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CORRELATION FUNCTIONS OF COULOMB PAIR

The correlation functions of two electrostatically interacting particles have been obtained for the first time, by using the direct algebraic method for finding the cross-correlation functions. The efficiency of this method has been demonstrated by finding almost all unknown elements of the decomposition matrices in the second-order approximation.

Keywords: secondary quantization, Coulomb pairing, correlation functions.

1. Introduction. Direct Algebraic Method to Determine Correlation Functions

This work is aimed at forming a basis for the exact theory of a Coulomb pair, i.e. a pair of free particles interacting electrostatically with each other. It is important to bear in mind that the particle pairing is a mere quantum-mechanical effect, and its description requires the development of exact methods for the solution of the corresponding nonlinear equations of motion for the creation and annihilation operators for each particle. The nonlinear component of such equations has the simplest form – with only one nonlinear operator – just in the case of a system consisting of two particles. This system is chosen below to avoid extra complications emerging at the solution of an obtained system of equations. We will consider a modification of the direct algebraic method (DAM) for the determination of correlation functions, which was proposed in work [1]. We recall that this method is based on the expansion of operator equations in a certain operator basis, which is selected with regard for the specific features of the problem concerned.

Let us consider the simplest case of expansion in the two-operator basis. After obtaining the equations for the operators and their commutators or anticommutators with the help of the decomposition matrices \hat{K}

and \hat{K}^+ , we will pass to the analysis of basic relations for correlation functions, which play the major role in the implementation of the direct algebraic method for the determination of correlation functions. For this purpose, we will consider two decomposition forms for the average values of operators with the help of matrices \hat{F} , \hat{F}^+ and \hat{G} , \hat{G}^+ , whose elements will be found by solving the obtained equations. The DAM is exact, because it enables the effective linearization of all operator equations and, as a result, the change from operator equations to a system of algebraic equations for unknown elements of the corresponding decomposition matrices to be performed. Those equations can be solved exactly, so that it is possible to find exact expressions for the correlation functions depending on the Hamiltonian parameters for the examined physical system. In this work, the results obtained with the use of the DAM are published for the first time.

2. Operator Equations

Let us consider a modification of the direct algebraic method for the determination of correlation functions, which was proposed in work [1]. For this purpose, the equations of motion for the creation and annihilation operators are used. In what follows, a system consisting of two particles interacting electrostatically is considered. The Hamiltonian of this system in the secondary quantization representation [2]

looks like

$$H = H_1 + H_2 + H_{12}, \quad (1)$$

where

$$H_i = \sum_p \varepsilon_{ip} a_{ip}^+ a_{ip}$$

is the Hamiltonian of a free particle of the i -th sort, and

$$H_{12} = \sum_{p_1+p_2=p'_1+p'_2} U_{p'_1 p'_2 p_2 p_1} a_{1p'_1}^+ a_{2p'_2}^+ a_{2p_2} a_{1p_1}$$

is the interaction Hamiltonian. Here, ε_{ip} is the kinetic energy, a_{ip}^+ are the creation operators, a_{ip} the annihilation ones, and $p = (s_z, \mathbf{p})$, where $\mathbf{p} = (p_x, p_y, p_z)$ are subscripts indicating the spin projections and the momenta of the particles. The quantity $U_{p'_1 p'_2 p_2 p_1}$ is the interaction potential in the momentum representation. Let the both particles be fermions, for which the following anticommutation relations hold:

$$a_{ip}^+ a_{iq} + a_{iq} a_{ip}^+ = \delta_{pq}, \quad (2)$$

$$a_{ip} a_{iq} + a_{iq} a_{ip} = 0, \quad (3)$$

$$a_{ip}^+ a_{iq}^+ + a_{iq}^+ a_{ip}^+ = 0, \quad (4)$$

where δ_{pq} is the Kronecker symbol. From the Hamiltonian, we obtain the following equations of motion, which form the basis of the method:

$$[a_{jq}, H] = K_{11q}^{(j)} a_{jq} + K_{12q}^{(j)} b_{jq}, \quad (5)$$

$$[b_{jq}, H] = K_{21q}^{(j)} a_{jq} + K_{22q}^{(j)} b_{jq}, \quad (6)$$

$$[a_{jq}^+, H] = -K_{11q}^{(j)} a_{jq}^+ - K_{12q}^{(j)} b_{jq}^+, \quad (7)$$

$$[b_{jq}^+, H] = K_{21q}^{(j)} a_{jq}^+ + K_{22q}^{(j)} b_{jq}^+. \quad (8)$$

Here,

$$b_{jq} = \frac{1}{K_{12q}^{(j)}} \sum_{p_1+p_2=p'_1+p'_2} U_{p'_1 p'_2 p_2 p_1} (\delta_{2j} \delta_{p'_2 q} a_{1p'_1}^+ + \delta_{1j} \delta_{p'_1 q} a_{2p'_2}^+) a_{2p_2} a_{1p_1}, \quad (9)$$

$$b_{jq}^+ = \frac{1}{K_{12q}^{(j)}} \sum_{p_1+p_2=p'_1+p'_2} U_{p'_1 p'_2 p_2 p_1} a_{1p'_1}^+ a_{2p'_2}^+ \times (a_{2p_2} \delta_{1j} \delta_{p_1 q} + a_{1p_1} \delta_{2j} \delta_{p_2 q}), \quad (10)$$

