

STRUCTURE OF FERMION AND BOSON EXCITATIONS IN ONE-BAND HUBBARD MODEL

YU.A. IZYUMOV, N.I. CHASCHIN

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Institute for Metal Physics, Ural Division of the Russian Acad. Sci.
(18, S. Kovalevskaya Str., Ekaterinburg 620219, Russia)

The Hubbard model in the X -operators representation is studied within the generating functional approach. In the boson sector, Green's functions of two collective excitations, magnons and doublons, are investigated. The equations for them include terms with functional derivatives with respect to the corresponding fluctuating fields of the normal and anomalous components of the electron Green's function. The solution of each equation can be presented through the self-energy and the terminal part which can be calculated by iterations on the electron hopping matrix element. It is shown that, at the half-filling, a Goldstone mode with wave vector $\mathbf{Q} = (\pi, \dots, \pi)$ appears. Expressions for spin and dielectric susceptibility are obtained in the hydrodynamic regime.

operators noncommuting on a c -value, GFs should be determined by one more quantity — the terminal part. At the first time, it was formulated by Bar'yakhtar, Krivoruchko, and Yablonsky [12] while analyzing the diagram technique for spin models. It turns out that this peculiarity has a general character, and one-particle GF \mathcal{G} in general case should have a multiplicative representation determined by two equations

$$\mathcal{G} = G\Lambda, \quad G^{-1} = G_0^{-1} - \Sigma.$$

Here, the quantity G is the propagator part of the GF \mathcal{G} , the quantity Σ is the self-energy part, and Λ is the terminal part. For the conventional Fermi-systems, $\Lambda \equiv 1$.

GFA allows one to derive the equation for a GF with functional derivatives and two separate equations for Σ and Λ following from it. It is possible to solve these equations by iterations. For strongly correlated models expressed in terms of X -operators, such iterations correspond to the perturbative theory near the atomic limit.

In this paper, we developed such an approach for the Hubbard model with the strong one-site Coulomb interaction U . We study a structure of GFs in both the fermion and boson sectors. In the last case, we deal with GFs of magnons (collective motion of a spin deviation) and doublons (the collective motion of a pair of electrons on a site as a complex). We do not present the details of calculations here, but we used the equations for electron and boson GFs derived by us earlier to find out the structure of GFs in the fermion and boson sectors and to determine the Goldstone magnon and doublon excitations.

1. Introduction

One of the methods in the many-body theory is the Generating Functional Approach (GFA) applied at first time to conventional Fermi-systems by Kadanoff and Baym [1]. The generating functional $Z[V]$ is a generalization of a partition function for the system in an external field fluctuating in space and time. Different Green's functions of the system can be presented as functional derivatives over these fields of $Z[V]$. It allows to derive formally closed equations for them in terms of functional derivatives.

Recently in [2–10], we generalized the Kadanoff-Baym approach for strongly correlated electron systems and spin models. A detailed description of the method is given in a book [10] and review [11]. Spin models (like the Heisenberg model) and electron models with strong correlation (like the Hubbard model, tJ -model, and periodic Anderson model) are described by operators not commuted on a c -value, contrary to the canonical Fermi-operators. The usual spin operators and X -operators describing a correlated motion of electrons are such types of operators.

Green's functions (GFs) constructed on such operators have a more complicated structure than the standard GFs constructed on the canonical Fermi-operators. The last ones are determined entirely by the self-energy introduced by the Dyson equation. For

2. Introduction of the Generating Functional

Let us consider the conventional Hubbard model for nondegenerate states. In terms of the Fermi operators, the model Hamiltonian is

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}(c_{i\sigma}^\dagger)$ is the operator of annihilation (creation) of an electron at the site i with spin σ , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the electron number at the same site with a given spin. Under the condition of strong on-site Coulomb repulsion $U > zt$ (where t is the hopping matrix element for the nearest neighbors and z is the coordination number) it is useful to express Hamiltonian (1) in terms of X -operators. The operator X_i^{pq} for the site i describes the transitions between four possible states $p = |0\rangle, |\sigma\rangle, |\bar{\sigma}\rangle, |2\rangle$ — without any electron, with one electron possessing the spin projection σ or $-\sigma \equiv \bar{\sigma}$, and a pair of electrons, respectively.

The X -operators can be represented through the conventional Fermi-operators by means of the relations

$$\begin{aligned} X_i^{\sigma 0} &= c_{i\sigma}^\dagger(1 - n_{i\bar{\sigma}}), & X_i^{2\sigma} &= \sigma c_{i\bar{\sigma}}^\dagger n_{i\sigma}, \\ X_i^{\sigma\bar{\sigma}} &= c_{i\sigma}^\dagger c_{i\bar{\sigma}}, & X_i^{20} &= \sigma c_{i\bar{\sigma}}^\dagger c_{i\sigma}^\dagger, \\ X_i^{\sigma\sigma} &= n_{i\sigma}(1 - n_{i\bar{\sigma}}), & X_i^{22} &= n_{i\sigma} n_{i\bar{\sigma}}, \end{aligned} \quad (2)$$

$$X_i^{00} = (1 - n_{i\sigma})(1 - n_{i\bar{\sigma}}).$$

Operators $X_i^{\sigma 0}$ and $X_i^{2\sigma}$ describe the creation of a correlated electron and are Fermi-like f -operators; $X_i^{\sigma\bar{\sigma}}$ and X_i^{20} describe the flip of a spin at a site and the creation of a pair; they are Bose-like b -operators, respectively. The remaining X 's are called diagonal. We note that there are the Hermitian-conjugate operators $(X_i^{pq})^\dagger = X_i^{qp}$. Sixteen X -operators comprise thus the whole set forming the algebra with the corresponding property of the product

$$X_i^{rs} X_i^{pq} = \delta_{sp} X_i^{rq}. \quad (3)$$

and the permutation relations of the anticommuting type for the f -operators and the commuting one for the b -operators. We note that the conventional Fermi operators are expressed through the linear combinations of X -operators of the f -type

$$c_{i\sigma}^\dagger = X_i^{\sigma 0} - \sigma X_i^{2\bar{\sigma}}, \quad c_{i\sigma} = X_i^{0\sigma} - \sigma X_i^{\bar{\sigma} 2}. \quad (4)$$

These relations express the motion of correlated electrons in two Hubbard subbands.

