cdots x_{R_N} = (-1)^R x_1 \cdots x_N$$

R is the permutation of the set $\{x_1, \cdots, x_N\}$, and belongs to the permutation group S_N ($R \in S_N$). It can be represented as:

$$R = \begin{pmatrix} 1 & 2 & \cdots & N \\ R_1 & R_2 & \cdots & R_N \end{pmatrix}$$

The first row corresponds to the original indices while the second row corresponds to the permuted indices. R can also be written in cyclic notation to easily determine the sign of the permutation. It is easiest to show this with an example:

$$x_2 x_3 x_1 x_5 x_4 = (-1)^R x_1 x_2 x_3 x_4 x_5$$

Permutation R can be expressed as:

$$R = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 3 & 1 & 5 & 4 \end{pmatrix}$$

where the permuted indices R_1 corresponds to index 2 in the original string and so on.

To determine the cyclic permutations, we pick one index and follow the permutations until we get back to that same index. We can see that here, index 1 turns to 2, index 2 turns to 3, and index 3 turns to 1. Thus, (123) represents a cyclic permutation. In the same way, index 4 becomes index 5, and index 5 becomes index 4, and (45) represents another cyclic permutation.

In cyclic notation, we can write:

$$R = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 3 & 1 & 5 & 4 \end{pmatrix} = (123)(45)$$

An odd number of elements in a particular cyclic permutation corresponds to a positive sign (+) for the permutation. An even number of elements in a particular cyclic permutation corresponds to a negative sign (−) for the permutation. In the above example, we have one cyclic permutation with a positive sign and one cyclic permutation with a negative sign, so the overall sign of the permutation is negative. We thus have:

$$x_2 x_3 x_1 x_5 x_4 = -x_1 x_2 x_3 x_4 x_5$$

Here is another example where one index does not change its place:

$$x_1 x_3 x_2 x_5 x_4 = (-1)^R x_1 x_2 x_3 x_4 x_5$$

$$R = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 2 & 5 & 4 \end{pmatrix} = (1)(23)(45) = (+)(-)(-) = (+)$$
$$x_1 x_3 x_2 x_5 x_4 = x_1 x_2 x_3 x_4 x_5$$

Cyclic permutations can also be referred to as "cycles".

2 Prerequisites to Wick's Theorem

Last time, we determined that much of the math we have to solve boils down to evaluating expectation values of strings of creation and annihilation operators in the true vacuum. Using anti-communtation rules to do this was tedious, and we wanted to find a more efficient way. Our answer is to use Wick's Theorem. We first need to introduce three concepts needed to present Wick's Theorem: normal products, contractions, and normal products with contractions.

2.1 Normal Products

A normal product is a product of creation and annihilation operators where all the creation operators are to the left of the expression. We say that a product in which all creation operators are to the left is "normal ordered". We denote a normal product of a string of operators $x_1 \cdots x_m$ (where x_i can represent a creation or annihilation operator) with the notation "$n[x_1 \cdots x_m]$", and formally define it as:

$$n[x_1 \cdots x_m] = (-1)^R a^\dagger_{R_1} \cdots a^\dagger_{R_j} a_{R_{j+1}} \cdots a_{R_m}$$
$$R = \begin{pmatrix} 1 & 2 & \cdots & j & j+1 & \cdots & m \\ R_1 & R_2 & \cdots & R_j & R_{j+1} & \cdots & R_m \end{pmatrix}$$

The normal product of an empty set is defined to be one:

$$n[\varnothing] = 1$$

2.1.1 Example 1

$$n[a^\dagger_p a_q a^\dagger_r] = (-)^R a^\dagger_p a^\dagger_r a_q$$

$$R = \begin{pmatrix} p & q & r \\ p & r & q \end{pmatrix} = (p)(qr) = (+)(-) = (-)$$

$$n[a^\dagger_p a_q a^\dagger_r] = -a^\dagger_p a^\dagger_r a_q$$

Equivalently, we can write:

$$n[a^\dagger_p a_q a^\dagger_r] = (-)^R a^\dagger_r a^\dagger_p a_q$$

$$R = \begin{pmatrix} p & q & r \\ r & p & q \end{pmatrix} = (prq) = (+)$$

$$n[a^\dagger_p a_q a_r] = a^\dagger_r a^\dagger_p a_q$$

Thus we see normal products can be written in different ways, which are equivalent due to antisymmetry.

