NOTES ON WICK’S THEOREM IN MANY-BODY THEORY

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I. INTRODUCTION

For bosons and fermions, destruction and creation operators of a particle in a state \(|i⟩\) annihilate the vacuum: \(\psi_i|\text{vac}⟩\) and \(⟨\text{vac}|\psi_i^†⟩ = 0\). Since observables have null expectation value in the vacuum state, it is convenient to construct them with creation operators on the left of destruction operators (normal order).

In a many body theory one usually makes reference to the ground state \(|gs⟩\) of some non-interacting or effective theory, which is filled with particles or quasi-particles. The theory is also supplied with a basis of canonical operators \(α_a, α_b^+: a, b = 1, 2, \ldots\)

\[
[α_a, α_b^+]_ν = 0, \quad [α_a^+, α_b^+]_ν = 0 \quad [α_a, α_b^+]_ν = δ_{ab}
\]

\(\prod [a, b]_ν = ab \mp ba\) that annihilate the reference state:

\[α_a|gs⟩ = 0, \quad ⟨gs|α_a^+ = 0. \quad (1)\]

Since they are a basis, operators \(ψ_i\) or \(ψ_i^†\), which will be here indifferently denoted as \(A_i\), have a decomposition

\[A_i = A_i^- + A_i^+\]

where the first term is a combination of operators \(α_a\), and the latter is a combination of operators \(α_a^+\). One term is not the adjoint of the other: the labels \(-\) and \(+\) refer to their action on the reference state \(|gs⟩\):

\[A_i^-|gs⟩ = 0, \quad ⟨gs|A_i^+ = 0 \quad (3)\]

Since the operators \(α_a\) and \(α_a^+\) are canonical, by construction one has

\[A_i^+A_i^- = 0, \quad [A_i^+, A_j^-]_ν = 0 \quad (4)\]

while mixed brackets \([A_i^+, A_j^+]_ν\) are in general non-zero. We require them to be c-numbers\footnote{since \([α_a, α_b^+]_ν = δ_{ab}\), this is certainly true if the operators \(A^±\) are linear combinations of the \(α_a^±\).}. This is a vital assumption, which makes the Wick’s theorem hold.

In a many particle theory one encounters the problem of expanding products of several field operators into normal-ordered expressions of the operators \(α_a\) and \(α_a^+\). The general problem of bringing products of field operators into a normal form was solved in 1950 by Gian Carlo Wick \(\Pi\) (1909-1992). He obtained his theorem while in Berkeley, in the effort to give a clear derivation of Feynman’s diagrammatic rules of perturbation theory.

II. EXAMPLES

The Hamiltonians in the examples below share a common property: they are all quadratic. They are diagonalized by a linear canonical transformation which assures us that \([A_i^+, A_j^-]_ν\) are c-numbers.

A. Independent fermions

This example is relevant for the perturbation theory with \(N\) interacting fermions. In the zero order description, the two-particle interaction is turned off and the independent fermions are described by a Hamiltonian of the form \(H = \sum_a \hbar \omega_a c_a^† c_a\) (\(a\) is a label for one-particle states, ordered so that \(\omega_1 ≤ ω_2 ≤ \ldots\)). The ground state \(|F⟩\) is obtained by filling the states \(a = 1 \ldots N\). The operators that annihilate \(|F⟩\) are:

\[
α_a = \begin{cases} 
    c_a^† & \text{if } a ≤ N, \\
    c_a & \text{if } a > N
\end{cases}, \quad α_a|F⟩ = 0 \quad (5)
\]

\[
α_a^+ = \begin{cases} 
    c_a & \text{if } a ≤ N, \\
    c_a^† & \text{if } a > N
\end{cases}, \quad (F|α_a^+ = 0 \quad (6)
\]