It is convenient to introduce two-component spinors for the f -operators:

$$\begin{aligned} \Psi(i\sigma) &= \begin{pmatrix} X_i^{0\sigma} \\ \bar{\sigma} X_i^{\bar{\sigma} 2} \end{pmatrix}, \\ \Psi^\dagger(i\sigma) &= (X_i^{\sigma 0}, \bar{\sigma} X_i^{2\bar{\sigma}}). \end{aligned} \quad (5)$$

Then Hamiltonian (1) is represented as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where

$$\mathcal{H}_0 = \sum_i \left(\sum_\sigma \varepsilon_\sigma X_i^{\sigma\sigma} + \varepsilon_2 X_i^{22} \right), \quad (6)$$

$$\mathcal{H}_1 = \sum_{ij\sigma} \sum_{\alpha_1\alpha_2} \Psi_{\alpha_1}^\dagger(i\sigma) t_{\alpha_1\alpha_2}(ij) \Psi_{\alpha_2}(j\sigma). \quad (7)$$

Here, we added the term $\sum_{i\sigma} (-\mu - \sigma \frac{h}{2}) n_{i\sigma}$ to

Hamiltonian (1), where μ is the chemical potential and h is the external magnetic field. That is why a new notation appears:

$$\varepsilon_\sigma = -\sigma \frac{h}{2} - \mu, \quad \varepsilon_2 = U - 2\mu.$$

In the quadratic form (7), $\Psi_\alpha(i\sigma)$ represents the component of the spinor $\Psi(i\sigma)$, ($\alpha = 1, 2$); in addition, we have introduced the matrix

$$t_{\alpha\beta}(ij) = t_{ij} \mathfrak{S}_{\alpha\beta}, \quad \mathfrak{S} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \quad (8)$$

Note that the index α numerates the Hubbard subbands. With the help of the rule of multiplication (3) for X -operators, one can write the permutation relations of the spinor f -operators:

$$\left. \begin{aligned} [\Psi(i\sigma) \otimes \Psi^\dagger(j\sigma)]_+ &= \delta_{ij} F_i^\sigma \\ [\Psi(i\sigma) \otimes \Psi^\dagger(j\bar{\sigma})]_+ &= \delta_{ij} X_i^{\bar{\sigma}\sigma} \tau^z \\ [\Psi(i\sigma) \otimes \Psi(j\bar{\sigma})]_+ &= \delta_{ij} \sigma X_i^{02}(i\tau^y) \end{aligned} \right\}, \quad (9)$$

where τ^x, τ^y, τ^z are the Pauli matrices, and F_i^σ is a 2×2 matrix composed of X -operators:

$$F_i^\sigma = \begin{pmatrix} X_i^{00} + X_i^{\sigma\sigma} & 0 \\ 0 & X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{22} \end{pmatrix}. \quad (10)$$

The permutation relations between f - and b -operators have a commutator character:

$$\left. \begin{aligned} [\Psi(i\sigma_1), X_j^{\sigma_2\bar{\sigma}_2}]_- &= \delta_{ij} \delta_{\sigma_1\sigma_2} \Psi(i\bar{\sigma}_1) \\ [\Psi(i\sigma_1), X_j^{20}]_- &= \delta_{ij} \bar{\sigma}_1 \Psi^\dagger(i\bar{\sigma}_1) \tau^x \end{aligned} \right\}. \quad (11)$$

In other cases of permutations, the relations of type (9) and (11) give zero.

Thus, an anticommutator of two Ψ -operators is expressed either through a diagonal or a b -operator, but the commutator of Ψ - and b -operators is naturally a Ψ -operator. Note the relations

$$(X_i^{pq})^\dagger = X_i^{qp}, \quad (12)$$

$$X_i^{00} + X_i^{\sigma\sigma} + X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{22} = 1 \quad (13)$$

which complete the algebra of X -operators.

Let us write the equation of motion for an f -operator. For the thermodynamical time τ ($-\beta \leq \tau \leq \beta$, $\beta = 1/kT$), we start from the Heisenberg equation

$$\dot{\Psi}(1\sigma) = -[\Psi(1\sigma), \mathcal{H}]$$

which can be written in the case of Hamiltonian (6)–(7) as

$$\begin{aligned} \dot{\Psi}(1\sigma_1) = & -E_1^{\sigma_1}\Psi(1\sigma_1) - F_1^{\sigma_1}\hat{t}(11')\Psi(1'\sigma_1) - \\ & - X_1^{\bar{\sigma}_1\sigma_1}\tau^z\hat{t}(11')\Psi(1'\bar{\sigma}_1) + \bar{\sigma}_1\Psi^\dagger(1'\bar{\sigma}_1)\hat{t}(1'1)it\tau^y X_1^{02}. \end{aligned} \quad (14)$$

Here, a double-row matrix with respect to the spinor index was introduced:

$$E_1^\sigma = \begin{pmatrix} \varepsilon_\sigma & 0 \\ 0 & \varepsilon_\sigma + U \end{pmatrix}. \quad (15)$$

Here and in the following, the numerical indices indicate the four-dimensional coordinates including the site and the time τ , i.e. $1 = (i_1, \tau_1), \dots$; a summation over the primed indices is understood (it is a summation over the sites i and an integration over the time τ). And finally, the value

$$\hat{t}(11') = \delta(\tau_1 - \tau_1')t_{i_1 i_1'}, \mathfrak{S} \equiv t(11')\mathfrak{S} \quad (16)$$

has been introduced representing the matrix over the spinor indices (the last circumstance has been specified by the symbol \hat{t}).

Thus, the operator $\hat{\Psi}$ represents a linear combination of f -operators, with the bosonic b -operators as the coefficients, and the matrices E and \hat{t} as well.

Following the method we have applied many times to different quantum models [2–11], we introduce the generating functional

$$Z[V] = \text{Tr} (e^{-\beta\mathcal{H}} T e^{-V}) \equiv e^{\Phi[V]}, \quad (17)$$

where T is the symbol of the chronological product and the trace is taken over the whole set of variables of the system.

