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Lower Subband Splitting and Superconductivity of 2D Hubbard Fermions with Strong Intersite Correlations

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Abstract—The effect of the strong intersite Coulomb correlations on the formation of an electron structure in the Shubin–Vonsowsky model in the regime of strong one-site correlations is studied. The results reveal a split-off band of the Fermi states. The spectral intensity of this band grows with the enhancement of the doping level and is determined by the mean-square fluctuation of occupation numbers. This changes the structure of the electron density of states qualitatively.

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Strong electron correlations (SECs) have been intensively studied since the second half of the 20th century, but these studies have so far been limited mainly to investigating one-site (Hubbard) correlations [1]. Revelations of the Coulomb interaction of electrons localized at different sites of a crystal lattice remain poorly studied. In the vast majority of works, the intersite Coulomb interaction of electrons has been ignored. Such an approach might be justified when the Coulomb interaction is strongly shielded. For weakly doped systems, however, in which the shielding radius becomes larger, ignoring the intersite Coulomb interaction can lead to inadequate description of the physical properties of compounds with SECs [2].

As was shown in [3, 4], strong intersite correlations can split the initial band of the Fermi states of a system with SECs. It should be noted that such splitting is not related to the well-known Hubbard formation of two subbands and manifests itself as an additional splitting of the lower (or upper) Hubbard subband (Fig. 1). The spectral intensity of a split-off band, as we show below, grows with the probability of deviation of the surrounding electron configuration from the nominal value.

In this study, we investigate the effect of the induction of a split-off band of the Fermi states on the superconducting properties of the Shubin–Vonsowsky model [5] in the regime of strong one-site electron correlations ($U = \infty$). The Hamiltonian of this model in the atomic representation is

$$H = \sum_{f\sigma}(\varepsilon_0 - \mu)X_f^{\sigma\sigma} + \sum_{fm\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma} + \frac{V}{2}\sum_{f\delta}\hat{n}_f\hat{n}_{f+\delta}. \quad (1)$$

Here, the first term describes the ensemble of noninteracting Hubbard fermions in the Wannier representation, the second term corresponds to the kinetic energy of Hubbard fermions, and the last term allows for the Coulomb interaction of electrons localized on neighboring sites f and $f + \delta$ (the intensity of this interaction is determined by parameter V). Below, we consider a case where the number of holes $h = (1/N)\sum_f \langle X_f^{00} \rangle$ in the system is low: $h = 1 - n \ll 1$.

Using the diagram technique for the Hubbard operators [6] under the condition that the hopping parameter is small, relative to the energy of the Coulomb repulsion of electrons on the neighboring sites of a lattice ($|t| \ll V$), we can obtain the expression for the one-particle Matsubara Green's function

$$D(k, i\omega_n) = \frac{(1 - n/2)(i\omega_n - \varsigma + \mu)}{(i\omega_n - \varepsilon_k + \mu)(i\omega_n - \varsigma + \mu) - 4h(1-h)V^2}, \quad (2)$$

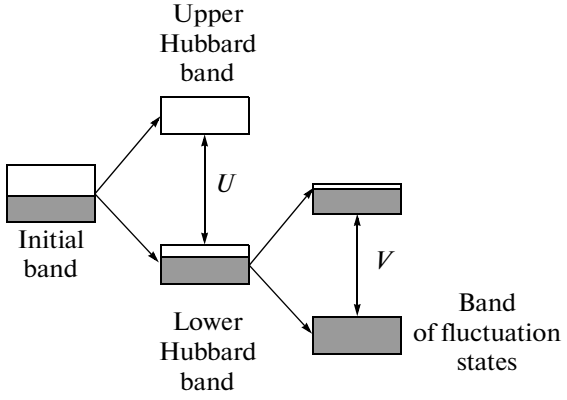

Fig. 1. Schematic of energy band splitting in a strongly correlated system with one-site and intersite Coulomb interactions of electrons.

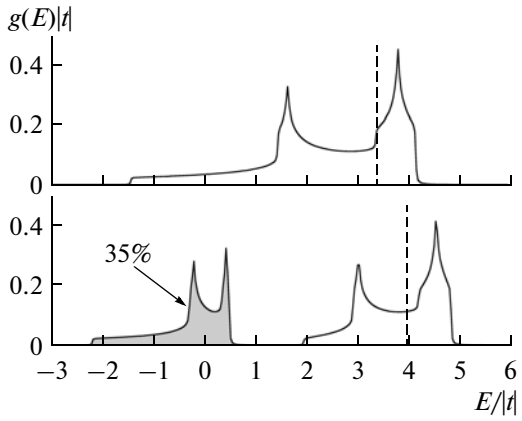

Fig. 2. Density of electron states calculated ignoring intersite correlations (at the top) and with allowance for them (at the bottom) at doping level $P = 0.2$. The dotted lines show the position of the chemical potential.

