GENERALIZED KONDO LATTICE MODEL AND ITS SPIN-POLARON REALIZATION BY THE PROJECTION METHOD FOR CUPRATES

V. V. Valkov,* **D. M. Dzebisashvili,***† **and A. F. Barabanov**‡

The spin–fermion model, which is an effective low-energy realization of the three-band Emery model after passing to the Wannier representation for the p_x and p_y orbitals of the subsystem of oxygen ions, reduces to the generalized Kondo lattice model. A specific feature of this model is the existence of spin-correlated hoppings of the current carriers between distant cells. Numerical calculations of the spectrum of spin-electron excitations highlight the important role of the long-range spin-correlated hoppings.

1. Introduction

The structure of quasiparticles of the normal phase of cuprate high-temperature superconductors (HTSC) and the nature of low-energy interactions play a key role in explaining the mechanism of Cooper instability, the anomalous temperature behavior of the kinetic coefficients, and many other anomalous properties [1], [2]. The far-from-perfect theory of a two-dimensional doped antiferromagnet (AFM) is primarily developed in terms of the Hubbard two-dimensional models, generalized t–J models, the three-band Emery model [3]–[7], and the spin–fermion model. We do not discuss the first two models and only mention that they differ substantially from the three-band Emery model and spin–fermion models because their charge and spin subsystems are formed by the same carriers. We therefore start with the more realistic models from our standpoint (the spin–fermion model and the three-band Emery model) where the spin-subsystem and the charge-subsystem carriers are respectively determined by d and p ions.

It is known that in the regime of strong electron correlations (SEC), the Hamiltonian of the three-band Emery model can be reduced to the spin–fermion model [8]–[11]. An attractive property of the spin–fermion model is that already in the simplest consideration, it allows obtaining the primary motif of the cuprate hole spectrum [8], [9]. In this case, the bottom of the carrier spectrum $E(k)$ is located in the vicinity of the boundary of the magnetic Brillouin zone, and the spectrum itself has the quasimomentum dependence $E(k) \sim (\cos k_x + \cos k_y)^2$.

Here, we reduce the Hamiltonians of the three-band Emery model and the spin–fermion model to a generalized Kondo lattice model that takes the long-range spin-correlated hoppings into account. Based on

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*Kirensky Institute of Physics, Siberian Branch, RAS, Krasnoyarsk, Russia, e-mail: vvv@iph.krasn.ru.

†Reshetnyov Siberian State Aerospace University, Krasnoyarsk, Russia, e-mail: ddm@iph.krasn.ru.

‡Institute for High Pressure Physics, RAS, Troitsk, Moscow Oblast, Russia.

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a comparison of the spectral dependences of spin-polaron quasiparticles for the Kondo lattice model and for its truncated version (where only interactions between the nearest ions remain), we conclude that the long-range spin-correlated hoppings are important.

2. The Hamiltonian of the three-band Emery model

The Hamiltonian of the three-band Emery model for the CuO_2 plane [3]–[6] can be written as

$$\hat{\mathscr{H}} = \hat{\mathscr{H}}_{pd} + \hat{\mathscr{H}}_I, \tag{1}$$

where

$$\hat{\mathscr{H}}_{pd} = \sum_f (\varepsilon_d \hat{n}_f^d + U_d \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d) + \sum_l (\varepsilon_p \hat{n}_l^p + U_p \hat{n}_{l\uparrow}^p \hat{n}_{l\downarrow}^p) +$$

$$+ V_{pd} \sum_{f,\delta} \hat{n}_f^d \hat{n}_{f+\delta}^p + t_{pd} \sum_{f,\delta,\sigma} (\vartheta(\delta) d_{f\sigma}^+ p_{f+\delta,\sigma} + \text{H.c.}) + \hat{T}, \tag{2}$$

$$\hat{T} = \sum_{l,\Delta,\sigma} t\varrho(\Delta) p_{l,\sigma}^+ p_{l+\Delta,\sigma}, \qquad \hat{\mathscr{H}}_I = \frac{I_1}{2} \sum_{f,g} \vec{S}_f \vec{S}_{f+g} + \frac{I_2}{2} \sum_{f,d} \vec{S}_f \vec{S}_{f+d}. \tag{3}$$

Here, ε_p and ε_d denote the energy of a hole on the respective oxygen and copper ions, U_p and U_d denote the energy of repulsion of two holes on oxygen and copper ions, V_{pd} is the energy of repulsion of two holes on nearest oxygen and copper sites, t_{pd} is the parameter of hybridization of nearest oxygen p and copper d orbitals. The vectors l show the positions of sites of oxygen ions. The vector δ in (2) takes the four values $\pm\delta_x$ and $\pm\delta_y$ ($\delta_x = (a/2, 0)$, $\delta_y = (0, a/2)$, and a is the lattice parameter of copper ions) and connects the nearest oxygen sites at positions $f + \delta$ with the copper ion at the site f. The function $\vartheta(\delta)$ takes the effect of correlations between the phases of copper and oxygen orbitals on hybridization processes into account. For commonly used orbitals, the function $\vartheta(\delta)$ takes the values $\vartheta(\delta) = \mp 1$ for $\delta = \pm\delta_x$ or $\delta = \pm\delta_y$.