For Hamiltonian (6) – (7), it is convenient to choose the operator V in the form

$$\begin{aligned} V = & v_1^{00} X_1^{00} + v_1^{22} X_1^{22} + v_1^{\sigma'\sigma'} X_1^{\sigma'\sigma'} + v_1^{\bar{\sigma}'\bar{\sigma}'} X_1^{\bar{\sigma}'\bar{\sigma}'} + \\ & + v_1^{02} X_1^{20} + v_1^{20} X_1^{02}. \end{aligned} \quad (18)$$

It represents the linear combination of the whole diagonal and b -operators with the single point fields v .

Thus, differentiating the equation $Z[V]$ (or $\Phi[V]$) with respect to the different v 's, we can express the different GFs through the functional derivatives with respect to the corresponding fields. For instance, for the single-particle Bose-like GFs of magnons and doublons, we have the expressions

$$\mathcal{D}^{\sigma\bar{\sigma}}(12) = -\langle T X_1^{\sigma\bar{\sigma}} X_2^{\bar{\sigma}\sigma} \rangle_V = -\frac{\delta^2 \Phi[V]}{\delta v_1^{\sigma\bar{\sigma}} \delta v_2^{\bar{\sigma}\sigma}}, \quad (19)$$

$$\mathcal{D}^{02}(12) = -\langle T X_1^{02} X_2^{20} \rangle_V = -\frac{\delta^2 \Phi[V]}{\delta v_1^{02} \delta v_2^{20}}. \quad (20)$$

Here and further, the symbol $\langle \dots \rangle_V \equiv \langle \dots e^{-V} \rangle$, where $\langle \dots \rangle$ means averaging over the Gibbs ensemble with Hamiltonian \mathcal{H} . Having been introduced in such a way, the GFs are functionals of the fluctuating fields. Directing these fields to zero after taking the functional derivatives, we obtain the actual GFs describing our system. The fermionic GF cannot be obtained by the differentiation of $Z[V]$ (or $\Phi[V]$) with respect to the single-point fields, and it is necessary to determine the equation of motion for them.

3. Equations of Motion for Electron Green's Function

We see that the equation for the GF $\langle T\Psi\Psi^\dagger \rangle_V$ contains the anomalous GF $\langle T\Psi^\dagger\Psi^\dagger \rangle_V$. Then, it is necessary to write the equation for it as well.

Let us introduce the matrix GF:

$$\begin{aligned} \mathcal{L}(\underline{1}\underline{2}) = & \\ = & - \begin{pmatrix} \langle T\Psi(1\sigma_1)\Psi^\dagger(2\sigma_2) \rangle_V & \langle T\Psi(1\sigma_1)\Psi(2\sigma_2) \rangle_V \\ \langle T\Psi^\dagger(1\sigma_1)\Psi^\dagger(2\sigma_2) \rangle_V & \langle T\Psi^\dagger(1\sigma_1)\Psi(2\sigma_2) \rangle_V \end{pmatrix}. \end{aligned} \quad (21)$$

The underlined numerical index $\underline{1}$ in the left part represents the cumulative index containing the space-time point 1 , the spin σ_1 , the spinor index α_1 and one more index ν_1 , accepting two values, specifying the matrix elements (21), so that $\underline{1} = \{1\sigma_1\alpha_1\nu_1\}$. The matrix $\mathcal{L}(\underline{1}\underline{2})$ is an 8×8 matrix with respect to the collection of discrete indices. A matrix of such a rank appears automatically in the Hubbard model. Its arising is described not only by the states with Cooper's pairs but also with normal states because Eq. (14) for the operator Ψ contains also the operator Ψ^\dagger . The equation for GFs in (21) has been derived earlier [8], and here we only reproduce the final result.

The set of four equations for the GFs in (21) can be written as a single matrix equation:

$$\left[L_{0V}^{-1} - (\hat{A}\Phi Y) - (\hat{A}Y) \right] (\underline{1}\underline{1}') \mathcal{L}(\underline{1}'\underline{2}) = (\hat{A}\Phi)(\underline{1}\underline{2}). \quad (22)$$

Here, we introduced the operator matrix

$$\hat{A}(\underline{1}\underline{2}) = \delta_{12} \begin{pmatrix} \hat{a}_1(\sigma_1\sigma_2) & -\sigma_1\delta_{\bar{\sigma}_1\sigma_2}i\tau^y\frac{\delta}{\delta v_1^{02}} \\ -\sigma_1\delta_{\bar{\sigma}_1\sigma_2}i\tau^y\frac{\delta}{\delta v_1^{20}} & \hat{a}_1(\sigma_2\sigma_1) \end{pmatrix}, \quad (23)$$

where each element represents the 2×2 matrix with respect to the spinor indices hidden in the Pauli matrices and the matrix \hat{a}_1 having the functional derivatives with respect to the fluctuating fields as its elements. In addition, Eq. (22) contains the matrices

$$\hat{a}(\sigma_1, \sigma_2) = -\delta_{\sigma_1, \sigma_2} \begin{pmatrix} \frac{\delta}{\delta v_1^{00}} + \frac{\delta}{\delta v_1^{\sigma\sigma}} & 0 \\ 0 & \frac{\delta}{\delta v_1^{\sigma\sigma}} + \frac{\delta}{\delta v_1^{22}} \end{pmatrix} - \delta_{\bar{\sigma}_1\sigma_2}\tau^z\frac{\delta}{\delta v_1^{\bar{\sigma}_1\sigma_1}}, \quad (24)$$

$$Y(\underline{1}\underline{2}) = \begin{pmatrix} \hat{t}(12) & 0 \\ 0 & -\hat{t}(12) \end{pmatrix}. \quad (25)$$

