WICK THEOREM AT FINITE T

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1. Static Wick theorem

Let $K_0 = \sum_r (\epsilon_r - \mu) c_r^\dagger c_r$. The "static" Wick theorem evaluates the thermal average of a product of creation and destruction operators of any state and in any order

$$\langle \psi_1 ... \psi_N \rangle = \mathrm{tr} \left[\frac{e^{-\beta K_0}}{Z_0} \psi_1 ... \psi_N \right]$$

• $\langle \psi_1 \psi_2 \dots \psi_N \rangle = 0$ if the number of creation operators is not equal to the number of destruction operators (in particular it is zero if N is odd).

• The τ-evolution of c_r and $c_r^\dagger$ is $c_r(\tau) = e^{-\frac{1}{\hbar}(\epsilon_r - \mu)\tau} c_r$ and $c_r^\dagger(\tau) = e^{+\frac{1}{\hbar}(\epsilon_r - \mu)\tau} c_r^\dagger$. In particular, with $\tau = \hbar\beta$ we obtain the useful relations

$$c_r e^{-\beta K_0} = e^{-\beta(\epsilon_r - \mu)} e^{-\beta K_0} c_r, \qquad c_r^\dagger e^{-\beta K_0} = e^{+\beta(\epsilon_r - \mu)\tau} e^{-\beta K_0} c_r^\dagger \tag{1}$$

Lemma 1. *Let $C_1 ... C_N$ be any choice of N (even) destruction and creation operators in the set c_r, $c_r^\dagger$. Then*

$$\langle C_1 C_2 \dots C_N \rangle = \sum_{k=2}^{N} \langle \overbracket{C_1 C_2 \dots C_k} \dots C_N \rangle \tag{2}$$

where the contraction is $\overbracket{C_1 C_k} = \langle C_1 C_k \rangle$.

Proof. The strategy is to bring C_1 to the right of C_N by repeated (anti)commutations (we use the same parenthesis). Then, by the cyclic property of the trace, C_1 is brought to the left of $e^{-\beta K_0}$. By means of the relations (**??**) C_1 and the state are exchanged, to obtain the initial correlator times a factor.

$$\begin{aligned} \langle C_1 C_2 \dots C_N \rangle &= \langle [C_1, C_2] C_3 \dots C_N \rangle \pm \langle C_2 C_1 C_3 \dots C_N \rangle \\ &= \langle [C_1, C_2] C_3 \dots C_N \rangle \pm \langle C_2 [C_1, C_3] \dots C_N \rangle + \langle C_2 C_3 C_1 \dots C_N \rangle \end{aligned}$$

The process continues until we reach C_N:

$$\begin{aligned} = \langle [C_1, C_2] C_3 \dots C_N \rangle &\pm \langle C_2 [C_1, C_3] C_4 \dots C_N \rangle + \langle C_2 C_3 [C_1, C_4] \dots C_N \rangle \\ \dots \quad &+ \langle C_2 C_3 C_4 \dots [C_1, C_N] \rangle \pm \langle C_2 C_3 \dots C_N C_1 \rangle \end{aligned}$$

The last term is $\langle C_2 \dots C_N C_1 \rangle = e^{\mp\beta(\epsilon_1 - \mu)} \langle C_1 C_2 \dots C_N \rangle$, where the upper sign refers to C_1 being a destruction operator, and the lower sign for a creator. Then:

$$\langle C_1 C_2 \dots C_N \rangle = \frac{1}{1 \mp e^{\mp\beta(\epsilon_1 - \mu)}} \Big[\langle [C_1, C_2] C_3 \dots C_N \rangle \pm ... + \langle C_2 C_3 \dots [C_1, C_N] \rangle \Big]$$

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Now we define the contraction of two operators (a c-number!):

$$\overbracket{C_r C_s} = \frac{[C_r, C_s]_\mp}{1 \mp e^{\mp\beta(\epsilon_r - \mu)}} = \langle C_r C_s \rangle \tag{3}$$

The contraction is extended to the case of p operators between:

$$\overbracket{C_r C_1 \dots C_p C_s} = (\pm 1)^p \overbracket{C_r C_s} C_1 \dots C_p \tag{4}$$

With this definition, the result follows. □

The non-zero contractions are:

$$\overbracket{c_r^\dagger c_s} = \frac{\delta_{rs}}{e^{+\beta(\epsilon_r - \mu)} \mp 1} = \delta_{rs} n_r \tag{5}$$

$$\overbracket{c_r c_s^\dagger} = \frac{\delta_{rs}}{1 \mp e^{-\beta(\epsilon_r - \mu)}} = \delta_{rs}(1 \pm n_r) \tag{6}$$

