The intersite interactions in the problem of energy structure of the strongly correlated electron systems

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Abstract. On the basis of the extended set of the irreducible operators orthogonal on Mori an effect of the intersite interactions on the formation of energy structure of the \( t - V \)–model has been studied. Qualitative new result consists in the appearance of an additional fluctuation band in the structure of energy spectrum. The formation of the fluctuation band is connected with the deviation of the occupation numbers from the nominal value. The spectral intensity of the fluctuation band depends on the carrier concentration and rises when the root-mean-square fluctuations of the occupation numbers are increased. Consequently at increase doping level there is a redistribution of the spectral weight between ordinary band and fluctuation band in favour of the last. This redistribution underlies a modification of integrated density of states.

1. Introduction
Coulomb repulsion of two electrons located on one site and possessing of the opposite spin moment projections plays a key role in the formation of the fundamental features of the strongly correlated electron systems. This interaction is the basis of the electron mechanism of Cooper instability which leads to the high-temperature transitions to the superconducting phase. Many theoretical studies of the last two decades have been aimed at investigation of the one-site correlations and their manifestation in the properties of the ground state and in the elementary excitation spectrum of high-temperature superconductors. However, not much attention has been focused on the intersite Coulomb interactions. Meanwhile, the simple analysis shows that at distances comparable with the lattice parameter, i.e., when the Coulomb interaction is not screened, the characteristic energy of the intersite interaction can be insignificantly lower than the energy of Hubbard’s repulsion. Therefore, the correct description of the strongly correlated systems requires the consideration of both intraionic and interionic correlations.

It should be noted that the intraionic correlations of the multiorbital systems can be effectively described by the method, which combines a cluster form of the perturbation theory and the atomic representation [1]. It is no surprise that in a number of studies the developed approach was also used for consideration of the intersite correlations. However, as was mentioned in [2], the cluster form of the perturbation theory causes some problems occurring upon including the intersite correlations and cannot be used, in particular, for obtaining the effective Hamiltonians. This fact was clearly demonstrated by calculation of the exchange integral of copper oxides with allowance made for the intersite interactions [2]. The intersite correlations that enhance the role played by the charge fluctuations were recently found to make an important contribution to the formation of Cooper instability [3].
The aforesaid factors provoke the study of the energy structure of the strongly correlated systems when the intersite interactions are considerable and, for this reason, cannot be described in the Hartree–Fock approximation (HFA), requiring a more correct approach. The problem can be solved using the gas approximation which is justified by the fact that in the area of weak doping of copper oxides a number of holes per unit cell of the CuO$_2$ plane is much less than one.

Hence, in the nearest neighborhood of copper ions there is not more than one hole on average on the nearest oxygen ions, which means that the concentration of holes can be considered as a gas parameter. Thus, upon extension of the basis set of Green’s functions, which must be accurately considered and do not allow uncoupling, one can limit the consideration to the functions describing the states with not more than one hole on the nearest copper ions.

In this study, using the principle of the selection of higher Green’s functions the energy structure is calculated for the $t–V$–model which brightly demonstrates the effects of the intersite correlations. The $t–V$–model is a Hubbard model [4] in the limit regime of the strong one-site correlations with the included Coulomb interaction of the electrons located on the neighboring lattice sites.

2. Hamiltonian of the $t–V$–model and equations of motion

Let us consider the Hamiltonian of the $t–V$–model

$$\hat{H} = \sum_{f,\sigma} \varepsilon_0 X^\sigma_f + \sum_{f,m,\sigma} t_{fm} X^\sigma_f X^{\bar{\sigma}}_m + \frac{1}{2} \sum_{f,m} V_{fm} \hat{n}_f \hat{n}_m. \quad (1)$$