2.1.2 Example 2

$$n[a^\dagger_p a^\dagger_q a^\dagger_r] = a^\dagger_p a^\dagger_q a^\dagger_r$$

Here, the string is already normal ordered, so we can just drop the normal product notation.

2.1.3 Properties of Normal Products

There are several properties of normal products that are useful to us:

1. A normal product of a normal ordered string of operators is just that string of operators:

$$n[a_1^\dagger \cdots a_j^\dagger a_{j+1} \cdots a_m] = a_1^\dagger \cdots a_j^\dagger a_{j+1} \cdots a_m$$

   We note that a string of only creation operators or only annihilation operators are already in normal order.

2. A normal product of a normal product is just the normal product:

$$n[n[x_1 \cdots x_m]] = n[x_1 \cdots x_m]$$

   This is simply a manifestation of property 1.

3. You can freely permute a string of operators, with an appropriate phase factor, as long as it is within the normal ordered form:

$$n[x_{R_1} \cdots x_{R_m}] = (-1)^R n[x_1 \cdots x_m]$$

   For example,

$$n[x_2 x_1] = -n[x_1 x_2]$$

2.2 Contractions of Operators

We *define* a contraction between 2 operators x_1 and x_2 where x_i can be either a creation or an annihilation operator, as the quantity:

$$\underbracket{x_1 x_2} = x_1 x_2 - n[x_1 x_2]$$

We can derive the value of the contraction for various combinations of creation and annihilation operators by evaluating the expression. We will make use of the properties listed above as well as remembering our anticommutation relations. We have four cases to consider:

1. $x_1 = a_p$, $x_2 = a_q$

$$\underbracket{a_p a_q} = a_p a_q - n[a_p a_q] = a_p a_q - a_p a_q = 0$$

2. $x_1 = a_p$, $x_2 = a_q^\dagger$

$$\underbracket{a_p a_q^\dagger} = a_p a_q^\dagger - n[a_p a_q^\dagger] = a_p a_q^\dagger + a_q^\dagger a_p = \delta_{pq}$$

3. $x_1 = a_p^\dagger$, $x_2 = a_q$

$$\underbracket{a_p^\dagger a_q} = a_p^\dagger a_q - n[a_p^\dagger a_q] = a_p^\dagger a_q - a_p^\dagger a_q = 0$$

4. $x_1 = a_p^\dagger$, $x_2 = a_q^\dagger$

$$\underbracket{a_p^\dagger a_q^\dagger} = a_p^\dagger a_q^\dagger - n[a_p^\dagger a_q^\dagger] = a_p^\dagger a_q^\dagger - a_p^\dagger a_q^\dagger = 0$$

2.3 Normal Products with Contractions

A normal products with contractions inside

$$\wick{n[x_1 \cdots \c1 x_{i_1} \cdots \c2 x_{i_\lambda} \cdots \c1 x_{j_1} \cdots \c2 x_{j_\lambda} \cdots x_m]}$$

can be rewritten as:

$$\wick{n[x_1 \cdots \c1 x_{i_1} \cdots \c2 x_{i_\lambda} \cdots \c1 x_{j_1} \cdots \c2 x_{j_\lambda} \cdots x_m]} = (-1)^R \wick{\c x_{i_1} \c x_{j_1}} \cdots \wick{\c x_{i_\lambda} \c x_{j_\lambda}} n[x_{k_1} \cdots x_{k_\mu}]$$

where

$$R = \begin{pmatrix} 1 & 2 & \cdots & 2\lambda - 1 & 2\lambda & 2\lambda + 1 & \cdots & m \\ i_1 & j_1 & \cdots & i_\lambda & j_\lambda & k_1 & \cdots & k_\mu \end{pmatrix}$$

