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**B. Westwański**

**PERTURBATION THEORY  
FOR HAMILTONIANS OF ANDERSON  
AND HUBBARD TYPE.**

**I. REALIZATION OF GENERAL STATISTICAL  
WICK THEOREM.**

**1973**

**ЛАБОРАТОРИЯ  
ТЕОРЕТИЧЕСКОЙ ФИЗИКИ**

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**PERTURBATION THEORY  
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WICK THEOREM.**

Объединенный институт  
ядерных исследований  
БИБЛИОТЕКА

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Вестваньски Б.

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Теория возмущений для гамильтонианов типа Андерсона и Хаббарда. I. Реализация обобщенной статистической теоремы Вика

Реализация обобщенной статистической теоремы Вика описана в терминах поперечных операторов восьмифермионного и четырехспинового типов. Получено диаграммное представление как для поперечных, так и для диагональных операторов.

Сообщение Объединенного института ядерных исследований  
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Westwański B.

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Perturbation Theory for Hamiltonians of Anderson and Hubbard Type. I. Realization of General Statistical Wick Theorem

Within a new perturbation theory the Coulomb interaction is included into zeroth-order Hamiltonian. The realization of the general statistical Wick theorem is described in terms of eight-Fermi and four-spin type transverse operators. Diagrammatic representation of both transverse and diagonal operators is obtained.

Communications of the Joint Institute for Nuclear Research.  
Dubna, 1973

## 1. Introduction

Insulator metal transitions are phenomena which have been known for quite a while in a wide variety of systems: metal vapour liquid system (mercury), metal ammonia solutions, disordered system (impurity bands), transition metal chalcogenides. In the last few years there has been considerable interest in transition metal oxides. These oxides form a very interesting class of materials<sup>/1-2/</sup>.

The Hubbard ideas<sup>/3/</sup> are central to the interpretation of the properties of many transition metal chalcogenides<sup>/4/</sup>. The Hubbard model<sup>/3/</sup> has been studied extensively in the approach of the equation of motion for the Green function<sup>/3-8/</sup>. The functional integration method is given in<sup>/9/</sup>. Moments method is developed in<sup>/10-13/</sup>.

Corresponding approaches to the Anderson model<sup>/14/</sup> are given and quoted in<sup>/15-17/</sup>.

This paper extends the ideas of<sup>/18-21/</sup>. We present here perturbation theory for Hamiltonians with the Coulomb repulsion of the type of the Anderson and Hubbard models, but using the general statistical Wick theorem (GSWT)<sup>/20-21/</sup>.

Following the Anderson model we include into the zeroth-order Hamiltonian the Coulomb interaction between two d-orbital electrons in addition to the single-particle d and conduction band energies. We pick out an analogous term in the Hubbard model case. The Coulomb interaction is in general the dominant term in both the above mentioned models. Therefore the perturbation theory presented here may be fruitful.

In § 2 the decomposition of Hamiltonian into unperturbed and interaction parts is given. In § 3 the realization of GSWT for transverse operators is achieved. In § 4 the diagrammatic representation of the transverse and diagonal operators is obtained.

## 2. Decomposition of Hamiltonian

Let us define

$$\langle X \rangle \equiv Z^{-1} \text{Tr} \{ X \exp[-\beta(H - \mu N)] \}; \quad (1)$$

$$Z \equiv \text{Tr} \{ \exp[-\beta(H - \mu N)] \},$$

where X is any operator, N total number operator,  $\mu$  - chemical potential, H any Hamiltonian of fermion systems (in magnetic field h) containing the Coulomb interaction U. We assume that operator  $H - \mu N$  can be written in the form

$$H - \mu N = H_0 + V, \quad (2)$$

where the "unperturbed" Hamiltonian

$$H_0 = \sum H_{0\kappa}, \quad (3)$$

in which a subsystem Hamiltonian

$$H_{0\kappa} = E_+ n_{\kappa+} + E_- n_{\kappa-} + U n_{\kappa+} n_{\kappa-} \quad (4)$$

with

$$E_{\sigma} = \epsilon + \sigma h - \mu \quad (5)$$

and  $\epsilon$  being some parameter. The operator  $n_{\kappa\sigma} = d_{\kappa\sigma}^+ d_{\kappa\sigma}$ , and  $d_{\kappa\sigma}^+$ ,  $d_{\kappa\sigma}$  are the creation and annihilation operators for an electron of spin  $\sigma$  ( $\sigma = \pm 1$ ) (at  $\kappa$ -th lattice side. The second term in (2), V, we will call an interaction).

