LET'S FORGET ABOUT THE PAIRING

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(Received June 04, 2013)

Abstract

The algebraic formulation of a Wick's theorem that allows one to present the vacuum or thermal averages of the chronological product of an arbitrary number of field operators as a determinant (permanent) of the matrix is proposed. Each element of the matrix is the average of the chronological product of only two operators. This formulation is extremely convenient for practical calculations in quantum field theory and statistical physics by the methods of symbolic mathematics using computers.

Wick's theorems are extensively used in quantum field theory [1–4] and statistical physics [5–7]. They allow one to use the Green's functions method and consequently to apply Feynman's diagrams for investigations [1–3]. The first of these, which can be referred to as Wick's Theorem for Ordinary Products, gives us the opportunity to reduce, in an almost automatic mode, the usual product of operators into a unique sum of normal products multiplied by c-numbers. It can be formulated as follows [4]. Let $A_i\left(x_i\right)$ $(i=1,2,\ldots,n)$ be "linear operators," i.e., some linear combinations of creation and annihilation operators. Then the ordinary product of linear operators is equal to the sum of all the corresponding normal products with all possible contractions, including the normal product without contractions, i.e.,

$$A_1\ldots A_n =: A_1\ldots A_n :+: \underbrace{A_1 A_2}\ldots A_n :+\ldots: \underbrace{A_1\ldots A_{n-1}} A_n :+: \underbrace{A_1\ldots A_n} :+: \underbrace{A_1 A_2}\,\underbrace{A_3 A_4}\ldots A_n :+\ldots ,$$

where $\underbrace{A_i A_j} = A_i A_j - : A_i A_j :$ $(i, j=1,2,\ldots,n)$ is the contraction between the factors A_i and A_j. Since the vacuum expectation value of the normal ordered product is zero, this theorem provides us a way of expressing the vacuum expectation values of n linear operators in terms of the vacuum expectation values of two operators.

Wick's Theorem for Chronological Products [4] asserts that the T-product of a system of n linear operators is equal to the sum of their normal products with all possible chronological contractions, including the term without contractions. It follows directly from the previous theorem and gives the opportunity to calculate the vacuum expectation values of the chronological products of linear operators.

Finally, from Wick's theorem for chronological products, the Generalized Wick's Theorem [4] can be obtained. It asserts that the vacuum expectation value of the chronological product of $n+1$ linear operators $A, B_1,\ldots,B_n$ can be decomposed into the sum of n vacuum expectation values of the same chronological products with all possible contractions of one of these operators (for example, A) with all others, i.e.,

$$\left\langle T\left(AB_1\ldots B_n\right)\right\rangle_0 = \sum_{1\le i\le n}\left\langle T\left(\overline{AB_1\ldots B_i}\ldots\ldots B_n\right)\right\rangle_0 \ . \qquad (1)$$

Here $\overline{A_i A_j} = T\left(A_i A_j\right) - :A_i A_j: = \left\langle T\left(A_i A_j\right)\right\rangle_0$ $(i, j = 1, 2, \ldots, n)$ is the chronological contraction between factors A_i and A_j. It should be noted that, in contrast to the usual Wick's theorem for chronological products, there are no expressions involving the number of contractions greater than one on the right-hand side of (1).

The Wick's theorem for chronological products or its generalized version is used for the calculation of matrix elements of the scattering matrix in each order of perturbation theory [1–4]. The procedure is reduced to calculation of the vacuum expectation of chronological products of the field operators in the interaction representation. A number of operators ψ_i of the Fermi fields and the same number of their "conjugate" operators $\bar{\psi}_i$, as well as operators of the Bose fields $\varphi_s = \varphi_s^{(+)} + \varphi_s^{(-)}$ may be used as factors in these products**.** Here, all continuous and discrete variables are included in the index. In the interaction, representation operators $\psi_i, \bar{\psi}_i$, and φ_s correspond to free fields and satisfy the commutation relationships of the form $\left[\psi_i, \psi_j\right]_+ = \left[\bar{\psi}_i, \bar{\psi}_j\right]_+ = 0$, $\left[\psi_i, \bar{\psi}_j\right]_+ = D^F_{rs\,ij}$, $\left[\varphi_r^{(+)}, \varphi_s^{(-)}\right]_- = D^B_{rs}$. Therefore, the averaging of the Fermi and Bose fields can be performed independently.