and the indices $2\lambda + \mu = m$. In words, a normal product with contractions can be written as a product of contractions outside the normal product multiplied by the uncontracted terms and a phase factor. It is important to note that when the contractions are taken out, you cannot flip the order of the contraction. In other words,

$$\wick{n[\c x_p \c x_q]} \neq \pm \wick{\c x_q \c x_p}$$

2.3.1 Example 1

$$\wick{n[\c a_p a_q \c a_r^\dagger]} = (-1)^R \wick{\c a_p \c a_r^\dagger} n[a_q]$$

$$R = \begin{pmatrix} p & q & r \\ p & r & q \end{pmatrix} = (p)(qr) = (-)$$

$$\wick{n[\c a_p a_q \c a_r^\dagger]} = -\wick{\c a_p \c a_r^\dagger} n[a_q] = -\delta_{pr} a_q$$

2.3.2 Two tips

There are two tips for faster evaluation of normal products with contractions.

The first tip is that neighboring contractions can be taken out of the normal product without considering the permutation. By "neighboring contraction", I mean contractions between operators that are next to each other. This is because the permutation associated with a neighboring pair is always positive. For example,

$$\wick{n[\c1 a_p \c2 a_q \c2 a_r^\dagger \c1 a_s a_t^\dagger a_u^\dagger]} = \wick{\c a_q \c a_r^\dagger} \wick{n[\c a_p \c a_s a_t^\dagger a_u^\dagger]}$$

The second tip is that for a *fully contracted* term, meaning that all operators are involved in a contraction, the phase factor can be obtained by counting the number of intersecting contraction lines ν:

$$(-1)^R = (-1)^\nu$$

For example, the term $\wick{n[\c1 a_p \c1 a_q^\dagger \c2 a_r \c2 a_s^\dagger \c3 a_t \c3 a_u^\dagger]}$ has 0 intersecting contraction lines, and will have an overall phase factor of (+1).

The term $\wick{n[\c1 a_p \c2 a_q \c1 a_r^\dagger \c2 a_s^\dagger \c3 a_t \c3 a_u^\dagger]}$ has 1 intersection, and will have an overall phase factor of (-1).

The term $\wick{n[\c1 a_p \c2 a_q \c1 a_r^\dagger \c3 a_s \c2 a_t^\dagger \c3 a_u^\dagger]}$ has 2 intersections, and will have an overall phase factor of (+1).

While we will not formally prove why this is true, the general idea is to reorder the string so there are only neighboring contractions. In order to do that, we have to permute the indices, and see that an intersection of contraction lines is gotten rid of by a permutation of operators (one sign factor).

We will use the following notation to denote a normal product which is fully contracted:

$$n\overline{\overline{[x_1 \cdots x_m]}}$$

The above three examples can all be expressed with this notation.

If you have a group of fully contracted operators within your normal product, you can take the full group out and use the number of intersecting contraction lines to determine the permutation associated with taking the group out.

For example, in the term

$$n[a_p a_q a_r^\dagger a_s a_t^\dagger a_u^\dagger a_v^\dagger a_w a_x a_y^\dagger]$$

the first six operators are fully contracted, and has an overall phase factor of $(+)$ because there are 2 intersections. As a result, we can take it out directly of the normal product:

$$n[a_p a_q a_r^\dagger a_s a_t^\dagger a_u^\dagger a_v^\dagger a_w a_x a_y^\dagger] = a_p a_r^\dagger a_q a_t^\dagger a_s a_u^\dagger n[a_v^\dagger a_w a_x a_y^\dagger]$$

2.4 Matrix elements of normal products with contractions

Remember that our ultimate goal is to know how to quickly evaluate matrix elements of strings of operators in the vacuum. We are now ready to prove some rules for determining how a normal ordered string of operators acts in the true vacuum.

- Rule 1: $n[x_1 \cdots x_m] |0\rangle = 0$ unless all $x_1 \cdots x_m$ are creation operators

  Proof: If all operators are creation operators,

  $$n[a_{p_1}^\dagger \cdots a_{p_m}^\dagger] |0\rangle = a_{p_1}^\dagger \cdots a_{p_m}^\dagger |0\rangle = |\Phi_{p_1 \cdots p_m}\rangle \neq 0$$

  If at least one x_i is an annihilation operator, it will be the rightmost term by the definition of the normal product, and will annihilate the vacuum. The overall result is zero.

