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A generating functional approach to the Hubbard model

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Abstract. The method of generating functional, suggested for conventional systems by Kadanoff and Baym, is generalized to the case of strongly correlated systems, described by the Hubbard X operators. The method has been applied to the Hubbard model with arbitrary value U of the Coulomb on-site interaction. For the electronic Green's function $\mathcal{G}$ constructed for Fermi-like X operators, an equation using variational derivatives with respect to the fluctuating fields has been derived and its multiplicative form has been determined. The Green's function is characterized by two quantities: the self energy Σ and the terminal part Λ. For them we have derived the equation using variational derivatives, whose iterations generate the perturbation theory near the atomic limit. Corrections for the electronic self-energy Σ are calculated up to the second order with respect to the parameter W/U (W width of the band), and a mean field type approximation was formulated, including both charge and spin static fluctuations. This approximation is actually equivalent to the one used in the method of Composite Operators, and it describes an insulator-metal phase transition at half filling reasonably well. The equations for the Bose-like Green's functions have been derived, describing the collective modes: the magnons and doublons. The main term in this equation represents variational derivatives of the electronic Green's function with respect to the corresponding fluctuating fields. The properties of the poles of the doublon Green's functions depend on electronic filling. The investigation of the special case $n = 1$ demonstrates that the doublon Green's function has a soft mode at the wave vector $\boldsymbol{Q} = (\pi, \pi, \dots)$, indicating possible instability of the uniform paramagnetic phase relatively to the two sublattices charge ordering. However this instability should compete with an instability to antiferromagnetic ordering. The generating functional method with the X operators could be extended to the other models of strongly correlated systems.

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1 Introduction

The Hubbard model is one of the basic models in the theory of strongly correlated systems. During its forty years of lifetime numerous approaches have been proposed for the investigation of the possible states of the system, the spectrum of its quasi-particles and the collective modes, the transport properties, the different types of ordered states and the phase transitions among them. Such long period of development of a model which could look simple at a first glance — since it contains only two parameters, the bare bandwidth W and the on-site Coulomb repulsion U — is determined by the circumstance that the case $U \geq W$ is of main physical significance. But just in this case the theory does not contain a small parameter. Already the first researchers tried to avoid perturbative theories and used different non-perturbative approaches. Starting from the pioneering works of Hubbard [1–3], the method of decoupling of the double-time Green's functions (GF) was treated successfully. The works based on projecting the equations of motion for the basic operators come here [4–6]. The most productive application of this approach has been done with the method of composite operators [7–10] used widely not only for the Hubbard model but also for many other models [11] of strongly correlated electronic systems. The method of the spectral density moments uses in essence the cut short of the equations of motions for the basic operators as well [12,13]. Also the variational method of Gutzwiller belongs to the non-perturbative approaches [14], and made it possible to investigate qualitatively the behavior of a vast class of strongly correlated systems during the last four decades. The method of slave particles (slave bosons) represents an important direction of investigation also [15–18]. The basic

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operators are expressed through a product of conventional Fermi and Bose operators with subsequent exclusion of unphysical states. The suitable choice of a slave particle representation makes it possible to catch the physics of low energy states in the scope of the mean field approximation. Unfortunately there is no standard recipe for constructing such representations, and it is not always clear which one among the possible representations is the most adequate.

During the last decade the method of the dynamical mean field theory (DMFT) has become quite popular [19,20]. By means of this method it has been possible to investigate the behavior of almost all the models in the theory of strongly correlated systems in the region of strong and intermediate interactions. Apparently DMFT is the most efficient method of investigation of these systems, although not exempt from some defects: it demands a huge amount of computations and has problems with the description of collective modes (see the review [21]). We do not mention here the numerical methods like Quantum Monte Carlo and small cluster diagonalization, because we concentrate our efforts on the analytical approaches.

We want to pay attention to one of the analytical approaches where there is a possibility to derive a consistent perturbative theory with respect to the parameter W/U. Definitely, such an approach corresponds to the perturbative theory near the atomic limit. The approach is based on the introduction of a generating functional $Z[V]$, describing the interaction of the system with fluctuating fields depending on space and time. This functional corresponds to the generalization of the partition function of the system for the case of interactions with external fluctuating fields. For a proper choice of the V operator the different GFs of the system are expressed through variational derivatives with respect to fluctuating fields.

At the beginning this method was developed for a weak interaction by Kadanoff and Baym [22,23] forty years ago. It could be generalized to a strongly correlated system when we express the Hamiltonian through some basic operators taking into account the correlations (for instance the Hubbard X operators) [3] instead of the conventional ones. The first time such an approach has been applied to the Hubbard model was in the limit $U \to \infty$ (with an additional small parameter $1/N$, where N is the degeneracy of the electronic states) [24]. Afterwards this approach has been developed farther in the works [25–27,32].

Recently we have provided a general framework for the generating functional approach (GFA) and we have applied it to a set of basic models of spin and strongly correlated electronic systems: Heisenberg model, Hubbard model for $U \to \infty$, tJ-model, sd-model, double exchange model [27,32]. The results of these investigations have been generalized in the monograph [33], published in Russian, and in the course of lectures delivered in an international school [34].

In this paper we apply the GFA to the Hubbard model with a finite Coulomb interaction U. Supposing that U is large but of the order of W we express the Hamiltonian of the model in terms of the X operators and calculate the electronic and bosonic GFs. The latter describes the two types of collective modes: magnons and doublons.

The electronic GF is a matrix with respect to the spin index σ, the index α, indicating the Hubbard subbands, and the index ν corresponding to the particle-hole representation. We have derived the equation in the variational derivatives with respect to fluctuating fields for it. Because the basic operators do not commute on c-values, the electronic Green's function is characterized by two functions of four-momenta: the self-energy Σ and the terminal part Λ. For Σ and Λ the equations with the variational derivatives have been derived too, whereas it is possible to make iterations with respect to the parameter W/U. Just these iterative series represent the perturbative theory near the atomic limit [35]. We have limited ourselves to the first and second order corrections for Σ and extracted from them a mean field type Σ_{MF} part, which includes contributions depending only on the wave vector $\boldsymbol{k}$, but not on the frequency. Σ_{MF} consists of a term giving a shift to the Hubbard subbands and renormalizing its width. The last term was extracted from the second order correction Σ_2', which is an "uncutable" term (with respect to the hopping matrix element), while a "cutable" term Σ_2 describes the dynamical interaction with boson-type excitations. A procedure of extraction of the static part from Σ_2' was borrowed from the Composite Operator Method (COM) [7–10]. The main idea of this approach is that bosonic correlators, describing for example static fluctuations of charge, spin and pair, should not be calculated by some uncontrollable approximation (like decoupling or use of the equation of motion), but must be determined by means of general properties of the electronic GF [10].

The GFA, restricted to the mean field approximation, and the COM, restricted to a two-pole approximation, have a different structure for the electronic GF. In spite of this, the results obtained by these two methods for different properties of the Hubbard model turned out to be in very good agreement. In particular, such mean field GFs give two quasiparticle subbands with a gap between them, which vanishes for half-filling at some critical value $U = U_c$, and an insulator-metal phase transition occurs. Detailed comparison of the mean field approximation in GFA and COM will be discussed below.

Using the electron GFs we found, we can calculate Bose-like GFs for plasmons, magnons and doublons. In this paper we study only doublons – collective modes, describing motion of double occupied states of the lattice sites. The equation for the doublon GF has been derived. This equation contains variational derivatives of the electronic GF with respect to the corresponding fluctuating fields, coupled with charge densities. In the mean field approximation for the electronic Σ we have obtained the closed equation for the doublon GF. For the paramagnetic state at half filling ($n = 1$) the doublon GF has a soft mode at momentum $\boldsymbol{Q} = \boldsymbol{\pi} = (\pi, \pi, \dots)$. It indicates a possible instability of the uniform state against a charge density wave formation. When the filling deviates from unity ($n < 1$), the pole of the doublon GF has a gap $U - 2\mu$, thus having the activative character.

The content of the paper is the following. In Section 2, based on the X operators formalism, the GFA is constructed. In Section 3 it is derived the equation of motion for the electronic GF in the form of equation with variational derivatives. This equation is decoupled into two: one for the self energy and one for the terminal part. In part 4 the iterations of these equations with respect to the parameter W/U are implemented and the GF in the "Hartree-Fock approximation" is calculated. In Section 5 we formulate a mean field approximation and compare GFA and COM approaches. A Bose-like GF for doublons is calculated in Section 6 with the electronic GF taken in the mean field approximation. In Section 7 we calculate the doublon susceptibility in the hydrodynamical regime. Finally in Section 8 we discuss the obtained results and propose suggestions for further study of the Hubbard model.

2 Introduction of the generating functional

Let us consider the conventional Hubbard model for non-degenerate states. In terms of the Fermi operators the model Hamiltonian is

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{2.1}$$

where $c_{i\sigma}(c^{\dagger}_{i\sigma})$ is the operator of annihilation (creation) of an electron on the site i with spin σ, $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the electron number on the same site with the given spin. Under the condition of a 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 the Hamiltonian (2.1) in terms of the X operators. The operator X_i^{pq} for the site i describes the transitions between the 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 $-\sigma$ and a pair of electrons, respectively.

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

$$\begin{aligned}
&X_i^{\sigma 0} = c^{\dagger}_{i\sigma}(1 - n_{i\bar{\sigma}}), && X_i^{2\sigma} = \sigma c^{\dagger}_{i\bar{\sigma}} n_{i\sigma},\\
&X_i^{\sigma\bar{\sigma}} = c^{\dagger}_{i\sigma} c_{i\bar{\sigma}}, && X_i^{20} = \sigma c^{\dagger}_{i\bar{\sigma}} c^{\dagger}_{i\sigma},\\
&X_i^{\sigma\sigma} = n_{i\sigma}(1 - n_{i\bar{\sigma}}), && X_i^{22} = n_{i\sigma} n_{i\bar{\sigma}},\\
&X_i^{00} = (1 - n_{i\sigma})(1 - n_{i\bar{\sigma}}).
\end{aligned} \tag{2.2}$$

The operators $X_i^{\sigma 0}$ and $X_i^{2\sigma}$ describe the correlated creation of an electron and are Fermi-like f-operators; $X_i^{\sigma\bar{\sigma}}$ and X_i^{20} describe the flip of a spin on 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 $(X_i^{pq})^{\dagger} = X_i^{qp}$. The sixteen X operators comprise thus the whole set, forming the algebra with the corresponding property of the product

$$X_i^{rs} X_i^{pq} = \delta_{sp} X_i^{rq}. \tag{2.3}$$

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

$$c^{\dagger}_{i\sigma} = X_i^{\sigma 0} - \sigma X_i^{2\bar{\sigma}}, \qquad c_{i\sigma} = X_i^{0\sigma} - \sigma X_i^{\bar{\sigma}2}. \tag{2.4}$$

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

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

$$\Psi(i\sigma) = \begin{pmatrix} X_i^{0\sigma} \\ \bar{\sigma} X_i^{\bar{\sigma}2} \end{pmatrix}, \qquad \Psi^{\dagger}(i\sigma) = \left(X_i^{\sigma 0},\, \bar{\sigma} X_i^{2\bar{\sigma}}\right). \tag{2.5}$$

Then the Hamiltonian (2.1) is represented as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where

$$\mathcal{H}_0 = \sum_i \left(\sum_{\sigma} \varepsilon_{\sigma} X_i^{\sigma\sigma} + \varepsilon_2 X_i^{22} \right), \tag{2.6}$$

$$\mathcal{H}_1 = \sum_{ij} \sum_{\sigma} \sum_{\alpha_1 \alpha_2} \Psi^{\dagger}_{\alpha_1}(i\sigma) t_{\alpha_1\alpha_2}(ij) \Psi_{\alpha_2}(j\sigma). \tag{2.7}$$

Here we added to Hamiltonian (2.1) the term $\sum_{i\sigma}(-\mu - \sigma\frac{h}{2}) n_{i\sigma}$, where μ is the chemical potential and h is the external magnetic field, that is why new notation appears: $\varepsilon_{\sigma} = -\sigma\frac{h}{2} - \mu$, $\varepsilon_2 = U - 2\mu$. In the quadratic form (2.7) $\Psi_{\alpha}(i\sigma)$ represents the component of the spinor $\Psi(i\sigma)$, $(\alpha = 1, 2)$; in addition we have introduced the matrix

$$t_{\alpha\beta}(ij) = t_{ij} \Im_{\alpha\beta}, \qquad \Im = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{2.8}$$

Note that the index α numerates the Hubbard subbands. With the help of the rule of multiplication (2.3) for X operators, one can write the permutation relations of the spinor f-operators:

$$\left.\begin{aligned}
&\left[\Psi(i\sigma) \otimes \Psi^{\dagger}(j\sigma)\right]_{+} = \delta_{ij} F_i^{\sigma} \\
&\left[\Psi(i\sigma) \otimes \Psi^{\dagger}(j\bar{\sigma})\right]_{+} = \delta_{ij} X_i^{\bar{\sigma}\sigma} \tau^z \\
&\left[\Psi(i\sigma) \otimes \Psi(j\bar{\sigma})\right]_{+} = \delta_{ij} \sigma X_i^{02} (i\tau^y)
\end{aligned}\right\}, \tag{2.9}$$

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

$$F_i^{\sigma} = \begin{pmatrix} X_i^{00} + X_i^{\sigma\sigma} & 0 \\ 0 & X_i^{\bar{\sigma}\bar{\sigma}} + X_i^{22} \end{pmatrix}. \tag{2.10}$$

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

$$\left.\begin{aligned}
&\left[\Psi(i\sigma_1), X_j^{\sigma_2\bar{\sigma}_2}\right]_{-} = \delta_{ij}\delta_{\sigma_1\sigma_2} \Psi(i\bar{\sigma}_1) \\
&\left[\Psi(i\sigma_1), X_j^{20}\right]_{-} = \delta_{ij}\bar{\sigma}_1 \Psi^{\dagger}(i\bar{\sigma}_1)\tau^x
\end{aligned}\right\}. \tag{2.11}$$

In other cases of permutations, relations of type (2.9) and (2.11) 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 two relations

$$(X_i^{pq})^\dagger = X_i^{qp}, \tag{2.12}$$

$$X_i^{00} + X_i^{\sigma\sigma} + X_i^{\bar\sigma\bar\sigma} + X_i^{22} = 1, \tag{2.13}$$

which complete the algebra of the X operators.

