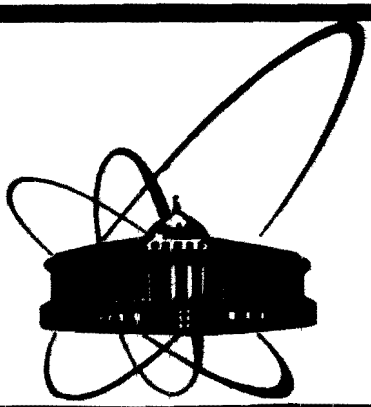

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CORRELATION EFFECTS IN THE EXTENDED HUBBARD MODEL

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INTRODUCTION

Up to the present, in papers concerning the investigation of the many-body effects within the Hubbard model, much attention has been paid to models with only interatomic integral U. Nevertheless, the intersite interactions may be important to the same degree as the intrasite interactions, especially if we take into consideration lattices with a relatively great number of the nearest-neighbours. Usually in models describing electrons in a single tight-binding band, electrons of an opposite spin interact by an on-site Coulomb repulsion and by nearest-neighbour sites Coulomb repulsion - it is the so-called extended Hubbard model. Hamiltonians with intersite interactions included have been investigated by a great number of authors and interesting results were obtained for these models. The importance of inter-site repulsion terms was soon realized, especially in attempts to describe metal-insulator transition in transition metal oxides [1]. Using the Green's function method R.Kishore and S.K.Joshi [2] have found that one band splits into three bands where the middle band occurs only upon introducing the interatomic Coulomb interactions. Their conclusions show that these interatomic correlations may be important for explaining the magnetic properties of transition metals. D.K.Ghosh [3] has computed the internal energy, chemical potential and a critical temperature corresponding to a nearest-neighbour Coulomb repulsion of electrons of opposite spins by means of Green's function method. R.A.Bari [4] has investigated the role of an electron-lattice interaction in a very narrow half-filled band on the basis of a Hamiltonian in which an electron part contains a term corresponding to interatomic Coulomb interactions. He was able to show the existence of the phase-transition to the insulating state characterized by a charge-density wave. The extended Hubbard Hamiltonian has also been investigated by B.Albani et al. [5] by functional integral methods in the context of generalized susceptibilities and phase transitions from the paramagnetic phase to ferromagnetic, antiferromagnetic or charge ordered phases. Their conclusion consists in that the extension of the Hubbard Hamiltinian by

including the interatomic Coulomb interactions permits one to obtain a long-range-ordered phase already in a simple approximation. Recently, an extended Hubbard model has also been analyzed for $U < 0$ in a series of papers [6,7,8], when U is thought of as an effective parameter taking into account either the interactions with phonon, or the coupling between electrons and intramolecular vibrations, or electronic excited states.

In recent years much attention has been paid to the theory of correlation effects in transition metals. The treatment of d-electrons in these metals faces serious preblems. We know that, for example, from photoemission spectra or magnetotransport experiments those electrons have to be described as delocalized band states, but at the same time we have at hand experiments which indicate rather an atomlike behaviour (existence of spin waves above T_c, and so on). A great number of papers has been devoted to the effect of the electron correlation on the magnetic properties of transition metals using the one-band Hubbard model, two-band or many band models within T-matrix approximation, a random phase approximation or irreducible Green's function methods [9,10,11,12]. J.Kanamori used T-matrix approximation in his investigation of the Hubbard model but did not obtain the effective exchange parameter $I(\vec{q})$ in the $\vec{q}$ -dependent static susceptibility as obtained by Lowde et al. [13] from the neutron scattering data for nickel. Only after the inclusion of interatomic interactions, the matrix element of the electron interaction becomes momentum-dependent as was obtained in works of E.Haga et al. [14,15] and T.Kato et al. [16]. The authors show, that the comparison with the experimental behaviour of $I(\vec{q})$ leads to the conclusion that the exchange interatomic interaction gives the contribution of about thirty percent to $I(0)$. The importance of interatomic interactions on the valence-band photoemission in Ni was also investigated by T.Aisaka et al. [17-20]. Especially, from several points of views, Ni is the case for which the many-electron correlation effect cannot be ignored. The experiments of the valence-band photoemission in Ni have shown that the bandwidth is narrower by about 30% than that given by the standard one-electron calculation and satellite peak exists about 6 eV below the Fermi level. By the including into consideration the interatomic interactions T.Aisaka et al. [17-20] have succeeded in affering the explanation for both the degree of the band narrowing and the position of the satellite peak. The problem of renormalization of the band width by the interatomic interactions was also investigated by E.Heiner and J.Schneider [21].