Since any operator ψ is a linear combination of operators c_r, and $\psi^\dagger$ is a linear combination of operators $c_r^\dagger$, the lemma extends by linearity to generic products of destruction and creation operators:

$$\langle \psi_1 \psi_2 \dots \psi_N \rangle = \sum_{k=2}^{N} \langle \overbracket{\psi_1 \psi_2 \dots \psi_k} \dots \psi_N \rangle \tag{7}$$

where the non-zero contractions are:

$$\overbracket{\psi_j^\dagger \psi_k} = \langle \psi_j^\dagger \psi_k \rangle \qquad \overbracket{\psi_j \psi_k^\dagger} = \langle \psi_j \psi_k^\dagger \rangle \tag{8}$$

The lemma gives a sum of terms with a single contraction; each term contains two less operators. By applying the lemma repeatedly to each term, the reduction comes to an end. The result is the static Wick theorem:

Theorem 2. *The thermal average of an equal number of creation and destruction operators is the sum on all possible contractions of all pairs in the product. The contraction of a pair is the thermal average of the pair.*

In this variant of the lemma, the pivot C_k is an operator not in first position.

Lemma 3. *For N even:*

$$\langle C_1 \dots C_N \rangle = \sum_{j=1}^{k-1} \langle C_1 \dots \overbracket{C_j \dots C_k} \dots C_N \rangle + \sum_{j=k+1}^{N} \langle C_1 \dots \overbracket{C_k \dots C_j} \dots C_N \rangle \tag{9}$$

Proof. By the KMS property we bring C_k in first position. Let $D_j = C_j(-\hbar\beta)$:

$$\begin{aligned} &\langle C_1 \dots C_k \dots C_N \rangle = \langle C_k \dots C_N D_1 \dots D_{k-1} \rangle \\ &= \sum_{j=k+1}^{N} \langle \overbracket{C_k \dots C_j} \dots C_N D_1 \dots D_{k-1} \rangle + \sum_{j=1}^{k-1} \langle \overbracket{C_k \dots C_N D_1 \dots D_j} \dots D_{k-1} \rangle \end{aligned}$$

The first sum is $\sum_{j=k+1}^{N} \langle C_1 \dots C_{k-1} \overbracket{C_k \dots C_j} \dots C_N \rangle$. A term in the other sum is:

$$\langle \overbracket{C_k \dots C_N D_1 \dots D_j} \dots D_{k-1} \rangle = \langle C_{j+1} \dots C_{k-1} \overbracket{C_k \dots C_N D_1 \dots D_j} \rangle$$

The $Q = j-1+N-k$ operators between C_k and D_j are taken out of the contraction and the KMS property is used:

$$= (\pm 1)^Q \langle C_1 \dots C_{j-1} C_{j+1} \dots C_{k-1} \overbracket{C_k D_j} C_{k+1} \dots C_N \rangle$$

Note that $\overbracket{C_k D_j} = \langle C_k C_j(-\hbar\beta)\rangle = \langle C_j C_k \rangle = \overbracket{C_j C_k}$ by the KMS property. Then:

$$= (\pm 1)^Q \langle C_1 \dots C_{j-1} C_{j+1} \dots C_{k-1} \overbracket{C_j C_k} C_{k+1} \dots C_N \rangle$$

$$= (\pm 1)^{Q+P} \langle C_1 \dots C_{j-1} \overbracket{C_j C_{j+1} \dots C_{k-1} C_k} C_{k+1} \dots C_N \rangle$$

where $P = N - j + k - 1$. Then $P + Q = 2(N-1)$, which is even. □

Example 4. (free fermions)

$$\begin{aligned}\langle a^\dagger_{\mathbf{k+q}\mu} a^\dagger_{\mathbf{p-q}\nu} a_{\mathbf{p}\nu} a_{\mathbf{k}\mu}\rangle =& \langle a^\dagger_{\mathbf{k+q}\mu} a_{\mathbf{k}\mu}\rangle \langle a^\dagger_{\mathbf{p-q}\nu} a_{\mathbf{p}\nu}\rangle - \langle a^\dagger_{\mathbf{k+q}\mu} a_{\mathbf{p}\nu}\rangle \langle a^\dagger_{\mathbf{p-q}\nu} a_{\mathbf{k}\mu}\rangle \\ =& \delta_{\mathbf{q},\mathbf{0}} n_k n_p - \delta_{\mu\nu}\delta_{\mathbf{q},\mathbf{p-k}} n_k n_p\end{aligned}$$

In particular, for the HEG it is: $\langle U_{ee}\rangle = -\frac{1}{V}\sum_{\mathbf{kp}} \frac{4\pi e^2}{|\mathbf{k-p}|^2} n_k n_p$.