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

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

which could be written in the case of the Hamiltonian (2.6)–(2.7) in the following form

$$\dot\Psi(1\sigma_1) = -E_1^{\sigma_1}\Psi(1\sigma_1) - F_1^{\sigma_1}\hat t(11')\Psi(1'\sigma_1) - X_1^{\bar\sigma_1\sigma_1}\tau^z\hat t(11')\Psi(1'\bar\sigma_1) + \bar\sigma_1\Psi^\dagger(1'\bar\sigma_1)\hat t(1'1)i\tau^y X_1^{02}. \tag{2.14}$$

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

$$E_1^\sigma = \begin{pmatrix} \varepsilon_\sigma & 0 \\ 0 & \varepsilon_\sigma + U \end{pmatrix}. \tag{2.15}$$

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

$$\hat t(11') = \delta(\tau_1 - \tau_1')t_{i_1 i_{1'}}\Im \equiv t(11')\Im, \tag{2.16}$$

has been introduced, representing the matrix over the spinor indexes (the last circumstance has been specified by the symbol $\hat t$).

Thus the operator $\dot\Psi$ represents the linear combination of the f-operators, with the bosonic b-operators as the coefficients, and the matrixes E and $\hat t$ too.

Following the method we have applied many times to different quantum models [27,32,33], we introduce the generating functional

$$Z[V] = \mathrm{Tr}\left(\mathrm{e}^{-\beta\mathcal{H}}T\mathrm{e}^{-V}\right) \equiv \mathrm{e}^{\Phi}, \tag{2.17}$$

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

For the Hamiltonian (2.6)–(2.7) it is convenient to choose the operator V in the form

$$V = v_{1'}^{00}X_{1'}^{00} + v_{1'}^{22}X_{1'}^{22} + v_{1'}^{\sigma'\sigma'}X_{1'}^{\sigma'\sigma'} + v_{1'}^{\sigma'\bar\sigma'}X_{1'}^{\bar\sigma'\sigma'} + v_{1'}^{02}X_{1'}^{20} + v_{1'}^{20}X_{1'}^{02}. \tag{2.18}$$

It represents the linear combination of the whole diagonal and b-operators with the single point fields v. Thus, differentiating the equation $Z[V]$ with respect to the different v's, we can express the different GFs through the variational derivatives with respect to the corresponding fields. For instance, for the single particle Bose-like GFs of the plasmons, magnons and the doublons we have the expressions:

$$\mathcal{N}^{\sigma_1\sigma_2}(12) = -\langle TX_1^{\sigma_1\sigma_1}X_2^{\sigma_2\sigma_2}\rangle_V = -\frac{1}{Z[V]}\frac{\delta^2 Z[V]}{\delta v_1^{\sigma_1\sigma_1}\delta v_2^{\sigma_2\sigma_2}}, \tag{2.19}$$

$$\mathcal{D}^{\sigma\bar\sigma}(12) = -\langle TX_1^{\sigma\bar\sigma}X_2^{\bar\sigma\sigma}\rangle_V = -\frac{\delta^2\Phi}{\delta v_1^{\sigma\bar\sigma}\delta v_2^{\bar\sigma\sigma}}, \tag{2.20}$$

$$\mathcal{D}^{02}(12) = -\langle TX_1^{02}X_2^{20}\rangle_V = -\frac{\delta^2\Phi}{\delta v_1^{02}\delta v_2^{20}}. \tag{2.21}$$

Here and further symbol $\langle\dots\rangle_V \equiv \langle\dots \mathrm{e}^{-V}\rangle$, where $\langle\dots\rangle$ means averaging over 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 variational derivatives, we shall obtain the actual GFs, describing our system. The fermionic GF cannot be obtained by differentiation of $Z[V](\Phi)$ 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 make use of the general equation of motion (see Appendix) and write it for the expression $((T\Psi_1\Psi_2^\dagger))$, determining the electronic GF:

$$\frac{\partial}{\partial\tau_1}(\!(T\Psi_{\alpha_1}(1\sigma_1)\Psi_{\alpha_2}^\dagger(2\sigma_2)e^{-V})\!) = (\!(T\{\Psi_{\alpha_1}(1\sigma_1), \Psi_{\alpha_2}^\dagger(2\sigma_2)\}_+ e^{-V})\!) + (\!(T\dot\Psi_{\alpha_1}(1\sigma_1)\Psi_{\alpha_2}^\dagger(2\sigma_2)e^{-V})\!) - (\!(T\{\Psi_{\alpha_1}(1\sigma_1), V\}_-\Psi_{\alpha_2}^\dagger(2\sigma_2)e^{-V})\!). \tag{3.1}$$

Let us calculate now the anticommutator and the commutator of the Ψ-operators in (3.1). According to relations (2.9) and (2.11), we have:

$$\{\Psi_{\alpha_1}(1\sigma_1), \Psi_{\alpha_2}^\dagger(2\sigma_2)\}_+ = \delta_{12}\left(\delta_{\sigma_1\sigma_2}(F_1^{\sigma_1})_{\alpha_1\alpha_2} + \delta_{\bar\sigma_1\sigma_2}\tau^z_{\alpha_1\alpha_2}X_1^{\bar\sigma_1\sigma_1}\right), \tag{3.2}$$

$$\{\Psi(1\sigma_1), V\}_- = W_1^{\sigma_1}\Psi(1\sigma_1) + v_1^{\bar\sigma_1\sigma_1}\Psi(1\bar\sigma_1) + \bar\sigma_1 v_1^{02}\Psi^\dagger(1\bar\sigma_1)\tau^x. \tag{3.3}$$

Here W is the double-row matrix composed with the fluctuating fields:

$$W_1^\sigma = \begin{pmatrix} v_1^{\sigma\sigma} - v_1^{00} & 0 \\ 0 & v_1^{22} - v_1^{\bar\sigma\bar\sigma} \end{pmatrix}. \tag{3.4}$$

After the substitution of expression (2.14) and the commutators in equation (3.1), the latter could be represented in the form:

$$\begin{aligned}G_{0V}^{-1}(1\sigma_1,1'\sigma_1')(\!(T\Psi(1'\sigma_1')\Psi^\dagger(2\sigma_2)e^{-V})\!) = \\ -\delta_{12}\left[\delta_{\sigma_1\sigma_2}(\!(TF_1^{\sigma_1}e^{-V})\!)+\delta_{\bar\sigma_1\sigma_2}\tau^z(\!(TX_1^{\bar\sigma_1\sigma_1}e^{-V})\!)\right] \\ +\bar\sigma_1 v_1^{02}\tau^x(\!(T\Psi^\dagger(1\bar\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V})\!) \\ +(\!(TF_1^{\sigma_1}\hat t(11')\Psi(1'\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V})\!) \\ +\tau^z\hat t(11')(\!(TX_1^{\bar\sigma_1\sigma_1}\Psi(1'\bar\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V})\!) \\ +\sigma_1(\!(TX_1^{02}\Psi^\dagger(1'\bar\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V})\!)\hat t(1'1)i\tau^y. \quad (3.5)\end{aligned}$$

Here the quantity

$$G_{0V}^{-1}(1\sigma_1,2\sigma_2) = \left\{\left(-\frac{\partial}{\partial\tau_1}-E_1^{\sigma_1}\right)\delta_{\sigma_1\sigma_2}-W_1^{\sigma_1}\delta_{\sigma_1\sigma_2}-v_1^{\bar\sigma_1\sigma_1}\tau^0\delta_{\bar\sigma_1\sigma_2}\right\}\delta_{12}, \quad (3.6)$$

has been introduced, which defines the zeroth-order approximation propagator of the electrons in the fluctuating single-point fields. This quantity is the 2×2 matrix with respect to spinor indexes. Expressing the mixed GFs through the variational derivatives of $Z[V]$, we can represent the obtained equation as

$$\begin{aligned}G_{0V}^{-1}(1\sigma_1,1'\sigma_1')(\!(T\Psi(1'\sigma_1')\Psi^\dagger(2\sigma_2)e^{-V})\!) = \\ -\delta_{12}\hat a_1(\sigma_1\sigma_2)Z[V]+\hat a_1(\sigma_1\sigma_1')\hat t(11')(\!(T\Psi(1'\sigma_1')\Psi^\dagger(2\sigma_2)e^{-V})\!) \\ -\sigma_1\left[v_1^{02}\tau^x\delta_{11'}-i\tau^y\hat{\tilde t}(11')\frac{\delta}{\delta v_1^{02}}\right](\!(T\Psi^\dagger(1'\bar\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V})\!). \quad (3.7)\end{aligned}$$

Here the double-row matrix is the differential operator with respect to the single point fluctuating fields:

$$\hat a_1(\sigma_1,\sigma_2) = \left(\delta_{\sigma_1\sigma_2}\hat F_1^{\sigma_1}-\delta_{\bar\sigma_1\sigma_2}\tau^z\frac{\delta}{\delta v_1^{\bar\sigma_1\sigma_1}}\right), \quad (3.8)$$

where

$$\hat F_1^\sigma = -\begin{pmatrix}\frac{\delta}{\delta v_1^{00}}+\frac{\delta}{\delta v_1^{\sigma\sigma}} & 0\\ 0 & \frac{\delta}{\delta v_1^{\bar\sigma\bar\sigma}}+\frac{\delta}{\delta v_1^{22}}\end{pmatrix}. \quad (3.9)$$

Also, let us note that $\hat{\tilde t}$ is the transposed matrix of $\hat t$.

As usual, we pass from the functional $Z[V]$ to the functional $\Phi[V]$ using the substitution:

$$Z[V] = e^{\Phi[V]}. \quad (3.10)$$

Then, the equation (3.5) results in a direct equation for the electronic GF:

$$\begin{aligned}[G_{0V}^{-1}(1\sigma,1'\sigma_1')-(\hat a_1(\sigma_1\sigma_1')\Phi)\hat t(11') \\ -\hat a_1(\sigma_1\sigma_1')\hat t(11')]\langle T\Psi(1'\sigma_1')\Psi^\dagger(2\sigma_2)e^{-V}\rangle = \\ -\delta_{12}[\hat a_1(\sigma_1\sigma_2)\Phi]-\sigma_1\delta_{11'}v_1^{02}\langle T\Psi^\dagger(1'\bar\sigma_1)\tau^x\Psi^\dagger(2\sigma_2)e^{-V}\rangle \\ -\sigma_1\left(\frac{\delta\Phi}{\delta v_1^{02}}+\frac{\delta}{\delta v_1^{02}}\right)\langle T\Psi^\dagger(1'\bar\sigma_1)\hat t(1'1)i\tau^y\Psi^\dagger(2\sigma_2)e^{-V}\rangle. \quad (3.11)\end{aligned}$$

We see that the equation for the GF $\langle T\Psi\Psi^\dagger e^{-V}\rangle$ contains the anomalous GF $\langle T\Psi^\dagger\Psi^\dagger e^{-V}\rangle$. Then, it is necessary to write the equation for it, too.

Let us introduce the matrix GF:

$$\mathcal{L}(\underline{1}\,\underline{2}) = -\begin{pmatrix}\langle T\Psi(1\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V}\rangle & \langle T\Psi(1\sigma_1)\Psi(2\sigma_2)e^{-V}\rangle \\ \langle T\Psi^\dagger(1\sigma_1)\Psi^\dagger(2\sigma_2)e^{-V}\rangle & \langle T\Psi^\dagger(1\sigma_1)\Psi(2\sigma_2)e^{-V}\rangle\end{pmatrix}. \quad (3.12)$$

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 (3.12), so that

$$\underline{1} = \{1\sigma_1\alpha_1\nu_1\}. \quad (3.13)$$

The matrix $\mathcal{L}(\underline{1}\,\underline{2})$ is an 8×8 matrix with respect to the collection of the discrete indexes. A matrix of such a rank appears automatically in the Hubbard model. Its arising is described "normal" states (without the Cooper's pairs) but also with broken symmetries as well.