In this paper we consider the effect of the most important class of interatomic interactions on the electronic properties

of the model Hamiltonian of the metal, especially on the electron self-energy. In the following we use the equation of motion method for a retarded Green function introduced by D.N.Zubariev [22]. But in contrast with the ordinary equation of motion, we introduce the self-energy operator and as a consequence obtained the Dyson-type equation for Green's function in the spirit of the method proposed by N.M.Plakida [23] and M.Ichiyanagi [24]. From a formal point of view this method may be thought as a combination of the projection operator method as the so-called irreducible Green's function method of N.M.Plakida [23]. In order to give a simple and transparent picture of the electronic correlation in transition metals, some approximations have to be made. First of all, we will assume that the metal can be described by one-band Hamiltonian but with inter-site Coulomb interaction included. We expect this model to be a reasonable qualitative description of 3d-series ferromagnetic transition metals. Secondly, in order to continue the calculations as far as possible we make a rather drastic approximation within the self-energy operator. This enables us to calculate the Green function and self-energy in a closed form.

The organization of the present paper is as follows. In the next section we introduce the model Hamiltonian. In Sec.3 we present the derivation of the Dyson equation for the Green function within a formalism of the equation of motion method connected with the projection operator method. In Sect.4 we present the electronic states in the mean-field approximation and expression for an electron self-energy.

2. THE HAMILTONIAN OF THE MODEL

The major feature of the Hubbard Hamiltonians is its explicit treatment of the one-site interaction U between electrons in the same band. Interband and intersite interactions do not appear explicitly and may enter only through the Hartree-Fock field. As has been mentioned in the Introduction we shall consider a model one-band Hamiltonian with the intersite Coulomb and exchange integrals explicitly included. This Hamiltonian may be written most generally in the tight-binding model as

$$H = \sum_{ij\sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma} + \frac{1}{2} \sum_{ijk\ell\sigma\sigma'} \langle ij|\frac{1}{r}|k\ell\rangle a^{+}_{i\sigma} a^{+}_{j\sigma'} a_{k\sigma'} a_{\ell\sigma} \quad , \qquad (1)$$

where $|i\rangle$ is a Wannier function at the i-th site $\Phi(\vec{r} - \vec{R}_i)$

$$\langle ij|\frac{1}{r}|k\ell\rangle = \iint d\vec{r}\,d\vec{r}\,'\Phi^*(\vec{r}-\vec{R}_i)\Phi^*(\vec{r}\,'-\vec{R}_j)\frac{1}{|\vec{r}-\vec{r}\,'|}\Phi(\vec{r}\,'-\vec{R}_k)\Phi(\vec{r}-\vec{R}_\ell), \tag{2}$$

$$t_{ij} = \int d\vec{r}\,\Phi^*(\vec{r}-\vec{R}_i)[\frac{p^2}{2m} + V(\vec{r})]\Phi(\vec{r}-\vec{R}_i)d\vec{r}, \tag{3}$$

and $V(\vec{r})$ is the effective potential composed of the ionic potentials of single atoms.

As a next step we retain in the Hamiltonian (1) only contributions coming from a one-centre and two-centre integrals of various kinds. Let us introduce the abbreviations for these integrals as follows:

$$\langle ii|\frac{1}{r}|ii\rangle \equiv U, \qquad \langle ij|\frac{1}{r}|ji\rangle \equiv U'_{ij} \tag{4a}$$

$$\langle ij|\frac{1}{r}|ij\rangle \equiv I'_{ij}, \qquad \langle ii|\frac{1}{r}|jj\rangle \equiv I''_{ij}, \tag{4b}$$

where relations (4a) correspond to the direct on-site and intersite Coulomb integrals and relations (4b) correspond to the exchange Coulomb interactions.