- Rule 2: $\langle 0|n[x_1 \cdots x_m]|0\rangle = 0$ for $m \geq 1$

  Proof: If all operators are creation operators, they will annihilate the vacuum because

  $$(a_p |0\rangle)^\dagger = \langle 0| a_p^\dagger = 0$$

  If one or more operators are annihilation operators, they will be on the right by the definition of the normal product and annihilate the vacuum.

- Rule 3. $n[x_1 \cdots x_{i_1} \cdots x_{i_\lambda} \cdots x_{j_1} \cdots x_{j_\lambda} \cdots x_m] |0\rangle = 0$ if there is at least 1 uncontracted annihilator among operators $x_1 \cdots x_m$.

  Proof:

  $$n[x_1 \cdots x_{i_1} \cdots x_{i_\lambda} \cdots x_{j_1} \cdots x_{j_\lambda} \cdots x_m] |0\rangle = (-1)^R x_{i_1} x_{j_1} \cdots x_{i_\lambda} x_{j_\lambda} n[x_{k_1} \cdots x_{k_\mu}] |0\rangle$$

  By Rule 1, $n[x_{k_1} \cdots x_{k_\mu}] |0\rangle = 0$ unless all operators $x_{k_1} \cdots x_{k_\mu}$ are creation operators.

- Rule 4. $\langle 0|n[x_1 \cdots x_{i_1} \cdots x_{i_\lambda} \cdots x_{j_1} \cdots x_{j_\lambda} \cdots x_m]|0\rangle = 0$ unless all operators are contracted. In other words, only a fully contracted normal product ($n[\overline{\overline{x_1 \cdots x_m}}]$) gives a nonzero expectation value in the true vacuum.

  Proof: This is easily see as an application of Rule 2. Contractions of operators reduces to a number which can be pulled out of the expectation value.The only case where the expectation value is nonzero is one in which there is no operators left in the normal product, $\langle 0|n[\varnothing]|0\rangle \neq 0$

  As a consequence of Rule 4, a vacuum expectation value of any normal product with contractions will be zero if there are a odd number of operators.

We now know how to quickly evaluate matrix elements of a normal ordered string, and a normal ordered string with contractions. Next, we need to know how to quickly put any string in normal order so we can take advantage of these shortcuts. This is what Wick's theorem provides us.

3 Wick's Theorem

We will first start by seeing what happens if we put specific strings of operators in normal order just by applying anticommutation relations.
Putting a product of 2 operators in normal order is a direct application of anticommuntation relations:

$$a_p a_q^\dagger = \delta_{pq} - a_q^\dagger a_p$$

The first term, δ_{pq}, can be re-expressed as $\underbracket{a_p a_q^\dagger}$, as shown in Section 2.3. We can equivalently write $n[\underbracket{a_p a_q^\dagger}]$. You will show that $\underbracket{a_p a_q^\dagger} = n[\underbracket{a_p a_q^\dagger}]$ in the exercises. The second term is simply the normal product $n[a_p a_q^\dagger]$. Thus, we can write (switching the order of the first and second terms):

$$a_p a_q^\dagger = n[a_p a_q^\dagger] + n[\underbracket{a_p a_q^\dagger}]$$

Let's try with a product of 3 operators, $a_p a_q^\dagger a_r^\dagger$:

$$\begin{aligned}
a_p a_q^\dagger a_r^\dagger &= (\delta_{pq} - a_q^\dagger a_p) a_r^\dagger \\
&= \delta_{pq} a_r^\dagger - a_q^\dagger a_p a_r^\dagger \\
&= \delta_{pq} a_r^\dagger - a_q^\dagger (\delta_{pr} - a_r^\dagger a_p) \\
&= \delta_{pq} a_r^\dagger - \delta_{pr} a_q^\dagger + a_q^\dagger a_r^\dagger a_p
\end{aligned}$$