The set of four equations for the GFs in (3.12) could be written as a single matrix equation:

$$\left[L_{0V}^{-1}(\underline{1}\,\underline{1}')-(\hat A\Phi Y)(\underline{1}\,\underline{1}')-(\hat A Y)(\underline{1}\,\underline{1}')\right]\mathcal{L}(\underline{1}'\underline{2}) = (\hat A\Phi)(\underline{1}\,\underline{2}). \quad (3.14)$$

Here we introduced the operator matrix

$$\hat A(\underline{1}\,\underline{2}) = \delta_{12}\begin{pmatrix}\hat a_1(\sigma_1\sigma_2) & -\sigma_1\delta_{\bar\sigma_1\sigma_2}i\tau^y\frac{\delta}{\delta v_1^{02}} \\ -\sigma_1\delta_{\bar\sigma_1\sigma_2}i\tau^y\frac{\delta}{\delta v_1^{20}} & \hat a_1(\sigma_2\sigma_1)\end{pmatrix}, \quad (3.15)$$

where each element represents the 2×2 matrix with respect to the spinor indexes, hidden in the Pauli matrices and the matrix $\hat a_1$, having the variational derivatives with respect to the fluctuating fields as its elements. Besides, the equation (3.14) contains the matrix

$$Y(\underline{1}\,\underline{2}) = \begin{pmatrix}\hat t(12) & 0\\ 0 & -\hat{\tilde t}(12)\end{pmatrix}. \quad (3.16)$$

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

$$L_{0V}^{-1}(\underline{1}\,\underline{2}) = \begin{pmatrix}G_{0V}^{-1}(1\sigma_1,2\sigma_2) & \sigma_1\delta_{\bar\sigma_1\sigma_2}\delta_{12}\tau^x v_1^{02} \\ -\sigma_1\delta_{\bar\sigma_1\sigma_2}\delta_{12}\tau^x v_1^{20} & \widetilde G_{0V}^{-1}(1\sigma_1,2\sigma_2)\end{pmatrix}, \quad (3.17)$$

where G_{0V}^{-1} is given by the expression (3.6), and $\widetilde G_{0V}^{-1}$ by its transposition:

$$\widetilde G_{0V}^{-1}(1\sigma_1,2\sigma_2) = \left\{\left(-\frac{\partial}{\partial\tau_1}+E_1^{\sigma_1}\right)\delta_{\sigma_1\sigma_2} + W_1^{\sigma_1}\delta_{\sigma_1\sigma_2}+v_1^{\sigma_1\bar\sigma_1}\tau^0\delta_{\bar\sigma_1\sigma_2}\right\}\delta_{12}.$$

If replace back in equation (3.14) term with by the mixture GFs one can see that the matrix equation (3.14) is equivalent that derived by Plakida [28,29]. The equation (3.14) is of the same type of the equation for the single particle GF, that we derived for the Hubbard model in the limit $U = \infty$ [27] and for the Heisenberg model as well. In the above models the matrix $\hat{A}$ degenerated into a scalar, but now it is a matrix with respect to the discrete indexes α and ν, likewise the other values in (3.15). By virtue of the noted similarity of the equation (3.14) 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 the electronic GFs. Let us represent them as a product of the propagator L and the terminal Π parts, respectively, namely:

$$\mathcal{L}(\underline{1}\,\underline{2}) = L(\underline{1}\,\underline{1}')\Pi(\underline{1}'\underline{2}). \tag{3.18}$$

The propagator part satisfies the Dyson equation

$$L^{-1}(\underline{1}\,\underline{2}) = L_{0V}^{-1}(\underline{1}\,\underline{2}) - \Sigma(\underline{1}\,\underline{2}). \tag{3.19}$$

Let us represent the equation for the self-energy part like the sum of the two terms:

$$\Sigma(\underline{1}\,\underline{2}) = \Sigma'(\underline{1}\,\underline{2}) + (\Pi Y)(\underline{1}\,\underline{2}), \tag{3.20}$$

which took place for the models considered before. Then, inserting (3.19) and (3.20) in (3.18) and comparing with the initial equation (3.14), we can obtain the two equations for Π and Σ':

$$\Pi(\underline{1}\,\underline{2}) = (\hat{A}\Phi)(\underline{1}\,\underline{2}) + (YL)(\underline{4}'\underline{3}')\hat{A}(\underline{1}\,\underline{4}')\Pi(\underline{3}'\underline{2}), \tag{3.21}$$

$$\Sigma'(\underline{1}\,\underline{2}) = -(YL)(\underline{4}'\underline{3}')\hat{A}(\underline{1}\,\underline{4}')\left(L_{0V}^{-1}(\underline{3}'\underline{2}) - \Sigma'(\underline{3}'\underline{2})\right). \tag{3.22}$$

In obtaining these equations we have taken into account the identity

$$(\hat{A}L)(\underline{1}\,\underline{2}) = -L(\underline{1}'\underline{2}')\left[\hat{A}(\underline{1}\,\underline{1}')L^{-1}(\underline{2}'\underline{3}')\right]L(\underline{3}'\underline{2}), \tag{3.23}$$

which is the generalization of the well known identity expressing the differentiation of a GF through the differentiation of its inverse:

$$\frac{\delta G}{\delta v} = -G\frac{\delta G^{-1}}{\delta v}G.$$

The equations (3.21) and (3.22) for the terminal and self-energy parts of the GF have a structure analogous to the respective equations of the other models. These are the equations for the variational derivatives for Π and Σ'. The contribution Σ' in the self-energy part Σ is not cutable through the "line of the interaction", representing the value Y. The cutable part Σ has been already extracted in the equation (3.20) like the second contribution.

From the set of the equations (3.18)–(3.20) it follows an important consequence, which could be represented in the form of the following equation for the GF $\mathcal{L}$:

$$\mathcal{L} = \mathcal{L}' + \mathcal{L}'Y\mathcal{L}. \tag{3.24}$$

Here $\mathcal{L}'$ is determined by the two relations:

$$\mathcal{L}' = L'\Pi, \qquad L'^{\,-1} = L_{0V}^{-1} - \Sigma'.$$

The solution of the equation (3.24) could be written as:

$$\mathcal{L}(\underline{1}\,\underline{2}) = \left[\mathcal{L}'^{-1} - Y\right]^{-1}(\underline{1}\,\underline{2}), \tag{3.25}$$

where

$$\mathcal{L}'^{\,-1} = \Pi^{-1}\left(L_{0V}^{-1} - \Sigma'\right). \tag{3.26}$$

As it follows from the definition, the value $\mathcal{L}'$ is not cutable through the line Y, therefore the equation (3.24) for the GF is the Larkin's equation, expressing a GF through an irreducible part (with respect to a line of "interaction"). From this equation it follows the locator representation (3.25) for the electronic GF, also.

So, this issue is a diagrammatic justification of the multiplicative representation (3.18) for one-particle electron GF. Similar representations for one-particle GFs in other models of strongly correlated electron and spin systems was discussed in details in a review [34].

The equations (3.21) and (3.22) could be solved by iterations. At the first orders with respect to Y we obtain:

$$\Pi(\underline{1}\,\underline{2}) = \hat{A}(\underline{1}\,\underline{2})\Phi + (YL)(\underline{4}'\underline{3}')\hat{A}(\underline{1}\,\underline{4}')\hat{A}(\underline{3}'\underline{2})\Phi + \ldots, \tag{3.27}$$

$$\begin{aligned}\Sigma'(\underline{1}\,\underline{2}) = &-(YL)(\underline{4}'\underline{3}')\left[\hat{A}(\underline{1}\,\underline{4}')L_{0V}^{-1}(\underline{3}'\underline{2})\right] \\ &+ (YL)(\underline{4}'\underline{3}')(YL)(\underline{6}'\underline{1}')\left[\hat{A}(\underline{1}\,\underline{4}')L_{0V}^{-1}(\underline{1}'\underline{2}')\right] \\ &\times L(\underline{2}'\underline{5}')\left[\hat{A}(\underline{3}'\underline{6}')L_{0V}^{-1}(\underline{5}'\underline{2})\right] + \ldots\end{aligned} \tag{3.28}$$

In (3.27) the operator $\hat{A}$, acting on Φ, brings the mean value of the diagonal and b-operators; a repeated action of the operator $\hat{A}$ will produce bosonic GFs of the different types. An action of the operator on L_{υ}^{-1} will result in expressions composed of different δ-symbols. The problem is contained in the multiplication of the matrices in the equations (3.27) and (3.28), taking into account that the matrix $\hat{A}(\underline{1}\,\underline{2})$ contains derivatives, which should act on the corresponding values. To fulfil the matrix multiplication accounting for the operator character of the several factors, we rewrite the expressions (3.27) and (3.28) in another form:

$$\Pi(\underline{1}\,\underline{2}) = \hat{A}(\underline{1}\,\underline{2})\Phi + \hat{A}(\underline{1}\,\underline{4}')(YL)(\underline{4}'\underline{3}')\hat{A}(\underline{3}'\underline{2})\Phi + \ldots, \tag{3.29}$$

$$\begin{aligned}\Sigma'(\underline{1}\,\underline{2}) = &-\hat{A}(\underline{1}\,\underline{4}')(YL)(\underline{4}'\underline{3}')L_V^{-1}(\underline{3}'\underline{2}) \\ &+ \hat{A}(\underline{1}\,\underline{4}')(YL)(\underline{4}'\underline{3}')\hat{A}(\underline{3}'\underline{6}')(YL)(\underline{6}'\underline{1}') \\ &\times L_V^{-1}(\underline{1}'\underline{2}')L(\underline{2}'\underline{5}')L_V^{-1}(\underline{5}'\underline{2}) + \ldots\end{aligned} \tag{3.30}$$

In these expressions all the factors are arranged in the order of the matrix multiplication, but we should not forget which factors the derivatives of the matrix $\hat{A}$ act on.

4 Iteration equation for the self-energy and terminal part

According to definition (3.12), the electronic GF $\mathcal{L}$ takes into account the possibility of states with coupled electrons. In this paper we shall consider the normal system, described completely by the matrix element of the electronic GF $\mathcal{L}(12)$, namely

$$\mathcal{G}(1\sigma_1\, 2\sigma_2\,) \equiv \mathcal{L}^{11}(1\sigma_1\, 2\sigma_2). \tag{4.1}$$

The normal GF $\mathcal{G}$ can be looked in the standard multiplicative form

$$\mathcal{G} = G\Lambda. \tag{4.2}$$

with G obeying the Dyson equation

$$G^{-1} = G_{0V}^{-1} - \Sigma, \tag{4.3}$$

and the self-energy part being a sum of two terms, uncutable Σ' and cutable $\Lambda\hat{t}$:

$$\Sigma = \Sigma' + \Lambda\hat{t}. \tag{4.4}$$

In equations (4.2) – (4.4) all quantities are 2×2 matrices with respect to spinor indexes, with arguments of the type $\mathcal{G}(1\sigma_1\, 2\sigma_2\,)$.

Iterations in general equations (3.21) and (3.22) allow to get series for Σ' and Λ, determined by equations (4.2)–(4.4). Calculations of these series are done in Appendix B, and here we present the results within the limit of the first two orders. We have, for the zeroth order of Λ:

$$\Lambda_0^\sigma(k) = \begin{pmatrix} 1-\langle n^{\bar\sigma}\rangle & 0 \\ 0 & \langle n^{\bar\sigma}\rangle \end{pmatrix}, \tag{4.5}$$

where

$$\langle n^\sigma\rangle = \langle X_i^{\sigma\sigma} + X_i^{22}\rangle = \langle c_{i\sigma}^\dagger c_{i\sigma}\rangle \tag{4.6}$$

is the average number of electrons on a site with spin σ. The first order correction for Λ is the following

$$\Lambda_1^\sigma(k) = \begin{pmatrix} \lambda_1^\sigma(k) & \lambda_2^\sigma(k) \\ -\lambda_1^\sigma(k) & -\lambda_2^\sigma(k) \end{pmatrix}, \tag{4.7}$$

where

$$\lambda_1^\sigma(k) = -\sum_q \varepsilon(\boldsymbol{k}+\boldsymbol{q})\Big[(G_{11}^\sigma + G_{21}^\sigma)(k+q)\mathcal{N}^{\bar\sigma\bar\sigma}(q) + (G_{11}^{\bar\sigma}+G_{21}^{\bar\sigma})(k+q)\mathcal{D}^{\sigma\bar\sigma}(q) + (G_{21}^{\bar\sigma}+G_{22}^{\bar\sigma})(-k-q)\mathcal{D}^{02}(q)\Big], \tag{4.8}$$

$$\lambda_2^\sigma(k) = \sum_q \varepsilon(\boldsymbol{k}+\boldsymbol{q})\Big[(G_{12}^\sigma + G_{22}^\sigma)(k+q)\mathcal{N}^{\bar\sigma\bar\sigma}(q) + (G_{12}^{\bar\sigma}+G_{22}^{\bar\sigma})(k+q)\mathcal{D}^{\sigma\bar\sigma}(q) + (G_{11}^{\bar\sigma}+G_{12}^{\bar\sigma})(-k-q)\mathcal{D}^{02}(q)\Big]. \tag{4.9}$$

The quantities $\mathcal{N}^{\bar\sigma\bar\sigma}(k)$, $\mathcal{D}^{\sigma\bar\sigma}(k)$ and $\mathcal{D}^{02}(k)$ are the Fourier transforms of the bosonic GFs, determined by relations (2.19)–(2.21) with 4-momentum q. Here $\varepsilon(\boldsymbol{k})$ is the Fourier transform of $t_{i_1 i_2}$, which is actually the bare electron energy in the lattice.

The contribution of the first order in Σ' is given by:

$$\Sigma_1'^\sigma = -\eta^\sigma \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \tag{4.10}$$

where

$$\eta^\sigma = \sum_k \varepsilon(\boldsymbol{k})\left[G_{11}^{\bar\sigma}(k) - G_{22}^{\bar\sigma}(k)\right]. \tag{4.11}$$

The second order correction is equal to:

$$\Sigma_2'^\sigma = \begin{pmatrix} \varphi_1^\sigma(k) & \varphi_2^\sigma(k) \\ -\varphi_1^\sigma(k) & -\varphi_2^\sigma(k) \end{pmatrix}, \tag{4.12}$$

where

$$\varphi_1^\sigma(k) = \sum_q \sum_{k_1} \varepsilon(\boldsymbol{k}+\boldsymbol{q})\varepsilon(\boldsymbol{k_1}+\boldsymbol{q}) \times \Big[G_{11}^\sigma(k_1) g^{\bar\sigma}(k+q) G_{11}^{\bar\sigma}(k_1+q) + G_{11}^{\bar\sigma}(k_1) g^{\sigma}(k+q) G_{11}^{\bar\sigma}(k_1+q) + \sum_{\sigma'} G_{22}^{\bar\sigma}(-k_1) g^{\sigma'}(k+q) G_{11}^{\bar\sigma'}(-k_1-q)\Big], \tag{4.13}$$

and the quantity $\varphi_2^\sigma(k)$ is given by a change of spinor indexes $1 \leftrightarrow 2$ in (4.13). Here $g^\sigma(k)$ is a linear combination of the matrix elements of the electronic GF:

$$g^\sigma(k) = G_{11}^\sigma(k) + G_{21}^\sigma(k) - G_{12}^\sigma(k) - G_{22}^\sigma(k) \tag{4.14}$$

Finally we write down the second order contribution in the cutable part of Σ, that is, the expression for $\Sigma_{red}^\sigma \equiv \Lambda^\sigma \hat{t}^\sigma$. Because in momentum representation $\hat{t}^\sigma$ is equal to $\varepsilon(\boldsymbol{k})\Im$, with $\Im$ being the 2×2 matrix determined in (2.8), we find, according to (4.8):

$$\Sigma_{red}^\sigma = \lambda^\sigma(k)\varepsilon(\boldsymbol{k}) \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \tag{4.15}$$

where

$$\lambda^\sigma(k) = \lambda_1^\sigma(k) + \lambda_2^\sigma(k) = -\sum_q \varepsilon(\boldsymbol{k}+\boldsymbol{q}) \times \Big[g^\sigma(k+q)\mathcal{N}^{\bar\sigma\bar\sigma}(q) \times + g^{\bar\sigma}(k+q)\mathcal{D}^{\sigma\bar\sigma}(q) + \widetilde{g}^{\bar\sigma}(k+q)\mathcal{D}^{02}(q)\Big], \tag{4.16}$$

$$\widetilde{g}^\sigma(k) = G_{21}^\sigma(-k) + G_{22}^\sigma(-k) - G_{11}^\sigma(-k) - G_{12}^\sigma(-k), \tag{4.17}$$

and

$$\widetilde{g}^\sigma(k) = -g^\sigma(-k).$$

We see that the correction $\Sigma_1'^{\sigma}$ depends neither on momentum nor on frequency and determines only a shift of electron spectrum, but it depends on spin. The second order corrections $\Sigma_2'^{\sigma}(k)$ and $\Sigma^{\sigma}_{red}(k)$ depend both on momentum and frequency. The contribution Σ^{σ}_{red} is determined by the interaction of electrons with bosonic excitations, while $\Sigma_2'^{\sigma}$ is determined by electronic GFs only.