The value L_{0V}^{-1} represents the double-row matrix

$$L_{0V}^{-1}(\underline{1}\underline{2}) = \begin{pmatrix} G_{0V}^{-1}(1\sigma_1, 2\sigma_2) & \sigma_1\delta_{\bar{\sigma}_1\sigma_2}\delta_{12}\tau^x v_1^{02} \\ -\sigma_1\delta_{\bar{\sigma}_1\sigma_2}\delta_{12}\tau^x v_1^{20} & \tilde{G}_{0V}^{-1}(1\sigma_1, 2\sigma_2) \end{pmatrix}, \quad (26)$$

where G_{0V}^{-1} is given by the expression

$$G_{0V}^{-1}(1\sigma_1, 2\sigma_2) = -\left[\left(\frac{\partial}{\partial \tau_1} + E_1^{\sigma_1} \right) \delta_{\sigma_1\sigma_2} + W_1^{\sigma_1}\delta_{\sigma_1\sigma_2} + v_1^{\bar{\sigma}_1\sigma_1}\tau^0\delta_{\bar{\sigma}_1\sigma_2} \right] \delta_{12} \quad (27)$$

and \tilde{G}_{0V}^{-1} by its transposition. Here, we use the 2×2 matrix

$$W_1^\sigma = \begin{pmatrix} -v_1^{00} + v_1^{\sigma\sigma} & 0 \\ 0 & v_1^{22} - v_1^{\bar{\sigma}\bar{\sigma}} \end{pmatrix}. \quad (28)$$

Equation (22) is of the same type as the equation for a single-particle GF that we derived for the Hubbard model in the limit $U = \infty$ and for the Heisenberg model as well [2–6,9]. In the above models, the matrix \hat{A} degenerates into a scalar, but now it is a matrix with respect to the discrete indices α and ν , likewise the other values in (22). The physical sense of this equation is compatible with that of equations derived in [13]. By virtue of the noted similarity of Eq. (22) with the respective equations of the models considered before, we could expect the same structure in the solutions of these equations, in particular the multiplicative character of electron GFs. Let us represent them as a product of the propagator L and the terminal Π part, respectively, namely:

$$\mathcal{L}(\underline{1}\underline{2}) = L(\underline{1}\underline{1}')\Pi(\underline{1}'\underline{2}). \quad (29)$$

The propagator part satisfies the Dyson equation

$$L^{-1}(\underline{1}\underline{2}) = L_{0V}^{-1}(\underline{1}\underline{2}) - \Sigma(\underline{1}\underline{2}). \quad (30)$$

Thus, the electron GF of the model is characterized by two quantities: the self-energy Σ and the terminal part Π . From Eq. (22), one can derive two equations for Σ and Π [10,11]. The iteration of these equations on powers of the hopping matrix element generates a series of perturbation theory near the atomic limit [10,11].

One comment should be done as for Eq. (22) with functional derivatives. In this equation, the normal components of the matrix GF (21) are coupled with perturbation anomalous ones. However, the last ones stand only under functional derivatives with respect to the fields v^{02} and v^{20} . In the normal phase, anomalous FGs equal zero, but the derivatives do not vanish. That is why we deal with the total matrix GF with anomalous components even for the normal phase.

4. Boson Green's Functions

The complete system of 16 X operators contains two Bose-like operators $X_1^{\sigma\bar{\sigma}}$ and X_1^{02} (and their conjugates $X_1^{\bar{\sigma}\sigma}$ and X_1^{20}) which determine two Bose-like GFs (19) and (20).

They describe the propagation of a spin-flip (magnon) and a dyad (doublon) representing two types of Bose-like collective modes. These GFs can be represented as the variational derivatives of Φ with respect to the fluctuating fields, see Eq. (19) and Eq. (20).

To write the equations of motion for the GFs $\mathcal{D}^{\sigma\bar{\sigma}}$ and \mathcal{D}^{02} , we need the equations of motion for the Bose-like operators:

$$\begin{aligned} \dot{X}_1^{\sigma\bar{\sigma}} &= -(\varepsilon_{\bar{\sigma}} - \varepsilon_{\sigma})X_1^{\sigma\bar{\sigma}} - \Psi_{\alpha'}^{\dagger}(1\sigma)\mathfrak{S}_{\alpha'\beta'}t(11')\Psi_{\beta'}(1'\bar{\sigma}) + \\ &+ \Psi_{\alpha'}^{\dagger}(1'\sigma)t(1'1)\mathfrak{S}_{\alpha'\beta'}\Psi_{\beta'}(1\bar{\sigma}), \end{aligned} \quad (31)$$

$$\begin{aligned} \dot{X}_1^{02} &= -(U - 2\mu)X_1^{02} + \\ &+ \sigma'(\tau^x\Psi)_{\alpha'}(1\bar{\sigma}')\mathfrak{S}_{\alpha'\beta'}t(11')\Psi_{\beta'}(1'\sigma'). \end{aligned} \quad (32)$$

We see that, on the right hand sides of these relations, Ψ -operators are present; therefore in the corresponding equations of motions for the magnon and doublon GFs, the T -mixed product of f - and b -operators will appear. They can be represented as the variational derivative of the electron GF with respect to the fluctuating field $v^{\sigma\bar{\sigma}}$ in the first case and v^{02} in the second. One of the important features of the doublon GF is that it includes the "anomalous" electron GF composed of the operators $\Psi(1\sigma)$ and $\Psi(2\bar{\sigma})$, whereas the equation for the magnon GF should include the normal electron GF composed of the operators $\Psi(1\sigma)$ and $\Psi^{\dagger}(2\bar{\sigma})$. These anomalous GFs by themselves are equal to zero when the fields are absent. However, their derivatives with respect to the fields $v^{\sigma\bar{\sigma}}$ and v^{02} are not equal to zero and determine the contribution in the equation of motion caused by the interactions of the electron and boson degrees of freedom.

By the method developed in [2–8], we come to the equation for the magnon GF

$$\begin{aligned} (K_{0V}^{\sigma\bar{\sigma}})^{-1}(1'1')\mathcal{D}^{\sigma\bar{\sigma}}(1'2) &= (n_1^{\sigma} - n_1^{\bar{\sigma}})\delta_{12} + \\ &+ \frac{\delta}{\delta v_2^{\sigma\bar{\sigma}}}\text{tr}(\mathfrak{S}[(t\mathcal{L}^{11})(1\bar{\sigma},1\sigma) - (\mathcal{L}^{11}t)(1\bar{\sigma},1\sigma)]), \end{aligned} \quad (33)$$

where \mathcal{L}^{11} is a matrix element of the electron GF (21) (normal component). Here,

$$(K_{0V}^{\sigma\bar{\sigma}})^{-1}(12) = -\left(\frac{\partial}{\partial\tau_1} + \sigma h + v_1^{\bar{\sigma}\bar{\sigma}} - v_1^{\sigma\sigma}\right)\delta_{12} \quad (34)$$

is a spin GF of the zero approximation in the fluctuating fields.