\(α_a^+\) creates a particle (above the Fermi level) or creates a hole (by removing a particle in the “Fermi sea” \(|F⟩\); \(α_a\) destroys a particle above the Fermi sea, or destroys a hole (by adding a particle in the Fermi sea). These particle-hole operators form a CAR. Any destruction or creation operator admits a decomposition in this basis into positive and negative parts:

\[
ψ_i = \sum_{a≤N} (i|a) c_a + \sum_{a>N} (i|a) c_a^†
\]

\[
= \sum_{a≤N} (i|a) α_a^+ + \sum_{a>N} (i|a) α_a = ψ_i^+ + ψ_i^-
\]

\[
ψ_i^† = \sum_{a≤N} (i|a) c_a^† + \sum_{a>N} (i|a) c_a = (ψ_i^†)^- + (ψ_i^†)^+
\]

with \((ψ_i^†)^- = (ψ_i^†)^-\) and \((ψ_i^†)^+ = (ψ_i^†)^+.\)

B. Bogoliubov transformation

In this example \(|gs⟩\) is the ground state \(|BCS⟩\) of the superconducting state at \(T = 0\) (Bardeen, Cooper and Schrieffer, 1957). It is filled of Cooper pairs of electrons
(spin singlets, with zero total momentum),

$$|BCS⟩ = \prod_k (u_k + v_k a_k^\dagger a_{-k,\downarrow}^\dagger) |\text{vac}\rangle$$

$u_k$ and $v_k$ are complex amplitudes, with $|u_k|^2 + |v_k|^2 = 1$ for the normalization of the state. The state is not an eigenstate of the total number operator. It is annihilated by the following operators (Bogoliubov and Valatin, 1958):

$$\alpha_k = u_k a_k^\dagger - v_k a_{-k,\downarrow}^\dagger, \quad \beta_{-k} = u_k a_{-k,\downarrow}^\dagger + v_k a_k^\dagger$$

$$\alpha_k |BCS⟩ = 0, \quad \beta_{-k} |BCS⟩ = 0$$

Together with their adjoint operators,

$$\langle BCS|\alpha_k^\dagger = 0 \quad \langle BCS|\beta_{-k}^\dagger = 0$$

they satisfy the CAR rules. They are obtained by a canonical transformation that mixes creation and destruction operators for spin-momentum states, in a way adapted to the BCS state.

Inversion gives the operators $\alpha_{k,\sigma}$ and $\alpha_{-k,\sigma}^\dagger$ as sums of a $-\sigma$ term (linear combination of $\alpha$ and $\beta$) and a $+\sigma$ term (linear combination of $\alpha^\dagger$ and $\beta^\dagger$ operators). Note that, although $\langle \alpha_{k,\sigma} \rangle = 0$, BCS-expectation values of pairs $aa$ or $a^\dagger a^\dagger$ may be different from zero (anomalous correlators).

The variational parameters $u_k$ and $v_k$ of $|BCS⟩$ are chosen to minimize the ground state energy $\langle H \rangle$. The evaluation is simplified by Wick’s theorem [2], which is proven in section III.

C. Independent Bosons

For independent bosons the ground state $|BEC⟩$ is a Bose-Einstein condensate $N$ particles in the lowest energy state, $a = 1$, and no particles in higher one-particle states, at $T = 0$. Since $\langle BEC|c_{1,\uparrow}c_{1,\downarrow}|BEC⟩ = N$, Bogoliubov suggested the rescaling $c_{1} = \sqrt{V}b$ and $c_{1}^\dagger = \sqrt{V}b^\dagger$, the other operators being left unchanged. Then

$$[b, b^\dagger] = \frac{1}{V}, \quad \langle BEC|b^\dagger b|BEC⟩ = \frac{N}{V}.$$ 

The operators $b$ and $b^\dagger$ may be treated as c-numbers in the thermodynamic limit [4], with $|b|^2 = N/V$. For any creation and destruction operator, one has the decomposition into a condensate term, and an excitation term:

$$\psi_n = \sum_a \langle i|α_a \rangle c_a^\dagger \sqrt{V}b + φ_i,$$

$$\psi_i^\dagger = \sum_a \langle i|α^\dagger_a \rangle c_a^\dagger \sqrt{V}b^\dagger + φ_i^\dagger$$

where $φ_i|BEC⟩ = 0$ and $⟨BEC|φ_i^\dagger⟩ = 0$.