In the expression for $\hat{\mathscr{H}}_{pd}$, the operators $p_{l\sigma}$ or $p_{l\sigma}^+$ respectively annihilate or create a hole on the oxygen ion with the site index l and spin projection σ, which takes the values $\uparrow$ or $\downarrow$. The operators $d_{f\sigma}$ or $d_{f\sigma}^+$ annihilate or create a hole on the copper ion with the index f and spin projection σ. The operators of the number of holes on the oxygen or copper ion at the site l or f with the spin σ are described by the expression $\hat{n}_{l\sigma}^p = \sum_\sigma p_{l\sigma}^+ p_{l\sigma}$ or $\hat{n}_{f\sigma}^d = \sum_\sigma d_{f\sigma}^+ d_{f\sigma}$. Moreover, $\hat{n}_l^p = \sum_\sigma \hat{n}_{l\sigma}^p$ and $\hat{n}_f^d = \sum_\sigma \hat{n}_{f\sigma}^d$.

The term $\hat{T}$ corresponds to the direct hoppings of the holes between nearest oxygen ions with the tunneling integral $t\varrho(\Delta)$. Its sign is defined by a function $\varrho(\Delta)$ that depends on the orientation of the line where the oxygen ions involved in the hoppings are located. The vector Δ takes the four values $(\pm a/2, \pm a/2)$ and connects the oxygen ion at the site l with the nearest oxygen ion with the number $l + \Delta$. For the selected oxygen orbital phases, we have $\varrho(\Delta) = 1$ if $\Delta = \pm(a/2, a/2)$. If $\Delta = \pm(a/2, -a/2)$, then $\varrho(\Delta) = -1$.

The second term $\hat{\mathscr{H}}_I$ in expression (1) corresponds to the superexchange interaction between the spin moments on the nearest and next-nearest sites ($d = \pm g_x \pm g_y$). The vectors of the nearest neighbors of the copper lattice are $g_x = (a, 0)$, $g_y = (0, a)$. In what follows, it is convenient to use the frustration parameter p and the effective exchange I: $I_1 = (1 - p)I$ and $I_2 = pI$, $0 \leq p \leq 1$, $I > 0$. According to this approach, it is assumed that considering the properties of the spin subsystem of copper ions, we can use the two-dimensional frustrated AFM Heisenberg model with $S = 1/2$. The AFM interaction between the nearest spins of Cu^{2+} ions in the CuO_2 plane is high (it has the order of $0.13\,\text{eV} \cong 1500\,\text{K}$) and is much higher than the interplane exchange. The interplane exchange is primarily responsible for the long-range order observed in the dielectric phase of the CuO_2 planes. For La_2CuO_4 (LSCO), the Neel temperature $T_N \sim 300\,\text{K}$. But with a comparatively weak doping of the system with holes, the long-range

AFM order disappears over the entire temperature interval. This behavior is adequately simulated by the introduction of frustration [12]. The cluster calculations indicate the existence of a sufficiently high frustration parameter $I_2/I_1 \sim 0.1$ even for the undoped LSCO [13]. The spin subsystem is considered quantitatively in the framework of a spherically symmetric self-consistent theory [14]–[16]. According to this theory, the subsystem of the spin moments localized on copper ions is considered in the state of an $SU(2)$-invariant quantum spin liquid, which has spherical symmetry in the spin space. This observation implies that the spin correlation functions $C_j = \langle \vec{S}_f \vec{S}_{f+r_j} \rangle$ (where r_j is the radius of jth coordination sphere) satisfy the relations $C_j = 3\langle S_f^x S_{f+r_j}^x \rangle = 3\langle S_f^y S_{f+r_j}^y \rangle = 3\langle S_f^z S_{f+r_j}^z \rangle$ and $\langle S_f^\alpha \rangle = 0$, where S_f^α is the spin operator along the direction $\alpha = x, y, z$ on the copper ion at the site f.

