Application of Symbolic Calculations for Wick's Theorem

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Wick's theorem for chronological products or its generalized version are used for the calculation of the scattering matrix in each order of perturbation theory [1-2]. The procedure is reduced to calculation of the vacuum expectation of chronological products of the field operators in the interaction representation. As factors in these products a number of operators a_i of the Fermi fields and the same number of their "conjugate" operators $\bar{a}_i$ are considered. Here all continuous and discrete variables are included in the index. In the interaction representation the operators a_i and $\bar{a}_i$ correspond to free fields and satisfy the commutation relationships of the form $[a_i, a_j]_+ = [\bar{a}_i, \bar{a}_j]_+ = 0, [a_i, \bar{a}_j]_+ = D_{ij}$.

Since we may rearrange the order of the operators inside of 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

$$\pm\langle T[(a_{i_1}\bar{a}_{j_1})(a_{i_2}\bar{a}_{j_2})\cdots(a_{i_n}\bar{a}_{j_n})]\rangle_0. \tag{1}$$

To calculate (1) we can use Wick's theorem for chronological products. However, while considering the higher-order perturbation theory, the number of pairs $a_i\bar{a}_i$ of the operators a_i and $\bar{a}_i$ 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 a_i and $\bar{a}_i$.

A consistent use of 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 (1) can be easily performed using a simple formula

$$\langle T[(a_{i_1}\bar{a}_{j_1})(a_{i_2}\bar{a}_{j_2})\cdots(a_{i_n}\bar{a}_{j_n})]\rangle_0 = det(\Delta_{i_\alpha j_\beta}), \tag{2}$$

$$\Delta_{i_\alpha j_\beta} = \langle T(a_{i_\alpha}\bar{a}_{j_\beta})\rangle_0, (\alpha, \beta = 1, 2, \cdots, n). \tag{3}$$

This result does not depend on the way how we divide the operators on the left hand of (2) into pairs. The proof of this theorem is by induction.

Obviously, the similar formula to (2) can be obtained also in the case of Bose fields.

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 to present this determinant as the sum of the elements and cofactors of one by any row or column, and thereafter to use again the indicated coincidence for the $(n-1)$-order determinant included in each summand, we will return to the generalized Wick's theorem. Alternatively, we can select arbitrary m rows or columns $(1 < m < n)$ in our n-order determinant and use the Generalized Laplace's Expansion [3] 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 equal to $n!/m!(n-m)!$. This decomposition can be useful for the summation of blocks of diagrams.

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 [4-5]. To calculate them in each order of perturbation theory, Wick's theorem is also used. Obviously, in this case the theorem also may be formulated in the form (2) convenient for practical calculation.

Representation (2) not only greatly simplify all calculation, but also allow one to perform them using a computer with programs of symbolic mathematics [6].

Bibliography

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