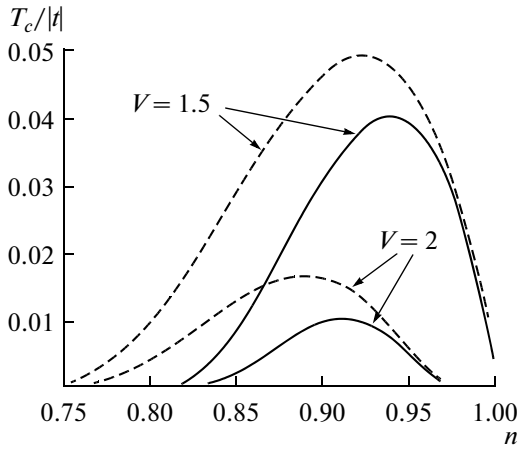

Fig. 3. Dependence of the temperature of the transition to the superconducting phase on electron concentration.

which, as can be seen, has a bipolar structure. Here, $\varepsilon_k = \tilde{\varepsilon} + (1 - n/2)t_k$, $\zeta = \tilde{\varepsilon} - V(1 - 2h)$, t_k is the Fourier image of the hopping integral, and μ is the chemical potential. The Fermi excitation spectrum is then

$$E_k^{\mp} = \frac{\varepsilon_k + \zeta}{2} \mp \nu_k,$$
$$\nu_k = \sqrt{\left(\frac{\varepsilon_k - \zeta}{2}\right)^2 + 4h(1-h)V^2}. \quad (3)$$

The upper energy band of this model corresponds to the motion of an electron over the lattice sites neighboring sites where there are no holes. The characteristic setting energy of such an electron is $\varepsilon + 4V$. The lower band describes the motion of an electron over the lattice sites that have one site with a hole arising in their neighborhood. The occurrence of a hole in the immediate environment reduces the setting energy of this electron to the characteristic value $\varepsilon_0 + 3V$. The formation of an additional band is due to the change in the energy of an electron on the site if the electron configurations deviate from nominal values nearby. The split-off band is therefore referred to as a fluctuation state band (FSB) [4].

The occurrence of an FSB qualitatively changes the form of the electron density of states of Hubbard fermions. The upper plot in Fig. 2 shows the density of states of the model under consideration with disregard of the intersite correlations. It can be seen that ignoring these correlations leads to a minor shift of the Hubbard fermion band. The lower plot in Fig. 2 shows the density of states of the model for the same set of parameters but with respect to the intersite correlations. A comparison of the plots shows that the allowance for these correlations qualitatively changes the form of the density of states: the FSB splits off and a gap is formed in the structure of the energy spectrum. For the sake of clarity, Fig. 2 shows the density of states of the FSB $g^-(E)$ as a line limiting the shaded area. The fraction of the FSB is 35% of the total number of states of the system; the fraction of the main band with the density of states $g^+(E)$ is 65%.

The change in the structure of the density of states leads to renormalization of the scattering amplitude pole in a Cooper channel and manifests itself in the dependence of the critical temperature of the transition to the superconducting state with the inhomogeneous electron concentration. The solid lines in Fig. 3 show the $T_c(n)$ dependences obtained with regard to the FSB. For comparison, dashed lines show the $T_c(n)$ dependences obtained with disregard of the effect of FSB induction. It can be seen that in the region of electron concentrations n close to unity, and the effect of the FSB is insignificant (the solid and dashed lines coincide). This comes as no surprise, since the spectral intensity of the FSB at $n \longrightarrow 1$ vanishes. If the concentration grows, the mean-square fluctuation of occupation numbers also grows. In this case, the spectral intensity for the FSB increases and the contribution from the FSB manifests itself fairly strongly. It can be seen from the figure that in the most interesting region of electron concentration $n \approx 0.8$–0.9, renormalization of the critical temperature is comparable to and even exceeds the value of T_c itself, calculated with disregard for the FSB contributions. FSB induction thus strongly affects the phase diagram of the system in the concentration region where the superconducting state is attained.

Our results on the influence of the intersite correlations on the energy structure and spectral characteristics of narrow-band Mott–Hubbard dielectrics at low doping levels demonstrate the presence of two qualitatively different effects. The first effect is related to the occurrence of a new energy band caused by charge fluctuations. The second effect is the redistribution of spectral intensity upon doping between the main band and FSB in favor of the latter. This modifies the den-

sity of states and the abovementioned renormalization of the temperature of the transition to the superconducting state with inhomogeneous electron concentration.

Note also that the considered modification of the energy structure due to strong intersite correlations is general and not limited merely by the Shubin–Vonsowsky model. We might expect that the effects disclosed in this study are of special importance for systems with variable valence.

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