Since we may rearrange the order of the operators inside T-products taking into account the change of the sign, which arises when the order of the Fermi operators is changed, we present our vacuum expectation value of the chronological product of the Fermi operators in the form

$$\pm\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\left(\psi_{i_2}\bar{\psi}_{j_2}\right)\ldots\left(\psi_{i_n}\bar{\psi}_{j_n}\right)\right]\right\rangle_0 . \qquad (2)$$

To calculate (2), we can use Wick's theorem for chronological products. However, while considering the higher-order perturbation theory, the number of pairs $\psi_i\bar{\psi}_j$ of operators ψ_i and $\bar{\psi}_j$ becomes so large that the direct application of this theorem begins to represent certain problems because it is very difficult to sort through all the possible contractions between ψ_i and $\bar{\psi}_j$.

A consistent use of the generalized Wick's theorem would introduce a greater accuracy in our actions. However, in this case, we expect very cumbersome and tedious calculations. Hereinafter, we show that the computation of (2) can be easily performed using a simple formula:

$$\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\left(\psi_{i_2}\bar{\psi}_{j_2}\right)\ldots\left(\psi_{i_n}\bar{\psi}_{j_n}\right)\right]\right\rangle_0 = \det\left(\Delta_{i_\alpha j_\beta}\right), \qquad (3)$$

where

$$\Delta_{i_\alpha j_\beta} = \overline{\psi_{i_\alpha}\bar{\psi}_{j_\beta}} = \left\langle T\left(\psi_{i_\alpha}\bar{\psi}_{j_\beta}\right)\right\rangle_0 \quad \left(\alpha, \beta = 1, 2, \ldots, n\right) . \qquad (4)$$

The proof of this theorem is provided by induction. Let us assume now that (3) is true for n pairs $\psi_i\bar{\psi}_j$ and consider it for the case of $n+1$. Using the generalized Wick's theorem, we have

$$\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\ldots\left(\psi_{i_{n+1}}\bar{\psi}_{j_{n+1}}\right)\right]\right\rangle_0 = -\Delta_{i_1 j_{n+1}}\left\langle T\left[\left(\psi_{i_{n+1}}\bar{\psi}_{j_1}\right)\left(\psi_{i_2}\bar{\psi}_{j_2}\right)\ldots\left(\psi_{i_n}\bar{\psi}_{j_n}\right)\right]\right\rangle_0$$
$$-\sum_{\gamma=2}^{n-1}\Delta_{i_\gamma j_{n+1}}\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\ldots\left(\psi_{i_{\gamma-1}}\bar{\psi}_{j_{\gamma-1}}\right)\left(\psi_{i_{n+1}}\bar{\psi}_{j_\gamma}\right)\left(\psi_{i_{\gamma+1}}\bar{\psi}_{j_{\gamma+1}}\right)\ldots\left(\psi_{i_n}\bar{\psi}_{j_n}\right)\right]\right\rangle_0$$
$$-\Delta_{i_n j_{n+1}}\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\ldots\left(\psi_{i_{n-1}}\bar{\psi}_{j_{n-1}}\right)\left(\psi_{i_{n+1}}\bar{\psi}_{j_n}\right)\right]\right\rangle_0 + \Delta_{i_{n+1} j_{n+1}}\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\ldots\left(\psi_{i_n}\bar{\psi}_{j_n}\right)\right]\right\rangle_0 .$$