$K_{11q}^{(j)} = \varepsilon_{jq}$, $K_{12q}^{(j)} = 1$, $K_{21q}^{(j)}$, $K_{22q}^{(j)}$, $K_{21q}^{+(j)}$, and $K_{22q}^{+(j)}$ are sought functions, and $[\dots, \dots]$ is the commutator. The main point of the direct algebraic method is the expansion of operators in a two-operator basis, which is similar to the vector expansion. In our case, the equations for the annihilation and creation operators are expanded in the bases (a_{ip}, b_{jq}) and (a_{ip}^+, b_{jq}^+) , respectively. Using the Jacobi identity for three operators,

$$[[A, B], C] + [[B, C], A] + [[C, A], B] = 0, \quad (11)$$

we obtain the following equations for the commutators $([\dots, \dots]_-)$ and anticommutators $([\dots, \dots]_+)$:

$$[a_{ip}, a_{jq}]_{\pm}, H] = (K_{11q}^{(j)} + K_{11p}^{(i)}) [a_{ip}, a_{jq}]_{\pm} + K_{12q}^{(j)} [a_{ip}, b_{jq}]_{\pm} + K_{12p}^{(i)} [b_{ip}, a_{jq}]_{\pm}, \quad (12)$$

$$[a_{ip}, b_{jq}]_{\pm}, H] = (K_{11p}^{(i)} + K_{22q}^{(j)}) [a_{ip}, b_{jq}]_{\pm} + K_{21q}^{(j)} [a_{ip}, a_{jq}]_{\pm} + K_{12p}^{(i)} [b_{ip}, b_{jq}]_{\pm}, \quad (13)$$

$$[b_{ip}, a_{jq}]_{\pm}, H] = (K_{22p}^{(i)} + K_{11q}^{(j)}) [b_{ip}, a_{jq}]_{\pm} + K_{21p}^{(i)} [a_{ip}, a_{jq}]_{\pm} + K_{12q}^{(j)} [b_{ip}, b_{jq}]_{\pm}, \quad (14)$$

$$[b_{ip}, b_{jq}]_{\pm}, H] = (K_{22q}^{(j)} + K_{22p}^{(i)}) [b_{ip}, b_{jq}]_{\pm} + K_{21p}^{(i)} [a_{ip}, b_{jq}]_{\pm} + K_{21q}^{(j)} [b_{ip}, a_{jq}]_{\pm}, \quad (15)$$

$$[a_{ip}^+, a_{jq}]_{\pm}, H] = (K_{11q}^{(j)} - K_{11p}^{(i)}) [a_{ip}^+, a_{jq}]_{\pm} + K_{12q}^{(j)} [a_{ip}^+, b_{jq}]_{\pm} - K_{12p}^{(i)} [b_{ip}^+, a_{jq}]_{\pm}, \quad (16)$$

$$[a_{ip}^+, b_{jq}]_{\pm}, H] = (K_{22q}^{(j)} - K_{11p}^{(i)}) [a_{ip}^+, b_{jq}]_{\pm} + K_{21q}^{(j)} [a_{ip}^+, a_{jq}]_{\pm} - K_{12p}^{(i)} [b_{ip}^+, b_{jq}]_{\pm}, \quad (17)$$

$$[b_{ip}^+, a_{jq}]_{\pm}, H] = (K_{22p}^{(i)} + K_{11q}^{(j)}) [b_{ip}^+, a_{jq}]_{\pm} + K_{21p}^{(i)} [a_{ip}^+, a_{jq}]_{\pm} + K_{12q}^{(j)} [b_{ip}^+, b_{jq}]_{\pm}, \quad (18)$$

$$[b_{ip}^+, b_{jq}]_{\pm}, H] = (K_{22q}^{(j)} + K_{22p}^{(i)}) [b_{ip}^+, b_{jq}]_{\pm} + K_{21p}^{(i)} [a_{ip}^+, b_{jq}]_{\pm} + K_{21q}^{(j)} [b_{ip}^+, a_{jq}]_{\pm}, \quad (19)$$

$$[a_{ip}^+, a_{jq}^+]_{\pm}, H] = -(K_{11q}^{(j)} + K_{11p}^{(i)}) [a_{ip}^+, a_{jq}^+]_{\pm} - K_{12q}^{(j)} [a_{ip}^+, b_{jq}^+]_{\pm} - K_{12p}^{(i)} [b_{ip}^+, a_{jq}^+]_{\pm}, \quad (20)$$

$$[a_{ip}^+, b_{jq}^+]_{\pm}, H] = (K_{22q}^{+(j)} - K_{11p}^{(i)})[a_{ip}^+, b_{jq}^+]_{\pm} + K_{21q}^{+(j)}[a_{ip}^+, a_{jq}^+]_{\pm} - K_{12p}^{(i)}[b_{ip}^+, b_{jq}^+]_{\pm}, \quad (21)$$

$$[b_{ip}^+, a_{jq}^+]_{\pm}, H] = (K_{22p}^{+(i)} - K_{11q}^{(j)})[b_{ip}^+, a_{jq}^+]_{\pm} + K_{21p}^{+(i)}[a_{ip}^+, a_{jq}^+]_{\pm} - K_{12q}^{(j)}[b_{ip}^+, b_{jq}^+]_{\pm}, \quad (22)$$

$$[b_{ip}^+, b_{jq}^+]_{\pm}, H] = (K_{22q}^{+(j)} + K_{22p}^{+(i)})[b_{ip}^+, b_{jq}^+]_{\pm} + K_{21p}^{+(i)}[a_{ip}^+, b_{jq}^+]_{\pm} + K_{21q}^{+(j)}[b_{ip}^+, a_{jq}^+]_{\pm}, \quad (23)$$