5 Mean field approximation

The simplest approximation of a mean field type is the Hubbard-I, which takes into account a term in Σ equal to $\Lambda_0\hat{t}$. To it, one can add a first order term Σ_1', not depending on frequency. The second order correction Σ_2' depends on the frequency, however we shall try to extract from it a static part by the following ansatz.

Let us consider that in Σ_2' both expressions for $\varphi_1^{\sigma}(k)$, $\varphi_2^{\sigma}(k)$ include a factor $\varepsilon(\boldsymbol{k}+\boldsymbol{q})$ in the summation over $\boldsymbol{q}$. So it can be factorized in the nearest neighbor approximation, and a term proportional to $\varepsilon(\boldsymbol{k})$ can be taken out from the static part of Σ_2' for the cubic lattice. Thus in the static approximation Σ_2' can be approximated by the expression

$$\Sigma_2'(\boldsymbol{k}) = \begin{pmatrix} p_1^{\sigma} & p_2^{\sigma} \\ -p_1^{\sigma} & -p_2^{\sigma} \end{pmatrix} \varepsilon(\boldsymbol{k}). \tag{5.1}$$

Here p_1^{σ} and p_2^{σ} are some spin dependent constants. Their expressions can be explicitly written out, but we will not do it, because we shall try to calculate them from some general conditions for electronic GFs, which should be satisfied. Such conditions were formulated in works by Mancini and coworkers (see general discussion in paper [10] and refs. therein), where it is developed a method using linearized equation of motion for composite operators. The condition is demanding that the electronic GF $\mathcal{G}_{12}$ is equal to zero when arguments coincide. Below we will use this idea for the determination of unknown parameters p_1^{σ} and p_2^{σ}.

First we write down the self-energy part in an approximation which includes the Hubbard-I term, the first order correction Σ' (4.10) and Σ_2' in the form (5.1). All these three contributions give Σ_{MF}, corresponding to a mean field approximation. So we have:

$$\Sigma^{\sigma}_{MF}(\boldsymbol{k}) = -\eta^{\sigma} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} + \begin{pmatrix} 1-\langle n^{\bar\sigma}\rangle + p_1^{\sigma} & 1-\langle n^{\bar\sigma}\rangle + p_2^{\sigma} \\ \langle n^{\bar\sigma}\rangle - p_1^{\sigma} & \langle n^{\bar\sigma}\rangle - p_2^{\sigma} \end{pmatrix} \varepsilon(\boldsymbol{k}). \tag{5.2}$$

It is clear that the first term is responsible for a shift of the Hubbard subbands, and the second one for a renormalization of their widths. The propagator part of the GF in the mean field approximation is determined by a matrix equation:

$$[G^{\sigma}(k)]^{-1} = [G_0^{\sigma}(k)]^{-1} - \Sigma^{\sigma}_{MF}(k).$$

We look for a solution of the form

$$G^{\sigma}_{\alpha\beta}(k) = \frac{(\mathcal{A}_1^{\sigma})_{\alpha\beta}(\boldsymbol{k})}{i\omega_n - E_1^{\sigma}(\boldsymbol{k})} + \frac{(\mathcal{A}_2^{\sigma})_{\alpha\beta}(\boldsymbol{k})}{i\omega_n - E_2^{\sigma}(\boldsymbol{k})}. \tag{5.3}$$

The poles $E_m^{\sigma}(\boldsymbol{k})$ and their residues $(\mathcal{A}_m^{\sigma})_{\alpha\beta}(\boldsymbol{k})$ are written in the form:

$$\left.\begin{aligned} (\mathcal{A}^{\sigma}_{1,2})_{11}(\boldsymbol{k}) &= \frac{1}{2}\left[1 \pm \frac{r^{\sigma}(\boldsymbol{k})}{2Q^{\sigma}(\boldsymbol{k})}\right] \\ (\mathcal{A}^{\sigma}_{1,2})_{22}(\boldsymbol{k}) &= \frac{1}{2}\left[1 \mp \frac{r^{\sigma}(\boldsymbol{k})}{2Q^{\sigma}(\boldsymbol{k})}\right] \\ (\mathcal{A}^{\sigma}_{1,2})_{12}(\boldsymbol{k}) &= \mp\frac{\eta^{\sigma} + (1-\langle n^{\bar\sigma}\rangle + p_2^{\sigma})\varepsilon(\boldsymbol{k})}{2Q^{\sigma}(\boldsymbol{k})} \\ (\mathcal{A}^{\sigma}_{1,2})_{21}(\boldsymbol{k}) &= \mp\frac{\eta^{\sigma} + (\langle n^{\bar\sigma}\rangle - p_1^{\sigma})\varepsilon(\boldsymbol{k})}{2Q^{\sigma}(\boldsymbol{k})} \end{aligned}\right\}, \tag{5.4}$$

$$E^{\sigma}_{1,2}(\boldsymbol{k}) = R^{\sigma}(\boldsymbol{k}) \mp Q^{\sigma}(\boldsymbol{k}). \tag{5.5}$$

Here

$$r^{\sigma}(\boldsymbol{k}) = U - [1 - 2\langle n^{\bar\sigma}\rangle + p_1^{\sigma} + p_2^{\sigma}]\varepsilon(\boldsymbol{k}),$$

whilst expressions for $R^{\sigma}(\boldsymbol{k})$ and $Q^{\sigma}(\boldsymbol{k})$ will be written later.

The electronic GF $\mathcal{G}^{\sigma}$ in the mean field approximation is found with the help of the general relation (4.2)

$$\mathcal{G}^{\sigma}(k) = G^{\sigma}(k)\Lambda_0^{\sigma}(k),$$

where $\Lambda_0^{\sigma}(k)$ is given by the matrix (4.5).

The electronic GF depends on parameters μ, η^{σ}, $\langle n^{\sigma}\rangle$, p_1^{σ} and p_2^{σ}, which must be determined in a self consistent way from the equations

$$\sum_{\sigma}\langle n_i^{\sigma}\rangle = n_i, \qquad \langle n_i^{\sigma}\rangle = \sum_{\alpha\beta}\mathcal{G}^{\sigma}_{\alpha\beta}(i,\tau\,;\,i,\tau+0),$$

and also from equation (4.11), determining the parameter η^{σ}. Parameters p_1^{σ} and p_2^{σ} will be determined [10] from conditions which follow from the properties of X operators, namely:

$$\left.\begin{aligned} \mathcal{G}^{\sigma}_{12}(i,\tau\,;\,i,\tau+0) &= \langle \bar\sigma X_i^{2\bar\sigma} X_i^{0\sigma}\rangle = 0 \\ \mathcal{G}^{\sigma}_{21}(i,\tau\,;\,i,\tau+0) &= \langle X_i^{\sigma 0} X_i^{\bar\sigma 2}\bar\sigma\rangle = 0 \end{aligned}\right\}. \tag{5.6}$$

Thus a complete system of equations for all five parameters can be written in the form:

$$\langle n^{\sigma}\rangle + \langle n^{\bar\sigma}\rangle = n, \tag{5.7}$$

$$\langle n^{\sigma}\rangle = \sum_k \left[\mathcal{G}^{\sigma}_{11}(k) + \mathcal{G}^{\sigma}_{22}(k)\right], \tag{5.8}$$

$$\eta^{\sigma} = \sum_k \varepsilon(\boldsymbol{k})\left[G^{\bar\sigma}_{11}(k) - G^{\bar\sigma}_{22}(k)\right], \tag{5.9}$$

$$\sum_k \mathcal{G}^{\sigma}_{12}(k) = 0, \tag{5.10}$$

$$\sum_k \mathcal{G}^{\sigma}_{21}(k) = 0 \tag{5.11}$$

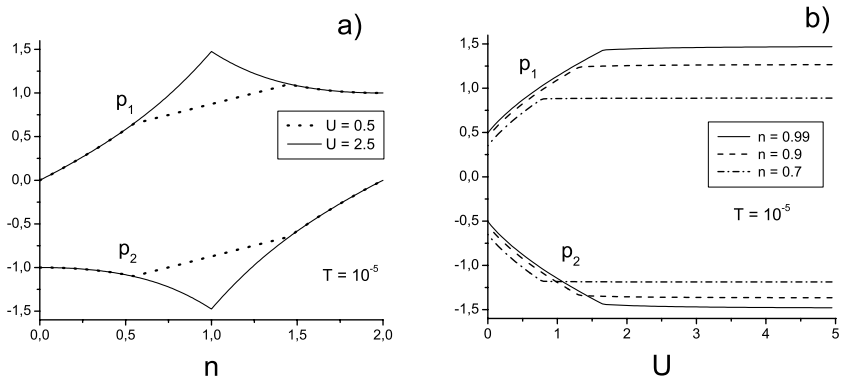

Fig. 1. Dependence of parameters p_1 and p_2 on (a) electron concentration n and (b) Coulomb interaction U.

(we assume homogeneous states, so all averages do not depend on site index).

From the comparison of the last two equations we find a relation between parameters p_1^σ and p_2^σ:

$$p_1^\sigma + p_2^\sigma = -(1 - 2\langle n^{\bar\sigma}\rangle). \tag{5.12}$$

Therefore, the parameter p_2^σ can be replaced in all the expressions above. Thus the equations (5.4) for the residues of GF are:

$$\left.\begin{aligned}(\mathcal{A}^\sigma_{1,2})_{11}(\boldsymbol{k}) &= \frac{1}{2}\left[1 \pm \frac{U}{2Q^\sigma(\boldsymbol{k})}\right]\\ (\mathcal{A}^\sigma_{1,2})_{22}(\boldsymbol{k}) &= \frac{1}{2}\left[1 \mp \frac{U}{2Q^\sigma(\boldsymbol{k})}\right]\\ (\mathcal{A}^\sigma_{1,2})_{12}(\boldsymbol{k}) = (\mathcal{A}^\sigma_{1,2})_{21}(\boldsymbol{k}) &= \mp\frac{\eta^\sigma + (\langle n^{\bar\sigma}\rangle - p_1^\sigma)\varepsilon(\boldsymbol{k})}{2Q^\sigma(\boldsymbol{k})}\end{aligned}\right\}. \tag{5.13}$$

Expressions for $R^\sigma(\boldsymbol{k})$ and $Q^\sigma(\boldsymbol{k})$, determining poles, are now equal to:

$$\left.\begin{aligned}R^\sigma(\boldsymbol{k}) &= -\sigma\frac{h}{2} - \eta^\sigma + (1 + p_1^\sigma - \langle n^{\bar\sigma}\rangle)\varepsilon(\boldsymbol{k}) + \frac{U}{2} - \mu\\ Q^\sigma(\boldsymbol{k}) &= \frac{1}{2}\sqrt{U^2 + 4\left[\eta^\sigma + (\langle n^{\bar\sigma}\rangle - p_1^\sigma)\varepsilon(\boldsymbol{k})\right]^2}\end{aligned}\right\}. \tag{5.14}$$

After the replacement of parameter p_2^σ, the two equations (5.10) and (5.11) reduce to only one, which allows to find the unknown parameter p_1^σ. Taking the summation over frequencies in all equations (5.8)–(5.11), we write our system in the form:

$$\langle n^\sigma\rangle = \frac{1}{2}(1 - \mathcal{K}_0^\sigma) - \frac{U}{2}\mathcal{F}_0^\sigma(1 - 2\langle n^{\bar\sigma}\rangle), \tag{5.15}$$

$$\eta^\sigma = -U\mathcal{F}_1^{\bar\sigma}, \tag{5.16}$$

$$\eta^\sigma\mathcal{F}_0^\sigma + (\langle n^{\bar\sigma}\rangle - p_1^\sigma)\mathcal{F}_1^\sigma = 0, \tag{5.17}$$

where we use the definitions of the paper [8]:

$$\mathcal{K}_n^\sigma = \frac{1}{2N}\sum_{\boldsymbol{k}}\varepsilon^n(\boldsymbol{k})\left[\mathrm{th}\left(\frac{E_1^\sigma(\boldsymbol{k})}{2T}\right) + \mathrm{th}\left(\frac{E_2^\sigma(\boldsymbol{k})}{2T}\right)\right], \tag{5.18}$$

$$\mathcal{F}_n^\sigma = \frac{1}{2N}\sum_{\boldsymbol{k}}\frac{\varepsilon^n(\boldsymbol{k})}{2Q^\sigma(\boldsymbol{k})}\left[\mathrm{th}\left(\frac{E_1^\sigma(\boldsymbol{k})}{2T}\right) - \mathrm{th}\left(\frac{E_2^\sigma(\boldsymbol{k})}{2T}\right)\right]. \tag{5.19}$$

We have to add to them equations (5.15)–(5.17) and equation (5.7) for chemical potential.

