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Abstract

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A THEOREM ON STATISTICAL AVERAGES FOR PAULI OPERATORS

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For statistical averages of products of Bose or Fermi operators over the states of the zero Hamiltonian of a system, the Wick–Bloch–Dominicis theorem holds ([1]). In the present note we establish an analogue of this theorem for averages of products of Pauli operators.

For the latter, the following commutation relations hold:

$$b_f b_g^+ - b_g^+ b_f = \delta_{f,g}\left(1 - 2b_f^+ b_g\right); \tag{1a}$$

$$b_f b_g - b_g b_f = 0; \qquad b_f^+ b_g^+ - b_g^+ b_f^+ = 0; \tag{1b}$$

$$b_f^2 = b_f^{+2} = 0. \tag{1c}$$

For the proof we shall use the following simple relations:

$$\langle b_g^+ A\rangle = \frac{1}{e^{\beta E_g} \pm 1}\langle [A, b_g^+]_\pm\rangle; \tag{2a}$$

$$\langle b_g A'\rangle = \frac{1}{1 \pm e^{-\beta E_g}}\langle [b_g, A']_\pm\rangle, \tag{2b}$$

where A and A' are arbitrary products of Pauli operators. The symbol $\langle \ldots \rangle$ denotes the statistical average:

$$\langle A\rangle = \mathrm{Sp}\, A e^{-\beta H_0} / \mathrm{Sp}\, e^{-\beta H_0}, \tag{3}$$

where

$$H_0 = \sum_g E_g b_g^+ b_g \tag{4}$$

is the Hamiltonian of the free system. Consider the average of the right-hand side of (2a):

$$\overline{m}_g\langle Ab_g^+ - b_g^+ A\rangle;\qquad \overline{m}_g = \frac{1}{e^{\beta E_g}-1}; \tag{5}$$

we move the operator b_g^+ of the first term in the bracket past all the operators in A, using relations (1a) and (1b). Since b_g^+ commutes with the operators b_f^+, we shall attend only to the operators b_f in A. Moving the operator b_g^+ past the rightmost operator b_i in A gives two terms:

$$\delta_{i,g} + b_g^+ b_i\left(1-2\delta_{i,g}\right).$$

Thus there arises the expression

$$\delta_{i,g}A_i + \left(1-2\delta_{i,g}\right)A_{gi}, \tag{6}$$

where the operator A_i is obtained by removing the operator b_i from the product A; A_{gi} is obtained if in A the operator b_g^+ is inserted next to and to the left of b_i.

In what follows we consider only the second term in (6). We again move the operator b_g^+ past the nearest left operator b_j of the form A_{gi}. In doing so⋯

there arises the sum:

$$\delta_{ig}(1-2\delta_{i,g})A_i + (1-2\delta_{j,g})(1-2\delta_{i,g})A_{gj}.$$

If the operator A contains n factors b_i, then, repeating the indicated procedure, we obtain

$$\begin{gathered}Ab_g^+ = \delta_{1,g}A_1 + \delta_{2,g}(1-2\delta_{1,g})A_2 + \ldots + \delta_{n,g}(1-2\delta_{1,g})(1-2\delta_{2g})\ldots\\ \ldots(1-2\delta_{n-1,g})A_n + (1-2\delta_{1,g})(1-2\delta_{2,g})\ldots(1-2\delta_{n,g})b_g^+A,\end{gathered}$$

where the indices $1, 2, \ldots, n$ number the operators b_f in the product A, counting from right to left. This form is valid for an arbitrary order of the operators in A. Thus expression (2a) can be represented in the form

$$\begin{gathered}\{1-\overline{m}_g[(1-2\delta_{1,g})(1-2\delta_{2,g})\ldots(1-2\delta_{n,g})-1]\}\langle b_g^+A\rangle =\\ = \overline{m}_g\{\delta_{1,g}\langle A_1\rangle + \delta_{2,g}(1-2\delta_{2,g})\langle A_2\rangle + \ldots\\ \ldots + \delta_{n,g}(1-2\delta_{1,g})(1-2\delta_{2,g})\ldots(1-2\delta_{n-1,g})\langle A_n\rangle\}.\end{gathered} \tag{7}$$