$$[a_{ip}^+, a_{jq}^+]_{\pm}, H] = (K_{11p}^{(i)} - K_{11q}^{(j)})[a_{ip}^+, a_{jq}^+]_{\pm} - K_{12q}^{(j)}[a_{ip}^+, b_{jq}^+]_{\pm} + K_{12p}^{(i)}[b_{ip}^+, a_{jq}^+]_{\pm}, \quad (24)$$

$$[a_{ip}^+, b_{jq}^+]_{\pm}, H] = (K_{11p}^{(i)} + K_{22q}^{+(j)})[a_{ip}^+, b_{jq}^+]_{\pm} + K_{21q}^{+(j)}[a_{ip}^+, a_{jq}^+]_{\pm} + K_{12p}^{(i)}[b_{ip}^+, b_{jq}^+]_{\pm}, \quad (25)$$

$$[b_{ip}^+, a_{jq}^+]_{\pm}, H] = (K_{22p}^{+(i)} - K_{11q}^{(j)})[b_{ip}^+, a_{jq}^+]_{\pm} + K_{21p}^{+(i)}[a_{ip}^+, a_{jq}^+]_{\pm} - K_{12q}^{(j)}[b_{ip}^+, b_{jq}^+]_{\pm}, \quad (26)$$

$$[b_{ip}^+, b_{jq}^+]_{\pm}, H] = (K_{22q}^{+(j)} + K_{22p}^{+(i)})[b_{ip}^+, b_{jq}^+]_{\pm} + K_{21p}^{+(i)}[a_{ip}^+, b_{jq}^+]_{\pm} + K_{21q}^{+(j)}[b_{ip}^+, a_{jq}^+]_{\pm}. \quad (27)$$

Since

$$[a_{1p}, a_{2q}] = 0, \quad (28)$$

a number of important relations can be obtained. In particular, Eq. (12) yields

$$K_{12p}^{(1)}[b_{1p}, a_{2q}] + K_{12q}^{(2)}[a_{1p}, b_{2q}] = 0. \quad (29)$$

Now, calculating once more the commutator of Eq. (29) with the Hamiltonian, we obtain

$$[b_{1p}, b_{2q}] = \frac{K_{11q}^{(2)} + K_{22p}^{(1)} - K_{11p}^{(1)} - K_{22q}^{(2)}}{2K_{12p}^{(1)}}[a_{1p}, b_{2q}]. \quad (30)$$

Finally, calculating once more the commutator of Eq. (30) with the Hamiltonian, we obtain

$$K_{12p}^{(1)}K_{21p}^{(1)} + \left(\frac{K_{22p}^{(1)} - K_{11p}^{(1)}}{2}\right)^2 = K_{12q}^{(2)}K_{21q}^{(2)} + \left(\frac{K_{22q}^{(2)} - K_{11q}^{(2)}}{2}\right)^2 = \text{const}. \quad (31)$$

In a similar way, the relation

$$[a_{1p}^+, a_{2q}^+] = 0 \quad (32)$$

yields

$$K_{12p}^{(1)}K_{21p}^{(1)+} - \left(\frac{K_{22p}^{(1)+} + K_{11p}^{(1)}}{2}\right)^2 = K_{12q}^{(2)}K_{21q}^{(2)+} - \left(\frac{K_{22q}^{(2)+} + K_{11q}^{(2)}}{2}\right)^2 = \text{const}. \quad (33)$$

In addition, the relation

$$[a_{1p}^+, a_{2q}] = 0, \quad (34)$$

yields the formula

$$K_{12p}^{(1)}K_{21p}^{(1)+} - \left(\frac{K_{22p}^{(1)+} + K_{11p}^{(1)}}{2}\right)^2 = -K_{12q}^{(2)}K_{21q}^{(2)} - \left(\frac{K_{11q}^{(2)} - K_{22q}^{(2)}}{2}\right)^2 = \text{const}'. \quad (35)$$

When comparing Eqs. (35) and (33), one can see that they are valid, if we put $K_{21q}^{(2)+} = -K_{21q}^{(2)}$ and $K_{22q}^{(2)+} = -K_{22q}^{(2)}$. Swapping the subscripts $1 \leftrightarrow 2$ in Eqs. (28), (32), and (34), one can see that we may put $K_{21q}^{(1)+} = -K_{21q}^{(1)}$ and $K_{22q}^{(1)+} = -K_{22q}^{(1)}$. In addition, $\text{const}' = -\text{const}$. Let us calculate the commutator of relation (2) with the Hamiltonian. Then it follows from Eq. (16), where $i = j$, that

$$b_p^+ a_q + a_q b_p^+ = a_p^+ b_q + b_q a_p^+. \quad (36)$$

Hereafter, in order to simplify the formulas, we omit the subscripts denoting the sort of particles if they are identical. Calculating the commutator of relation (36) with the Hamiltonian, we obtain

$$2(b_p^+ b_q + b_q b_p^+) = 2K_{21p}\delta_{pq} + (K_{22p} + K_{22q} - K_{11p} - K_{11q})(a_p^+ b_q + b_q a_p^+). \quad (37)$$