The energy of the system can be found by averaging the Hamiltonian (2.6)–(2.7) over a Gibbs ensemble. It is quite easy to express it by means of electronic GFs:

$$\frac{1}{N}\langle\mathcal{H}\rangle = \sum_{k\sigma}\varepsilon(\boldsymbol{k})\sum_{\alpha\beta}\mathcal{G}^\sigma_{\alpha\beta}(k) + U\langle X^{22}\rangle \tag{5.20}$$

where

$$\langle X^{22}\rangle \equiv D = \frac{1}{2}\sum_{k\sigma}\mathcal{G}^\sigma_{22}. \tag{5.21}$$

After substituting here the expressions for the matrix elements $\mathcal{G}^\sigma_{\alpha\beta}$, we find the expressions for the energy $\langle\mathcal{H}\rangle$ and the double occupation parameter D:

$$\frac{1}{N}\langle\mathcal{H}\rangle = U\langle X^{22}\rangle + \sum_\sigma\left[-\eta^\sigma\langle n^\sigma\rangle - \frac{1}{2}\mathcal{K}_1^\sigma - \frac{U}{2}\mathcal{F}_1^\sigma + \eta^\sigma\mathcal{F}_1^\sigma + (\langle n^{\bar\sigma}\rangle - p_1^\sigma)\mathcal{F}_2^\sigma\right], \tag{5.22}$$

$$\langle X^{22}\rangle \equiv D = \frac{1}{4}\sum_\sigma\langle n^{\bar\sigma}\rangle(1 - \mathcal{K}_0^\sigma + U\mathcal{F}_0^\sigma). \tag{5.23}$$

In Figure 1 the parameters p_1 and p_2 are plotted as functions of electron concentration at different U. Such results are typical for other fixed parameters of the system. For all different n and U the parameter p_1 is positive and p_2 is negative. A negative solution for parameter p_1 was not found. The behavior of p_1 is rather similar to the COM1 solution for the parameter p in works [8,9] (COM1 is a name authors [8,9] gave for the solution with $p > 0$). In Figure 2 the concentration dependence of chemical potential is given for two values of U. In the same figure a COM1 solution, that we found from equations of paper [8], is presented for two variants of density of states for the bare electron band: a two-dimensional square lattice with nearest-neighbor hopping and a model density

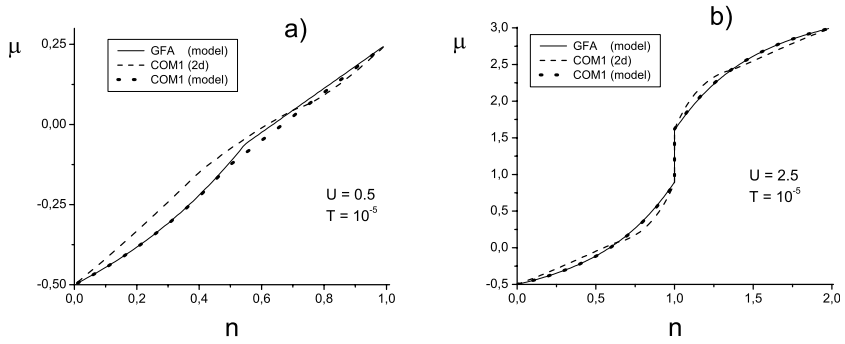

Fig. 2. Chemical potential μ as a function of electron concentration n for two intervals (a) $0 < n < 1$ and (b) $0 < n < 2$.

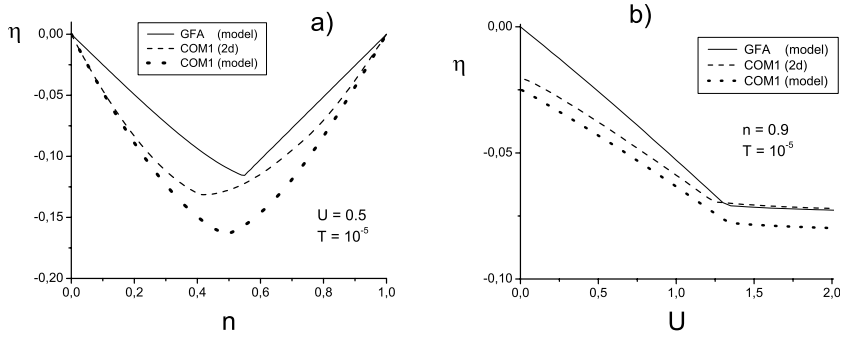

Fig. 3. Parameter η as function of n and U.

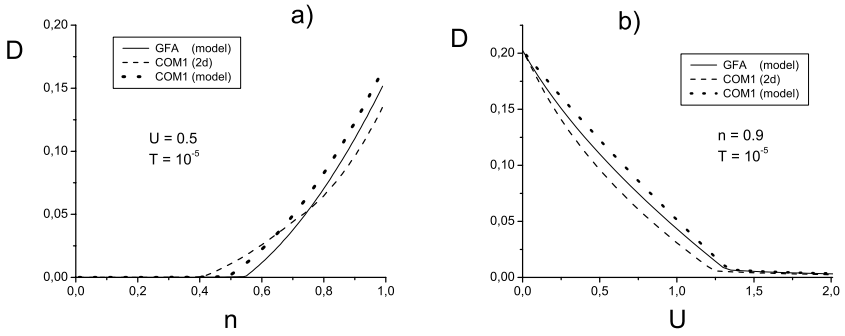

Fig. 4. Parameter $D = \langle n^{\sigma} n^{\bar{\sigma}} \rangle$ of double occupation depending on n and U.

of states of this type:

$$\rho(\varepsilon) = \begin{cases} 1, & |\varepsilon| < W/2 \\ 0, & |\varepsilon| > W/2 \end{cases}. \tag{5.24}$$

We see that COM and our GFA give similar results. The COM1 solution for the 2D-system and for the model density of states are quantitatively very close, and because of this we shall use hereafter for simplicity the model density of states (5.24).

Slightly worse is the comparison of results for η (Fig. 3), however there is a qualitative coincidence of COM1 and GFA calculations. The parameter of double occupation D gives again a satisfactory coincidence of the two approaches (Fig. 4). It is useful to show the dependence of η on n in a whole electron concentration interval at different values of U (Fig. 5). When decreasing U a part of the curve denoted by dash lines approaches to the

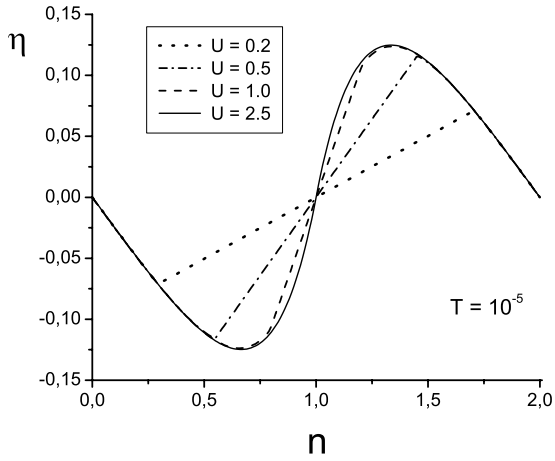

Fig. 5. Dependence of parameter η on n at different values of U.

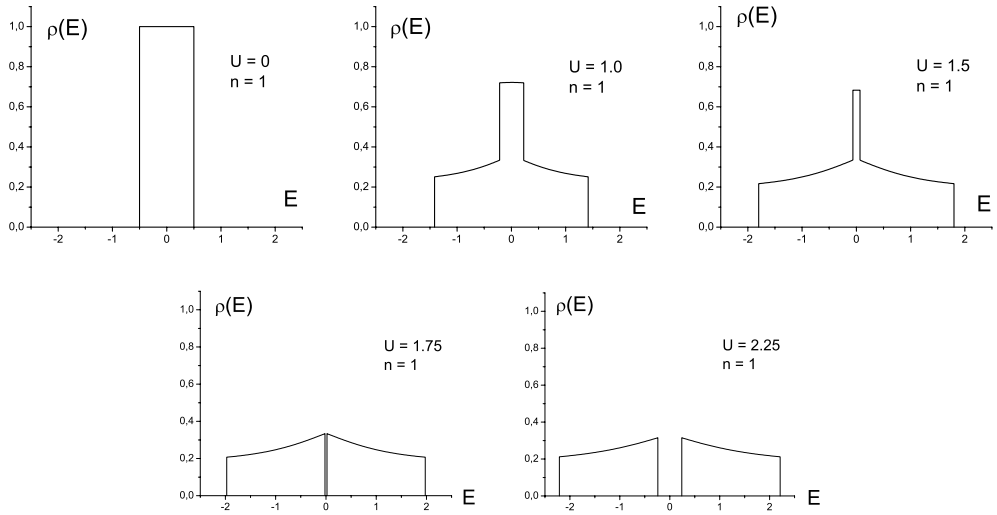

Fig. 6. Evolution of the quasiparticle density of states at half filling depending on U for a model density of states (5.24) in the bare band.

abscess line, and when $U \to 0$ one can see that $\eta \to 0$, as it should be in the case of noninteracting electrons.

Calculations show that when U decreases, the value of the jump of the chemical potential at $n = 1$ decreases too, and at the same critical value $U_c \approx 1.73\,W$ becomes equal to zero. This corresponds to the closing up the two Hubbard subbands, and the insulator-metal phase transition occurs. The evolution of the density of states of the quasiparticle spectrum when U changes is shown for two different bare density of states: the model one (5.24), Figure 6, and the semielliptic one

$$\rho(\varepsilon) = \begin{cases} \frac{4}{\pi W}\sqrt{1-\left(\frac{2\varepsilon}{W}\right)^2} & , \quad |\varepsilon| < W/2 \\ 0 & , \quad |\varepsilon| > W/2 \end{cases}, \qquad (5.25)$$

Figure 7. In COM1 the critical value is $U_c \approx 1.68W$ [8], which is close to our value $U_c \approx 1.73\,W$, obtained for the density of states (5.24).

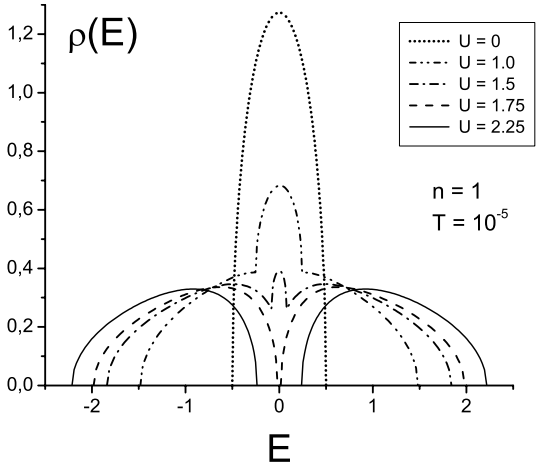

Fig. 7. The same as in Figure 6 but for a semielliptic density of states (5.25).

At half-filling it is easy to get an expression for the gap between the two Hubbard subbands with energies $E_1(\boldsymbol{k})$ and $E_2(\boldsymbol{k})$:

$$\Delta E = -\left(\frac{1}{2}+p_1\right)W + \sqrt{U^2+\left(\frac{1}{2}-p_1\right)^2 W^2}. \quad (5.26)$$

From here follows the critical value U_c, when $\Delta E = 0$. It is equal to

$$U_c = \sqrt{2p_1}\,W, \qquad (5.27)$$

so that when $U > U_c$ the system is an insulator, and when $U < U_c$ a metal.

Compare now the two approaches for the Hubbard model: GFA and COM. The mean field approximations in the framework of these approaches are close to each other both as what regards the GFs structure and physical properties of the model calculated with their help. In both cases the electronic GF has a two-poles structure. The COM approach includes only the parameter p, which has to be found from the equation $\mathcal{G}_{12} = 0$. In the GFA two parameters, (p_1 and p_2), appear, determined through two equations: $\mathcal{G}_{12} = 0$ and $\mathcal{G}_{21} = 0$. Due to this pair of equations one of these parameters can be eliminated, and as a result we have only one parameter, p_1.

The physical meanings of the parameters p and p_1 are close. In the COM approach the parameter p describes the static fluctuation of charge, spin and pair. In GFA the parameter p_1 includes traces of static charge and spin fluctuations as well. Corrections for the self-energy due to dynamical interaction of electrons with bosons in both approaches practically coincide and correspond to SCBA.

The equations for the determination of parameters μ, $\langle n^\sigma\rangle$, η, p_1 in GFA and μ, $\langle n^\sigma\rangle$, Δ, p in COM are rather similar, but have different solutions. In COM at fixed external parameters (n, U, W) one has two solutions: with $p > 0$ and $p < 0$, while in GFA there is only one solution with $p_1 > 0$ (the second parameter p_2 is always negative, but it does not enter in the electronic GF explicitly; but

it only guarantees the satisfaction of the two conditions $\mathcal{G}_{12}=0$ and $\mathcal{G}_{21}=0$, simultaneously). A remarkable conclusion follows from numerical calculations with different sets of external parameters. In spite of some difference in GFA and COM, the calculated quantities of the model are rather close to each other, if in COM only COM1 solutions with $p>0$ are taken into account. The two-poles GF of this approximation can be used farther for the calculation of corrections to the self-energy $\Sigma(\boldsymbol{k},\omega)$ from the dynamical fluctuations [30] and for bosonic GFs (magnon, plasmon, doublon), describing these fluctuations [31].

6 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 the two Bose-like GFs (2.15) and (2.16).