Rewriting the terms in a similar way as for the product of 2 operators, we obtain:

$$a_p a_q^\dagger a_r^\dagger = n[a_p a_q^\dagger a_r^\dagger] + n[\underbracket{a_p a_q^\dagger} a_r^\dagger] + n[\underbracket{a_p a_q^\dagger a_r^\dagger}]$$

In these two examples, we observe that the products of the creation and annihilations operators could be expressed as its normal product plus all possible contractions of its normal product form. Wick's theorem simply generalizes this observation to any string of creation and annihilation operators. Formally defined, Wick's theorem states:

$$
\begin{aligned}
x_1 \cdots x_m = {} & n[x_1 \cdots x_m] \\
& + \sum_{i<j} n[x_1 \cdots \wick{\c x_i \cdots \c x_j} \cdots x_m] \\
& + \sum_{\substack{i_1<j_1, i_2<j_2 \\ i_1<i_2, j_1 \neq j_2}} n[x_1 \cdots \wick{\c1 x_{i_1} \cdots \c2 x_{i_2} \cdots \c1 x_{j_1} \cdots \c2 x_{j_2}} \cdots x_m] \\
& + \cdots \\
& + \sum_{f.c.} n\overline{\overline{[x_1 \cdots x_m]}}
\end{aligned}
$$

where "f.c." stands for fully contracted. In words, a string of operators can be written as its normal product plus all contractions of the normal product. We will adopt a shorthand notation for expressing all possible contractions of the normal product and write Wick's theorem as:

$$
x_1 \cdots x_m = n[x_1 \cdots x_m] + \sum_{a.c.} n\overline{[x_1 \cdots x_m]}
$$

where "a.c." stands for all contractions. Let's explicitly write out Wick's theorem for a general product of 4 operators for a more concrete example:

$$
\begin{aligned}
x_1x_2x_3x_4 = {} & n[x_1x_2x_3x_4] \\
& + n[\wick{\c x_1 \c x_2}x_3x_4] + n[\wick{\c x_1 x_2 \c x_3}x_4] + n[\wick{\c x_1 x_2 x_3 \c x_4}] + n[x_1\wick{\c x_2 \c x_3}x_4] + n[x_1\wick{\c x_2 x_3 \c x_4}] + n[x_1x_2\wick{\c x_3 \c x_4}] \\
& + n[\wick{\c1 x_1 \c1 x_2 \c2 x_3 \c2 x_4}] + n[\wick{\c1 x_1 \c2 x_2 \c1 x_3 \c2 x_4}] + n[\wick{\c1 x_1 \c2 x_2 \c2 x_3 \c1 x_4}]
\end{aligned}
$$

Wick's theorem is proved generally in the next set of lecture notes.

3.1 Generalized Wick's Theorem

In some cases, substrings of operator strings are already in the normal product form. This will allow us to simplify the terms we need to consider for Wick's theorem.

Let's begin with an example:

$$
x_1 n[x_2x_3]
$$

Wick's theorem for x_2x_3 is

$$
x_2x_3 = n[x_2x_3] + n[\wick{\c x_2 \c x_3}]
$$

We can rearrange this as:

$$
n[x_2x_3] = x_2x_3 - n[\wick{\c x_2 \c x_3}]
$$

We can substitute this into our original expression:

$$
\begin{aligned}
x_1 n[x_2x_3] &= x_1(x_2x_3 - n[\wick{\c x_2 \c x_3}]) \\
&= x_1x_2x_3 - x_1 n[\wick{\c x_2 \c x_3}] \\
&= x_1x_2x_3 - x_1\wick{\c x_2 \c x_3} \\
&= n[x_1x_2x_3] + n[\wick{\c x_1 \c x_2}x_3] + n[\wick{\c x_1 x_2 \c x_3}] + n[x_1\wick{\c x_2 \c x_3}] - x_1\wick{\c x_2 \c x_3} \\
&= n[x_1x_2x_3] + n[\wick{\c x_1 \c x_2}x_3] + n[\wick{\c x_1 x_2 \c x_3}] + \wick{\c x_2 \c x_3}n[x_1] - x_1\wick{\c x_2 \c x_3} \\
&= n[x_1x_2x_3] + n[\wick{\c x_1 \c x_2}x_3] + n[\wick{\c x_1 x_2 \c x_3}] + x_1\wick{\c x_2 \c x_3} - x_1\wick{\c x_2 \c x_3} \\
&= n[x_1x_2x_3] + n[\wick{\c x_1 \c x_2}x_3] + n[\wick{\c x_1 x_2 \c x_3}]
\end{aligned}
$$

We observe that the contraction between the operators originally in normal ordered form cancel out in the final expression.