In the following  $\langle \dots \rangle_0$  denotes the average (1-2) with  $V=0$  and

$$X(\tau) \equiv \exp[\tau H_0] X \exp[-\tau H_0], \quad (6)$$

$$|\tau| \leq \beta. \quad (7)$$

Hamiltonians, in which a part of the type (3-4) occurs being of great physical significance, have been introduced by Anderson<sup>/14/</sup>:

$$H_0 = H_{0d} + H_{0s}; \quad (8)$$

$$H_{0d} = \epsilon_{d+} n_{d+} + \epsilon_{d-} n_{d-} + U n_{d+} n_{d-}, \quad (9)$$

$$H_{0s} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma}, \quad (10)$$

$$\epsilon_{(\mathbf{k})\sigma} = \epsilon_{(\mathbf{k})} + \sigma h - \mu,$$

$$V = \sum_{\mathbf{k}} (V_{\mathbf{k}d}^* d_{\sigma}^+ c_{\mathbf{k}\sigma} + V_{\mathbf{k}d} c_{\mathbf{k}\sigma}^+ d_{\sigma}) \quad (11)$$

and by Hubbard<sup>/3/</sup>:

$H_0$  has the form (3-5) with  $\epsilon = T_{\kappa\kappa}$ ,

$$V \equiv V_H = \sum_{\substack{\kappa \neq \kappa' \\ \sigma}} T_{\kappa\kappa'} d_{\kappa\sigma}^+ d_{\kappa'\sigma}. \quad (12)$$

The other types of the interaction have been given in<sup>/3,13/</sup>. A most general form of interaction will be discussed in § 4.

The first who introduced the decomposition of Anderson Hamiltonian into "unperturbed" and interaction parts in the way (8-11) is just Scalapino<sup>/15/</sup>. He initiated finite-order perturbation theory for the partition function. Keiter and Kimball<sup>/16/</sup> following Scalapino have formulated infinite diagram summation. These authors applied the usual Wick theorem to k-electron operators only, and the thermodynamic expectation values of products of d electron operators were evaluated in the representation, where  $H_{0d}$  in (9) is diagonal.

It should be noted that, Kaschenko et al. <sup>/22/</sup> were trying to formulate an analog of the Wick theorem, when "unperturbed" Hamiltonian contains single-ion anisotropy in addition to the Zeeman term <sup>/18/</sup>. However they conclude that an analog of the Wick theorem in this case does not exist. According to <sup>/20-21/</sup>, their conclusion is not valid. In <sup>/20/</sup> GSWT was given for an arbitrary unperturbed Hamiltonian. Application of GWST to spin Hamiltonian with  $S=1$  is discussed in <sup>/21/</sup>. This discussion contains two interesting physical cases - single ion anisotropy and more complicated crystal fields as described for example in <sup>/23, 24/</sup>. It seems, that recently (Report on the International Conference on Magnetism, Moscow, August 1973) the authors of <sup>/22/</sup> (and additional collaborators: V.N.Kitaev, Yu.A.Emelianov) have changed their opinion and get the result, which is a special case of that in <sup>/20, 21/</sup>.

Now we present here the general principles of diagram technique for Hamiltonians of the type of that by Anderson and Hubbard, on the basis of GSWT <sup>/20-21/</sup> for operators, commutators or anticommutators of which are not c-numbers. According to GSWT when it is possible to extract from Hamiltonian that part, which has the form of the sum (3), we can treat it as unperturbed Hamiltonian and the remaining part as an interaction.