The Hubbard operators $X^\sigma_f$ correspond to the transitions between the one-ion states of electrons; the first term describes one-site energy of electrons; the second term reflects their kinetic energy, $t$ is the hopping integral between nearest neighbours; the third term describes the intersite Coulomb interaction with parameter $V$. Using the condition of completeness of the Hubbard operators in the reduced Hilbert space $X^{00}_f + X^{\uparrow\downarrow}_f + X^{\downarrow\uparrow}_f = 1$, we can write the Hamiltonian of the $t–V$–model as follows:

$$\hat{H} = E_0 + \sum_{f,\sigma} \varepsilon - 4Vh X^\sigma_f + \sum_{f,m,\sigma} t_{fm} X^\sigma_f X^{\bar{\sigma}}_m + \frac{1}{2} \sum_{f,m} V_{fm} (X^\sigma_f - h)(X^{\bar{\sigma}}_m - h), \quad (2)$$

where $E_0 = -2NV(1 - h)^2$, $\varepsilon = \varepsilon_0 + 4V$ and $h = \frac{1}{N} \sum_f (X^{00}_f)$ is the average holes number.

The main reason for isolation of the obvious mean-field effects is the need for presentation of the intersite interaction in the form which explicitly reflects the correlation effects. After some simple identical transformations the last Hamiltonian term describing the intersite correlations is written in the desired form. One can see that this term will contribute to the energy structure only in the presence of noticeable fluctuations of the occupation numbers. The energy $E_0$ originates from isolation of the mean-field effects.

In order to determine the energy structure of the system under consideration we write the exact equations of motion in the Heisenberg representation:

$$i \frac{d}{dt} X^\sigma_f = (\varepsilon - 4Vh) X^\sigma_f + \sum_{m} t_{fm} \left( (X^{00}_f + X^{\bar{\sigma}}_f) X^{\sigma}_m + X^{\bar{\sigma}}_f X^{\sigma}_m \right) - V_{fm} \hat{\Phi}_f,$$

$$i \frac{d}{dt} \Phi_f = (\varepsilon - 4Vh) \Phi_f + \sum_{m,\delta} t_{fm} \left( (X^{00}_f + X^{\bar{\sigma}}_f) X^{\sigma}_m + X^{\bar{\sigma}}_f X^{\sigma}_m \right) (X^{\sigma}_{f+\delta} - h) \quad (3)$$

$$+ \sum_{m,\delta,\sigma'} t_{m,f+\delta} (X^{\sigma}_m X^{\sigma'}_{f+\delta} - X^{\bar{\sigma}}_f X^{\sigma'}_{f+\delta} X^{\sigma}_m) - \sum_{m,\delta} V_{fm} X^{\sigma}_m (X^{\sigma}_m - h)(X^{\sigma}_{f+\delta} - h),$$
where \( \hat{\Phi}_f^\sigma = \sum \delta X^0_\sigma (X^0_f + \delta - h) \). This system of equations contains terms of the highest order which are product of the different-site operators. When \( V \gg t \), the energy coefficients before such operators are different. Generalizing the Hubbard concept \([4]\) for consideration of the one-site correlations to the intersite correlations, we see that in the operators that are not preceded by large energy parameter ordinary uncoupling of the HFA type can be performed. At the same time, the multisite operators that appear in (3) with a large energy coefficient must be taken into account exactly and need in corresponding equations of motion. In our case, the number of such new equations is significantly reduced due to the use of the gas approximation. This simplification is justified, because upon weak doping the condition \( h \ll 1 \) should be met. In practice, this reflects in the fact that the equations (3) should be projected \([5, 6]\) onto orthogonal basis \( \{ X^0_\sigma, \hat{\Phi}_f^\sigma \} \).