3. Basic Relations

The following operators can be introduced for an arbitrary operator A :

$$\tilde{A} = \rho^{-1} A \rho \quad (38)$$

and

$$\widehat{A} = \rho A \rho^{-1}, \quad (39)$$

where ρ is the statistical operator of the system. Then the following expansions can be used:

$$\widetilde{a}_{ip} = F_{11p}^{(i)} a_{ip} + F_{12p}^{(i)} b_{ip}, \quad (40)$$

$$\widetilde{b}_{ip} = F_{21p}^{(i)} a_{ip} + F_{22p}^{(i)} b_{ip}, \quad (41)$$

$$\widehat{a}_{ip} = G_{11p}^{(i)} a_{ip} + G_{12p}^{(i)} b_{ip}, \quad (42)$$

$$\widehat{b}_{ip} = G_{21p}^{(i)} a_{ip} + G_{22p}^{(i)} b_{ip}, \quad (43)$$

$$\widetilde{a}_{ip}^+ = F_{11p}^{+(i)} a_{ip}^+ + F_{12p}^{+(i)} b_{ip}^+, \quad (44)$$

$$\widetilde{b}_{ip}^+ = F_{21p}^{+(i)} a_{ip}^+ + F_{22p}^{+(i)} b_{ip}^+, \quad (45)$$

$$\widehat{a}_{ip}^+ = G_{11p}^{+(i)} a_{ip}^+ + G_{12p}^{+(i)} b_{ip}^+, \quad (46)$$

$$\widehat{b}_{ip}^+ = G_{21p}^{+(i)} a_{ip}^+ + G_{22p}^{+(i)} b_{ip}^+, \quad (47)$$

which play the essential role in applications of the method. Here, as well as in Eq. (8), the sign + marks those matrix elements that correspond to the creation operators and does not denote the conjugation ! For the averaged operators, we obtain

$$\langle \widetilde{a}_{ip} \rangle = F_{11p}^{(i)} \langle a_{ip} \rangle + F_{12p}^{(i)} \langle b_{ip} \rangle, \quad (48)$$

$$\langle \widetilde{b}_{ip} \rangle = F_{21p}^{(i)} \langle a_{ip} \rangle + F_{22p}^{(i)} \langle b_{ip} \rangle, \quad (49)$$

and

$$\langle \widehat{a}_{ip} \rangle = G_{11p}^{(i)} \langle a_{ip} \rangle + G_{12p}^{(i)} \langle b_{ip} \rangle, \quad (50)$$

$$\langle \widehat{b}_{ip} \rangle = G_{21p}^{(i)} \langle a_{ip} \rangle + G_{22p}^{(i)} \langle b_{ip} \rangle. \quad (51)$$

Here, the notation

$$\langle A \rangle = \text{Sp}(\rho A), \quad (52)$$

where Sp is the operator trace, is used. In view of the relation

$$\text{Sp}(AB) = \text{Sp}(BA), \quad (53)$$

we obtain

$$\langle \widetilde{a}_{ip} \rangle = F_{11p}^{(i)} \langle a_{ip} \rangle + F_{12p}^{(i)} \langle b_{ip} \rangle = \langle a_{ip} \rangle, \quad (54)$$

$$\langle \widetilde{b}_{ip} \rangle = F_{21p}^{(i)} \langle a_{ip} \rangle + F_{22p}^{(i)} \langle b_{ip} \rangle = \langle b_{ip} \rangle, \quad (55)$$

$$\langle \widehat{a}_{ip} \rangle = G_{11p}^{(i)} \langle a_{ip} \rangle + G_{12p}^{(i)} \langle b_{ip} \rangle = \langle a_{ip} \rangle, \quad (56)$$

$$\langle \widehat{b}_{ip} \rangle = G_{21p}^{(i)} \langle a_{ip} \rangle + G_{22p}^{(i)} \langle b_{ip} \rangle = \langle b_{ip} \rangle. \quad (57)$$

From whence, we immediately find that

$$\langle b_{ip} \rangle = \frac{1 - F_{11p}^{(i)}}{F_{12p}^{(i)}} \langle a_{ip} \rangle = \frac{1 - G_{11p}^{(i)}}{G_{12p}^{(i)}} \langle a_{ip} \rangle \quad (58)$$

provided the following conditions for the decomposed matrices:

$$F_{21p}^{(i)} F_{12p}^{(i)} = (1 - F_{22p}^{(i)})(1 - F_{11p}^{(i)}), \quad (59)$$

$$G_{21p}^{(i)} G_{12p}^{(i)} = (1 - G_{22p}^{(i)})(1 - G_{11p}^{(i)}), \quad (60)$$

$$\frac{1 - F_{11p}^{(i)}}{F_{12p}^{(i)}} = \frac{1 - G_{11p}^{(i)}}{G_{12p}^{(i)}}, \quad (61)$$

$$\frac{1 - F_{22p}^{(i)}}{F_{21p}^{(i)}} = \frac{1 - G_{22p}^{(i)}}{G_{21p}^{(i)}}. \quad (62)$$

Simple combinations give rise to

$$F_{21p}^{(i)} G_{12p}^{(i)} = (1 - F_{22p}^{(i)})(1 - G_{11p}^{(i)}) \quad (63)$$

and

$$G_{21p}^{(i)} F_{12p}^{(i)} = (1 - G_{22p}^{(i)})(1 - F_{11p}^{(i)}). \quad (64)$$