The Hamiltonian defined by Eq.(1) now takes the following form:

$$H = \sum_{ij\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} + \frac{1}{2}U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + \frac{1}{2}\sum_{ij\sigma}(1-\delta_{ij})(U'_{ij}-I'_{ij})n_{i\sigma}n_{j\sigma} +$$

$$+ \frac{1}{2}\sum_{ij\sigma}(1-\delta_{ij})U'_{ij}\,n_{i\sigma}n_{j-\sigma} + \frac{1}{2}\sum_{ij\sigma}(1-\delta_{ij})I''_{ij}\,a^+_{i\sigma}a^+_{i-\sigma}a_{j-\sigma}a_{j\sigma}; \tag{5}$$

where we omitted the intersite exchange interactions with $\sigma = -\sigma'$, called spin-flip terms [25], and where $I'_{ij} = I''_{ij}$ for working with a real Wannier functions. In addition to the intrasite Coulomb interaction U which is the only interaction present in the Hubbard model, the Hamiltonian given by Eq.(5) contains three more intersite interactions, namely the intersite Coulomb and intersite exchange interactions. As has been mentioned in Hubbard's paper [11], especially term with U'_{ij} can be very important in describing the correlation effects in metals. If we consider only the short-range interactions such as $\langle ij|\frac{1}{r}|k\ell\rangle = U\,\delta_{ij}\,\delta_{k\ell}\,\delta_{i\ell}$, the Hamiltonian (5) just reduces to the form of the Hubbard Hamiltonian.

3. THE DYSON EQUATION FOR THE ONE-ELECTRON TWO-TIME GREEN FUNCTIONS

In the following, we consider the so-called band limit, i.e. $U/W \ll 1$, W - the band width, and for that reason it is convenient to work with the two-time Green functions defined by [22]:

$$G^\sigma_{ij}(t-t') = \langle\langle a_{i\sigma}(t); a^+_{j\sigma}(t')\rangle\rangle = -i\theta(t-t')\langle[a_{i\sigma}(t), a^+_{j\sigma}(t')]_+\rangle, \tag{6}$$

where $\theta(t)$ is the step function, unity for positive and zero for negative value of time, $\langle\ldots\rangle$ denote an average with respect to the canonical density matrix of the system described by time-independent Hamiltonian (5) and temperature T:

$$\langle A\rangle = Z^{-1}\,\mathrm{Tr}\,e^{-\beta H}A, \qquad Z = \mathrm{Tr}\,e^{-\beta H}, \qquad \beta = 1/k_B T,$$
$$A(t) = e^{iHt}\,A\,e^{-iHt}. \tag{7}$$

In practice it is convenient to work with the Fourier transform of the Green function $G^\sigma_{ij}(t)$ with respect to the energy E:

$$\langle\langle a_{i\sigma}|a^+_{j\sigma}\rangle\rangle_{E^+} \equiv G^\sigma_{ij}(E) = \int_{-\infty}^{+\infty} e^{-iE^+t}\,G^\sigma_{ij}(t)\,dt, \quad E^+ = E + iO, \tag{8}$$

for which we obtain equation of motion in the form:

$$E\,G^\sigma_{ij}(E) = \langle[a_{i\sigma}, a^+_{j\sigma}]_+\rangle + \langle\langle ia_{i\sigma}|a^+_{j\sigma}\rangle\rangle. \tag{9}$$

The righ-hand side of Eq.(9) contains higher-order Green functions and now we could go further and write the latter Green functions again in terms of higher ones, and generally speaking we would obtain a sequence of coupled equations. In order to obtain an approximate solution one tries to truncate this system of equations at a certain level by decoupling the higher-order Green functions into the lower-order ones. In practice it is rather difficult to make such a decoupling and this decoupling process is of course an approximation, the meaning of which is not immediately transparent. For these reasons, the equation of motion method for the two-time Green functions has been generally criticized for being based on weakly defined decoupling schemes and thus producing ambiguous results [26]. Despite of these difficulties, a great number of papers appeared in which the method of equations for Green's functions was

applied and decoupling process at various stages of the hierarchy of equations was done. Taking into consideration the discussion given above, there are methods in which one is trying to obtain Dyson-type equations for Green's function in an exact way. For example applying the projection operator method Yu.A.Tsercovnikov obtained an infinite system of equations of the Dyson type and explicit formulas for correlation functions which enter into the mass operator of the equations of the chain under consideration. N.M.Plakida [23] obtained the Dyson-type equation for Green's function introducing the so-called irreducible parts of some operators and was able to give a closed equation for the mass operator. The same method was applied by A.L.Kuzemsky [29] for a simple Hubbard model (see, e.g., also [12,27-28]).

In the following we adopt the method presented by M.Ichiyanagi [24]. Strictly speaking, this method is a certain combination of the equation of motion method with differentiation with respect to the first and second time variable, the projection operator method and irreducible Green's function method. It allows us to obtain a Dyson equation which determines an irreducible proper self-energy part. The resulting representation for the self-energy operator is not exact [32], and further calculation requires some approximations. Neverthless, these approximations will be done on a later stage of calculations [12,27-29] in comparison with the ordinary equation of motion method. For the sake of completeness, a brief review showing the way of obtaining the Dyson eq. along the projection operator and Ichiyanagi [24] methods is given below.