### 3. Realization of GSWT

To determine the realization of GSWT <sup>/20, 21/</sup> it is sufficient to find the solutions for eigenvalues  $H_{0K}^{+ij}$  and eigenoperators  $J_K^{ij}$  ( $i \neq j$ ) of superpropagator  $H_{0K}^x$

$$H_{0K}^x J_K^{+ij} = [H_{0K}, J_K^{+ij}] = H_{0K}^{+ij} J_K^{+ij};$$

$$H_{0K}^{+ij} = H_{0K}^i - H_{0K}^j = H_{0K}^{ji} = -H_{0K}^{ij};$$

$$J_K^{+ij} = J_K^{ji} \quad (13)$$

Physical meaning of such eigenoperators is described in <sup>/25/</sup>. In contrast with <sup>/20/</sup> we define here (for convenience) the operators  $J_K^{13}$ ,  $J_K^{14}$  in the following way

$$J_K^{13} = -|3\rangle_K \langle 1|_K, \quad J_K^{14} = -|4\rangle_K \langle 1|_K \quad (13a)$$

Four eigenstates of  $H_{0K}$

$$\begin{aligned} |1\rangle_K &= |11\rangle_K, & |2\rangle_K &= |01\rangle_K, \\ |3\rangle_K &= |10\rangle_K, & |4\rangle_K &= |00\rangle_K \end{aligned} \quad (14)$$

with two electrons, with a  $d_{K-}$ -electron, a  $d_{K+}$ -electron and no electron, respectively <sup>/15, 16/</sup> have properties

$$|1\rangle_K = d_{K+}^+ d_{K-}^+ |4\rangle_K \quad (15)$$

$$|2\rangle_K = d_{K-}^+ |4\rangle_K$$

$$|3\rangle_K = d_{K+}^+ |4\rangle_K \quad (16)$$

In this representation (4) may be rewritten as the 4x4 matrix

$$H_{0K} = \begin{pmatrix} H_{0K}^1 & 0 & 0 & 0 \\ 0 & H_{0K}^2 & 0 & 0 \\ 0 & 0 & H_{0K}^3 & 0 \\ 0 & 0 & 0 & H_{0K}^4 \end{pmatrix} \quad (17)$$

with eigenvalues  $H_{0K}^1 = E_+ + E_- + U$ ,  $H_{0K}^2 = E_-$ ,  $H_{0K}^3 = E_+$ ,  $H_{0K}^4 = 0$ . Hence due to (13) it suffices to write down  $H_{0K}^{+ij}$  for  $i < j$ :

$$H_{0K}^{+12} = E_+ + E_-, \quad H_{0K}^{+13} = E_- + U, \quad H_{0K}^{+23} = -2h, \quad (18)$$

$$\overset{+}{H}_{0\kappa}^{34} = E_+, \quad \overset{+}{H}_{0\kappa}^{24} = E_-, \quad \overset{+}{H}_{0\kappa}^{14} = E_+ + E_- + U.$$

According to (13a-16) and <sup>/20/</sup> the operators  $J_{\kappa}^{ij}$  ( $i < j$ ) take the form <sup>/3/</sup>:

$$\left. \begin{aligned} J_{\kappa}^{12} &= d_{\kappa+} n_{\kappa-}, & J_{\kappa}^{34} &= d_{\kappa+} (1 - n_{\kappa-}), \\ J_{\kappa}^{13} &= n_{\kappa+} d_{\kappa-}, & J_{\kappa}^{24} &= (1 - n_{\kappa+}) d_{\kappa-}, \end{aligned} \right\} \quad (19)$$

$$J_{\kappa}^{23} = d_{\kappa+}^+ d_{\kappa-}, \quad J_{\kappa}^{14} = d_{\kappa+} d_{\kappa-}. \quad (20)$$

For convenience we denote by  $F_{\kappa}$  and  $S_{\kappa}$  the sets of pseudo-fermion and pseudo-spin operators, correspondingly:

$$F_{\kappa} \equiv \{ J_{\kappa}^{12}, J_{\kappa}^{+12}, J_{\kappa}^{34}, J_{\kappa}^{+34}, J_{\kappa}^{13}, J_{\kappa}^{+13}, J_{\kappa}^{24}, J_{\kappa}^{+24} \} \quad (19a)$$

$$S_{\kappa} \equiv \{ J_{\kappa}^{23}, J_{\kappa}^{+23}, J_{\kappa}^{14}, J_{\kappa}^{+14} \}. \quad (20a)$$