One can see that basis (4) does not contain the operators describing more than one hole on sites in the nearest neighborhood of particular site. After the transition to the quasi-momentum space by the Fourier transformation a closed system of equations for Green’s functions was obtained which determines the dynamics of the Fermi excitations of the system under study:

\[
\begin{align*}
(\omega - \varepsilon_{\vec{k}}) \langle \langle X_{\vec{k}\sigma} \vert X_{\vec{k}\sigma}^\dagger \rangle \rangle &= \frac{1 + h}{2} - \gamma_{\vec{k}} \langle \langle \Phi_{\vec{k}\sigma} \vert X_{\vec{k}\sigma}^\dagger \rangle \rangle, \\
(\omega - \xi_{\vec{k}}) \langle \langle \Phi_{\vec{k}\sigma} \vert X_{\vec{k}\sigma}^\dagger \rangle \rangle &= -4h(1 - h)\gamma_{\vec{k}} \langle \langle X_{\vec{k}\sigma} \vert X_{\vec{k}\sigma}^\dagger \rangle \rangle.
\end{align*}
\]

Here the notations are used

\[
\begin{align*}
\varepsilon_{\vec{k}} &= (\varepsilon - 4Vh) + \left( \frac{1 + h}{2} \right) t_{\vec{k}}, \\
\gamma_{\vec{k}} &= V - \frac{t_{\vec{k}}}{8}, \\
\xi_{\vec{k}} &= (\varepsilon - 4Vh) - V(1 - 2h) + \left( \frac{2 + h}{8} \right) t_{1\vec{k}}, \\
t_{\vec{k}} &= 2t(\cos k_x + \cos k_y).
\end{align*}
\]

3. Energy structure

The solving of the system of equations (5) shows, that the correct account for the intersite correlations leads to the appearance of additional energy level in the energy structure of the \( t - V \)–model (figure 1). The formation of the additional energy level is caused by changing energy of the electron located on a site if near this site the electronic configurations deviate from nominal ones. Consequently, the occurrence of the new level is related to the density fluctuations. The hopping processes lead to spreading the fluctuation level into energy band (figure 1, bottom), which we name the band of the fluctuation states (BFS). The spectral intensity depends on both the carrier concentration in the conduction band and the intensity of the hybridization processes.

It should be emphasized that the occurrence of the BFS in the \( t - V \)–model due to the intersite correlations is qualitatively similar to the occurrence of two Hubbard subbands at the strong intra-atomic repulsion. Obviously, upon weak doping the spectral intensity of the BFS will be small and its contribution to the integrated energy structure will be insignificant. However, if the concentration of holes in the system increases, then at the doping levels \( P = 0.2 \div 0.3 \) the picture becomes qualitative different. With an increase in number of holes in the system or in intensity of the hopping processes the spectral intensity of the BFS, determined by the root-mean-square fluctuations of the occupation numbers increases and the new band starts playing an important role. As a result, with an increase in doping level the spectral weight is redistributed between the ordinary band and the BFS in favour of the latter. This induces the occurrence of an additional peak of the density of states (figure 2, on bottom).
Figure 1. Band picture of the $t-V$–model with account for the intersite correlations in the HFA (top) and with account for the BFS (bottom) for the set of parameters $\varepsilon_0 = -2$, $V = 1.5$ (in terms of $|t|$) at $h = 0.21$. Dashed lines show the chemical potential.

Figure 2. Density of states of the $t-V$–model with account for the intersite correlations in the HFA (top) and with account for the BFS (bottom) for the set of parameters $\varepsilon_0 = -2$, $V = 1.5$ (in terms of $|t|$) at $h = 0.21$. Dashed lines show the chemical potential.

4. Conclusion
The study of the energy structure of the $t-V$–model carried out has shown that the inclusion of the intersite correlations effects yields not only quantitative changes but also a number of qualitatively new features. It should be emphasized that we are speaking of the intersite correlations and not of the intersite interaction. Indeed, the most part of the interaction which is reduced to the mean-field effects is easily described by the above-mentioned renormalization of the one-site energies of the copper and oxygen orbitals, whereas the description of the correlation effects would demand the higher irreducible Green’s functions.

The qualitatively new effects found are the following. The first one is the occurrence of new energy band due to the charge fluctuations. The second effect is redistribution of the spectral intensity between the ordinary band and fluctuation band, which is especially important as it can induce the pseudogap state of a strongly correlated system upon doping.

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