We represent the operator $i\dot{a}_{i\sigma}$ from the righ-hand side of Eq.(9) in the form resulting from using the projection operator P of Ichiyanagi or Tsercovnikov having the property of projecting out that part of any operator which is contained in the Hilbert space spanned by variables $a_{i\sigma}$. We have:

$$i\dot{a}_{i\sigma} \equiv P(i\dot{a}_{i\sigma}) + (1-P)(i\dot{a}_{i\sigma}) = \sum_j \omega_{ij}^{\sigma} a_{j\sigma} + (1-P)i\dot{a}_{i\sigma}, \tag{10}$$

where ω_{ij}^{σ} will be given below. Now Eq.(9) may be represented in the form:

$$\sum_j \mathcal{H}_{ij}^{\sigma} G_{jn}^{\sigma}(E) = \delta_{in} + \langle\langle (1-P)i\dot{a}_{i\sigma} | a_{n\sigma}^{+} \rangle\rangle, \tag{11}$$

where

$$\mathcal{H}_{ij}^{\sigma} = E - \omega_{ij}^{\sigma}. \tag{12}$$

Writing, in turn, equation of motion for $\langle\langle (1-P)i\dot{a}_{i\sigma} | a_{j\sigma}^{+} \rangle\rangle$, we obtain:

$$E\langle\langle (1-P)i\dot{a}_{i\sigma} | a_{j\sigma} \rangle\rangle = \langle [(1-P)i\dot{a}_{i\sigma}, a_{j\sigma}^{+}]_{+} \rangle + \langle\langle (1-P)i\dot{a}_{i\sigma} | (i\dot{a}_{j\sigma})^{+} \rangle\rangle, \tag{13}$$

The projection operator is defined in such a way that the first term in the right-hand side of Eq.(13) disappears [24] (see also [23,27-29]), i.e., ω_{ij}^{σ} from Eq.(12) takes the form:

$$\omega_{ij}^{\sigma} = t_{ij} + U_{ij}^{(1)} \langle n_{i-\sigma} \rangle + \sum_{\ell} U_{i\ell}^{(2)} \delta_{ij} \langle n_{\ell\sigma} \rangle + U_{ij}^{(2)} \langle a_{i\sigma} a_{j\sigma}^{+} \rangle + \sum_{\ell} U_{i\ell}^{(3)} \delta_{ij} \langle n_{\ell-\sigma} \rangle + U_{ij}^{(4)} \langle a_{j-\sigma} a_{i-\sigma}^{+} \rangle, \tag{14}$$

where

$$U_{ij}^{(1)} = U\delta_{ij}, \qquad U_{ij}^{(2)} = (1-\delta_{ij})(U_{ij}' - I_{ij}'),$$
$$U_{ij}^{(3)} = (1-\delta_{ij})U_{ij}', \qquad U_{ij}^{(4)} = -(1-\delta_{ij})I_{ij}''. \tag{15}$$

If one introduces the projection operator into the right-hand side of Eq.(9), then after introducing the generalized mean-field Green functions $G_{ij}^{o\sigma}(E)$ defined by equation:

$$\sum_j \mathcal{H}_{ij}^{\sigma} G_{jn}^{o\sigma} = \delta_{in} \tag{16}$$

for full Green functions $G_{ij}^{\sigma}(E)$ we have:

$$G_{ij}^{\sigma}(E) = G_{ij}^{o\sigma}(E) + \sum_{\ell n} G_{i\ell}^{o\sigma} T_{\ell n}^{\sigma}(E) G_{nj}^{o\sigma}(E), \tag{17}$$

where the scattering operator $T_{\ell n}^{\sigma}(E)$ reads:

$$T_{\ell n}^{\sigma}(E) = \langle\langle (1-P)\dot{a}_{\ell\sigma} | (1-P)\dot{a}_{n\sigma}^{+} \rangle\rangle_{E^+}. \tag{18}$$