For the Hermitian-conjugate creation operators, we obtain

$$\langle b_{ip}^+ \rangle = \frac{1 - F_{11p}^{+(i)}}{F_{12p}^{+(i)}} \langle a_{ip}^+ \rangle = \frac{1 - G_{11p}^{+(i)}}{G_{12p}^{+(i)}} \langle a_{ip}^+ \rangle, \quad (65)$$

so that

$$F_{21p}^{+(i)} F_{12p}^{+(i)} = (1 - F_{22p}^{+(i)})(1 - F_{11p}^{+(i)}), \quad (66)$$

$$G_{21p}^{+(i)} G_{12p}^{+(i)} = (1 - G_{22p}^{+(i)})(1 - G_{11p}^{+(i)}), \quad (67)$$

$$\frac{1 - F_{11p}^{+(i)}}{F_{12p}^{+(i)}} = \frac{1 - G_{11p}^{+(i)}}{G_{12p}^{+(i)}}, \quad (68)$$

$$\frac{1 - F_{22p}^{+(i)}}{F_{21p}^{+(i)}} = \frac{1 - G_{22p}^{+(i)}}{G_{21p}^{+(i)}}, \quad (69)$$

$$F_{21p}^{+(i)} G_{12p}^{+(i)} = (1 - F_{22p}^{+(i)})(1 - G_{11p}^{+(i)}), \quad (70)$$

$$G_{21p}^{+(i)} F_{12p}^{+(i)} = (1 - G_{22p}^{+(i)})(1 - F_{11p}^{+(i)}). \quad (71)$$

Using relation (53), it is possible to find the following relations for the products of two operators:

$$\langle BA \rangle = \langle \widehat{A\widetilde{B}} \rangle = \langle \widetilde{A\widehat{B}} \rangle. \quad (72)$$

These basic relations between the correlation functions can be used to determine the unknown matrices \hat{F} and \hat{G} .

Let us consider the case of non-zero correlations. For example, in the case where $\langle a_p a_q \rangle \neq 0$ and $i = j$, we have

$$-\langle a_p a_q \rangle = \langle a_q a_p \rangle = \langle \tilde{a}_p a_q \rangle = F_{11p} \langle a_p a_q \rangle + F_{12p} \langle b_p a_q \rangle, \quad (73)$$

$$-\langle a_p a_q \rangle = \langle a_q a_p \rangle = \langle a_p \hat{a}_q \rangle = G_{11q} \langle a_p a_q \rangle + G_{12q} \langle a_p b_q \rangle. \quad (74)$$

From whence, we obtain

$$\langle b_p a_q \rangle = -\frac{1 + F_{11p}}{F_{12p}} \langle a_p a_q \rangle, \quad (75)$$

$$\langle a_p b_q \rangle = -\frac{1 + G_{11q}}{G_{12q}} \langle a_p a_q \rangle. \quad (76)$$

Using the remaining relations

$$\begin{aligned} \langle a_q b_p \rangle &= F_{21p} \langle a_p a_q \rangle + F_{22p} \langle b_p a_q \rangle = \\ &= G_{11q} \langle b_p a_q \rangle + G_{12q} \langle b_p b_q \rangle, \end{aligned} \quad (77)$$

$$\begin{aligned} \langle b_q a_p \rangle &= F_{11p} \langle a_p b_q \rangle + F_{12p} \langle b_p b_q \rangle = \\ &= G_{21q} \langle a_p a_q \rangle + G_{22q} \langle a_p b_q \rangle, \end{aligned} \quad (78)$$

we have

$$\langle b_p b_q \rangle = \frac{1 - \text{Sp} \hat{F} - F_{22p} + G_{11q}(1 + F_{11p})}{F_{12p} G_{12q}} \langle a_p a_q \rangle \quad (79)$$

and

$$\langle b_p b_q \rangle = \frac{1 - \text{Sp} \hat{G} - G_{22q} + F_{11p}(1 + G_{11q})}{F_{12p} G_{12q}} \langle a_p a_q \rangle. \quad (80)$$

From whence, we obtain

$$\text{Sp} \hat{G} = \text{Sp} \hat{F} \quad (81)$$

and

$$\langle b_p b_q \rangle = \frac{1 - F_{22p} - G_{22q} + F_{11p} G_{11q}}{F_{12p} G_{12q}} \langle a_p a_q \rangle. \quad (82)$$

Finally, we obtain

$$\langle a_q b_p \rangle = \frac{1 - \text{Sp} \hat{F} - F_{22p}}{F_{12p}} \langle a_p a_q \rangle, \quad (83)$$

$$\langle b_q a_p \rangle = \frac{1 - \text{Sp} \hat{G} - G_{22q}}{G_{12q}} \langle a_p a_q \rangle, \quad (84)$$

$$\langle b_q b_p \rangle = \frac{(G_{22q} + \text{Sp} \hat{G} - 1)G_{11p} - 1 - G_{11q}}{G_{12p} G_{12q}} \langle a_p a_q \rangle. \quad (85)$$

In a completely identical way, we can determine the following relations for the matrices \hat{F}^+ and \hat{G}^+ if $\langle a_p^+ a_q^+ \rangle \neq 0$:

$$\langle b_p^+ a_q^+ \rangle = -\frac{1 + F_{11p}^+}{F_{12p}^+} \langle a_p^+ a_q^+ \rangle, \quad (86)$$

$$\langle a_p^+ b_q^+ \rangle = -\frac{1 + G_{11q}^+}{G_{12q}^+} \langle a_p^+ a_q^+ \rangle, \quad (87)$$

$$\text{Sp} \hat{F}^+ = \text{Sp} \hat{G}^+, \quad (88)$$

and

$$\langle b_p^+ b_q^+ \rangle = \frac{1 - F_{22p}^+ - G_{22q}^+ + F_{11p}^+ G_{11q}^+}{F_{12p}^+ G_{12q}^+} \langle a_p^+ a_q^+ \rangle, \quad (89)$$

$$\langle a_q^+ b_p^+ \rangle = \frac{1 - \text{Sp} \hat{F}^+ - F_{22p}^+}{F_{12p}^+} \langle a_p^+ a_q^+ \rangle, \quad (90)$$

$$\langle b_q^+ a_p^+ \rangle = \frac{1 - \text{Sp} \hat{G}^+ - G_{22q}^+}{G_{12q}^+} \langle a_p^+ a_q^+ \rangle, \quad (91)$$

$$\langle b_q^+ b_p^+ \rangle = \frac{(G_{22q}^+ + \text{Sp} \hat{G}^+ - 1)G_{11p}^+ - 1 - G_{11q}^+}{G_{12p}^+ G_{12q}^+} \langle a_p^+ a_q^+ \rangle. \quad (92)$$