Taking into account (3), we obtain

$$\left\langle T\left[\left(\psi_{i_1}\bar{\psi}_{j_1}\right)\ldots\left(\psi_{i_{n+1}}\bar{\psi}_{j_{n+1}}\right)\right]\right\rangle_0 = -\Delta_{i_1 j_{n+1}}\begin{vmatrix}\Delta_{i_{n+1}j_1} & \Delta_{i_{n+1}j_2} & \cdots & \Delta_{i_{n+1}j_n}\\ \Delta_{i_2 j_1} & \Delta_{i_2 j_2} & \cdots & \Delta_{i_2 j_n}\\ \vdots & \vdots & \ddots & \vdots\\ \Delta_{i_n j_1} & \Delta_{i_n j_2} & \cdots & \Delta_{i_n j_n}\end{vmatrix}$$
$$-\Delta_{i_2 j_{n+1}}\begin{vmatrix}\Delta_{i_1 j_1} & \Delta_{i_1 j_2} & \cdots & \Delta_{i_1 j_n}\\ \Delta_{i_{n+1}j_1} & \Delta_{i_{n+1}j_2} & \cdots & \Delta_{i_{n+1}j_n}\\ \vdots & \vdots & \ddots & \vdots\\ \Delta_{i_n j_1} & \Delta_{i_n j_2} & \cdots & \Delta_{i_n j_n}\end{vmatrix} - \ldots - \Delta_{i_n j_{n+1}}\begin{vmatrix}\Delta_{i_1 j_1} & \Delta_{i_1 j_2} & \cdots & \Delta_{i_1 j_n}\\ \vdots & \vdots & \cdots & \vdots\\ \Delta_{i_{n-1}j_1} & \Delta_{i_{n-1}j_2} & \ddots & \Delta_{i_{n-1}j_n}\\ \Delta_{i_{n+1}j_1} & \Delta_{i_{n+1}j_2} & \cdots & \Delta_{i_{n+1}j_n}\end{vmatrix} \qquad (5)$$
$$+\Delta_{i_{n+1} j_{n+1}}\begin{vmatrix}\Delta_{i_1 j_1} & \Delta_{i_1 j_2} & \cdots & \Delta_{i_1 j_n}\\ \Delta_{i_2 j_1} & \Delta_{i_2 j_2} & \cdots & \Delta_{i_2 j_n}\\ \vdots & \vdots & \ddots & \vdots\\ \Delta_{i_n j_1} & \Delta_{i_n j_2} & \cdots & \Delta_{i_n j_n}\end{vmatrix}.$$

Rearranging the rows in the determinants in (5), it is easy to see that the right hand side is the expansion of the

$$\det\left(\Delta_{i_\alpha j_\beta}\right) = \begin{vmatrix}\Delta_{i_1 j_1} & \Delta_{i_1 j_2} & \cdots & \Delta_{i_1 j_{n+1}}\\ \Delta_{i_2 j_1} & \Delta_{i_2 j_2} & \cdots & \Delta_{i_2 j_{n+1}}\\ \vdots & \vdots & \ddots & \vdots\\ \Delta_{i_{n+1}j_1} & \Delta_{i_{n+1}j_2} & \cdots & \Delta_{i_{n+1}j_{n+1}}\end{vmatrix} \qquad \left(\alpha,\beta = 1,2,\ldots,n+1\right)$$

along the last column [8]. The validity of (3) for $n=1$ follows from the definition $\Delta_{i_\alpha j_\beta}$ in (4).

Note that this result does not depend on the way how we divide the operators on the left hand side of (3) into pairs $\psi_{i_\alpha}\bar{\psi}_{j_\beta}$. Indeed, if on the left hand side of (3) we permute, for example, $\bar{\psi}_{j_\beta}$ and $\bar{\psi}_{j_\gamma}$ ($\beta \neq \gamma$), it changes its sign. The same happens on the right hand side of (3) since this change leads to the permutation of two columns in the determinant, and it also changes its sign. Similarly, in the case of a permutation of ψ_{i_α} and ψ_{i_δ} ($\alpha \neq \delta$). Obviously, when the whole pair $\psi_{i_\alpha}\bar{\psi}_{j_\beta}$ is transposed, the left and right hand sides of (3) do not change.

The above theorem has an important consequence. In fact, it establishes a perfect coincidence between the vacuum expectation values of the chronological products of n pairs of field operators and the n-order determinant. If we present this determinant as the sum of the elements and cofactors of one any row or column and thereafter use again the indicated coincidence for the $(n-1)$-order determinants included in each summand, we will return to the generalized Wick's theorem. Alternatively, in our n-order determinant, we can select arbitrary m rows or columns ($1<m<n$) and use the *Generalized Laplace's Expansion* [8] for its presentation as the sum of the products of all m-rowed minors using these rows (or columns) and their algebraic complements. Then, taking into account our theorem, we obtain a representation of the vacuum expectation values of the chronological products of n pairs of field operators as the sum of the products of vacuum expectation values of the chronological products of m pairs of operators and vacuum expectation values of the chronological products of $n-m$ pairs. The number of terms in this sum is $n!/m!(n-m)!$. This decomposition can be useful for the summation of blocks of diagrams.