They describe propagation of a spin flip (magnon) and a dyad (doublon), representing the two types of the Bose-like collective modes. These GFs could be represented as the variational derivatives of $Z[V]$ with respect to the fluctuating fields:

$$\mathcal{D}^{\sigma\bar{\sigma}}(12)=-\frac{\delta^2\Phi}{\delta v_1^{\sigma\bar{\sigma}}v_2^{\bar{\sigma}\sigma}}, \tag{6.1}$$

$$\mathcal{D}^{02}(12)=-\frac{\delta^2\Phi}{\delta v_1^{02}v_2^{20}}. \tag{6.2}$$

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:

$$\dot{X}_1^{\sigma\bar{\sigma}}=-(\varepsilon_{\bar{\sigma}}-\varepsilon_{\sigma})X_1^{\sigma\bar{\sigma}}-\Psi^{\dagger}_{\alpha'}(1\sigma)\Im_{\alpha'\beta'}t(11')\Psi_{\beta'}(1'\bar{\sigma}) + \Psi^{\dagger}_{\alpha'}(1'\sigma)t(1'1)\Im_{\alpha'\beta'}\Psi_{\beta'}(1\bar{\sigma}), \tag{6.3}$$

$$\dot{X}_1^{02}=-(U-2\mu)X_1^{02}+\sigma'(\tau^x\Psi)_{\alpha'}(1\bar{\sigma}')\Im_{\alpha'\beta'}t(11')\Psi_{\beta'}(1'\sigma'). \tag{6.4}$$

We see that in the right hand sides of these relations Ψ-operators occur; therefore in the corresponding equations of motions for the magnon and the doublon GFs the T-mixed product of f- and b-operators will appear. They could be represented as the the variational derivative of the electronic 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 feature of the doublon GF is that it includes the "anomalous" electronic GF, composed of the two operators $\Psi(1\sigma)$ and $\Psi(2\bar{\sigma})$, while the equation for the magnon GF should include the normal electronic GF, composed of the operators $\Psi(1\sigma)$ and $\Psi^{\dagger}(2\bar{\sigma})$. By itself these anomalous GFs 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 electronic and bosonic degrees of freedom. Now our task is to determine the equations of motion for the magnon and doublon GFs and to obtain their approximate solution. This will let us determine the spectrum of the corresponding collective modes. In this paper we study only the doublon GF.

Let us derive the equation of motion for the doublon GF (2.21); to this purpose we write the equation of motion for the mean value of the operator X_1^{02}:

$$\frac{\partial}{\partial\tau_1}(\!(TX_1^{02}e^{-V})\!)=(\!(T\dot{X}_1^{02}e^{-V})\!)-(\!(T\{X_1^{02},V\}e^{-V})\!). \tag{6.5}$$

We substitute in it the expression (6.4) for $\dot{X}_1^{02}$, and also the relation

$$\{X_1^{02},V\}=-v_1^{00}X_1^{02}+v_1^{22}X_1^{02}+v_1^{02}(X_1^{00}-X_1^{22}).$$

Then our initial equation could be rewritten in the form:

$$\left(K_{0V}^{02}\right)^{-1}(11')(\!(TX_{1'}^{02}e^{-V})\!)=-v_1^{02}(\!(T(X_1^{22}-X_1^{00})e^{-V})\!) +\sigma' t(11')\Im_{\alpha'\beta'}(\!(T\Psi_{\beta'}(1'\sigma')(\tau^x\Psi)_{\alpha'}(1\bar{\sigma}')e^{-V})\!),$$

where

$$\left(K_{0V}^{02}\right)^{-1}(12)=-\left(\frac{\partial}{\partial\tau_1}+U-2\mu+v_1^{22}-v_1^{00}\right)\delta_{12}. \tag{6.6}$$

Taking into account the definition of the electronic GF we write its last term in the form

$$-Z\sigma'\,\mathrm{Tr}\left[\Im\left(t\mathcal{L}^{12}\right)(1\sigma',1\bar{\sigma}')\right],$$

where

$$\mathcal{L}^{12}_{\alpha\beta}(1\sigma_1,2\sigma_2)=-\langle T\Psi_{\alpha}(1\sigma_1)\Psi_{\beta}(2\sigma_2)\rangle \tag{6.7}$$

is the anomalous component of the electronic GF.

The mean values $(\!(\dots)\!)$ of X operators are expressed through the variational derivative of the functional $\Phi[V]$, and we come to the final form of the equation for the generating functional:

$$\left(K_{0V}^{02}\right)^{-1}(11')\frac{\delta\Phi}{\delta v_{1'}^{02}}=-v_1^{02}\left(\frac{\delta\Phi}{\delta v_1^{22}}-\frac{\delta\Phi}{\delta v_1^{00}}\right) +\sigma'\,\mathrm{Tr}\left[\Im\left(t\mathcal{L}^{12}\right)(1\sigma',1\bar{\sigma}')\right]. \tag{6.8}$$

In the same way it is possible to write the equation for $(\!(TX_1^{20}e^{-V})\!)$ and reduce it to the form

$$\frac{\delta\Phi}{\delta v_{1'}^{20}}\left(K_{0V}^{02}\right)^{-1}(1'1)= -v_1^{20}\left(\frac{\delta\Phi}{\delta v_1^{22}}-\frac{\delta\Phi}{\delta v_1^{00}}\right)+\sigma'\,\mathrm{Tr}\left[\Im\left(\mathcal{L}^{21}t\right)(1\bar{\sigma}',1\sigma')\right]. \tag{6.9}$$

Differentiating now the equation (6.8) with respect to v_2^{20}, and the equation (6.9) with respect to v_2^{02}, we come to the pair of conjugate equations for the doublon GF:

$$\left(K_{0V}^{02}\right)^{-1}(11')\mathcal{D}^{02}(1'2)=(1-n_1)\delta_{12}-\sigma'\frac{\delta}{\delta v_2^{20}} \times\,\mathrm{Tr}\left[\Im\left(t\mathcal{L}^{12}\right)(1\sigma',1\bar{\sigma}')\right]. \tag{6.10}$$

$$\mathcal{D}^{02}(12')\left(K_{0V}^{02}\right)^{-1}(2'2) = (1-n_1)\delta_{12} - \sigma'\frac{\delta}{\delta v_2^{02}} \times \mathrm{Tr}\left[\Im\left(\mathcal{L}^{21}t\right)(2\bar{\sigma}',2\sigma')\right]. \quad (6.11)$$

Here we introduced the number of electrons on the site, $n_1 = n_1^{\sigma} + n_1^{\bar{\sigma}}$, where $n_1^{\sigma} = \langle c_{1\sigma}^{\dagger} c_{1\sigma}\rangle$. We see that the exact equations for the doublon GF contain terms with variational derivatives of anomalous electronic GF with respect to the fields v_1^{02} and v_1^{20}. To obtain a close equation for doublon GF we have to calculate these terms by the same approximate way.

Let us calculate the derivative of off-diagonal (with respect to the upper spinor indexes) electronic GFs $\mathcal{L}^{12}$ and $\mathcal{L}^{21}$. We use the multiplicative representation (3.18). In the normal state we could use the expression for the variational derivative.

$$\frac{\delta\mathcal{L}^{12}(34)}{\delta v_2^{20}} = -L^{11}(33')\frac{\delta\left[L^{-1}(3'4')\right]^{12}}{\delta v_2^{20}} \times \mathcal{L}^{22}(4'4) + L^{11}(33')\frac{\delta\Pi^{12}(3'4)}{\delta v_2^{20}}. \quad (6.12)$$

We take the inverse propagator GF L^{-1} in the approximation, when in the general expression (3.20) the term Σ' is neglected, and Π is taken in the zeroth order approximation. It is easy to obtain the relations:

$$\frac{\delta\left[L_{0V}^{-1}(3\sigma_3,4\sigma_4)\right]^{12}}{\delta v_2^{20}} = \sigma_3\delta_{\bar{\sigma}_3\sigma_4}\delta_{23}\delta_{34}\tau^x,$$

$$\frac{\delta\Pi_0^{12}(3\sigma_3,4\sigma_4)}{\delta v_2^{20}} = -\sigma_3\delta_{\bar{\sigma}_3\sigma_4}\delta_{34}\frac{\delta^2\Phi}{\delta v_3^{02}v_2^{20}}i\tau^y.$$

Then, within the first order approximation with respect to t the equation (6.10) is determined by the expression

$$\frac{\delta\mathcal{L}^{12}(3\sigma_3,4\sigma_4)}{\delta v_2^{20}} = -\sigma_3\delta_{\bar{\sigma}_3\sigma_4}\Big\{G^{\sigma_3}(32)\tau^x\widetilde{\mathcal{G}}^{\bar{\sigma}_3}(24) - G^{\sigma_3}(33')\left[\delta_{3'4}i\tau^y - i\tau^y\Im(\tilde{t}\,\widetilde{\mathcal{G}}^{\bar{\sigma}_3})(3'4)\right]\mathcal{D}^{02}(3'2)\Big\}. \quad (6.13)$$

After substituting this relation into the equation (6.10), we represent equation for the doublon GF in the form

$$\left[\left(K_{0V}^{02}\right)^{-1}(11') - \mathcal{M}_l^{02}(11')\right]\mathcal{D}^{02}(1'2) = (1-n_1)\delta_{12} + \mathcal{P}_l^{02}(12), \quad (6.14)$$

$$\mathcal{P}_l^{02}(12) = \mathrm{Tr}\left[\Im(tG^{\sigma'})(12)\tau^x\widetilde{\mathcal{G}}^{\bar{\sigma}'}(21)\right], \quad (6.15)$$

$$\mathcal{M}_l^{02}(12) = -\mathrm{Tr}\left[\Im(tG^{\sigma'})(12)\left(i\tau^y\delta_{12} - i\tau^y\Im(\tilde{t}\,\widetilde{\mathcal{G}}^{\bar{\sigma}'})(21)\right)\right]. \quad (6.16)$$

The index l of the terminal and the self-energy part indicates the "left" form of the equations for $\mathcal{D}^{02}$. In the same way starting from the equation (6.11), it is possible to come to the "right" form of the equation for $\mathcal{D}^{02}$:

$$\mathcal{D}^{02}(12')\left[\left(K_{0V}^{02}\right)^{-1}(2'2) - \mathcal{M}_r^{02}(2'2)\right] = (1-n_1)\delta_{12} + \mathcal{P}_r^{02}(12), \quad (6.17)$$

$$\mathcal{P}_r^{02}(12) = \mathrm{Tr}\left[\Im\widetilde{G}^{\bar{\sigma}'}(21)\tau^x(\mathcal{G}^{\sigma'}t)(12)\right], \quad (6.18)$$

$$\mathcal{M}_r^{02}(12) = \mathrm{Tr}\left[\Im\widetilde{G}^{\bar{\sigma}'}(21)\left(i\tau^y t_{12} + i\tau^y\Im(t\mathcal{G}^{\sigma'}t)(12)\right)\right]. \quad (6.19)$$

To recover the symmetry of the doublon GF let us symmetrize the equations (6.14) and (6.17) making their sum. Then, the doublon GF is equal to

$$\mathcal{D}^{02}(q) = \frac{(1-n) + \mathcal{P}^{02}(q)}{i\omega_n - (U-2\mu) - \mathcal{M}^{02}(q)}, \quad (6.20)$$

where

$$\mathcal{M}^{02}(q) = \frac{1}{2}\left[\mathcal{M}_l^{02}(q) + \mathcal{M}_r^{02}(q)\right],$$
$$\mathcal{P}^{02}(q) = \frac{1}{2}\left[\mathcal{P}_l^{02}(q) + \mathcal{P}_r^{02}(q)\right].$$

The self-energy and the terminal part are equal to

$$\mathcal{M}^{02}(q) = -\frac{1}{2}\sum_{k\sigma}\varepsilon(\boldsymbol{k})\Big\{\mathrm{Tr}[\Im\,G^{\sigma}(k)\,i\tau^y] - \mathrm{Tr}[\Im\,\widetilde{G}^{\sigma}(k-q)\,i\tau^y]\Big\} + \frac{1}{2}\sum_{k\sigma}\varepsilon(\boldsymbol{k})\Big\{\varepsilon(\boldsymbol{k}-\boldsymbol{q})\mathrm{Tr}[\Im\,G^{\sigma}(k)\,i\tau^y\,\Im\,\widetilde{\mathcal{G}}^{\bar{\sigma}}(k-q)] + \varepsilon(\boldsymbol{k})\mathrm{Tr}[i\tau^y\,\Im\,\mathcal{G}^{\sigma}(k)\,\Im\,\widetilde{G}^{\bar{\sigma}}(k-q)]\Big\}, \quad (6.21)$$

$$\mathcal{P}^{02}(q) = \frac{1}{2}\sum_{k\sigma}\varepsilon(\boldsymbol{k}) \times\Big\{\mathrm{Tr}[\Im\,G^{\sigma}(k)\,\tau^x\,\widetilde{\mathcal{G}}^{\bar{\sigma}}(k-q)] + \mathrm{Tr}[\Im\,\widetilde{G}^{\sigma}(k-q)\,\tau^x\,\mathcal{G}^{\bar{\sigma}}(k)]\Big\}. \quad (6.22)$$

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

$$\mathcal{D}^{20}(q) = \frac{-(1-n) + \mathcal{P}^{20}(q)}{i\omega_n + (U-2\mu) - \mathcal{M}^{20}(q)}, \quad (6.23)$$

where the values $\mathcal{P}^{20}(q)$ and $\mathcal{M}^{20}(q)$ are expressed through $\mathcal{P}^{02}(q)$ and $\mathcal{M}^{02}(q)$:

$$\mathcal{P}^{20}(q) = -\mathcal{P}^{02}(-q),$$
$$\mathcal{M}^{20}(q) = -\mathcal{M}^{02}(-q). \quad (6.24)$$

Thus we see that the condition of symmetry is fulfilled

$$\mathcal{D}^{20}(q) = \mathcal{D}^{02}(-q), \quad (6.25)$$

or $\mathcal{D}^{20}_{12} = \mathcal{D}^{02}_{21}$ in the coordinate space, which follows directly from the definition (6.2) for the doublon GF.