From (19) and (20) we see that for  $\kappa \neq \kappa'$  1° operators from  $F_{\kappa}$  and  $F_{\kappa'}$  anticommute, 2° operators from  $S_{\kappa}$  and  $S_{\kappa'}$  (or  $F_{\kappa'}$ ) commute. This is why we have to introduce the following set  $Q_{\kappa} \equiv \{ Q_{\kappa}^{ij} \}$  of diagonal operators

$$Q_{\kappa}^{ij} \equiv [J_{\kappa}^{ij}, J_{\kappa}^{+ij}]_{-\eta}; \quad \eta = \begin{cases} -1 & \text{for } J_{\kappa}^{ij} \in F_{\kappa} \\ +1 & \text{for } J_{\kappa}^{ij} \in S_{\kappa} \end{cases}, \quad i < j, \quad (21)$$

i.e.,

$$\begin{aligned} Q_{\kappa}^{12} &= n_{\kappa-}, & Q_{\kappa}^{34} &= 1 - n_{\kappa-}, \\ Q_{\kappa}^{13} &= n_{\kappa+}, & Q_{\kappa}^{24} &= 1 - n_{\kappa+}, \\ Q_{\kappa}^{23} &= Q_{\kappa}^{13} - Q_{\kappa}^{12}, \\ Q_{\kappa}^{14} &= 1 - (Q_{\kappa}^{13} + Q_{\kappa}^{12}). \end{aligned}$$

The operators (21) commute with both transverse operators from  $F_{\kappa'}$  and  $S_{\kappa'}$  for different lattice site indices. Let now by definition

$$\Theta_{\kappa} = F_{\kappa} \cup S_{\kappa} \cup Q_{\kappa}. \quad (22)$$

The corresponding anticommutators (or commutators) of any pair of operators from  $\Theta_{\kappa}$  are obtained from table of products given in Appendix A.

According to 1°, 2° and <sup>/20/</sup> we have to introduce two types of the following free Green functions (FGF): Fermi FGF's ( $\eta = -1$ ) corresponding to pseudo-fermi operators (19a) and Bose FGF's ( $\eta = +1$ ) corresponding to pseudo-spin operators (20a), i.e.,

$$\begin{aligned} G_{ij}^{+}(\tau - \tau') &= \exp[(\tau - \tau') \overset{+}{H}_{0\kappa}^{ij}] [\eta n(ij) \Theta(\tau - \tau') + \\ &+ (\eta n(ij) + 1) \Theta(\tau - \tau')] = \beta^{-1} \sum_m \exp[-i\lambda_m(\tau - \tau')] G_{ij}^{+}(i\lambda_m), \end{aligned} \quad (23)$$

where

$$\begin{aligned} n(ij) &\equiv (\exp[\beta \overset{+}{H}_{0\kappa}^{ij}] - \eta)^{-1}, \\ G_{ij}^{+}(i\lambda_m) &\equiv (i\lambda_m + \overset{+}{H}_{0\kappa}^{ij})^{-1} \end{aligned}$$

and  $i\lambda_m$  is the imaginary Fermi or Bose frequency due to the kind of operator  $J_{\kappa}^{ij}$ . FGF's (23) relate the "unperturbed" (the word "unperturbed" will be omitted in the following) average of T-ordered product of operators  $J_{\ell}^{ij}(\tau')$  and  $J_{\ell}^{ij}(\tau)$  to that of  $[J_{\ell}^{ij}, J_{\ell}^{+ij}]_{-\eta}$  in the following way:

$$\langle T J_{\ell'}^{ij}(\tau') J_{\ell}^{+ij}(\tau) \rangle_0 = G_{ij}^{+}(\tau - \tau') \delta_{\ell, \ell'} \langle [J_{\ell}^{ij}, J_{\ell}^{+ij}]_{-\eta} \rangle_0, \quad (24)$$

where  $J(\tau)$  is defined in (6).