From the expression

$$\langle a_p a_q \rangle = F_{11q} \langle a_q a_p \rangle + F_{12q} \langle b_q a_p \rangle, \quad (93)$$

we obtain the relation

$$G_{12q}(1 + F_{11q}) + (G_{22q} + \text{Sp} \hat{G} - 1)F_{12q} = 0. \quad (94)$$

Moreover, the expression

$$\langle a_p a_q \rangle = G_{11p} \langle a_q a_p \rangle + G_{12p} \langle a_q b_p \rangle \quad (95)$$

yields the relation

$$F_{12q}(1 + G_{11q}) + (F_{22q} + \text{Sp} \hat{F} - 1)G_{12q} = 0. \quad (96)$$

From whence,

$$G_{12q} = -F_{12q} \quad (97)$$

and

$$(1 - F_{22q})G_{12q} = (1 - G_{22q})F_{12q}, \quad (98)$$

which gives rise to

$$G_{22q} + F_{22q} = 2, \quad (99)$$

$$G_{22q} + \text{Sp}\hat{G} - 1 = 1 + F_{11q}, \quad (100)$$

$$F_{22q} + \text{Sp}\hat{F} - 1 = 1 + G_{11q}. \quad (101)$$

Finally, it follows from Eqs. (61) and (97) that

$$G_{11q} - 1 = 1 - F_{11q}. \quad (102)$$

Hence, Eq. (100) yields

$$\begin{aligned} G_{22q} + \text{Sp}\hat{G} - 1 &= 2G_{22q} + G_{11q} - 1 = \\ &= 2G_{22q} - F_{11q} + 1 = 1 + F_{11q}. \end{aligned} \quad (103)$$

Ultimately, it follows from Eq. (103) that

$$F_{11q} = G_{22q}. \quad (104)$$

Similarly, Eq. (101) yields

$$G_{11q} = F_{22q}. \quad (105)$$

From the last relations and Eqs. (100) and (101), we have

$$\text{Sp}\hat{F} = \text{Sp}\hat{G} = 2. \quad (106)$$

Analogously,

$$G_{12p}^+ = -F_{12p}^+, \quad (107)$$

$$G_{22p}^+ + F_{22p}^+ = 2, \quad (108)$$

$$G_{11p}^+ - 1 = 1 - F_{11p}^+, \quad (109)$$

$$F_{11p}^+ = G_{22p}^+, \quad (110)$$

$$G_{11p}^+ = F_{22p}^+, \quad (111)$$

$$\text{Sp}\hat{F}^+ = \text{Sp}\hat{G}^+ = 2. \quad (112)$$

Now, let us use the following relations for a product of two operators:

$$\begin{aligned} \langle AB \rangle^+ &= [\text{Sp}(\rho AB)]^+ = \text{Sp}\{(\rho AB)^+\rho^+\} = \\ &= \text{Sp}\{(\rho AB)^+\rho\} = \text{Sp}\{\rho(\rho AB)^+\} = \\ &= \langle (\rho AB)^+ \rangle = \langle B^+ A^+ \rangle. \end{aligned} \quad (113)$$

Then

$$\langle AB \rangle^+ = \langle B^+ A^+ \rangle. \quad (114)$$

Let us assume that all unknown matrix elements are real. Then, from Eqs. (83) and (86), we obtain

$$(1 + F_{11p}^+)F_{12p} = (1 - \text{Sp}\hat{F} - F_{22p})F_{12p}^+. \quad (115)$$

In turn, Eqs. (84), (87), (97), and (107) yield

$$(1 + G_{11p}^+)F_{12p} = (1 - \text{Sp}\hat{G} - G_{22p})F_{12p}^+. \quad (116)$$

From whence, taking Eq. (106) into account, we ultimately obtain

$$(1 + G_{22p})(1 + F_{11p}^+) = (1 + F_{22p})(1 + G_{11p}^+), \quad (117)$$

if one of the following conditions is satisfied (we consider only the versions, in which the non-diagonal elements of decomposition matrices with a superscript of 12 are non-zero):

$$1 + F_{22p} \neq 0, \quad (118)$$

$$1 + G_{11p}^+ \neq 0, \quad (119)$$

$$1 + G_{22p} \neq 0, \quad (120)$$

$$1 + F_{11p}^+ \neq 0. \quad (121)$$

Taking Eqs. (104), (105), (110), and (111) into account, Eq. (117) gives to

$$F_{11p}^+ = F_{22p}, \quad (122)$$

$$F_{22p}^+ = F_{11p}, \quad (123)$$

$$G_{11p}^+ = G_{22p}, \quad (124)$$

$$G_{22p}^+ = G_{11p}. \quad (125)$$

Finally, from Eq. (115) with regard for Eqs. (97) and (107), we have

$$F_{12p}^+ = -F_{12p} = G_{12p} = -G_{12p}^+. \quad (126)$$

This relation and Eqs. (60), (63), (66), and (67) yield the following useful relations:

$$G_{21q}G_{12q} = -(1 - F_{11q})^2, \quad (127)$$

$$F_{21q}G_{12q} = (1 - F_{11q})^2, \quad (128)$$

$$F_{21p}^+G_{12p} = -(1 - F_{11p})^2, \quad (129)$$

$$G_{21p}^+G_{12p} = (1 - F_{11p})^2. \quad (130)$$

We also have

$$\begin{aligned} \delta_{pq} - \langle a_p^+ a_q \rangle &= \langle a_q a_p^+ \rangle = F_{11p}^+ \langle a_p^+ a_q \rangle + \\ &+ F_{12p}^+ \langle b_p^+ a_q \rangle = G_{11q} \langle a_p^+ a_q \rangle + G_{12q} \langle a_p^+ b_q \rangle. \end{aligned} \quad (131)$$