After the computation of the trace in the expressions (6.21) and (6.22), we can represent them in the form:

$$\mathcal{M}^{02}(q) = -\frac{1}{2}\sum_{k\sigma}\varepsilon(\boldsymbol{k})[g^{\sigma}(k) - \widetilde{g}^{\sigma}(k-q)] + \frac{1}{2}\sum_{k\sigma}\varepsilon(\boldsymbol{k})\Bigg[\varepsilon(\boldsymbol{k}-\boldsymbol{q})g^{\sigma}(k)\sum_{\alpha\beta}\widetilde{\mathcal{G}}^{\bar{\sigma}}_{\alpha\beta}(k-q) + \varepsilon(\boldsymbol{k})\widetilde{g}^{\sigma}(k-q)\sum_{\alpha\beta}\mathcal{G}^{\bar{\sigma}}_{\alpha\beta}(k)\Bigg]. \quad (6.26)$$

$$\mathcal{P}^{02}(q) = -\frac{1}{2}\sum_{k\sigma}\varepsilon(\boldsymbol{k}) \times \Big\{[G^{\sigma}_{11}(k) + G^{\sigma}_{21}(k)]\,[\mathcal{G}^{\bar{\sigma}}_{12}(-k+q) + \mathcal{G}^{\bar{\sigma}}_{22}(-k+q)] + [G^{\sigma}_{12}(k) + G^{\sigma}_{22}(k)]\,[\mathcal{G}^{\bar{\sigma}}_{11}(-k+q) + \mathcal{G}^{\bar{\sigma}}_{21}(-k+q)] + [G^{\sigma}_{11}(-k+q) + G^{\sigma}_{12}(-k+q)]\,[\mathcal{G}^{\bar{\sigma}}_{21}(k) + \mathcal{G}^{\bar{\sigma}}_{22}(k)] + [G^{\sigma}_{21}(-k+q) + G^{\sigma}_{22}(-k+q)]\,[\mathcal{G}^{\bar{\sigma}}_{11}(k) + \mathcal{G}^{\bar{\sigma}}_{12}(k)]\Big\}. \quad (6.27)$$

Now we calculate the expression (6.26) in the mean field approximation for the electronic GF. Substituting here the formula (5.3) and summing over frequencies, we write the result as a sum of two contributions of the first and second order with respect to t:

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

where

$$\mathcal{M}^{02}_1(\boldsymbol{q}) = -\frac{U}{2}\sum_{\boldsymbol{k}\sigma}\frac{\varepsilon(\boldsymbol{k}) + \varepsilon(\boldsymbol{k}-\boldsymbol{q})}{2Q^{\sigma}(\boldsymbol{k})}\Big[f\,[E^{\sigma}_1(\boldsymbol{k})] - f\,[E^{\sigma}_2(\boldsymbol{k})]\Big], \quad (6.28)$$

$$\mathcal{M}^{02}_2(q) = \frac{1}{2}\sum_{\boldsymbol{k}\sigma}\varepsilon(\boldsymbol{k}-\boldsymbol{q})\frac{\varepsilon(\boldsymbol{k}) + \varepsilon(\boldsymbol{k}-\boldsymbol{q})}{2Q^{\sigma}(\boldsymbol{k})} \times \sum_{nm}C^{\sigma}_{nm}(\boldsymbol{k},\boldsymbol{k}-\boldsymbol{q}) \times \frac{1 - f\,[E^{\sigma}_n(\boldsymbol{k})] - f\,\big[E^{\bar{\sigma}}_m(\boldsymbol{k}-\boldsymbol{q})\big]}{i\omega_{\nu} - E^{\sigma}_n(\boldsymbol{k}) - E^{\bar{\sigma}}_m(\boldsymbol{k}-\boldsymbol{q})}. \quad (6.29)$$

where $(n, m = 1, 2)$

$$C^{\sigma}_{nm}(\boldsymbol{k},\boldsymbol{k}-\boldsymbol{q}) = [(\mathcal{A}^{\sigma}_n)_{11} - (\mathcal{A}^{\sigma}_n)_{22}](\boldsymbol{k}) \times \Big\{\big[(\mathcal{A}^{\bar{\sigma}}_m)_{11} + (\mathcal{A}^{\bar{\sigma}}_m)_{21}\big](\boldsymbol{k})\big(\Lambda^{\bar{\sigma}}_{11} + \Lambda^{\bar{\sigma}}_{12}\big) + \big[(\mathcal{A}^{\bar{\sigma}}_m)_{12} + (\mathcal{A}^{\bar{\sigma}}_m)_{22}\big](\boldsymbol{k})\big(\Lambda^{\bar{\sigma}}_{21} + \Lambda^{\bar{\sigma}}_{22}\big)\Big\} \quad (6.30)$$

and here $(\mathcal{P}^{\sigma}_m)$, Λ^{σ} are determined by formulas (5.13) and (4.5) Remarkable is the fact that expressions $\mathcal{M}_1$ and $\mathcal{M}_2$ vanish at wave vector $\boldsymbol{Q} = (\pi, \pi, \dots)$. Because $\mathcal{M}^{02}(q)$ is nothing but the self-energy of a doublon, we see from equation (6.23), that at half-filling, when $U - 2\mu = 0$, a doublon is a soft mode in the vicinity of the point $(\pi, \pi, \dots)$. This observation pushes to study its dispersion law and attenuation.

We postpone the study of doublons at arbitrary electron concentration and fix ourselves on the case $n = 1$. We are limited now to the hydrodynamical regime.

7 Dynamical fluctuations in the hydrodynamical regime

It is well known that collective modes in a disordered (symmetrical) phase in the hydrodynamical regime are ruled by the conservation laws [36]. 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 [37–40]. The three pseudospin components

$$P^{+} = \sum_i e^{i\boldsymbol{Q}\cdot\boldsymbol{R}_i}c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}, \quad P^{-} = \sum_i e^{-i\boldsymbol{Q}\cdot\boldsymbol{R}_i}c_{i\downarrow}c_{i\uparrow}, \quad P^{z} = \sum_i \frac{1}{2}(n_i - 1) \quad (7.1)$$

with $\boldsymbol{Q} = (\pi\,\pi\,\dots)$ obey permutation relations

$$[P^{+}, \mathcal{H}] = (2\mu - U)P^{+}, \quad [P^{-}, \mathcal{H}] = -(2\mu - U)P^{-}, \quad [P^{z}, \mathcal{H}] = 0, \quad (7.2)$$

from which it is clear that at 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 $\chi^{02}(\boldsymbol{q}, \omega)$. According to Kubo-Mori theory, this susceptibility is expressed through the memory function $\mathcal{M}^{02}(\boldsymbol{q}, \omega)$ by the relation

$$\chi^{02}(\boldsymbol{q}, \omega) = \langle\langle X^{02}_i \big| X^{20}_j\rangle\rangle_{\boldsymbol{q},\omega} = \frac{M^{02}(\boldsymbol{q}, \omega)}{\omega - \dfrac{M^{02}(\boldsymbol{q}, \omega)}{\chi^{02}_{\boldsymbol{q}}}}, \quad (7.3)$$

where we introduce a notation for the static susceptibility, $\chi^{02}_{\boldsymbol{q}} \equiv \chi^{02}(\boldsymbol{q}, 0)$.

On the other hand the memory function is expressed through the irreducible retarded GF of pseudospin currents (see [41]):

$$M^{02}(\boldsymbol{q}, \omega) = -\sum_{ij}e^{-i\boldsymbol{q}\boldsymbol{R}_{ij}}\int_{-\infty}^{+\infty}\frac{d\omega'}{\pi}\,\frac{\mathrm{Im}\langle\langle i\dot{X}^{02}_i \big| -i\dot{X}^{20}_j\rangle\rangle^{irr}_{\omega'}}{\omega'(\omega - \omega' + i\delta)}. \quad (7.4)$$

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

$$i\dot{X}^{02}_i = [X^{02}_i, \mathcal{H}] = (U - 2\mu)X^{02}_i - \sigma'(\tau^{x}\Psi)_{\alpha'}(i\bar{\sigma}')(\hat{t}\Psi)_{\alpha'}(i\sigma'). \quad (7.5)$$

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

$$\langle\langle i\dot{X}_i^{02}(t)\big|-i\dot{X}_j^{20}(0)\rangle\rangle^{irr} = \langle\langle(\tau^x\Psi)_{\alpha'}(i\bar{\sigma}',t)(\hat{t}\Psi)_{\alpha'}(i\sigma',t)\big|(\Psi^+\hat{t})_{\beta'}(j\sigma')(\Psi^+\tau^x)_{\beta'}(j\bar{\sigma}')\rangle\rangle^{irr} - \langle\langle(\tau^x\Psi)_{\alpha'}(i\bar{\sigma}',t)(\hat{t}\Psi)_{\alpha'}(i\sigma',t)\big|(\Psi^+\hat{t})_{\beta'}(j\bar{\sigma}')(\Psi^+\tau^x)_{\beta'}(j\sigma')\rangle\rangle^{irr}. \tag{7.6}$$

Now we use the approximation of interacting modes, well known in the relaxation theory, by Mori [42]: the two-particle electron correlations in expression (7.6) are decomposed into pair correlators and then expressed through the imaginary parts of the retarded electron GFs. As a result we come to the following expression, determining the memory function:

$$M^{02}(\boldsymbol{q},\omega) = 2\sum_{\boldsymbol{k}}\big[\varepsilon(\boldsymbol{k}) + \varepsilon(\boldsymbol{k}-\boldsymbol{q})\big]^2 \times \int d\omega' \int d\omega_1 \big[f(\omega_1-\omega') - f(\omega_1)\big] \times \frac{\mathrm{tr}\big\{[\mathrm{Im}\mathcal{G}^{\bar{\sigma}'}(\boldsymbol{q}-\boldsymbol{k},\omega'-\omega_1)][\mathrm{Im}(\Im\mathcal{G}^{T\sigma'}(\boldsymbol{k},\omega_1)\Im)]\big\}}{\omega'(\omega-\omega'+i\delta)}. \tag{7.7}$$

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

Expression (7.7) is similar to those obtained in the interacting modes approximation for other dynamical susceptibilities. For example, the spin susceptibility is:

$$\chi^{\sigma\bar{\sigma}}(\boldsymbol{q},\omega) = \langle\langle X_i^{\sigma\bar{\sigma}}\big|X_j^{\bar{\sigma}\sigma}\rangle\rangle_{\boldsymbol{q},\omega} = -\frac{M^{\sigma\bar{\sigma}}(\boldsymbol{q},\omega)}{\omega - \dfrac{M^{\sigma\bar{\sigma}}(\boldsymbol{q},\omega)}{\chi_{\boldsymbol{q}}^{\sigma\bar{\sigma}}}}. \tag{7.8}$$

By similar decoupling of the irreducible GFs of the currents we obtain:

$$M^{\sigma\bar{\sigma}}(\boldsymbol{q},\omega) = 4\sum_{\boldsymbol{k}}\big[\varepsilon(\boldsymbol{k}) - \varepsilon(\boldsymbol{k}-\boldsymbol{q})\big]^2 \times \int d\omega' \int d\omega_1 \big[f(\omega_1-\omega') - f(\omega_1)\big] \times \frac{\mathrm{tr}\big\{[\mathrm{Im}\mathcal{G}^{\sigma}(\boldsymbol{k}-\boldsymbol{q},\omega_1-\omega')][\mathrm{Im}(\Im\mathcal{G}^{\bar{\sigma}}\Im)(\boldsymbol{k},\omega]\big\}}{\omega'(\omega-\omega'+i\delta)}. \tag{7.9}$$

It is remarkable that the memory GF for the spin susceptibility vanishes at $\boldsymbol{q} = 0$, while for the doublon susceptibility it vanishes at $\boldsymbol{q} = \boldsymbol{Q}$. This difference originates from the total spin conservation law (Fourier component of the spin density at $\boldsymbol{q} = 0$), while the component of the pseudospin density is conserved at $\boldsymbol{q} = \boldsymbol{Q}$ and only for half-filling. There is another important difference in expressions (7.7) and (7.9). 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 (doublone) is formed through excitations of two particles (or two holes).

Consider now the hydrodynamical limit corresponding to small frequencies ω and small wave point $\boldsymbol{q}$ (for expression (7.7)). In the hydrodynamical limit $\omega \ll vq$, where v is a characteristic electron velocity on the Fermi surface. Under these conditions from equations (7.7) and (7.9) the asymptotic expressions follow:

$$\mathrm{Im}\mathcal{M}^{02}(\boldsymbol{q},\omega) = -D^{02}p^2, \qquad \mathrm{Re}\mathcal{M}^{02}(\boldsymbol{q},\omega) = 0, \tag{7.10}$$

$$\mathrm{Im}\mathcal{M}^{\sigma\bar{\sigma}}(\boldsymbol{q},\omega) = -D^{\sigma\bar{\sigma}}q^2, \qquad \mathrm{Re}\mathcal{M}^{\sigma\bar{\sigma}}(\boldsymbol{q},\omega) = 0, \tag{7.11}$$

where the coefficients of spin and pseudospin stiffness are equal

$$D^{02} = 2\pi\sum_{\boldsymbol{k}}\big(v(\boldsymbol{k})\boldsymbol{e}\big)^2 \int d\omega_1 f'(\omega_1) \times \mathrm{tr}\Big\{\mathrm{Im}\mathcal{G}^{\bar{\sigma}'}(-\boldsymbol{k},-\omega_1)\mathrm{Im}\big[\Im\mathcal{G}^{T\sigma'}(\boldsymbol{k},\omega_1)\Im\big]\Big\}, \tag{7.12}$$

$$D^{\sigma\bar{\sigma}} = 4\pi\sum_{\boldsymbol{k}}\big(v(\boldsymbol{k})\boldsymbol{e}\big)^2 \int d\omega_1 f'(\omega_1) \times \mathrm{tr}\Big\{\mathrm{Im}\mathcal{G}^{\sigma}(\boldsymbol{k},\omega_1)\mathrm{Im}\big[\Im\mathcal{G}^{\bar{\sigma}}(\boldsymbol{k},\omega_1)\Im\big]\Big\}. \tag{7.13}$$

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

Expression (7.13) is valid at arbitrary U; in the case of $U \gg W$ it is consistent with the result of [41] for the tJ-model.

Notice that if we use the electron GF in the mean field approximation (without attenuation of quasiparticles) both expressions (7.12) and (7.13) 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 (7.7) and (7.9) for the memory function give in the hydrodynamical limit correct asymptotic values, therefore the susceptibilities have the diffusion form, which is

$$\frac{1}{\omega}\mathrm{Im}\chi(\boldsymbol{q},\omega) = \chi_{\boldsymbol{q}}\frac{\widetilde{D}q^2}{\omega^2 + \big(\widetilde{D}q^2\big)^2}, \tag{7.14}$$

where $\widetilde{D} = D/\chi_{\boldsymbol{q}}$.