Consider expression (2b). We take into account that

$$A'b_g = \delta_{1,g}A'_1 + \delta'_{2,g}(1-2\delta_{1,g})A'_2 + \dots$$
$$\dots + \delta_{n,g}(1-2\delta_{1,g})(1-2\delta_{2,g})\dots(1-2\delta_{n,g})A'_n +$$
$$+(1-2\delta_{1,g})(1-2\delta_{2,g})\dots(1-2\delta_{n,g})b_gA',$$

where the operator A'_i is obtained if the operator b_i^+ is removed from A', and the indices $1, 2, \dots, n$ number the n operators b_f^+ in A', counting from right to left. Thus we have

$$\{1-(1+\overline{m}_g)[1-(1-2\delta_{1,g})(1-2\delta_{2,g})\dots(1-2\delta_{n,g})]\}\langle b_gA'\rangle =$$
$$= -(1+\overline{m}_g)\{\delta_{1,g}\langle A'_1\rangle + \delta_{2,g}(1-2\delta_{1,g})\langle A'_2\rangle + \dots$$
$$\dots + \delta_{n,g}(1-2\delta_{1,g})(1-2\delta_{2,g})\dots(1-2\delta_{n-1,g})\langle A'_n\rangle\}. \quad (8)$$

Formulas (7) and (8) are rules for calculating averages of a product of operators by reducing them to averages of a simpler form, containing one pair of operators fewer than in the initial expression. This result is a generalized Wick—Bloch—de Dominicis theorem.

Let us give formulas (7), (8) a more customary form. For this purpose we note that

$$\langle b_g^+b_1\rangle = \frac{\overline{m}_g}{1+2\overline{m}_g}\,\delta_{1,g} = \overline{n}_g\delta_{1,g},$$
$$\langle b_gb_1^+\rangle = -\frac{(1+\overline{m}_g)}{1-2(1+\overline{m}_g)}\,\delta_{1,g} = (1-\overline{n}_g)\delta_{1,g}, \quad (9)$$

where

$$\overline{n}_g = (e^{\beta E_g}+1)^{-1}. \quad (10)$$

Using (9), we obtain

$$\langle b_g^+A\rangle = C_g^{-1}(n,\dots,2,1)\{\langle b_g^+b_1\rangle\langle A_1\rangle + (1-2\delta_{1,g})\langle b_g^+b_2\rangle\langle A_2\rangle + \dots$$
$$\dots + (1-2\delta_{1,g})(1-2\delta_{2,g})\dots(1-2\delta_{n-1,g})\langle b_g^+b_n\rangle\langle A_n\rangle\}, \quad (11)$$

$$C_g(n,\dots,1) = (1+2\overline{m}_g)^{-1}\{1-\overline{m}_g[(1-2\delta_{1,g})\dots(1-2\delta_{n,g})-1]\}$$

and, analogously,

$$\langle b_gA'\rangle = D_g^{-1}(n,\dots,1)\{\langle b_gb_1^+\rangle\langle A'_1\rangle + (1-2\delta_{1,g})\langle b_gb_2^+\rangle\langle A'_2\rangle + \dots$$

$$\dots + (1-2\delta_{1,g})(1-2\delta_{2,g})\dots(1-2\delta_{n-1,g})\langle b_g b_n^+\rangle\langle A_n'\rangle\}, \tag{12}$$

$$D_g(n,\dots,1) =$$
$$= \{1-2(1+\overline{m}_g)\}^{-1}\{1-(1+\overline{m}_g)[1-(1-2\delta_{1,g})\dots(1-2\delta_{n,g})]\}.$$

Finally, let us introduce the functions

$$\begin{aligned}
&\alpha_1(n,\dots,1) = C_1^{-1}(n_1,\dots,1);\\
&\alpha_2(n,\dots,1) = (1-2\delta_{1,2})\,C_2^{-1}(n,\dots,1);\\
&\alpha_3(n,\dots,1) = (1-2\delta_{1,3})(1-2\delta_{2,3})\,C_3^{-1}(n,\dots,1);\\
&\qquad\dots\\
&\alpha_n(n,\dots,1) = (1-2\delta_{1,n})(1-2\delta_{2,n})\cdots(1-2\delta_{n-1,n})\,C_n^{-1}(n,\dots,1),
\end{aligned} \tag{13}$$

and also the functions

$$\begin{aligned}
&\beta_1(n,\dots,1) = D_1^{-1}(n,\dots,1);\\
&\beta_2(n,\dots,1) = (1-2\delta_{1,2})\,D_2^{-1}(n,\dots,1);\\
&\qquad\dots\\
&\beta_n(n,\dots,1) = (1-2\delta_{1,n})(1-2\delta_{2,n})\cdots(1-2\delta_{n-1,n})\,D_n^{-1}(n,\dots,1),
\end{aligned} \tag{14}$$

where, according to (11), (12) and (5), (10),

$$\begin{aligned}
C_1(n,\dots,1) &= 1+\bar{n}_1\big[(1-2\delta_{2,1})(1-2\delta_{3,1})\cdots(1-2\delta_{n-1})-1\big],\\
D_1(n,\dots,1) &= 1+(1-\bar{n}_1)\big[(1-2\delta_{2,1})(1-2\delta_{3,1})\cdots(1-2\delta_{n,1})-1\big],
\end{aligned} \tag{15}$$

and so on.