It follows from definition (19) that the magnon GF has a symmetry:

$$\mathcal{D}^{\sigma\bar{\sigma}}(12) = \mathcal{D}^{\bar{\sigma}\sigma}(21), \quad \mathcal{D}^{\sigma\bar{\sigma}}(q) = \mathcal{D}^{\bar{\sigma}\sigma}(-q). \quad (35)$$

The solution of the obtained equation can be written as

$$\mathcal{D}^{\sigma\bar{\sigma}}(q) = \frac{n^{\sigma} - n^{\bar{\sigma}} + \mathcal{P}^{\sigma\bar{\sigma}}(q)}{i\omega_n - \sigma h - \mathcal{M}^{\sigma\bar{\sigma}}(q)}, \quad (36)$$

where the self-energy $\mathcal{M}^{\sigma\bar{\sigma}}$ and the terminal part $\mathcal{P}^{\sigma\bar{\sigma}}$ obey the symmetry relations

$$\mathcal{M}^{\sigma\bar{\sigma}}(q) = -\mathcal{M}^{\bar{\sigma}\sigma}(-q), \quad \mathcal{P}^{\sigma\bar{\sigma}}(q) = -\mathcal{P}^{\bar{\sigma}\sigma}(-q). \quad (37)$$

We see that the crucial term in Eq. (33) for the magnon GF contains a term which is a derivative of the normal component of the electron GF. By iteration of the equation for it to the second order in the hopping, we get the self-energy of the magnon GF as

$$\begin{aligned} \mathcal{M}^{\sigma\bar{\sigma}}(q) &= \frac{1}{2} \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k} - \mathbf{q})] \times \\ &\times \sum_{\alpha\beta} \left([(G^{\bar{\sigma}}(\mathbf{k}) - G^{\sigma}(\mathbf{k}))\tau^z]_{\alpha\beta} + \right. \\ &+ \varepsilon(\mathbf{k} - \mathbf{q}) [G^{\bar{\sigma}}(\mathbf{k})\tau^+]_{\alpha\beta} \sum_{\alpha'\beta'} \mathcal{G}_{\alpha'\beta'}^{\sigma}(k - q) + \\ &+ \varepsilon(\mathbf{k}) [G^{\sigma}(\mathbf{k})\tau^+]_{\alpha\beta} \sum_{\alpha'\beta'} \mathcal{G}_{\alpha'\beta'}^{\bar{\sigma}}(k - q) \left. \right). \end{aligned} \quad (38)$$

Here, $G^{\sigma} \equiv \mathcal{L}^{11}$ and G^{σ} is the propagator part, $\tau^{\pm} = \tau^x \pm i\tau^y$; and $\varepsilon(\mathbf{k})$ is the Fourier transform of the hopping matrix element t_{ij} . A similar equation can be obtained for the terminal part $\mathcal{P}^{\sigma\bar{\sigma}}(q)$ [8]. Finally, we present the self-energy part in the mean field approximation for the electron GF $\mathcal{G}^{\sigma\bar{\sigma}}$ as

$$\begin{aligned} \mathcal{M}^{\sigma\bar{\sigma}}(q) &= \sigma \frac{U}{2N} \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k} - \mathbf{q})] \times \\ &\times \sum_{\sigma} \sigma \frac{f[E_1^{\sigma}(\mathbf{k})] - f[E_2^{\sigma}(\mathbf{k})]}{E_1^{\sigma}(\mathbf{k}) - E_2^{\sigma}(\mathbf{k})} + \\ &+ \frac{U}{2N} \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k} - \mathbf{q})] \sum_{\nu\mu} (-1)^{\nu+\mu} C_{\nu\mu}^{\sigma\bar{\sigma}}(\mathbf{k}, \mathbf{k} - \mathbf{q}) \times \\ &\times \frac{f[E_{\nu}^{\sigma}(\mathbf{k})] - f[E_{\mu}^{\bar{\sigma}}(\mathbf{k})]}{i\omega_n + E_{\nu}^{\sigma}(\mathbf{k}) - E_{\mu}^{\bar{\sigma}}(\mathbf{k})}. \end{aligned} \quad (39)$$

Here, $E_\nu^\sigma(\mathbf{k})$ is the quasiparticle energy, the index $\nu = 1, 2$ numerates two Hubbard subbands, $f[E]$ is the Fermi-function, and $C_{\nu\mu}^{\sigma\bar{\sigma}}$ are some dimensionless coefficients [8].

For the doublon GF (20), we can derive the equation [8]

$$(K_{0V}^{02})^{-1} (11')\mathcal{D}^{02}(1'2) = (1 - n_1)\delta_{12} - \sigma' \frac{\delta}{\delta v_1^{20}} \text{Tr} [\Im (t\mathcal{L}^{12}) (1\sigma', 1\bar{\sigma}')], \quad (40)$$

where K_{0V}^{02} is a propagator in the zero approximation but with the corresponding fluctuating fields:

$$(K_{0V}^{02})^{-1} (12) = - \left(\frac{\partial}{\partial \tau_1} + U - 2\mu + v_1^{22} - v_1^{00} \right) \delta_{12}. \quad (41)$$

A solution of Eq. (40) is sought in the form where the self-energy \mathcal{M}^{02} and the terminal part \mathcal{P}^{02} can be obtained by iterations of the GF, similarly to the case of the magnon GF.

$$\mathcal{D}^{02}(q) = \frac{(1 - n) + \mathcal{P}^{02}(q)}{i\omega_n - (U - 2\mu) - \mathcal{M}^{02}(q)}. \quad (42)$$

In the same way, we can calculate the conjugated doublon GF \mathcal{D}_{12}^{20} . It is possible to represent the result of computations in the form

$$\mathcal{D}^{20}(q) = \frac{-(1 - n) + \mathcal{P}^{20}(q)}{i\omega_n + (U - 2\mu) - \mathcal{M}^{20}(q)}, \quad (43)$$

where the values $\mathcal{P}^{20}(q)$ and $\mathcal{M}^{20}(q)$ are connected with $\mathcal{P}^{02}(q)$ and $\mathcal{M}^{02}(q)$ by the relations

$$\mathcal{P}^{20}(q) = -\mathcal{P}^{02}(-q), \quad \mathcal{M}^{20}(q) = -\mathcal{M}^{02}(-q). \quad (44)$$