III. NORMAL ORDERING AND CONTRACTIONS

A product of operators $A_i^\pm$ is normally ordered if all factors $A_i^−$ are at the right of the factors $A_i^+$:

$$A_i^+ \cdots A_k^+ A_{k+1}^- \cdots A_n^-$$

In particular, a product of operators of the same type, $A_i^+ \cdots A_k^+ \sqrt{V}$ or $A_i^- \cdots A_k^-$, is normally ordered. The very usefulness of the definition is the obvious property that the expectation value on $⟨gs⟩$ of a normally ordered operator is always zero:

$$⟨gs|A_i^+ \cdots A_n^-|gs⟩ = 0$$

It is clear that any product of operators $A_1 A_2 \ldots A_n$ can be written as a sum of normally ordered terms. One first writes every factor as $A_i^+ + A_i^−$ and gets $2^n$ terms. In each term, the components $A_i^−$ are brought to the right by successive commutations (bosons) or anticommutations (fermions). After much boring work, the desired expression will be obtained. Wick’s theorem is an efficient answer to this precise problem: to write a product $A_1 \ldots A_n$ as a sum of normally ordered terms. The theorem is an extremely useful operator identity, with important corollaries. To state and prove it, we need some technical tools.

The normal ordering operator brings a generic product into a normal form. If the product contains $k$ factors $A_i^+$ mixed with $n - k$ factors $A_i^-$, it is:

$$N[A_i^+ \cdots A_k^+] = (±1)^P A_i^+ \cdots A_k^+ A_k^− \cdots A_n^-$$

where for bosons $(±)^P = 1$, while for fermions $(−1)^P$ is the parity of the permutation that brings the sequence $1 \ldots n$ to the sequence $i_1 \ldots i_n$ (another frequently used notation for normal ordering is $A_i^+ \cdots A_k^+$).

It may appear that normal ordering is not unique, since within $+$ operators or $-$ operators one can choose different orderings. However the different expressions are actually the same operator, because $A^+$ operators commute or anticommute exactly among themselves, and the same is for $−$ operators. For example $N[A_1 A_2 A_3^+]$ can be written as $A_1^+ A_2^+ A_3^−$, or with the factors exchanged: $±A_2^+ A_1^+ A_3^−$: the two operators coincide.

The action of $N$-ordering is extended by linearity from products of components $A_i^±$ to products of operators $A_i$. For example:

$$N[A_1 A_2] = N[A_1^- A_2^-] (A_2^+ + A_2^-)$$

$$= N[A_1^+ A_2^+] + N[A_1^+ A_2^-] + N[A_1^- A_2^+] + N[A_1^- A_2^-]$$

$$= A_1^+ A_2^+ + A_1^- A_2^- + A_1^+ A_2^- \pm A_2^+ A_1^-.$$ 

The following property follows from [14]:

$$N[A_1 \cdots A_n] = (±1)^P N[A_{i_1} \cdots A_{i_n}]$$

A product $A_1 \ldots A_n$ can be written as a sum of normally ordered terms. For two operators the process is
straightforward:

$$A_1 A_2 = (A_1^+ + A_1^-) (A_2^+ + A_2^-)$$
$$= A_1^+ A_2^+ + A_1^+ A_2^- + A_1^- A_2^+ + A_1^- A_2^-$$
$$= N[A_1 A_2] + [A_1^-, A_2^+]$$  

(16)

The last term $[A_1^-, A_2^+] = 0$, it follows that

**Lemma IV.1.**

A contraction, denoted by a bracket, of two operators is defined as

$$\overrightarrow{A_1 A_2} = A_1 A_2 - N[A_1 A_2]$$  

(17)

Combining the contraction definition with (16) yields

$$\overrightarrow{A_1 A_2} = [A_1^-, A_2^+]_\pm.$$  

(18)

Also, since the $gs$-expectation value of a normal ordered operator is zero, it follows that

$$\overrightarrow{A_1 A_2} = \langle gs | \overrightarrow{A_1 A_2} | gs \rangle = \langle gs | A_1 A_2 | gs \rangle$$  

(19)

The following definition extends the contraction of two operators to the case where there is a product of $n$ operators in between:

$$\overrightarrow{A(A_1 \cdots A_n)A'} = (\pm 1)^n \overrightarrow{A'}(A_1 \cdots A_n)$$  

(20)

**IV. Wick’s Theorem**

We begin by proving three Lemmas - each one is a generalization of the former. In the first one, a single $A^-$ operator is at the left of $A^+$ operators, and normal ordering is achieved by bringing it to the right of them by repeated (anti)commutations.