As a next step we want to obtain the Dyson-type equation for the Green functions $G_{ij}^{\sigma}(E)$ and an explicit expression for the self-energy operator. Following the method of M.Ichiyanagi [24] after introducing "the force" $K_i(t) = (1-P)i\dot{a}_i(t)$ and considering the time evolution equation for it, we obtain:

$$T_{ij}^{\sigma}(E) = M_{ij}^{\sigma}(E) + \sum_{j_1} \langle\langle (1-P)i\dot{a}_{i\sigma} | a_{j_1\sigma}^{+} \rangle\rangle M_{j_1 j}^{\sigma}(E), \tag{19}$$

where $M^{\sigma}_{ij}(E)$ is the Fourier transform of $M^{\sigma}_{ij}(t)$

$$M^{\sigma}_{ij}(E) = \int_{-\infty}^{+\infty} dt\, M^{\sigma}_{ij}(t)\, e^{-i\omega t}, \tag{20}$$

and

$$M^{\sigma}_{ij}(t-t') = -i\theta(t-t') < [e^{i(1-P)Lt} K_i(0), \{e^{i(1-P)Lt'} K_j(0)\}^{+}]_{+} > . \tag{21}$$

Eq. (19) permits one to rewrite Eq.(11) in the form of the Dyson equation

$$G^{\sigma}_{ij}(E) = G^{0\sigma}_{ij}(E) + \sum_{k\ell} G^{0\sigma}_{ik} M^{\sigma}_{k\ell}(E) G^{\sigma}_{\ell j}(E). \tag{22}$$

From these formulas we can say that $M^{\sigma}_{ij}(E)$ contains, in the language of the diagram method, the irreducible diagrams whose representation yields the reducible expression $T^{\sigma}_{ij}(E)$ [24] (see also [23,27-29]). The self-energy formulae entering into the Dyson eq. requires considerable approximations. Approximations are possible and these are made to obtain results which are relatively easy to calculate and analyze. In the following, in order to give a simple and transparent picture of the electronic correlations, we approximate the Fourier transform of $M^{\sigma}_{ij}(t-t')$ by (in a symbolic notation)

$$M^{\sigma}_{ij}(E) \rightarrow \ll i\dot{a}_{i\sigma} | (i\dot{a}_{j\sigma})^{+} \gg^{c}_{E^{+}}. \tag{23}$$

Eq.(23) denotes, unfortunately, that we remove from self-energy given by Eq.(21) almost all information which has been introduced by the projection operator. Some information in a Dyson equation about the way of introducing the projection operator remains in the form of the mean fields contained in $G^{0\sigma}_{ij}(E)$.

It should be noticed that the above approximation is equivalent to the one used in papers [12,27-29]. Further discussion of the validity of this approximation will be given in the next section.

After all the manipulations have been performed, we can represent the self-energy operator in the form:

$$M^{\sigma}_{\ell k}(E) = \sum_{ij} \{U^{(1)}_{\ell j}[\mathcal{D}^{(1,1)}_{jjj,iii} U^{(1)}_{ik} + \mathcal{D}^{(1,2)}_{jjj,kii} U^{(2)}_{ik} + \mathcal{D}^{(1,3)}_{jjj,kii} U^{(3)}_{ik} +$$

$$+ \mathcal{D}^{(1,4)}_{jjj,iik} U^{(4)}_{ik}] + U^{(2)}_{\ell j}[\mathcal{D}^{(2,1)}_{\ell jj,iii} U^{(1)}_{ik} + \mathcal{D}^{(2,2)}_{\ell jj,kii} U^{(2)}_{ik} + \mathcal{D}^{(2,3)}_{\ell jj,kii} U^{(3)}_{ik} +$$

$$+ \mathcal{D}^{(2,4)}_{\ell jj,iik} U^{(4)}_{ik}] + U^{(3)}_{\ell j}[\mathcal{D}^{(3,1)}_{\ell jj,iii} U^{(1)}_{ik} + \mathcal{D}^{(3,2)}_{\ell jj,kii} U^{(2)}_{ik} + \mathcal{D}^{(3,3)}_{\ell jj,kii} U^{(3)}_{ik} + \tag{24}$$

$$+ \mathcal{D}^{(3,4)}_{\ell jj,iik} U^{(4)}_{ik}] + U^{(4)}_{\ell j}[\mathcal{D}^{(4,1)}_{j\ell j,iii} U^{(1)}_{ik} + \mathcal{D}^{(4,2)}_{j\ell j,kii} U^{(2)}_{ik} +$$

$$+ \mathcal{D}^{(4,3)}_{j\ell j,kii} U^{(3)}_{ik} + \mathcal{D}^{(4,4)}_{j\ell j,iik} U^{(4)}_{ik}]\},$$

where we denoted

$$\mathcal{D}^{(n,m)}_{i_1 i_2 i_3, i_4 i_5 i_6} \equiv \ll a_{i_1\sigma_1} a^{+}_{i_2\sigma_2} a_{i_3\sigma_3} | a^{+}_{i_4\sigma_4} a^{+}_{i_5\sigma_5} a_{i_6\sigma_6} \gg^{c}. \tag{25}$$