Thus, we see that the condition of symmetry

$$\mathcal{D}^{20}(q) = \mathcal{D}^{02}(-q) \quad (45)$$

is fulfilled, or $\mathcal{D}_{12}^{20} = \mathcal{D}_{21}^{02}$ in the coordinate space, which follows directly from the definition of a doublon GF. In the mean field approximation for the electron GF, we can obtain the doublon self-energy up to the second order in the hopping:

$$\mathcal{M}^{02}(q) = \mathcal{M}_1^{02}(q) + \mathcal{M}_2^{02}(q),$$

$$\mathcal{M}_1^{02}(q) = -\frac{U}{2} \sum_{\mathbf{k}\sigma} \frac{\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k} - \mathbf{q})}{2Q^\sigma(\mathbf{k})} \times$$

$$\times \left[f[E_1^\sigma(\mathbf{k})] - f[E_2^\sigma(\mathbf{k})] \right], \quad (46)$$

$$\begin{aligned} \mathcal{M}_2^{02}(q) = & -\frac{1}{2} \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k} - \mathbf{q}) \frac{\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k} - \mathbf{q})}{2Q^\sigma(\mathbf{k})} \times \\ & \times \sum_{\mu\nu} C_{\mu\nu}^\sigma(\mathbf{k}, \mathbf{k} - \mathbf{q}) \times \\ & \times \frac{1 - f[E_\mu^\sigma(\mathbf{k})] - f[E_\nu^\sigma(\mathbf{k} - \mathbf{q})]}{i\omega_n - E_\mu^\sigma(\mathbf{k}) - E_\nu^\sigma(\mathbf{k} - \mathbf{q})}. \end{aligned} \quad (47)$$

Here, $C_{\mu\nu}^\sigma$ is some dimensionless coefficients, and $2Q^\sigma(\mathbf{k}) = E_2^\sigma(\mathbf{k}) - E_1^\sigma(\mathbf{k})$.

Let us now compare the equations of motion and their solutions for the magnon and doublon GFs. Eq. (36) and Eq. (42) have a common structure, and the interaction of the corresponding boson modes with the electron system is described by a term with the functional derivative with respect to the corresponding fields of the electron GF. For magnons, such a field is $v^{\bar{\sigma}\sigma}$ coupled with the operator $X^{\sigma\bar{\sigma}}$ of a spin deviation at the site; for doublons, it is the field v^{20} coupled with the operator X^{02} creating an electron pair at an unoccupied site. In the first or second case, the equation includes, respectively, the normal component \mathcal{L}^{11} of the electron GF or the anomalous one \mathcal{L}^{12} .

Solutions (36) for magnons and (42) for doublons express the fact that the boson GFs as well as electron ones have the self-energy and the terminal part which can be calculated by iterations on the electron hopping. In the zero approximation, the nominator of the magnon GF is just equal to magnetization, while that of the doublon GF is equal to a deviation from the half-filling ($n = 1$). In the denominators of both GFs, the quantity σh or $U - 2\mu$ stands which vanishes in the paramagnetic phase in the case of magnons and at the half-filling, whereas $U - 2\mu = 0$ in the case of doublons.

Now we return to expressions (38) and (46)–(47) for the self-energy of magnons and doublons. It is explicitly seen that $\mathcal{M}^{\sigma\bar{\sigma}}(q)$ vanishes when $\mathbf{q} = 0$ and $\mathcal{M}^{02}(q)$ vanishes when $\mathbf{q} = \mathbf{Q} = (\pi, \dots, \pi)$. Thus, similarly to the fact that a magnon with the momentum $\mathbf{q} = 0$ is a Goldstone mode, a doublon is a Goldstone mode as well, only with the momentum $\mathbf{q} = \mathbf{Q}$. Moreover, similarly to the fact that a magnetic field creates a gap h in the magnon spectrum, a deviation from the half-filling produces a gap $U - 2\mu$ in the doublon spectrum. When a Goldstone mode is condensed, a homogeneous ordered

phase (ferromagnetic) or two-subband (dielectric) phase can appear.

We see that the half-filling ($n = 1$) for doublons is a peculiar point, and strong dielectric fluctuations should exist in a vicinity of the wave vector \mathbf{Q} . We will study them now in the hydrodynamic regime.

5. Dynamical Fluctuations in the Hydrodynamic Regime

It is well known that collective modes in a disordered (symmetric) phase in the hydrodynamic regime are ruled by the conservation laws [14]. Thus, the spin GF $\mathcal{D}^{\sigma\bar{\sigma}}$ should be determined by the total spin conservation law, while the pseudospin GF \mathcal{D}^{02} is determined by the pseudospin conservation law [16–18]. The three pseudospin components

$$P^+ = \sum_i e^{i\mathbf{Q}\cdot\mathbf{R}_i} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger,$$

$$P^- = \sum_i e^{-i\mathbf{Q}\cdot\mathbf{R}_i} c_{i\uparrow} c_{i\downarrow},$$

$$P^z = \sum_i \frac{1}{2}(n_i - 1) \tag{48}$$

with $\mathbf{Q} = (\pi \pi \dots)$ obey the permutation relations

$$[P^+, \mathcal{H}] = (2\mu - U)P^+,$$

$$[P^-, \mathcal{H}] = -(2\mu - U)P^-,$$

$$[P^z, \mathcal{H}] = 0, \tag{49}$$

from which it is clear that, at the half-filling ($n = 1$), all pseudospin components are conserved. This leads to the diffusion form of the pseudospin (doublon) susceptibility, which is the retarded doublon GF $\chi^{02}(\mathbf{q}, \omega)$. According to the Kubo–Mori theory, this susceptibility is expressed through the memory function $\mathcal{M}^{02}(\mathbf{q}, \omega)$ by the relation

$$\chi^{02}(\mathbf{q}, \omega) = \langle\langle X_i^{02} | X_j^{20} \rangle\rangle_{\mathbf{q}, \omega} = \frac{M^{02}(\mathbf{q}, \omega)}{\omega - \frac{M^{02}(\mathbf{q}, \omega)}{\chi_{\mathbf{q}}^{02}}}, \tag{50}$$

where we introduce the notation for static susceptibility: $\chi_{\mathbf{q}}^{02} \equiv \chi^{02}(\mathbf{q}, 0)$.