**Lemma IV.1.**

$$A_0^+(A_1^+ \cdots A_n^+)^n = N[A_0^- A_1^- \cdots A_n^-] + \sum_{i=1}^n N[A_0 \cdots \hat{A_i} \cdots A_n^-]$$  

(21)

**Proof.**

$$A_0^+(A_1^+ \cdots A_n^+)^n = \langle [A_0^-, A_1^+]_\pm \cdots [A_0^-, A_n^+]_\pm \rangle + A_0^+ A_1^+ \cdots A_n^+ + A_0^+ A_1^- A_2^+ \cdots A_n^+ + A_0^+ A_1^- A_2^- A_3^+ \cdots A_n^+ + \cdots$$

$$= \sum_{i=1}^n A_0^+ A_1^+ \cdots \hat{A_i} \cdots A_n^+ + (\pm 1)^n A_1^+ \cdots A_n^+ A_0^-$$

$$= N[A_0^- A_1^- \cdots A_n^-] + \sum_{i=1}^n N[A_0 \cdots \hat{A_i} \cdots A_n^-].$$

**Lemma IV.2.**

$$A_0^+ N[A_1 \cdots A_n] = N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^n N[A_0 \cdots \hat{A_i} \cdots A_n^-].$$  

(22)

**Proof.** The proof is by induction. Eq. (22) holds for $n = 1$. If, by hypothesis, it holds for $n$ operators, it is now proven for $n + 1$ operators (we write $1^k$ in place of $A_1^+$):

$$0^{-1} N[\cdots (n + 1)]$$

$$= 0^{-1} N[\cdots (n + 1)] + (\pm 1)^0 0^{-1} N[\cdots (n + 1)]$$

$$= 0^{-1} N[\cdots (n + 1)] + (\pm 1)^0 0^{-1} N[\cdots (n + 1)]$$

$$= N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^n N[A_i \cdots A_n^-].$$

The hypothesis of induction is now used in the second and third terms:

$$= N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^n N[A_i \cdots A_n^-]$$

$$= N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^n N[A_i \cdots A_n^-]$$

$$= N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^n N[A_i \cdots A_n^-]$$

The last line is (22) with $n + 1$ operators.

**Lemma IV.3.**

$$A_0 N[A_1 \cdots A_n] = N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^n N[A_0 \cdots \hat{A_i} \cdots A_n^-].$$  

(23)

**Proof.** This is achieved by adding $A_0^+ N[A_1 \cdots A_n]$ to both sides of Lemma IV.2.

Wick’s theorem gives the practical rule to express a product of creation and destruction operators as a sum of normally ordered terms. It is an operator identity. Each contraction, being a c-number, reduces by two the operator content.
**Theorem IV.4** (Wick’s Theorem).

\[
A_1 A_2 \cdots A_n = N[A_1 \cdots A_n] + \sum_{(ij)} N[A_1 \cdots A_i A_j \cdots A_n] + \sum_{(ij)(rs)} N[A_1 \cdots A_i A_r A_j A_s \cdots A_n] + \cdots
\]

(24)

The first sum runs on single contractions of pairs, the second sum runs on double contractions, and so on. If \( n \) is even, the last sum contains terms which are products of contractions (c-numbers). If \( n \) is odd, the last sum has terms with single unpaired operators (see examples).

**Proof.** The theorem is proven by induction. For \( n = 2 \) it is true. Next, suppose that the statement is true for a product of creation/destruction operators \( A_0 A_1 \cdots A_n \); it is shown that it is true for a product \( A_0 A_1 \cdots A_n \).