The spin indices have signs as follows (in a symbolic notation):

$$\mathcal{D}_{\sigma_1\sigma_2\sigma_3,\sigma_4\sigma_5\sigma_6} \rightarrow \begin{vmatrix} \ll\uparrow\downarrow\downarrow|\uparrow\downarrow\downarrow\gg & \ll\uparrow\downarrow\downarrow|\uparrow\uparrow\uparrow\gg & \ll\uparrow\downarrow\downarrow|\downarrow\uparrow\downarrow\gg & \ll\uparrow\downarrow\downarrow|\downarrow\uparrow\downarrow\gg \\ \ll\uparrow\uparrow\uparrow|\uparrow\downarrow\downarrow\gg & \ll\uparrow\uparrow\uparrow|\uparrow\uparrow\uparrow\gg & \ll\uparrow\uparrow\uparrow|\uparrow\downarrow\downarrow\gg & \ll\uparrow\uparrow\uparrow|\downarrow\uparrow\downarrow\gg \\ \ll\uparrow\downarrow\downarrow|\uparrow\downarrow\downarrow\gg & \ll\uparrow\downarrow\downarrow|\uparrow\uparrow\uparrow\gg & \ll\uparrow\downarrow\downarrow|\uparrow\downarrow\downarrow\gg & \ll\uparrow\downarrow\downarrow|\downarrow\uparrow\downarrow\gg \\ \ll\downarrow\downarrow\uparrow|\uparrow\downarrow\downarrow\gg & \ll\downarrow\downarrow\uparrow|\uparrow\uparrow\uparrow\gg & \ll\downarrow\downarrow\uparrow|\uparrow\downarrow\downarrow\gg & \ll\downarrow\downarrow\uparrow|\downarrow\uparrow\downarrow\gg \end{vmatrix}$$

4. ELECTRONIC STATES IN MEAN-FIELD APPROXIMATION AND ELECTRONIC QUASI-PARTICLES

Now we are going to consider the renormalized spectrum of the mean-field Green functions $G^{0\sigma}_{ij}(E)$ and damping of the quasiparticle resulting from full Green functions $G^{\sigma}_{ij}(E)$. It is a convenient pass with the help of the Fourier transform to the momentum space using the transformations of the creation and annihilation operators as well as $G^{\sigma}_{ij}(E)$, $G^{0\sigma}_{ij}(E)$ and $M^{\sigma}_{ij}(E)$ according to the formulas:

$$a_{i\sigma} = N^{-1/2} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_i} a_{\vec{k}\sigma}, \qquad a^{+}_{i\sigma} = N^{-1/2} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}_i} a^{+}_{\vec{k}\sigma},$$

$$a_{\vec{k}\sigma} = N^{-1/2} \sum_{i} e^{-i\vec{k}\cdot\vec{R}_i} a_{i\sigma}, \qquad a^{+}_{\vec{k}\sigma} = N^{-1/2} \sum_{i} e^{i\vec{k}\cdot\vec{R}_i} a^{+}_{i\sigma}, \tag{26}$$

$$G_{ij}^{\sigma}(E) = N^{-1}\sum_{\vec{k}} G^{\sigma}(\vec{k};E)\, e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)},$$
$$G^{\sigma}(\vec{k};E) = N^{-1}\sum_{ij} e^{-i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} G_{ij}^{\sigma}(E), \qquad (27)$$

and similar transformation for $G_{ij}^{0\sigma}(E)$ and $M_{ij}^{\sigma}(E)$. This transformation to momentum space enables us to rewrite Eq.(16) in the form:

$$G^{0\sigma}(\vec{k};E) = \{E^{+} - \epsilon(\vec{k}) + N^{-1}\sum_{\vec{q}} [U'(\vec{k}-\vec{q}) - I'(\vec{k}-\vec{q})] \times$$
$$\times \langle n_{\vec{q}\sigma}\rangle - N^{-1}\sum_{\vec{q}} I''(\vec{k}+\vec{q})\langle n_{\vec{q}-\sigma}\rangle - [U+U'(0)]\langle n_{-\sigma}\rangle - [U'(0)-I'(0)]\langle n_{\sigma}\rangle\}^{-1}, \qquad (28)$$

where

$$\epsilon(\vec{k}) = N^{-1}\sum_{ij} t_{ij}\, e^{-i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} \qquad (29)$$

and $U'(\vec{k})$, $I'(\vec{k})$, $I''(\vec{k})$ are Fourier transforms of interatomic integrals.