From whence, we obtain

$$\begin{aligned} \langle b_p^+ a_q \rangle &= \frac{\delta_{pq} - (1 + F_{11p}^+) \langle a_p^+ a_q \rangle}{F_{12p}^+} = \\ &= \frac{\delta_{pq} + (F_{11p} - 3) \langle a_p^+ a_q \rangle}{G_{12p}}, \end{aligned} \quad (132)$$

$$\begin{aligned} \langle a_p^+ b_q \rangle &= \frac{\delta_{pq} - (1 + G_{11q}) \langle a_p^+ a_q \rangle}{G_{12q}} = \\ &= \frac{\delta_{pq} + (F_{11q} - 3) \langle a_p^+ a_q \rangle}{G_{12q}}. \end{aligned} \quad (133)$$

From the formula

$$\begin{aligned} \langle a_p^+ a_q \rangle &= G_{11p}^+ \langle a_q a_p^+ \rangle + G_{12p}^+ \langle a_q b_p^+ \rangle = \\ &= F_{11q} \langle a_q a_p^+ \rangle + F_{12q} \langle b_q a_p^+ \rangle, \end{aligned} \quad (134)$$

we obtain

$$\langle b_q a_p^+ \rangle = \frac{F_{11q} \delta_{pq} - (1 + F_{11q}) \langle a_p^+ a_q \rangle}{G_{12q}}, \quad (135)$$

$$\langle a_q b_p^+ \rangle = \frac{F_{11p} \delta_{pq} - (1 + F_{11p}) \langle a_p^+ a_q \rangle}{G_{12p}}. \quad (136)$$

Analogously, from formula

$$\langle b_q a_p^+ \rangle = F_{11p}^+ \langle a_p^+ b_q \rangle + F_{12p}^+ \langle b_p^+ b_q \rangle, \quad (137)$$

we have

$$\langle b_p^+ b_q \rangle = \frac{F_{11p} F_{11q} - 3(F_{11p} + F_{11q}) + 5}{G_{12p} G_{12q}} \langle a_p^+ a_q \rangle. \quad (138)$$

Moreover, the formula

$$\langle b_p^+ a_q \rangle = F_{11q} \langle a_q b_p^+ \rangle + F_{12q} \langle b_q b_p^+ \rangle \quad (139)$$

yields

$$\langle b_q b_p^+ \rangle = \{(F_{11p}^2 - 1) \delta_{pq} + (3 - F_{11p} - F_{11q} - F_{11p} F_{11q}) \langle a_p^+ a_q \rangle\} \div (G_{12p} G_{12q}). \quad (140)$$

Finally, from formula

$$\langle b_p^+ b_q \rangle = F_{21q} \langle a_q b_p^+ \rangle + F_{22q} \langle b_q b_p^+ \rangle, \quad (141)$$

we obtain

$$F_{11q} = 1. \quad (142)$$

By averaging Eq. (36), we find that

$$G_{12q} = G_{12p} = G_{12} \neq 0 \quad (143)$$

are constants. At the same time, averaging Eq. (37), we obtain

$$\langle a_p^+ a_q \rangle = \frac{K_{21p} G_{12} + 2(K_{22p} - K_{11p}) \delta_{pq}}{4(K_{22p} - K_{11p})} \delta_{pq}. \quad (144)$$

Taking into account that the operators with different indices marking the sort of particles commute and repeating the previous calculations for the case $j \neq i$, we obtain the following general relations:

$$\langle a_{jq} b_{ip} \rangle = \langle b_{ip} a_{jq} \rangle = \frac{1 - F_{11p}^{(i)}}{F_{12p}^{(i)}} \langle a_{ip} a_{jq} \rangle = 0, \quad (145)$$

$$\langle b_{jq} a_{ip} \rangle = \langle a_{ip} b_{jq} \rangle = \frac{1 - G_{11q}^{(j)}}{G_{12q}^{(j)}} \langle a_{ip} a_{jq} \rangle = 0, \quad (146)$$

$$\langle b_{jq} b_{ip} \rangle = \langle b_{ip} b_{jq} \rangle = \frac{(1 - F_{11p}^{(i)})(1 - G_{11q}^{(j)})}{F_{12p}^{(i)} G_{12q}^{(j)}} \langle a_{ip} a_{jq} \rangle = 0, \quad (147)$$

$$\langle a_{jq} b_{ip}^+ \rangle = \langle b_{ip}^+ a_{jq} \rangle = \frac{1 - F_{11p}^{+(i)}}{F_{12p}^{+(i)}} \langle a_{ip}^+ a_{jq} \rangle = 0, \quad (148)$$

$$\langle b_{jq} a_{ip}^+ \rangle = \langle a_{ip}^+ b_{jq} \rangle = \frac{1 - G_{11q}^{(j)}}{G_{12q}^{(j)}} \langle a_{ip}^+ a_{jq} \rangle = 0, \quad (149)$$