This is an example of the generalized Wick's theorem, which formally states:

$$x_1 \cdots x_m = n[x_1 \cdots x_m] + \sum_{a.c.}{}' n\overline{[x_1 \cdots x_m]}$$

where $\sum_{a.c.}{}'$ denotes skipping contractions of operators that originated from the same normal ordered group.

Thus, we see it is to our benefit to have as many operators as we can in normal ordered form because then we do not have to consider contractions between the normal ordered operators. The generalized Wick's theorem is proved in the next set of lecture notes.

3.2 Expectation values with Wick's theorem

In Section 2.4 we proved some rules for quickly evaluating normal products or normal products with contractions acting in the true vacuum. We have now introduced Wick's theorem (WT), which is a clever bookkeeping method to express any product of operators as normal products and normal products with contractions. We will now apply WT with the rules developed in Section 2.4 to start seeing how we can take advantage of WT when evaluating matrix elements of operator strings.

We list the four previous rules here for easy reference:

- Rule 1: $n[x_1 \cdots x_m]\,|\rangle\rangle = 0$ unless all $x_1 \cdots x_m$ are creation operators

- Rule 2: $\langle 0|n[x_1 \cdots x_m]|0\rangle = 0$ for $m \geq 1$

- Rule 3. $n[x_1 \cdots x_{i_1} \cdots x_{i_\lambda} \cdots x_{j_1} \cdots x_{j_\lambda} \cdots x_m]\,|0\rangle = 0$ if there is at least 1 uncontracted annihilator among operators $x_1 \cdots x_m$.

- Rule 4. $\langle 0|n[x_1 \cdots x_{i_1} \cdots x_{i_\lambda} \cdots x_{j_1} \cdots x_{j_\lambda} \cdots x_m]|0\rangle = 0$ unless all operators are contracted. A vacuum expectation value of any normal product with contractions will be zero if there are a odd number of operators.

We can use Rules 1–4 in conjunction with Wick's theorem to develop some more rules:

- Rule 5 $\langle 0|x_1 \cdots x_{2m+1}|0\rangle = 0$

  Proof:
  $$\langle 0|x_1 \cdots x_{2m+1}|0\rangle = \langle 0|n[x_1 \cdots x_{2m+1}]|0\rangle + \sum_{a.c.} \langle 0|n\overline{[x_1 \cdots x_{2m+1}]}|0\rangle$$
  The first term is zero by Rule 2 and the second term is zero by Rule 4

- Rule 6 $\langle 0|x_1 \cdots x_{2m}|0\rangle = \sum_{f.c.} \langle 0|\overline{\overline{n[x_1 \cdots x_{2m}]}}|0\rangle = \sum_{f.c.}(-1)^R x_{i_1} x_{j_1} \cdots x_{i_m} x_{i_m}$

  $$R = \begin{pmatrix} 1 & 2 & \cdots & 2m-1 & 2m \\ i_1 & j_1 & \cdots & i_m & j_m \end{pmatrix}$$

  Proof:
  $$\langle 0|x_1 \cdots x_{2m}|0\rangle = \langle 0|n[x_1 \cdots x_{2m}]|0\rangle + \sum_{a.c.} \langle 0|n\overline{[x_1 \cdots x_{2m}]}|0\rangle$$

The first term is 0 by Rule 2 and the second term is $\sum_{f.c.} \langle 0|\overline{\overline{n[x_1 \cdots x_{2m}]}}|0\rangle$ by Rule 4.