On the other hand, the memory function is expressed through the irreducible retarded GF of pseudospin currents (see [19]):

$$M^{02}(\mathbf{q}, \omega) = - \sum_{ij} e^{-i\mathbf{q}\cdot\mathbf{R}_{ij}} \times \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{Im \langle\langle i \dot{X}_i^{02} | -i \dot{X}_j^{20} \rangle\rangle_{\omega'}}{\omega'(\omega - \omega' + i\delta)}. \tag{51}$$

Here, \dot{X}_i^{02} means the real time derivative of the operator X_i^{02} :

$$i \dot{X}_i^{02} = [X_i^{02}, \mathcal{H}] = (U - 2\mu)X_i^{02} - \sigma'(\tau^x \Psi)_{\alpha'}(i\bar{\sigma}')(\hat{t}\Psi)_{\alpha'}(i\sigma'). \tag{52}$$

Further, we consider the half-filling case where $U - 2\mu = 0$. Then

$$\begin{aligned} \langle\langle i \dot{X}_i^{02}(t) | -i \dot{X}_j^{20}(0) \rangle\rangle^{irr} = & \langle\langle (\tau^x \Psi)_{\alpha'}(i\bar{\sigma}', t)(\hat{t}\Psi)_{\alpha'}(i\sigma', t) | \times \\ & \times (\Psi^+ \hat{t})_{\beta'}(j\sigma')(\Psi^+ \tau^x)_{\beta'}(j\bar{\sigma}') \rangle\rangle^{irr} - \\ & - \langle\langle (\tau^x \Psi)_{\alpha'}(i\bar{\sigma}', t)(\hat{t}\Psi)_{\alpha'}(i\sigma', t) | \times \\ & \times (\Psi^+ \hat{t})_{\beta'}(j\bar{\sigma}')(\Psi^+ \tau^x)_{\beta'}(j\sigma') \rangle\rangle^{irr}. \end{aligned} \tag{53}$$

Now we use the approximation of interacting modes well known in the relaxation theory [17, 18]: the two-particle electron correlations in expression (53) are decomposed into pair correlators and then expressed through the imaginary parts of retarded electron GFs. As a result, we come to the following expression determining the memory function:

$$\begin{aligned} M^{02}(\mathbf{q}, \omega) = 2 \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k} - \mathbf{q})]^2 \times \\ \times \int d\omega' \int d\omega_1 \frac{f(\omega_1 - \omega') - f(\omega_1)}{\omega'(\omega - \omega' + i\delta)} \times \\ \times \text{tr}([\text{Im}\mathcal{G}^{\bar{\sigma}'}(\mathbf{q} - \mathbf{k}, \omega' - \omega_1)][\text{Im}(\mathfrak{S}\mathcal{G}^{T\sigma'}\mathfrak{S})(\mathbf{k}, \omega_1)]). \end{aligned} \tag{54}$$

Here, $\mathcal{G}^{T\sigma}$ is the transposed matrix \mathcal{G}^σ . The quantity $\mathcal{G}^\sigma(\mathbf{k}, \omega)$ is the retarded electron GF. It can be obtained from the Matsubara GFs by analytical continuation from discrete imaginary frequencies into real ones: $i\omega_n \rightarrow \omega + i\delta$.

Expression (54) is similar to those obtained in the interacting modes approximation for other dynamical susceptibilities. For example, the spin susceptibility is

$$\chi^{\sigma\bar{\sigma}}(\mathbf{q}, \omega) = \langle\langle X_i^{\sigma\bar{\sigma}} | X_j^{\bar{\sigma}\sigma} \rangle\rangle_{\mathbf{q}, \omega} = -\frac{M^{\sigma\bar{\sigma}}(\mathbf{q}, \omega)}{\omega - \frac{M^{\sigma\bar{\sigma}}(\mathbf{q}, \omega)}{\chi_q^{\sigma\bar{\sigma}}}}. \quad (55)$$

By a similar decoupling of the irreducible GFs of the currents, we obtain

$$\begin{aligned} M^{\sigma\bar{\sigma}}(\mathbf{q}, \omega) &= 4 \sum_{\mathbf{k}} [\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k} - \mathbf{q})]^2 \times \\ &\times \int d\omega' \int d\omega_1 \frac{f(\omega_1 - \omega') - f(\omega_1)}{\omega'(\omega - \omega' + i\delta)} \times \\ &\times \text{tr}([\text{Im}\mathcal{G}^\sigma(\mathbf{k} - \mathbf{q}, \omega_1 - \omega')] [\text{Im}(\Im\mathcal{G}^{\bar{\sigma}\sigma})(\mathbf{k}, \omega)]). \end{aligned} \quad (56)$$

It is remarkable that the memory GF for the spin susceptibility vanishes at $\mathbf{q} = 0$, while it vanishes at $\mathbf{q} = \mathbf{Q}$ for the doublon susceptibility. This difference originates from the total spin conservation law (Fourier component of the spin density at $\mathbf{q} = 0$), while the component of the pseudospin density is conserved at $\mathbf{q} = \mathbf{Q}$ and only for the half-filling. There is another important difference in expressions (54) and (56). Arguments of the electron GFs appear in a different way in these expressions. This reflects the fact that the spin collective mode is formed through excitations of a particle and a hole, while the pseudospin collective mode (doublon) is formed through excitations of two particles (or two holes).