Obviously, the formula similar to (3) can be obtained and in the case of Bose fields:

$$\left\langle T\left[\left(\varphi_{i_1}^{(+)}\varphi_{j_1}^{(-)}\right)\left(\varphi_{i_2}^{(+)}\varphi_{j_2}^{(-)}\right)\ldots\left(\varphi_{i_n}^{(+)}\varphi_{j_n}^{(-)}\right)\right]\right\rangle_0=\operatorname{perm}\left(\bar{\Delta}_{i_\alpha j_\beta}\right),$$
$$\bar{\Delta}_{i_\alpha j_\beta}=\overline{\varphi_{i_\alpha}^{(+)}\varphi_{j_\beta}^{(-)}}=\left\langle T\left(\varphi_{i_\alpha}^{(+)}\varphi_{j_\beta}^{(-)}\right)\right\rangle_0\quad(\alpha,\beta=1,2,\ldots,n)\ . \tag{6}$$

Representations (3) and (6) not only greatly simplify all calculations, but also allow one to perform them using a computer with programs of symbolic mathematics [9].

In quantum statistics the n-body thermal, or imaginary-time, Green's functions in the Grand Canonical Ensemble are defined as the thermal trace of a time-ordered product of the field operators in the imaginary-time Heisenberg representation [5–7]. To calculate them in each order of perturbation theory, the Wick's theorem is also used. Obviously, in this case, the theorem also may be formulated in the form of (3) and (6) convenient for practical calculation.

In order to demonstrate the usability of the proposed formulation of the Wick's theorem, we find the first-order correction to the one- and two-particle thermal Green's functions for the Fermi system described in the interaction representation by the Hamiltonian

$$H_{\text{int}}(\tau)=\frac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2\,\bar{\psi}_\alpha(\mathbf{r}_1,\tau)\bar{\psi}_\beta(\mathbf{r}_2,\tau)U(\mathbf{r}_1-\mathbf{r}_2)\psi_\beta(\mathbf{r}_2,\tau)\psi_\alpha(\mathbf{r}_1,\tau),$$

that contains the product of the field operators $\psi_\alpha(\mathbf{r}_1,\tau)$ and $\bar{\psi}_\alpha(\mathbf{r}_1,\tau)$ in this representation (parameter α indicates the spin projections, τ is the imaginary-time). The one-particle Green's function can be represented as [6, 7]

$$\mathcal{G}_I(x_1,x_2)=-\frac{\left\langle T_\tau\left[\psi(x_1)\bar{\psi}(x_2)\mathcal{S}\right]\right\rangle_0}{\left\langle\mathcal{S}\right\rangle_0},$$

where $\langle\ldots\rangle_0$ is the symbol for the Gibbs average over the states of a system of noninteracting particles, $x\equiv(\mathbf{r},\tau,\alpha)$ and

$$\mathcal{S}(\tau)=T_\tau\exp\left\{-\int_0^\tau d\tau' H_{\text{int}}(\tau')\right\}.$$

We obtain

$$\mathcal{G}_I(x_1,x_2) = -\left\langle T_\tau\left[\psi(x_1)\bar{\psi}(x_2)\right]\right\rangle_0 + \frac{1}{2\langle\mathcal{S}\rangle_0}\int dz_1 dz_2\,\mathcal{V}(z_1-z_2)$$

$$\times\left\langle T_\tau\left[\left(\psi(x_1)\bar{\psi}(x_2)\right)\left(\psi(z_1)\bar{\psi}(z_1)\right)\left(\psi(z_2)\bar{\psi}(z_2)\right)\right]\right\rangle_0 \tag{7}$$

$$= -\Delta(x_1,x_2) + \frac{1}{2\langle\mathcal{S}\rangle_0}\int dz_1 dz_2\,\mathcal{V}(z_1-z_2)\begin{vmatrix}\Delta(x_1,x_2) & \Delta(x_1,z_1) & \Delta(x_1,z_2)\\ \Delta(z_1,x_2) & \Delta(z_1,z_1) & \Delta(z_1,z_2)\\ \Delta(z_2,x_2) & \Delta(z_2,z_1) & \Delta(z_2,z_2)\end{vmatrix},$$

where $\mathcal{V}(x_1-x_2) = U(\mathbf{r}_1-\mathbf{r}_2)\delta(\tau_1-\tau_2)$. We can immediately take into account the reduction of the disconnected diagrams, if we assume in (7) that $\langle\mathcal{S}\rangle_0 = 1$ and $\Delta(x_1,x_2)=0$ [6]. Then,

$$\mathcal{G}_I(x_1,x_2) = -\Delta(x_1,x_2) + \frac{1}{2}\int dz_1 dz_2\,\mathcal{V}(z_1-z_2)$$