$$\sum_{f.c.} \langle 0|\overline{\overline{n[x_1 \cdots x_{2m}]}}|0\rangle = \sum_{f.c.} (-1)^R x_{i_1} x_{j_1} \cdots x_{i_m} x_{i_m} \langle 0|n[\varnothing]|0\rangle = \sum_{f.c.} (-1)^R x_{i_1} x_{j_1} \cdots x_{i_m} x_{i_m}$$

- Rule 7: $x_1 \cdots x_m |0\rangle = \sum_{annihilator f.c.} n\overline{[x_1 \cdots x_m]}\,|0\rangle$ where "annihilator f.c" denotes all contractions with the annihilation operator fully contracted.

  Proof:

  $$x_1 \cdots x_m |0\rangle = n[x_1 \cdots x_m]\,|0\rangle + \sum_{a.c.} n\overline{[x_1 \cdots x_m]}\,|0\rangle$$

  The first term is 0 unless it is all creation operators by Rule 1, and the second is 0 unless all annihilation operators are contracted by Rule 3.

It is not important to remember which rule you are using when applying Wick's theorem to solve problems. Rather, we are simply listing the rules to document the important consequences of Wick's theorem that allow us to take shortcuts. As long as you understand Wick's theorem and how we obtained the rules, you should be able to naturally apply them to problems.

4 Derivation of Slater's first rule using Wick's Theorem

We showed in class that using anticommutation relations to derive Slater's first rule was too much work. We could only show that Slater's rule is true for Slater determinants with a few spin orbitals, but could not prove it generally without spending a lot of tedious time. Now, with Wick's theorem, we can prove Slater's first rule generally.

$$\langle \Phi_{p_1 \cdots p_N}| \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} \langle pq|rs\rangle\, a_p^\dagger a_q^\dagger a_s a_r |\Phi_{p_1 \cdots p_N}\rangle = \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle$$

4.1 One-body operator

$$\langle \Phi_{p_1 \cdots p_N}| \sum_{pq} h_{pq} a_p^\dagger a_q |\Phi_{p_1 \cdots p_N}\rangle = \sum_{pq} h_{pq} \langle 0| a_{p_N} \cdots a_{p_1} a_p^\dagger a_q a_{p_1}^\dagger \cdots a_{p_N}^\dagger |0\rangle$$

We know from Wick's theorem that the only nonzero terms will be the fully contracted terms. Furthermore, we know that we do not have to consider contractions within normal ordered groups. Thus, we do not consider contractions within the terms in blue, orange, or red, but only contractions between the different colors.

$a_p^\dagger$ will only form nonzero contractions with $a_{p_N} \cdots a_{p_1}$, and a_q will only form nonzero contractions with $a_{p_1}^\dagger \cdots a_{p_N}^\dagger$. After forming those two contractions, the remaining terms in orange and red have to form contractions with each other. However, the only nonzero contractions that they can form are between terms with the same indices ($\underbrace{a_p a_q^\dagger} = \delta_{pq}$) This means that $a_p^\dagger$ and a_q can only form nonzero contractions if their respective orange and red contraction partners have the same indices as each other.

To summarize, the only terms in the expectation value that does not vanish are ones in which the operators in blue are contracted with orange and red operators with the same indices (a_{p_i} and $a_{p_i}^\dagger$), and the remaining orange and red operators form contractions between operators with the same indices. There will be N contractions that can be formed, since the operators in blue can form contractions with any operators in the red and orange set as long as the red and orange operators have the same indices.

We can express this in the following way:

$$\langle \Phi|\hat{O}_1|\Phi\rangle = \sum_{pq} h_{pq} \sum_i^N \langle 0| a_{p_N} \cdots a_{p_i} \cdots a_{p_1} a_p^\dagger a_q a_{p_1}^\dagger \cdots a_{p_i}^\dagger \cdots a_{p_N}^\dagger |0\rangle$$

We notice 2 things:

1. The number of intersecting contraction lines will always be even, and so the phase factor to move all contractions out of the expectation value is positive.