By hypothesis of induction for \( n \) operators:

\[
A_1 A_2 \cdots A_n = \sum_{k=0}^{n/2} N_{n,k}
\]

(25)

where \( N_{n,k} \) is the sum of normally ordered products of \( n \) operators with \( k \) contractions. By Lemma 4.3,

\[
A_0 N_{n,k} = N[A_0 N_{n,k}] + N[A_0 N_{n,k}].
\]

(26)

where \( \overrightarrow{N_{n,k}} \) means the sum of all contractions of \( A_0 \) with unpaired operators \( A_i \) contained in \( N_{n,k} \). The following relation takes place:

\[
N[A_0 N_{n,k}] + N[A_0 N_{n,k+1}] = N_{n+1,k+1}.
\]

(27)

Using the induction hypothesis and the last two identities we find,

\[
A_0 A_1 \cdots A_n = A_0 N_{n,0} + A_0 N_{n,1} + A_0 N_{n,2} + \cdots
\]

\[= N[A_0 N_{n,0}] + N[A_0 N_{n,1}] + N[A_0 N_{n,1}] + N[A_0 N_{n,1}] + N[A_0 N_{n,2}] + \cdots
\]

\[= N_{n+1,0} + N_{n+1,1} + \cdots
\]

which expresses Wick’s theorem for \( n + 1 \) operators. \( \Box \)

**Example IV.5.**

\[
A_1 A_2 A_3
\]

\]

\[= N[123] + (12) A_3 \pm (13) A_2 + (23) A_1
\]

(28)

Understanding Wick’s theorem is a rule for the expectation value of the product of even number of destruction and creation operators:

**Corollary IV.6.**

\[
\langle gs | A_1 \cdots A_{2n} | gs \rangle = \sum (\pm 1)^P \langle A_{i_1} A_{j_1} \cdots A_{i_n} A_{j_n} \rangle
\]

(30)

The sum is over all partitions of 1, \ldots, 2n into pairs \( \{(i_1, j_1), \ldots, (i_n, j_n)\} \) with \( i_\# < j_\# \). \( P \) is the permutation that takes 1, \ldots, 2n to the sequence \( i_1, j_1, \ldots, i_n, j_n \).

**Example IV.7.**

\[
\langle gs | 123 | gs \rangle = 0
\]

(31)

\[
\langle gs | 1234 | gs \rangle = (12) \langle 34 \rangle \pm (13) \langle 24 \rangle + (14) \langle 23 \rangle
\]

(32)

This is a general rule: two-point correlators determine all n-point correlators.

In thermal theory there is no distinguished state to define a normal ordering, and thus no Wick’s theorem in the form of an operator identity. Nevertheless, one can prove a thermal analogue of the corollary: for non-interacting particles: the thermal average of a product of one-particle creation and destruction operators is the sum of all possible thermal contractions of pairs. The thermal contraction of two operators is the thermal average of their product.\[4 \[3 \].

**V. WICK’S THEOREM WITH TIME-ORDERING**

An important variant of Wick’s theorem deals with the normal-ordering of a time-ordered product. A necessary condition is that the time evolution of the operators \( \alpha_q \) and \( \alpha^+_q \) is a multiplication by some time-dependent phase factor (c-number). Then, the discussion on normal ordering and contraction of operators \( A_i(t_i) \) remains unaltered.
A. T-contractions

Let us begin with two operators, and apply Wick’s theorem:

\[ T A_1(t_1) A_2(t_2) \]
\[ = \theta(t_1 - t_2) \{ N[A_1(t_1) A_2(t_2)] + A_1(t_1) A_2(t_2) \} \]
\[ \pm \theta(t_2 - t_1) \{ N[A_2(t_2) A_1(t_1)] + A_2(t_2) A_1(t_1) \} \]
\[ = \theta(t_1 - t_2) N[A_1(t_1) A_2(t_2)] + \theta(t_2 - t_1) N[A_1(t_1) A_2(t_2)] \]
\[ + \theta(t_1 - t_2) A_1(t_1) A_2(t_2) \pm \theta(t_2 - t_1) A_1(t_1) A_2(t_2) \]
\[ = N[A_1(t_1) A_2(t_2)] + A_1(t_1) A_2(t_2) \] (33)

The last term is a c-number. We define the time-ordered contraction (T-contraction):

\[ A_1(t_1) A_2(t_2) = \langle gs | T A_1(t_1) A_2(t_2) | gs \rangle \] (34)