The renormalized energies $E^{\sigma}(\vec{k})$ have the form:

$$E^{\sigma}(\vec{k}) = E - \epsilon(\vec{k}) - U\langle n_{-\sigma}\rangle + N^{-1}\sum_{\vec{q}} [U'(\vec{k}-\vec{q}) - I'(\vec{k}-\vec{q})]\langle n_{\vec{q}\sigma}\rangle$$
$$- N^{-1}\sum_{\vec{q}} I''(\vec{k}+\vec{q})\langle n_{\vec{q}-\sigma}\rangle - U'(0)\langle n_{-\sigma}\rangle - [U'(0)-I'(0)]\langle n_{\sigma}\rangle, \qquad (30)$$

where

$$\langle n_{\sigma}\rangle = N^{-1}\sum_{\vec{q}} \langle n_{\vec{q}\sigma}\rangle.$$

The band splitting now reads as

$$E^{\uparrow}(\vec{k}) - E^{\downarrow}(\vec{k}) = [U - I'(0)](\langle n_{\downarrow}\rangle - \langle n_{\uparrow}\rangle) + N^{-1}\sum_{\vec{q}} [U'(\vec{k}-\vec{q}) -$$
$$- I'(\vec{k}-\vec{q}) + I''(\vec{k}+\vec{q})]\langle n_{\vec{q}\downarrow} - n_{\vec{q}\uparrow}\rangle. \qquad (31)$$

In the case of $I' = U' = I'' = 0$ we obtain $\vec{k}$-independent result of the Hartree-Fock theory. Eqs.(30)-(31) generalize the Hartree-Fock renormalized energies and band-splitting.

Now we are going to consider the electronic quasiparticles and their damping. We can write the formal solution of the Dyson Eq.(22) (in $\vec{k}$-representation) as follows:

$$G^{\sigma}(\vec{k};E) = [G^{0\sigma}(\vec{k};E)^{-1} - M^{\sigma}(\vec{k};E)]^{-1}. \qquad (32)$$

To find an expression for the mass operator we proceed in the same way as previously[12], i.e. we express the Green function entering into the operator $M^{\sigma}(k;E)$ through the correlation functions using the spectral theorem[22]. These correlation functions are decoupling in the pair approximation (valid for a small density of quasiparticles) in the following way:

$$\langle a^{+}_{\vec{k}_1\sigma_1}(t)a_{\vec{k}_2\sigma_2}(t)a^{+}_{\vec{k}_3\sigma_3}(t)|a_{\vec{k}_4\sigma_4}a^{+}_{\vec{k}_5\sigma_5}a_{\vec{k}_6\sigma_6}\rangle^{c} \approx \langle a^{+}_{\vec{k}_1\sigma_1}(t)a_{\vec{k}_1\sigma_1}\rangle \times$$
$$\times \langle a_{\vec{k}_2\sigma_2}(t)a^{+}_{\vec{k}_2\sigma_2}\rangle\langle a^{+}_{\vec{k}_3\sigma_3}(t)a_{\vec{k}_3\sigma_3}\rangle\, \delta_{\vec{k}_1\vec{k}_4}\delta_{\vec{k}_2\vec{k}_5}\delta_{\vec{k}_3\vec{k}_6}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_5}\delta_{\sigma_3\sigma_6} + \qquad (33)$$
$$+ \langle a^{+}_{\vec{k}_3\sigma_3}(t)a_{\vec{k}_3\sigma_3}\rangle\langle a_{\vec{k}_2\sigma_2}(t)a_{\vec{k}_2\sigma_2}\rangle\langle a_{\vec{k}_1\sigma_1}(t)a_{\vec{k}_1\sigma_1}\rangle \times$$
$$\times \delta_{\vec{k}_3\vec{k}_4}\delta_{\vec{k}_2\vec{k}_5}\delta_{\vec{k}_1\vec{k}_6}\delta_{\sigma_3\sigma_4}\delta_{\sigma_2\sigma_5}\delta_{\sigma_1\sigma_6},$$

where we form all possible one-particle averages with different times. The simultaneous averages have been taken into account by using the projection operators. As previously noted, we do not retain spin-flip-type correlation functions.