On the basis of above consideration and that in <sup>/20-21/</sup> applying the Gaudin method <sup>/26,18,27/</sup> we obtain a modification of GSWT <sup>/20/</sup> for the case considered here (when

there are two types of the reducers (19a) and (20a)). Namely the average of T-ordered product of  $n+1$  operators may be reduced to that of T-product of  $m$  operators with  $m < n+1$  according to the formulae (GSWT)

$$\begin{aligned} < T \prod_{\kappa_1}^{l_{\kappa_1}}(\tau_1) \dots \prod_{\kappa_f}^{l_{\kappa_f}}(\tau_f) J_{\kappa_p}^{l_{\kappa_p}}(\tau_p) \prod_{\kappa_{f+1}}^{l_{\kappa_{f+1}}}(\tau_{f+1}) \dots \\ \prod_{\kappa_n}^{l_{\kappa_n}}(\tau_n) >_0 = \sum_{j=1}^n (-1)^{P_j} \delta_{\kappa_j, \kappa_p} G^{l_{\kappa_p}}(\tau_p, -\tau_j) < \prod_{\kappa_1}^{l_{\kappa_1}}(\tau_1) \dots \\ \prod_{\kappa_{j-1}}^{l_{\kappa_{j-1}}}(\tau_{j-1}) [I_{\kappa_j}^{l_{\kappa_j}} J_{\kappa_p}^{l_{\kappa_p}}]_{-\eta}(\tau_j) * \\ * \prod_{\kappa_{j+1}}^{l_{\kappa_{j+1}}}(\tau_{j+1}) \dots \prod_{\kappa_n}^{l_{\kappa_n}}(\tau_n) >_0, \end{aligned} \quad (25)$$

where

a)  $G_{\kappa_p}^{l_{\kappa_p}}$  is of the Fermi type (Bose type) if

$$J_{\kappa_p}^{l_{\kappa_p}} \in F_{\kappa_p} (S_{\kappa_p}),$$

b) anticommutator should be taken if  $I_{\kappa_i}$  and  $J_{\kappa_p}^{l_{\kappa_p}}$  belong to  $F_{\kappa_j}$  and  $F_{\kappa_p}$ , correspondingly, otherwise - commutator (i.e.,  $J_{\kappa_p}^{l_{\kappa_p}} \in F_{\kappa_p}$  and  $I_{\kappa_j}^{l_{\kappa_j}} \in S_{\kappa_j} \cup Q_{\kappa_j}$ ,  $J_{\kappa_p}^{l_{\kappa_p}} \in S_{\kappa_p}$  and  $I_{\kappa_j}^{l_{\kappa_j}} \in \Theta_{\kappa_j}$ ),

c) factor  $(-1)^{P_j}$  arises when  $J_{\kappa_p}^{l_{\kappa_p}} \in F_{\kappa_p}$ ;  $P_j$  is the number of transpositions of the operator  $J_{\kappa_p}^{l_{\kappa_p}}$  with other operators  $I$  on the left-hand side of (25) which is required to set up this operator on the right of  $I_{\kappa_j}^{l_{\kappa_j}}$ . In this procedure the operators  $I_{\kappa_k}^{l_{\kappa_k}} \in S_{\kappa_k} \cup Q_{\kappa_k}$  may be treated as the product of two Fermi operators, and this procedure then gives factor  $(-1)^2$ .

FGF's (23) satisfy the relation

$$G_{ij}^{\dagger}(\tau - \tau') = -G_{ij}(\tau' - \tau). \quad (26)$$

If in (25)  $l_{\kappa_p} = ij_{\kappa_p}$ , i.e., we reduce the average on the left-hand side of (25) with the help of operators  $J_{\kappa_p}^{ij_{\kappa_p}}$  using  $G_{ij_{\kappa_p}}(\tau_p, -\tau_j)$ , then from (26) it follows that the same FGF with transposed time arguments, i.e.,  $G_{ij_{\kappa_p}}^{\dagger}(\tau_j, -\tau_p)$  can be used if  $l_{\kappa_p} = ij_{\kappa_p}$  in (25) but at the same time we have  $[J_{\kappa_p}^{ij_{\kappa_p}}, I_{\kappa_j}^{l_{\kappa_j}}]_{-\eta}(\tau_j)$  on the right-hand side of (25)