2. The contractions $a_j a_j^\dagger = \delta_{jj}$ will collapse to products of 1 for all j.

This means we are left with:

$$\begin{aligned}
\langle \Phi | \hat{O}_1 | \Phi \rangle &= \sum_i^N \sum_{pq} h_{pq} \delta_{pp_i} \delta_{qp_i} \langle 0|0 \rangle \\
&= \sum_i^N h_{p_i p_i} \quad \text{or just} \\
&= \sum_i^N h_{ii}
\end{aligned}$$

4.2 Two-body operator

$$\langle \Phi_{p_1 \cdots p_N} | \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \, a_p^\dagger a_q^\dagger a_s a_r | \Phi_{p_1 \cdots p_N} \rangle = \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \, \langle 0 | a_{p_N} \cdots a_{p_1} a_p^\dagger a_q^\dagger a_s a_r a_{p_1}^\dagger \cdots a_{p_N}^\dagger |0\rangle$$

In a similar manner as before, we are limited in the nonzero contractions we can form. Operators a_s and a_r can form contractions with $a_{p_i}^\dagger$ and $a_{p_j}^\dagger$, and operators $a_p^\dagger$ and $a_q^\dagger$ can form contractions with a_{p_i} and a_{p_j}. There are four total combinations of contractions between these 8 operators. The remaining uncontracted operators will form contractions between operators with the same indices and collapse to products of 1. We will write the four types of contractions that can formed (contractions between red and orange operators assumed and not written explicitly):

$$\begin{aligned}
\langle \Phi_{p_1 \cdots p_N} | \hat{O}_2 | \Phi_{p_1 \cdots p_N} \rangle &= \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \sum_{i<j} \langle 0 | \cdots a_{p_j} \cdots a_{p_i} \cdots a_p^\dagger a_q^\dagger a_s a_r \cdots a_{p_i}^\dagger \cdots a_{p_j}^\dagger \cdots |0\rangle \\
&+ \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \sum_{i<j} \langle 0 | \cdots a_{p_j} \cdots a_{p_i} \cdots a_p^\dagger a_q^\dagger a_s a_r \cdots a_{p_i}^\dagger \cdots a_{p_j}^\dagger \cdots |0\rangle \\
&+ \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \sum_{i<j} \langle 0 | \cdots a_{p_j} \cdots a_{p_i} \cdots a_p^\dagger a_q^\dagger a_s a_r \cdots a_{p_i}^\dagger \cdots a_{p_j}^\dagger \cdots |0\rangle \\
&+ \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \sum_{i<j} \langle 0 | \cdots a_{p_j} \cdots a_{p_i} \cdots a_p^\dagger a_q^\dagger a_s a_r \cdots a_{p_i}^\dagger \cdots a_{p_j}^\dagger \cdots |0\rangle \\
&= \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \sum_{i<j} \left[\delta_{pp_i} \delta_{qp_j} \delta_{rp_i} \delta_{sp_j} - \delta_{pp_j} \delta_{qp_i} \delta_{rp_i} \delta_{sp_j} - \delta_{pp_i} \delta_{qp_j} \delta_{rp_j} \delta_{sp_i} + \delta_{pp_j} \delta_{qp_i} \delta_{rp_j} \delta_{sp_i} \right] \\
&= \frac{1}{2} \sum_{i<j} \left[\langle p_i p_j | p_i p_j \rangle - \langle p_j p_i | p_i p_j \rangle - \langle p_i p_j | p_j p_i \rangle + \langle p_j p_i | p_j p_i \rangle \right] \\
&= \frac{1}{2} \sum_{i<j} 2 \left[\langle p_i p_j | p_i p_j \rangle - \langle p_i p_j | p_j p_i \rangle \right] \\
&= \frac{1}{2} \sum_{ij} \frac{1}{2} (2) \left[\langle p_i p_j | p_i p_j \rangle - \langle p_i p_j | p_j p_i \rangle \right] \\
&= \frac{1}{2} \sum_{ij} \langle p_i p_j || p_i p_j \rangle \quad \text{or just} \\
&= \frac{1}{2} \sum_{ij} \langle ij || ij \rangle
\end{aligned}$$