$$\langle b_{jq} b_{ip}^+ \rangle = \langle b_{ip}^+ b_{jq} \rangle = \frac{(1 - F_{11p}^{+(i)})(1 - G_{11q}^{(j)})}{F_{12p}^{+(i)} G_{12q}^{(j)}} \langle a_{ip}^+ a_{jq} \rangle = 0, \quad (150)$$

$$\langle a_{jq}^+ b_{ip}^+ \rangle = \langle b_{ip}^+ a_{jq}^+ \rangle = \frac{1 - F_{11p}^{+(i)}}{F_{12p}^{+(i)}} \langle a_{ip}^+ a_{jq}^+ \rangle = 0, \quad (151)$$

$$\langle b_{jq}^+ a_{ip}^+ \rangle = \langle a_{ip}^+ b_{jq}^+ \rangle = \frac{1 - G_{11q}^{(j)}}{G_{12q}^{(j)}} \langle a_{ip}^+ a_{jq}^+ \rangle = 0, \quad (152)$$

$$\langle b_{jq}^+ b_{ip}^+ \rangle = \langle b_{ip}^+ b_{jq}^+ \rangle = \frac{(1 - F_{11p}^{+(i)})(1 - G_{11q}^{(j)})}{F_{12p}^{+(i)} G_{12q}^{(j)}} \langle a_{ip}^+ a_{jq}^+ \rangle = 0. \quad (153)$$

4. Energy of Elementary Excitations in the Case of Triangular Decomposition Matrices

We recall that it follows from Eqs. (104), (105), (110), (111), (122)–(125), and (142) that

$$G_{22} = F_{22} = G_{11} = F_{11} = G_{22}^+ = F_{22}^+ = G_{11}^+ = F_{11}^+ = 1. \quad (154)$$

Let us consider some consequences of the results obtained. From Eqs. (58) and (65), we obtain

$$\langle b_{ip}^+ \rangle = \langle b_{iq} \rangle = 0. \quad (155)$$

From Eqs. (127)–(130), (142), and (143), it follows that

$$G_{21} = G_{21}^+ = F_{21} = F_{21}^+ = 0. \quad (156)$$

Let us use formula (3.4.12) from work [1] written in the form

$$K_{21p} \langle a_p a_p^+ \rangle + (K_{22p} - K_{11p}) \langle a_p b_p^+ \rangle - K_{12p} \langle b_p b_p^+ \rangle = 0. \quad (157)$$

From whence, in view of the results obtained above, we have

$$\langle a_p^+ a_p \rangle = \frac{K_{21p} G_{12} + K_{22p} - K_{11p}}{K_{21p} G_{12} + 2(K_{22p} - K_{11p})}. \quad (158)$$

Finally, from Eq. (144), we have

$$\langle a_p^+ a_q \rangle = \frac{\delta_{pq}}{2}, \quad (159)$$

as well as

$$K_{21} = 0. \quad (160)$$

Taking Eq. (31) into account, we obtain

$$K_{22p}^{(i)} = K_{11p}^{(i)} \pm K, \quad (161)$$

where K is an unknown constant.

Note that Eq. (158) is applicable only if $K \neq 0$. Otherwise, if we put simultaneously $K_{21} = 0$ and $K_{22p} = K_{11p}$ in Eq. (157), it is satisfied automatically, and $\langle a_p^+ a_p \rangle$ remains indefinite! Therefore, we will consider only one of the possible cases where Eq. (159) is satisfied. Then, from Eqs. (143), (154), (156), and (160), we see that all decomposition matrices are triangular in this case. According to author's concept of the DAM, the eigenvalues of the decomposition matrix determine the energy of elementary excitations of the Coulomb pair [1]. If the matrix is triangular, its eigenvalues are equal to its diagonal elements. From Eq. (161), one can see that the energy of elementary excitations either is equal to the kinetic energy of particles or differs from it by a constant.

5. Conclusions

Since the quantity $n_{ip} = \langle a_{ip}^+ a_{ip} \rangle$ corresponds to the average number of i -th particles in the state with a definite spin projection s_z and a definite momentum $\mathbf{p} = (p_x, p_y, p_z)$, we see from Eq. (159) that there are only two possible states for each of the particles with a definite spin and a definite momentum of the pair. We recall that, in this work, only the case of non-zero anomalous distribution functions was considered, when $\langle a_{ip} a_{iq} \rangle \neq 0$ and $\langle a_{ip}^+ a_{iq}^+ \rangle \neq 0$, which is a condition for the particle pairing. It is of interest to pay attention to the case where the total momentum of the pair equals zero, i.e. the momenta of the particles are directed oppositely. Then, the total current of the pair will be different from zero, and we will obtain a magnetic field as a result of the Coulomb pairing.

The obtained results allow us to conclude that the DAM is an effective method for the description of correlations in a system of two particles, which interact electrostatically. Even in the second order, it allows almost all unknown components of the decomposition matrices and a relation for the correlation functions to be determined. However, for the determination of the average energy of the system, the correlation functions of the fourth order have to be known. Therefore, only a basis of the exact theory for the Coulomb pair was laid in this work. Note that the explicit form for the potential energy of interaction – it is important only for results obtained for the third, fourth, and higher orders of correlation functions – has not been used.

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КОРЕЛЯЦІЙНІ ФУНКЦІЇ КУЛОНІВСЬКОЇ ПАРИ

Резюме

Вперше публікуються результати, що отримані прямим алгебраїчним методом, для кореляційних функцій двох частинок із кулонівською взаємодією. Ефективність цього методу продемонстрована знаходженням в другому порядку майже всіх невідомих матричних елементів матриць розкладання.