Example 5. $\langle n_r n_s \rangle = \langle c^\dagger_r c_r c^\dagger_s c_s \rangle = n_r n_s + \langle c^\dagger_r c_s\rangle\langle c_r c^\dagger_s\rangle = n_r n_s + \delta_{rs} n_r (1 \pm n_r)$. In particular:

$$\langle n_r^2 \rangle - \langle n_r \rangle^2 = n_r(1 \pm n_r) = \frac{e^{\beta(\epsilon_r - \mu)}}{(e^{\beta(\epsilon_r-\mu)} \mp 1)^2} = -\frac{1}{\beta}\frac{\partial n_r}{\partial \epsilon_r}$$

2. T-ordered wick theorem

With generator K_0 the τ-evolution of the operators c_r and $c^\dagger_r$ is a c-factor. We define the T-ordered contraction of two operators:

$$\overbrace{C_r(\tau) C_s(\tau')} = \langle \mathsf{T} C_r(\tau) C_s(\tau')\rangle \tag{10}$$

and extend the definition to the case with p operators between.

Lemma 6.

$$\langle \mathsf{T} C_1(\tau_1) \dots C_N(\tau_N)\rangle = \sum_{j=2}^N \langle \mathsf{T} C_1 \overbrace{(\tau_0) \dots C_j}(\tau_j) \dots C_N(\tau_N)\rangle \tag{11}$$

Proof. The action of T is to permute the operators putting times in a decreasing sequence

$$\langle \mathsf{T} C_1(\tau_1) \dots C_N(\tau_N)\rangle = (\pm 1)^\pi \langle C_{\pi_1}(\tau_{\pi_1}) \dots C_1(\tau_1) \dots C_{\pi_N}(\tau_{\pi_N})\rangle$$

We apply Lemma **??** of the static Wick theorem, with the notation $C_k(\tau_k) = C_k$:

$$= (\pm 1)^\pi \sum\nolimits_j [\theta(\tau_{\pi_j} - \tau_1)\langle C_{\pi_1} \dots \overbracket{C_{\pi_j} \dots C_1} \dots \rangle + \theta(\tau_1 - \tau_{\pi_j})\langle \dots \overbracket{C_1 \dots C_{\pi_j}} \dots C_{\pi_N}\rangle]$$

Since operators are τ-ordered, the symbol T is introduced in both thermal averages and the operators are permuted back to the initial order. In doing so, in the first sum, the order in the contraction (a c-number is not subject to T) is exchanged, which amounts to a sign for fermions:

$$= \sum_j [\pm\theta(\tau_j - \tau_1)\langle \mathsf{T} \overline{C_1(\tau_1)\dots C_j}(\tau_j)\dots\rangle + \theta(\tau_1 - \tau_j)\langle \mathsf{T} \overline{C_1(\tau_1)\dots C_j}(\tau_j)\dots\rangle]$$

$$= \sum_{j=2}^N \langle \mathsf{T} \overbrace{C_1(\tau_1)\dots C_j}(\tau_j)\dots C_N(\tau_N)\rangle$$

$\square$

By linearity, the result extends to any set of one-particle creation and destruction operators. The non-zero τ-ordered contractions are Green functions up to a sign:

$$\overline{\psi(1)\psi^\dagger}(2) = \langle \mathsf{T}\psi(1)\psi^\dagger(2)\rangle = -\mathscr{G}^0(1,2) \tag{12}$$

$$\overline{\psi^\dagger(1)\psi}(2) = \langle \mathsf{T}\psi^\dagger(1)\psi(2)\rangle = \mp\mathscr{G}^0(2,1) \tag{13}$$

Theorem 7 (The T-ordered Wick theorem)**.** *A τ-ordered correlator for non-interacting particles is the sum of full τ-ordered contractions.*

Example 8. Green functions are combinations of one-particle Green functions.

$$\begin{aligned} (-1)^2\mathscr{G}^0(1234) &= \langle \mathsf{T}\psi(1)\psi(2)\psi^\dagger(4)\psi^\dagger(3)\rangle \\ &= \langle \mathsf{T}\psi(1)\psi^\dagger(3)\rangle\langle \mathsf{T}\psi(2)\psi^\dagger(4)\rangle \pm \langle \mathsf{T}\psi(1)\psi^\dagger(4)\rangle\langle \mathsf{T}\psi(2)\psi^\dagger(3)\rangle \\ &= (-1)^2[\mathscr{G}^0(13)\mathscr{G}^0(24) \pm \mathscr{G}^0(14)\mathscr{G}^0(23)] \end{aligned} \tag{14}$$

Example 9.

$$\begin{aligned} -\mathscr{D}^0(x,y) =& \langle \mathsf{T}\delta n(x)\delta n(y)\rangle = \sum_{\mu\nu}\langle \mathsf{T}\psi^\dagger_\mu(x)\psi_\mu(x)\psi^\dagger_\nu(y)\psi_\nu(y)\rangle_{conn} \\ =& \sum_{\mu\nu}\langle \mathsf{T}\psi_\mu(x)\psi^\dagger_\nu(y)\rangle\langle \mathsf{T}\psi^\dagger_\mu(x)\psi_\nu(y)\rangle \\ =& \pm\sum_{\mu\nu}\mathscr{G}^0_{\mu\nu}(x,y)\mathscr{G}^0_{\nu\mu}(y,x) \end{aligned} \tag{15}$$