Due to this fact two reduction processes can be carried out, in one of which only FGF's  $G_{ij}^{\dagger}$  ( $i < j$ ) arise and  $G_{ij}$ 's ( $i < j$ ) - in the other. It is easy to see that FGF's (23) are not all independent and hence the way of reduction in (25) is not the only one. However in every case we obtain the same result. Therefore we can separate one of all these ways. We propose the following process of the reduction. Let us consider the averages like those on the left-hand side of (25). Firstly for the reduction we take an arbitrary transverse operator, say  $J_{\kappa_p}^{l_{\kappa_p}}(\tau_p)$ . Then we obtain  $n$  terms on the right-hand side of (25). We define the second stage as follows: if  $[I_{\kappa_j}^{l_{\kappa_j}}, J_{\kappa_p}^{l_{\kappa_p}}]_{-\eta}$  is (according to realization of GSWT and Appendix A) a transverse operator, then it is to be used for the reduction of  $j$ -th term, otherwise, i.e., if  $[I_{\kappa_j}^{l_{\kappa_j}}, J_{\kappa_p}^{l_{\kappa_p}}]_{-\eta}$  is a diagonal operator we reduce the  $j$ -th

average by means of an arbitrary transverse operator. We define the next stages as the repetition of second one. This repetition is continued as long as there are transverse operators and at the end (25) becomes a sum of the products of FGF's (23) ( $i \neq j = 1, 2, 3, 4$ , and  $ji \equiv ij$ ) and averages of product of diagonal operators only.

#### 4. Diagrammatic Representation of Operators from $\Theta_K$

From the definition of the reduction process there follows diagrammatic representation of transverse operators given in Appendix B, where directed lines

$$\begin{array}{l} \tau_p \xrightarrow{ij^+} \tau_j, \\ \tau_p \xrightarrow{\ell_k} \tau_i \end{array} \quad (27)$$

denote the FGF's (23)  $G_{ij^+}^{\dagger}(\tau_p, -\tau_j)$  and  $G_{\ell_k}^{\dagger}(\tau_p, -\tau_i)$ , respectively. Here we introduce a generalization of usual particle-hole picture<sup>/28/</sup> calling the operators  $J_{ij^+}^{\dagger}$ ,  $J_{\ell_k}^{\dagger}$  correspondingly the creation (annihilation) and annihilation (creation) ones of "particle (hole)  $ij$ ". Such a picture in the case  $ij=23$  ( $H_{0K}^{\dagger,23} = -H_{0K}^{\dagger,23}$  is independent of chemical potential) is adopted here only for generality. These operators playing the role of creation and annihilation ones of "particle  $ij$ " are represented in the following manner

$$\textcircled{ij^+} \xrightarrow{ij^+} \quad (28)$$

$$\xrightarrow{ij^+} \textcircled{ij} \quad (29)$$

i.e., the operator  $J_{ij^+}^{\dagger}$  by the  $\textcircled{ij^+}$  with one outgoing line  $\xrightarrow{ij^+}$  and  $J_{\ell_k}^{\dagger}$  by  $\textcircled{ij}$  with one incoming line  $\xrightarrow{ij^+}$ . The other possibilities of representation of above operators in the "particle" case are of two types: with one incoming and one outgoing line

$$\xrightarrow{\ell_k} \textcircled{ij^+} \xrightarrow{pq} \quad (28a)$$

$$\xrightarrow{\ell_k'} \textcircled{ij} \xrightarrow{p'q'} \quad (29a)$$

or with two incoming and one outgoing line

$$\begin{array}{l} \xrightarrow{\ell_k} \\ \xrightarrow{ij^+} \end{array} \textcircled{ij} \xrightarrow{\ell_k} \quad (30)$$

The kind of incoming and outgoing line in (28a, 29a) is determined by corresponding conditions:

$$[J_{K}^{ij^+}, J_{K}^{\ell_k}]_{-\eta} = (\pm) J_{K}^{pq} \quad (28b)$$

$$H_{0K}^{\dagger, pq} - H_{0K}^{\dagger, \ell_k} = H_{0K}^{\dagger, ij}$$

$$[J_{K}^{ij^+}, J_{K}^{\ell_k'}]_{-\eta} = (\pm) J_{K}^{p'q'} \quad (29b)$$

$$H_{0K}^{\dagger, \ell_k'} - H_{0K}^{\dagger, p'q'} = H_{0K}^{\dagger, ij}$$

In (30) the line  $\xrightarrow{\ell_k}$  occurs if

$$[Q_{K}^{ij}, J_{K}^{\ell_k}]_{-1} = (\pm) J_{K}^{\ell_k} \quad (30a)$$

The sign  $(\pm)$  in (28b-30a) given by  $[ , ]_{-\eta}$  is indicated on the figures in Appendix B.