In the new notation formulas (11) and (12) take the form:

$$\begin{aligned}
\langle b_g^+ A\rangle = \alpha_1(n,\dots,1)\langle b_g^+ b_1\rangle\langle A_1\rangle + \alpha_2(n,\dots,1)\langle b_g^+ b_2\rangle\langle A_2\rangle + \cdots\\
\cdots + \alpha_n(n,\dots,1)\langle b_g^+ b_n\rangle\langle A_n\rangle;
\end{aligned} \tag{16}$$

$$\begin{aligned}
\langle b_g A'\rangle = \beta_1(n,\dots,1)\langle b_g b_1^+\rangle\langle A_1'\rangle + \beta_2(n,\dots,1)\langle b_g b_2^+\rangle\langle A_2'\rangle + \cdots\\
\cdots + \beta_n(n,\dots,1)\langle b_g b_n^+\rangle\langle A_n'\rangle.
\end{aligned} \tag{17}$$

The expressions obtained so far did not take into account the property (1b) of the operators b_f, b_f^+. Therefore this property must be additionally brought into the formulas given above, for which one may use the identities

$$b_1 b_2 = (1-\delta_{1,2})\, b_1 b_2; \qquad b_1^+ b_2^+ = (1-\delta_{1,2})\, b_1^+ b_2^+;$$
$$b_1 b_2 b_3 = (1-\delta_{1,2})(1-\delta_{1,3})(1-\delta_{2,3})\, b_1 b_2 b_3 \tag{18}$$

and so on.

In a number of cases these additional projection factors simplify equalities (16), (17).

Indeed, suppose that in the products b^+A and bA' all creation and annihilation operators are not intermingled with one another. By virtue of the identities (18), the indices of the operators within each of these two groups are distinct, which allows one to omit, in the functions α_i and β_i, the symbols $\delta_{i,i'}$, as a result of which they become equal to unity. Thus, we have:

$$\begin{aligned}\langle b_g^+ b_1^+ \cdots b_{n-1}^+ b_{n'} b_{n'-1} \cdots b_1 \rangle &= (1-\delta_{1'2'})(1-\delta_{1'3'})\cdots \\ &\cdots(1-\delta_{n'-1,n'})\{\langle b_g^+ b_{1'}\rangle \langle b_1^+ \cdots b_{n-1}^+ b_{n'} \cdots b_{2'}\rangle + \cdots \\ &\cdots + \langle b_g^+ b_{n'}\rangle\langle b_1^+ \cdots b_{n-1}^+ b_{n'-1} \cdots b_1\rangle\}, \\ \langle b_g\, b_1 \cdots b_{n-1} b_{n'}^+ \cdots b_1^+\rangle &= \\ &= (1-\delta_{1',2'})(1-\delta_{1',3'})\cdots(1-\delta_{n'-1,n'})\{\langle b_g b_{1'}^+\rangle\langle b_1 \cdots b_{n-1} b_{n'}^+ \cdots \\ &\cdots b_2^+\rangle + \cdots + \langle b_g b_{n'}^+\rangle\langle b_1 \cdots b_{n-1} b_{n'-1}^+ \cdots b_1^+\rangle\}.\end{aligned} \tag{19}$$

This theorem is analogous to the corresponding theorem for Bose operators, but with the simplest pairings of fermionic type.

In conclusion we note that repeated application of the generalized theorem (16), (17) will lead to the formation of complete systems of pairings, which will be present-

to apply the Wick–Bloch–Dominicis theorem to Pauli operators. The appearance of the factors α_i, β_i obviously greatly complicates the graphical representation of statistical averages, since the contributions of the diagrams will contain additional factors depending on the vertex indices. This will lead, in particular, to a revision of the concept of connectedness of diagrams.

Finally, let us note that theorems (16), (17) may prove useful in carrying out approximate decouplings for many-particle Green' s functions of ferromagnetic systems.

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[1] C. Bloch, C. de Dominicis, Nucl. Phys., **7**, 459 (1958).

Note: Figure translations are in progress. See original paper for figures.