$$\left[\Delta(x_1,z_2)\begin{vmatrix}\Delta(z_1,x_2) & \Delta(z_1,z_1)\\ \Delta(z_2,x_2) & \Delta(z_2,z_1)\end{vmatrix} - \Delta(x_1,z_1)\begin{vmatrix}\Delta(z_1,x_2) & \Delta(z_1,z_2)\\ \Delta(z_2,x_2) & \Delta(z_2,z_2)\end{vmatrix}\right]$$

$$= -\Delta(x_1,x_2) - \int dz_1 dz_2\,\Delta(x_1,z_1)\mathcal{V}(z_1-z_2)\begin{vmatrix}\Delta(z_1,x_2) & \Delta(z_1,z_2)\\ \Delta(z_2,x_2) & \Delta(z_2,z_2)\end{vmatrix}$$

$$= -\Delta(x_1,x_2) + \int dz_1 dz_2\,\Delta(x_1,z_1)\mathcal{V}(z_1-z_2)\Delta(z_1,z_2)\Delta(z_2,x_2)$$

$$-\int dz_1\,\Delta(x_1,z_1)\left[\int dz_2\mathcal{V}(z_1-z_2)\Delta(z_2,z_2)\right]\Delta(z_1,x_2).$$

Taking into account $\mathcal{G}^{(0)}(x_1,x_2) = -\Delta(x_1,x_2)$, we finally obtain

$$\mathcal{G}_I(x_1,x_2) = \mathcal{G}^{(0)}(x_1,x_2) + \int dz_1 dz_2\,\mathcal{G}^{(0)}(x_1,z_1)\Sigma^{(1)}(z_1,z_2)\mathcal{G}^{(0)}(z_2,x_2),$$

$$\Sigma^{(1)}(z_1,z_2) = -\mathcal{V}(z_1-z_2)\mathcal{G}^{(0)}(z_1,z_2) + \delta(z_1-z_2)\int dz\,\mathcal{V}(z_1-z)\mathcal{G}^{(0)}(z,z).$$

Similarly, for the two-particle Green's function

$$\mathcal{G}_{II}(x_1,x_2,x_3,x_4) = -\frac{\left\langle T_\tau\left[\psi(x_1)\psi(x_2)\bar{\psi}(x_3)\bar{\psi}(x_4)\mathcal{S}\right]\right\rangle_0}{\langle\mathcal{S}\rangle_0},$$

we have

$$\mathcal{G}_{II}(x_1,x_2,x_3,x_4) = \left\langle T_\tau\left[\left(\psi(x_1)\bar{\psi}(x_3)\right)\left(\psi(x_2)\bar{\psi}(x_4)\right)\right]\right\rangle_0$$

$$-\frac{1}{2\langle\mathcal{S}\rangle_0}\int dz_1 dz_2\,\mathcal{V}(z_1-z_2)\left\langle T_\tau\left[\left(\psi(x_1)\bar{\psi}(x_3)\right)\left(\psi(x_2)\bar{\psi}(x_4)\right)\left(\psi(z_1)\bar{\psi}(z_1)\right)\left(\psi(z_2)\bar{\psi}(z_2)\right)\right]\right\rangle$$

$$= \begin{vmatrix}\Delta(x_1,x_3) & \Delta(x_1,x_4)\\ \Delta(x_2,x_3) & \Delta(x_2,x_4)\end{vmatrix} - \frac{1}{2}\int dz_1 dz_2\,\mathcal{V}(z_1-z_2)\begin{vmatrix}0 & 0 & \Delta(x_1,z_1) & \Delta(x_1,z_2)\\ 0 & 0 & \Delta(x_2,z_1) & \Delta(x_2,z_2)\\ \Delta(z_1,x_3) & \Delta(z_1,x_4) & \Delta(z_1,z_1) & \Delta(z_1,z_2)\\ \Delta(z_2,x_3) & \Delta(z_2,x_4) & \Delta(z_2,z_1) & \Delta(z_2,z_2)\end{vmatrix}$$

$$= \mathcal{G}^{(0)}(x_1, x_3)\mathcal{G}^{(0)}(x_2, x_4) - \mathcal{G}^{(0)}(x_1, x_4)\mathcal{G}^{(0)}(x_2, x_3)$$

$$-\int dz_1 dz_2\, \mathcal{G}^{(0)}(x_1, z_1)\mathcal{G}^{(0)}(x_2, z_2)\mathcal{V}(z_1 - z_2)\left[\mathcal{G}^{(0)}(z_1, x_3)\mathcal{G}^{(0)}(z_2, x_4) - \mathcal{G}^{(0)}(z_1, x_4)\mathcal{G}^{(0)}(z_2, x_3)\right]_0 .$$

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