The T-contraction of two operators with a product of n operators in between inherits the property of ordinary contractions

\[ A_1(t_1) \cdots A_2(t_2) = (\pm 1)^n A_1(t_1) A_2(t_2) \cdots \] (35)

T-contractions have a new property, not shared by an ordinary contraction:

\[ A_1(t_1) A_2(t_2) = \pm A_2(t_2) A_1(t_1) \] (36)

For field operators we have the explicit expressions:

\[ \psi(1) \psi^\dagger(2) = \langle T \psi(1) \psi^\dagger(2) \rangle = iG^0(1, 2) \] (37)
\[ \psi(1) \psi(2) = \langle T \psi(1) \psi(2) \rangle = iF^0(1, 2) \] (38)
\[ \psi^\dagger(1) \psi^\dagger(2) = \langle T \psi^\dagger(1) \psi^\dagger(2) \rangle = iF^{\dagger0}(1, 2) \] (39)

If |gs⟩ has a definite number of particles, the anomalous correlators \( F^0 \) and \( F^{\dagger0} \) are equal to zero. They are non-zero in the BCS theory.

B. Wick’s theorem for time-ordered products

For the time-ordered product of several operators, Wick’s theorem retains the same structure as in (24), with T-contractions replacing ordinary ones. The statement is:

**Theorem V.1** (Wick’ theorem, with time-ordering).

\[ T[A_1(t_1) \cdots A_n(t_n)] = N[A_1(t_1) \cdots A_n(t_n)] \] (40)
\[ + \sum_{(ij)} N[A_1(t_1) \cdots A_i(t_i) \cdots A_j(t_j) \cdots A_n(t_n)] \]
\[ + \sum N[ \cdots \text{double T-contractions} \cdots ] \]
\[ + \cdots \]

Proof. \( T(1 \cdots n) \) corresponds to a time ordered sequence (±1)\(^P\)\(_{i_1 \cdots i_n}\) (we put \( i = A_i(t_i) \)), to which the previous formulation of Wick’s theorem applies:

\[ T[12 \cdots n] = (\pm 1)^P N[i_1 \cdots i_n] \]
\[ + (\pm 1)^P \sum_{(ij)} N[i_1 \cdots i \cdots j \cdots i_n] \]
\[ + (\pm 1)^P \sum_{(ij)(rs)} N[i_1 \cdots i \cdots j \cdots s \cdots i_n] \]
\[ + \cdots \]

The factor \((\pm 1)^P\) is compensated by restoring the sequence 1 \cdots n inside the normal ordering. Then the first term is \( N[1 \cdots n] \). In doing so, a contraction \( ij \) remains unaltered if \( i_t > t_j \) otherwise it is twisted to \( ji \) (\( j \) precedes \( i \) in the sequence 1 \cdots n). Therefore:

\[ (\pm 1)^P N[i_1 \cdots i \cdots j \cdots i_n] = N[1 \cdots i \cdots j \cdots n] \]

As an interesting application, consider an n-particle Green function

\[ i^n G(x_1, \ldots, x_n, y_1, \ldots, y_n) = (gs | T \psi(x_1) \cdots \psi(x_n) \psi(y_1) \cdots \psi(y_n) | gs) \] (41)

where \( x \) denotes a complete set of quantum numbers and time (the Heisenberg evolution with the Hamiltonian whose ground state is \( |gs⟩ \)). For independent particles, Wick’s theorem applies. The average is evaluated as a sum of total T-contractions of field operators, i.e. propagators (we now exclude anomalous propagators):

\[ G^0(x_1, \ldots, x_n, y_1, \ldots, y_n) = \sum_P (\pm 1)^P G^0(x_1, y_{i_1}) \cdots G^0(x_n, y_{i_n}) \] (42)

where \( P \) is the permutation \( P(1 \cdots n) = (i_1 \cdots i_n) \). The sum corresponds to the evaluation of the permanent (bosons) or determinant (fermions) of the matrix \( G^0(x_i, x_j) \), \( i, j = 1, \ldots, n \).

**Remark V.2.** A free theory is a many-particle theory where, in some basis, n-particle Green functions are determined solely by one-particle Green functions.

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**REFERENCES**