The "hole" case representation of operators  $J_{ij^+}^{\dagger}$ ,  $J_{\ell_k}^{\dagger}$  can be considered analogically.

According to accepted above reduction process we will represent the diagonal operators  $Q^{ij}$  by  $\boxed{ij}$  with the same incoming and outgoing line  $\xrightarrow{\ell_k}$

$$\xrightarrow{\ell_k} \boxed{ij} \xrightarrow{\ell_k} \quad (31)$$

where all possible lines are determined by the condition (30a). Corresponding representation table for diagonal operators is to be obtained from that given in Appendix B, when here one replaces  $\textcircled{ij^+}$  by  $\boxed{ij}$  on the figures

of the type (30). Besides (31) we will represent diagonal operators  $Q^{ij}$  simply by

$$\boxed{ij} \quad (32)$$

Obviously

$$\begin{array}{l} \boxed{ij^+} = \boxed{ij} \quad \text{for } ij = 12, 34, 13, 24, \\ \boxed{ij^+} = -\boxed{ij} \quad \text{for } ij = 23, 14. \end{array}$$



It should be pointed out here that described above diagrammatic representation of operators from  $\Theta_K$  is valid for arbitrary structure of interaction. From (19-21) it follows what types of interactions with hopping integrals similar to that of Hubbard<sup>13/</sup> we can introduce (if they can have the physical meaning). Namely denoting

such integrals by  $T_{K,K'}^{l_K, k_K}$ , where the index  $l_K(k_K)$  denotes the kind of the operator in  $\Theta_K(\Theta_{K'})$ , we can write down the class of interactions mentioned in §2 in the form

$$\sum_{K \neq K'} T_{K,K'}^{l_K, k_K} I_K^{l_K} I_{K'}^{k_K}. \quad (33)$$

Frequently we obtain the interaction of the type of (33) by a diagonalization analogous to (17-21).

In conclusion we would like to point out that in the second part of this paper (referred to as II) we shall formulate an analog of GSWT for diagonal operators and use the presented approach to study of the Anderson and Hubbard model.

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#### Appendix A. Table of Products of Operators from $\Theta$

$$J^{+12} J^{12} = J^{+13} J^{13} = J^{+14} J^{14} = Q^{13} Q^{12}$$

$$J^{+23} J^{23} = J^{+24} J^{24} = J^{12} J^{+12} = Q^{24} Q^{12}$$

$$J^{+34} J^{34} = J^{13} J^{+13} = J^{23} J^{+23} = Q^{13} Q^{34}$$

$$J^{14} J^{+14} = J^{24} J^{+24} = J^{34} J^{+34} = Q^{24} Q^{34}$$

$$J^{12} Q^{13} = Q^{24} J^{12} = -J^{+23} J^{13} = -J^{+24} J^{14} = J^{12}$$

$$J^{34} Q^{13} = Q^{24} J^{34} = J^{24} J^{+23} = J^{14} J^{+13} = J^{34}$$

$$J^{13} Q^{12} = Q^{34} J^{13} = -J^{23} J^{12} = J^{+34} J^{14} = J^{13}$$

$$J^{23} Q^{12} = Q^{34} J^{23} = Q^{13} J^{23} = J^{23} Q^{24} = J^{34} J^{24} = -J^{13} J^{+12} = J^{23}$$

$$J^{14} Q^{12} = Q^{34} J^{14} = Q^{24} J^{14} = J^{14} Q^{13} = J^{34} J^{13} = -J^{24} J^{12} = J^{14}$$

$$J^{24} Q^{12} = Q^{34} J^{24} = -J^{14} J^{+12} = J^{34} J^{23} = J^{24}$$



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