8 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 electronic correlations $U > W$. We have derived the exact equation for the electronic GF in terms of the variational derivatives with respect to the fluctuating fields $v^{\sigma\sigma'}$, $v^{\sigma\bar{\sigma}}$, v^{20} coupled with the spin and charge densities. The electronic GFs represent generally an 8×8 matrix with respect to

the three discrete indexes σ, α, ν. In the matrix representation the equation has the same structure with the GF for the Hubbard model in the limit $U \to \infty$, for the tJ- and sd-models and for the GFs of the transverse spin components in the Heisenberg model as well.

The electronic 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. From the equation for $\mathcal{G}$, a pair of equations with variational derivatives for Σ and Λ follow. Their iteration generates a power series in the parameter W/U. This corresponds to the perturbation theory close to the atomic limit. The iteration corrections of the first two orders allow to formulate a mean field approximation essentially equivalent to that of COM.

Taking the electronic 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 electronic 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 $n \to 1$, $U - 2\mu \to 0$. The investigation of the special case $n = 1$ reveals that a soft mode with $\boldsymbol{Q} = (\pi, \pi, \dots)$ may exist. However at $\boldsymbol{Q} = (\pi, \pi, \dots)$ the paramagnetic phase of the Hubbard model has an instability to antiferromagnetic ordering. It means that two possible instabilities – doublon and magnon ones – should compete, and a final result concurring a type of ordering at half filling demands a farther investigations. It will be a subject of next study.

The other direction is to investigate magnetically ordered states. We should go out of the scope of the mean field approximation and take into account the second order correction Σ_2, including the interaction of electrons with magnons. The preliminary analysis reveals that it contains a singular Kondo-like term $\sim \ln \mid \omega - E_F \mid$, which, as it has been pointed out in the works [43][44], leads to a stable ferromagnetism. After the extraction of the relevant term in the second order correction we could write a more exact equation for the magnon GF and calculate the spin-wave spectrum. All of this will form the subject of a next paper.

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Appendix A

Equation of motion for an arbitrary Green's function

Consider an average of an arbitrary T-product of the operators A_1, B_2, C_3, D_4,... (it could be X operators, spin operators or other), taken in the Heiseberg representation:

$$A_1 \equiv \mathrm{e}^{\mathcal{H}\tau} A_{i_1} \mathrm{e}^{-\mathcal{H}\tau}, \qquad 1 = \{i_1, \tau_1\}, \tag{A.1}$$

and so on. Then the following identity is valid:

$$\begin{aligned}\frac{\partial}{\partial\tau_1}(\!(TA_1B_2C_3D_4\dots\mathrm{e}^{-V})\!) &= (\!(T\dot{A}_1B_2C_3D_4\dots\mathrm{e}^{-V})\!)\\ &+ (\!(T\{A_1,B_2\}C_3D_4\dots\mathrm{e}^{-V})\!)\\ &+ (\!(T\{A_1,C_3\}B_2D_4\dots\mathrm{e}^{-V})\!) + \dots\\ &- (\!(T\{A_1,V\}B_2C_3D_4\dots\mathrm{e}^{-V})\!).\end{aligned} \tag{A.2}$$

Here the average over the Gibbs statistical ensemble is denoted by

$$(\!(T\dots\mathrm{e}^{-V})\!) \equiv \mathrm{Tr}\{\mathrm{e}^{-\beta\mathcal{H}}T\dots\mathrm{e}^{-V}\}. \tag{A.3}$$

The relation (A.2) represents the result of the differentiation of the initial average with respect to the time τ_1 ascribed to the operator A_1. In the right hand side of the relation (A.1) $\dot{A}_1$ represents the time derivative

$$\dot{A}_1 = -[A_1, \mathcal{H}]. \tag{A.4}$$

The curl brackets of the kind $\{A_1, B_2\}$ mean

$$\{A_1, B_2\} = \delta(\tau_1 - \tau_2)[A_{i_1}, B_{i_2}]_{\pm}(\tau_1), \tag{A.5}$$

where $[\dots,\dots]_{\pm}$ is an anticommutator or a commutator depending on the kind of the A and B operators. The signs of the terms in the second line of equation (A.2) are determined by the signs of the transpositions of f-operators in the T-product from their original place to the second one in the energy term. In the last term of equation (A.2) the expression $\{A_1, V\}$ is a commutator because the operator V is implied to be boson-like. Formally this term and the first one could be merged and $\mathcal{H} + V$ may be considered in a sense as the Hamiltonian of a system immersed in fluctuating fields.

The identity (A.2) could be proved by differentiating the T-product expressed through the $\theta(\tau - \tau')$ functions and the expansion of the exponent e^{-V} in a series, with subsequent recollection of all the terms back to the exponent. This identity serves as a basis for the derivation of the GFs in the fluctuating fields, defined as

$$\langle TA_1B_2\dots\mathrm{e}^{-V}\rangle_V = \frac{(\!(TA_1B_2\dots\mathrm{e}^{-V})\!)}{(\!(T\mathrm{e}^{-V})\!)}, \tag{A.6}$$

where $(\!(T\mathrm{e}^{-V})\!) = Z[V]$ is the generating functional.

Appendix B

Expansion of self-energy and terminal part of the electronic Green's function

The normal GF $\mathcal{G}(12)$ can be represented in a multiplicative form similar to that of (3.18) for the whole GF, namely

$$\mathcal{G}(\mathbf{12}) = G(\mathbf{11'})\Lambda(\mathbf{1'2}) \tag{B.1}$$

where bold indexes mean $\mathbf{1} = \{1, \alpha, \sigma_1\}$. Thus quantities $\mathcal{G}$, G, Λ and Σ' (determined by Dyson equation (4.3)) are 2×2 matrices with respect to the spinor index α.

We find the equations for Λ and Σ from the general matrix equations (3.21) and (3.22) by writing down the equation for the matrix element Σ'^{11}:

$$\begin{aligned}\Sigma'^{11}(\mathbf{12}) = &- \Big[(\hat{t}L^{11})(\mathbf{4'3'})\hat{A}^{11}(\mathbf{14'}) - (\hat{\tilde{t}}L^{21})(\mathbf{4'3'})\hat{A}^{12}(\mathbf{14'})\Big] \\ &\quad \cdot \Big[\big(L_{0V}^{-1}\big)^{11}(\mathbf{3'2}) - \Sigma'^{11}(\mathbf{3'2})\Big] \\ &- \Big[(\hat{t}L^{12})(\mathbf{4'3'})\hat{A}^{11}(\mathbf{14'}) - (\hat{\tilde{t}}L^{22})(\mathbf{4'3'})\hat{A}^{12}(\mathbf{14'})\Big] \\ &\quad \cdot \Big[\big(L_{0V}^{-1}\big)^{21}(\mathbf{3'2}) - \Sigma'^{21}(\mathbf{3'2})\Big] \quad \text{(B.2)}\end{aligned}$$

$$\begin{aligned}\Sigma'^{21}(\mathbf{12}) = &- \Big[(\hat{t}L^{11})(\mathbf{4'3'})\hat{A}^{21}(\mathbf{14'}) - (\hat{\tilde{t}}L^{21})(\mathbf{4'3'})\hat{A}^{22}(\mathbf{14'})\Big] \\ &\quad \cdot \Big[\big(L_{0V}^{-1}\big)^{11}(\mathbf{3'2}) - \Sigma'^{11}(\mathbf{3'2})\Big] \\ &- \Big[(\hat{t}L^{12})(\mathbf{4'3'})\hat{A}^{21}(\mathbf{14'}) - (\hat{\tilde{t}}L^{22})(\mathbf{4'3'})\hat{A}^{22}(\mathbf{14'})\Big] \\ &\quad \cdot \Big[\big(L_{0V}^{-1}\big)^{21}(\mathbf{3'2}) - \Sigma'^{21}(\mathbf{3'2})\Big]. \quad \text{(B.3)}\end{aligned}$$

For the normal phase, matrix elements $L^{12} = L^{21} = 0$, however the derivatives of them with respect to the fields v^{02} and v^{20} should not vanish, therefore in equations (B.2) and (B.3) we must keep such derivatives.

In the first order in $\hat{t}$ equations (B.2) and (B.3) lead respectively to an equation for the self-energy of the normal GF ($\Sigma'^{11} \equiv \Sigma'$). Matrix operators $\hat{A}^{11}$ and $\hat{A}^{12}$ include the derivatives with respect to fluctuating fields which act on $(L_{0V}^{-1})^{11}$ and $(L_{0V}^{-1})^{12}$, and therefore we come to the expression:

$$\begin{aligned}\Sigma'_1(1\sigma,2\sigma) \equiv \Sigma'^{\sigma}_1(12) &= -\delta_{12}\Big[(\tau^z\hat{t}G)(1\bar{\sigma},2\bar{\sigma}) + (i\tau^y\hat{\tilde{t}}\widetilde{G}\tau^x)(1\bar{\sigma},2\bar{\sigma})\Big] \\ &= -\delta_{12}\Big[(tG^{\bar{\sigma}}_{11})(11) - (tG^{\bar{\sigma}}_{22})(11)\Big]\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}.\end{aligned} \quad \text{(B.4)}$$

Here in the last line we have used a more concise definition of $G = G^{\sigma}$, and also made use of the expression for the transposed matrix

$$\widetilde{G}(12) = -G(21). \quad \text{(B.5)}$$

The calculation of second order contribution in the uncutable part Σ'_2 demands much more efforts, but it involves nothing else then standard and straightforward iterations of equations (B.2) and (B.3). We present the final result:

$$\Sigma'^{\sigma}_2(12) = -\sum_{\sigma'}(tg^{\sigma'})(12)\begin{pmatrix} B_1^{\bar{\sigma}\bar{\sigma}'}(21) & B_2^{\bar{\sigma}\bar{\sigma}'}(21) \\ -B_1^{\bar{\sigma}\bar{\sigma}'}(21) & -B_2^{\bar{\sigma}\bar{\sigma}'}(21)\end{pmatrix}, \quad \text{(B.6)}$$

where

$$\left.\begin{aligned}B_1^{\sigma\sigma'}(21) &= (\hat{t}G^{\sigma}_{11})(21)G^{\sigma'}_{11}(12) - G^{\sigma}_{22}(21)(G^{\sigma'}_{22}\hat{t})(12)\\ B_2^{\sigma\sigma'}(21) &= (\hat{t}G^{\sigma}_{22})(21)G^{\sigma'}_{22}(12) - G^{\sigma}_{11}(21)(G^{\sigma'}_{11}\hat{t})(12)\end{aligned}\right\}. \quad \text{(B.7)}$$

In a similar way we calculate the terminal part Λ of the electronic GF. Firstly we write down the expression for a matrix element $\Pi^{11} \equiv \Lambda$ from equation (3.29). This element is coupled with the off-diagonal element Π^{21}. We have the following pair of coupled equations

$$\begin{aligned}\Lambda(\mathbf{12}) = &(\hat{A}^{11}\Phi)(\mathbf{12}) \\ &+ \Big[(\hat{t}L^{11})(\mathbf{4'3'})\hat{A}^{11}(\mathbf{14'}) - (\hat{\tilde{t}}L^{21})(\mathbf{4'3'})\hat{A}^{12}(\mathbf{14'})\Big]\Lambda(\mathbf{3'2}) \\ &+ \Big[(\hat{t}L^{12})(\mathbf{4'3'})\hat{A}^{11}(\mathbf{14'}) - (\hat{\tilde{t}}L^{22})(\mathbf{4'3'})\hat{A}^{12}(\mathbf{14'})\Big]\Pi^{21}(\mathbf{3'2}),\end{aligned} \quad \text{(B.8)}$$

$$\begin{aligned}\Pi^{21}(\mathbf{12}) = &(\hat{A}^{21}\Phi)(\mathbf{12}) \\ &+ \Big[(\hat{t}L^{11})(\mathbf{4'3'})\hat{A}^{21}(\mathbf{14'}) - (\hat{\tilde{t}}L^{21})(\mathbf{4'3'})\hat{A}^{22}(\mathbf{14'})\Big]\Lambda(\mathbf{3'2}) \\ &+ \Big[(\hat{t}L^{12})(\mathbf{4'3'})\hat{A}^{21}(\mathbf{14'}) - (\hat{\tilde{t}}L^{22})(\mathbf{4'3'})\hat{A}^{22}(\mathbf{14'})\Big]\Pi^{21}(\mathbf{3'2}).\end{aligned} \quad \text{(B.9)}$$

From here we find the zeroth order expressions for Π^{11} and Π^{21}

$$\Lambda_0(1\sigma_1,2\sigma_2) = \delta_{12}\big(\hat{a}_1(\sigma_1\sigma_2)\Phi\big), \quad \text{(B.10)}$$

$$\Pi_0^{21}(1\sigma_1,2\sigma_2) = -\delta_{12}\sigma_1(i\tau^y)\frac{\delta\Phi}{\delta v_1^{20}}. \quad \text{(B.11)}$$

Substituting these expressions in equations (B.8) and (B.9) leads to the first order correction for the terminal part:

$$\begin{aligned}\Lambda_1(1\sigma,2\sigma) = &(\tau^z\hat{t}G\tau^z)(1\sigma,2\sigma)\langle Tn_2^{\bar{\sigma}}n_1^{\bar{\sigma}}\rangle_c \\ &+ (\tau^z\hat{t}G\tau^z)(1\bar{\sigma},2\bar{\sigma})\langle TX_2^{\sigma\bar{\sigma}}X_1^{\bar{\sigma}\sigma}\rangle \\ &+ (i\tau^y\hat{\tilde{t}}\widetilde{G}i\tau^y)(1\bar{\sigma},2\bar{\sigma})\langle TX_2^{02}X_1^{20}\rangle,\end{aligned} \quad \text{(B.12)}$$

which includes bosonic GFs determined by definitions (2.19)–(2.21).

Fourier transformations of expressions (B.4), (B.6), (B.10) and (B.12) give the final results for the self-energy and the terminal part of the electronic GF. They are given by formulas (4.10), (4.12), (4.5) and (4.7), respectively.

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