Consider now the hydrodynamic limit corresponding to small frequencies ω , a small wave point $\mathbf{p} = \mathbf{Q} - \mathbf{q}$ (for expression (54)), and small \mathbf{q} (for expression (56)). In the hydrodynamic limit, $\omega \ll vp$ and $\omega \ll vq$, where v is a characteristic electron velocity on the Fermi surface. Under these conditions, Eqs. (54) and (56) yield the asymptotic expressions

$$\text{Im}\mathcal{M}^{02}(\mathbf{q}, \omega) = -D^{02}p^2, \quad \text{Re}\mathcal{M}^{02}(\mathbf{q}, \omega) = 0, \quad (57)$$

$$\text{Im}\mathcal{M}^{\sigma\bar{\sigma}}(\mathbf{q}, \omega) = -D^{\sigma\bar{\sigma}}q^2, \quad \text{Re}\mathcal{M}^{\sigma\bar{\sigma}}(\mathbf{q}, \omega) = 0, \quad (58)$$

where the coefficients of the spin and pseudospin stiffnesses are equal to

$$\begin{aligned} D^{02} &= 2\pi \sum_{\mathbf{k}} (v(\mathbf{k})\mathbf{e})^2 \int d\omega_1 f'(\omega_1) \times \\ &\times \text{tr}([\text{Im}\mathcal{G}^{\bar{\sigma}'}(-\mathbf{k}, -\omega_1)] [\text{Im}(\Im\mathcal{G}^{T\sigma'}\Im)(\mathbf{k}, \omega_1)]), \end{aligned} \quad (59)$$

$$\begin{aligned} D^{\sigma\bar{\sigma}} &= 4\pi \sum_{\mathbf{k}} (v(\mathbf{k})\mathbf{e})^2 \int d\omega_1 f'(\omega_1) \times \\ &\times \text{tr}([\text{Im}\mathcal{G}^\sigma(\mathbf{k}, \omega_1)] [\text{Im}(\Im\mathcal{G}^{\bar{\sigma}}\Im)(\mathbf{k}, \omega_1)]). \end{aligned} \quad (60)$$

Here, \mathbf{e} is the unit wave vector, and $f'(\omega)$ is the derivative of the Fermi-function.

Expression (60) is valid at arbitrary U ; in the case of $U \gg W$, it is consistent with the result for the tJ -model [15].

Notice that if we use the electron GF in the mean field approximation (without attenuation of quasiparticles), both expressions (59) and (60) vanish. It is easy to show that if the attenuation of quasiparticles γ obeys the condition $\gamma \gg vq$, both expressions become finite. In the general case, expressions (54) and (56) for the memory function give correct asymptotic values in the hydrodynamical limit. Therefore, the susceptibilities have the diffusion form

$$\frac{1}{\omega} \text{Im}\chi(\mathbf{q}, \omega) = \chi_q \frac{\tilde{D}q^2}{\omega^2 + (\tilde{D}q^2)^2}, \quad (61)$$

where $\tilde{D} = D/\chi_q$.

6. Conclusions

We have applied the GFA to investigate the Hubbard model in the X -operator representation. This means that we discussed the case of sufficiently strong electron correlations $U > W$. We have derived the exact equation for the electron GF in terms of the functional derivatives with respect to the fluctuating fields $v^{\sigma\sigma'}$, $v^{\sigma\bar{\sigma}}$, v^{20} coupled with the spin and charge densities. The electron GFs represent generally an 8×8 matrix with respect to three discrete indices σ, α, ν . In the matrix representation, the equation has the same structure with the GF for the Hubbard model in the limit $U \rightarrow \infty$, for the tJ - and sd -models, and for the GFs of the transverse spin components in the Heisenberg model as well.

The electron GF \mathcal{G} has a multiplicative character in the sense that it is expressed by a product of two

quantities, $\mathcal{G} = G\Lambda$, where G is the propagator satisfying the Dyson equation with the self-energy Σ , and Λ is the terminal part. Their iteration generates a power series in the parameter W/U . This corresponds to the perturbation theory close to the atomic limit.

Taking the electron GF in the mean field approximation, we derived an equation for the doublon GF. The properties of the poles of the doublon GF depends substantially on the electron concentration n . For $n < 1$, there is a pole which has a real part $U - 2\mu > 0$ corresponding to the activated mode with the quadratic dispersion law. For $n \rightarrow 1$, $U - 2\mu \rightarrow 0$. The investigation of the special case $n = 1$ reveals that a soft mode with $\mathbf{Q} = (\pi, \dots, \pi)$ may exist. However it is known that the paramagnetic phase of the Hubbard model has an instability to the antiferromagnetic ordering. This means that two possible instabilities – doublon and magnon ones – should compete, and a final result concurring a type of ordering at the half-filling demands further investigations.

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СТРУКТУРА ФЕРМІОННИХ І БОЗОННИХ ЗБУДЖЕНЬ В ОДНОЗОННІЙ МОДЕЛІ ХАББАРДА

Ю.А. Ізюмов, Н.І. Чащин

Резюме

Досліджено модель Хаббарда у представленні X -операторів методом генеруючого функціонала і вивчено два колективні збудження, магнонів та дублонів, у бозоновому секторі функцій Гріна. Їх рівняння містять функціональні похідні по відповідних флуктуаційних полях нормальної та аномальної електронної функції Гріна. Розв'язок кожного рівняння може бути записаний через власну енергію і термінальну частину, які можуть бути обчислені шляхом ітерацій за електронними стрічковими матричними елементами. Показано, що голдстоунівська мода з хвильовим вектором $\mathbf{Q} = (\pi, \dots, \pi)$ виникає в разі половинного заповнення. Вирази для спинові та електронної сприйнятливостей отримано у гідродинамічному наближенні.

СТРУКТУРА ФЕРМИОННЫХ И БОЗОННЫХ ВОЗБУЖДЕНИЙ В ОДНОЗОННОЙ МОДЕЛИ ХАББАРДА

Ю.А. Изюмов, Н.И. Чащин

Резюме

Исследована модель Хаббарда в представлении X -операторов методом производящего функционала и рассмотрены два коллективные возбуждения, магнонов и дублонов, в бозоновом секторе функций Грина. Их уравнения включают функциональные производные по соответствующим флуктуационным полям нормально и аномальной электронной функции Грина. Решения каждого уравнения могут быть представлены с помощью собственной энергии и терминальной части, которые могут быть вычислены путем итераций по электронным прыжковым матричным элементам. Показано, что голдстоуновская мода с волновым вектором $\mathbf{Q} = (\pi, \dots, \pi)$ возникает при половинном заполнении. Выражения для спиновой и электронной восприимчивостей получены в гидродинамическом приближении.