After lengthy algebraic manipulations, the resulting expression for a self-energy can be written as follows:

$$M^{\sigma}(\vec{k};E) = N^{-2}\sum_{\vec{p}\vec{q}} [\mathfrak{M}_{-\sigma\sigma-\sigma}(\vec{k};E)f_1(\vec{k},\vec{p},\vec{q}) + \mathfrak{M}_{-\sigma-\sigma\sigma}(\vec{k};E)\times$$
$$\times f_2(\vec{k},\vec{p},\vec{q}) + \mathfrak{M}_{\sigma\sigma\sigma}(\vec{k};E)f_3(\vec{k},\vec{p},\vec{q})], \qquad (34)$$

where

$$\mathfrak{M}_{\sigma_1\sigma_2\sigma_3}(\vec{k};E) = \frac{1}{\pi^3}\iiint_{-\infty}^{+\infty}\frac{d\omega_1 d\omega_2 d\omega_3}{E^{+}+\omega_1-\omega_2-\omega_3}\{n(\omega_1)[1-n(\omega_2)]\times \qquad (35)$$

$$\times[1-n(\omega_3)]+[1-n(\omega_1)]\,[1-n(\omega_2)]n(\omega_3)\}\mathrm{Im}\,G^{\sigma_1}(\vec{p}+\vec{k};\omega_1)\times$$

$$\times\,\mathrm{Im}\,G^{\sigma_2}(\vec{p}+\vec{q};\omega_2)\cdot\mathrm{Im}\,G^{\sigma_3}(\vec{q};\omega_3),$$

and

$$f_1(\vec{k},\vec{p},\vec{q})=U^2+UU'(\vec{p})+UI'(\vec{k}+\vec{p}+\vec{q})+UU'(\vec{p})+U(\vec{p})^2+U(\vec{p})I''(\vec{k}+\vec{p}+\vec{q}),$$

$$f_2(\vec{k},\vec{p},\vec{q})=UI''(\vec{k}+\vec{p}+\vec{q})+I''(\vec{k}+\vec{p}+\vec{q})U'(\vec{k}-\vec{q})+I''(\vec{k}+\vec{p}+\vec{q})^2, \qquad (36)$$

$$f_3(\vec{k},\vec{p},\vec{q})=[I'(\vec{p})-U'(\vec{p})][U'(\vec{k}-\vec{q})-I'(\vec{k}-\vec{q})]+[U'(\vec{p})-I'(\vec{p})]^2.$$

In the case of a simple Hubbard model we obtain from Eqs.(34--36) the self-energy in the form found in /29/. In order to determine the Green function in a fully self-consistent treatment of the correlation problem for our Hamiltonian one would require the solution of a set of complex coupled equations (22) and (24) or (within a pair-decoupling scheme) Eqs.(22) and (34). It is a very difficult problem to find a solution of these two coupled equations. We must remember that the expression for a self-energy involves tedious integrations in a 9-dimensional space (6-dimensional integral in $\vec{k}$ -space and 3-dimensional in energy space for 3-dimensional systems). In principle, we can try to obtain a solution of this problem by starting with the initial approximation for a Green function, then calculate the self-energy and as a next step calculate a Green function and so on. If for the first step we take simple one-pole expression (this is a rather reasonable starting point):

$$-\frac{1}{\pi}\,\mathrm{Im}\,G^{\sigma}(\vec{k};E)\sim\delta(E-E^{\sigma}(\vec{k})), \qquad (37)$$

where $E^{\sigma}(\vec{k})$ is given by Eq.(30), than the 9-dimensional integral appearing in self-energy reduces to 6-dimensional ones, and in principle, we can obtain the self-energy in a relatively simple way (it is true for the first iteration step only). If this first step is sufficient for the problem under consideration, for example for $U/W \ll 1$, then we can finish the iteration process at the first stage and obtain the Green function in an approximate way. Such a method of an approximate calculation of the self-energy and spectral density of states was used in the case of a simple Hubbard model in /29/ and for the multi-band Hubbard model in /12/. In order to give a short explanation of an approximation accepted in Eqs.(23) and (33) we insert Eq.(37) with substitution $E^{\sigma} \to \epsilon(\vec{k})$ into Eq.(34). As a result, we obtain, for example in the case of a simple Hubbard Hamiltonian, an expression for self-energy the same as in the second-order-perturbation theory - see for comparison formulas in /30/ and /31/. Then our approximation contained in Eqs.(23) and (33) may in this manner be justified to some extent. The numerical results and discussion will be given in a separate paper.

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