3. Generalized Kondo lattice model

For simplicity, we consider the case $U_p = V_{pd} = t = 0$. Under these conditions, the Hamiltonian of three-band Emery model (1) is substantially simplified:

$$\hat{\mathscr{H}}_{pd} = \sum_f (\varepsilon_d \hat{n}_f^d + U_d \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d) + \varepsilon_p \sum_l \hat{n}_l^p + t_{pd} \sum_{f,\delta,\sigma} (\vartheta(\delta) d_{f\sigma}^+ p_{f+\delta,\sigma} + \text{H.c.}). \tag{4}$$

As is known [8], [9], in the SEC regime where $U_d > \varepsilon_{pd} = \varepsilon_p - \varepsilon_d \gg t_{pd}$, operator (4) is reducible to the Hamiltonian of the spin–fermion model, and the corresponding Hilbert space is characterized by the homeopolar states of copper ions:

$$\hat{\mathscr{H}}_{\text{sp-f}} = N(\varepsilon_d - 4\tau) + \varepsilon_p \sum_f (\hat{n}_{f+\delta_x}^p + \hat{n}_{f+\delta_y}^p) + 2\tau(1-\eta) \sum_{f,\delta,\delta_1,\sigma} u_{\delta\delta_1} p_{f+\delta,\sigma}^+ p_{f+\delta_1,\sigma} +$$

$$+ 4\tau(1+\eta) \sum_{f,\delta,\delta_1,\sigma,\sigma',\alpha} u_{\delta\delta_1} p_{f+\delta,\sigma}^+ (S_f^\alpha \hat{\sigma}_{\sigma\sigma'}^\alpha) p_{f+\delta_1,\sigma'}, \tag{5}$$

where we introduce the notation $\tau = t_{pd}^2/\varepsilon_{pd}$, $\eta = \varepsilon_{pd}/(U_d - \varepsilon_{pd})$, and $u_{\delta\delta_1} = \vartheta(\delta)\vartheta(\delta_1)/4$. In (5), N is the number of unit cells in the CuO$_2$ plane, and $\hat{\sigma}^{x(y,z)}$ are the Pauli matrices.

For the operators $p_{f+\delta_{x(y)},\sigma}$, we pass to the quasimomentum representation,

$$p_{k,\delta_x,\sigma} = \frac{1}{\sqrt{N}} \sum_f e^{-ikf} p_{f+\delta_x,\sigma}, \qquad p_{k,\delta_y,\sigma} = \frac{1}{\sqrt{N}} \sum_f e^{-ikf} p_{f+\delta_y,\sigma}, \tag{6}$$

and define new operators ϕ and ψ as [17]–[20]

$$\phi_{k\sigma} = \frac{s_{kx} p_{k,\delta_x,\sigma} + s_{ky} p_{k,\delta_y,\sigma}}{s_k}, \qquad \psi_{k\sigma} = \frac{s_{ky} p_{k,\delta_x,\sigma} - s_{kx} p_{k,\delta_y,\sigma}}{s_k}, \tag{7}$$

where

$$s_{kx} = \sin \frac{k_x}{2}, \qquad s_{ky} = \sin \frac{k_y}{2}, \qquad s_k = \sqrt{s_{kx}^2 + s_{ky}^2}. \tag{8}$$

Using the inverse Fourier transform, we introduce the operators $\phi_{f\sigma}$ and $\psi_{f\sigma}$ in the Weiner representation:

$$\phi_{k\sigma} = \frac{1}{\sqrt{N}} \sum_f e^{-ikf} \phi_{f\sigma}, \qquad \psi_{k\sigma} = \frac{1}{\sqrt{N}} \sum_f e^{-ikf} \psi_{f\sigma}. \tag{9}$$

The effective Hamiltonian of the cuprate HTSC in the second order of the perturbation theory in t_{pd} in the Wannier representation is then written as

$$\hat{\mathscr{H}}_{\text{eff}}^\phi = N(\varepsilon_d - 4\tau) + \tilde{\varepsilon}_\phi \sum_{f,\sigma} \phi_{f\sigma}^+ \phi_{f\sigma} + \varepsilon_p \sum_{f,\sigma} \psi_{f\sigma}^+ \psi_{f\sigma} - t_g \sum_{f,g,\sigma} \phi_{f\sigma}^+ \phi_{f+g,\sigma} +$$

$$+ 4\tau(1+\eta) \sum_{f,n,m,\sigma,\sigma_1,\alpha} (s_n s_m^*) \phi_{f-m,\sigma}^+ (S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha) \phi_{f-n,\sigma_1}, \tag{10}$$

where $\tilde{\varepsilon}_\phi = \varepsilon_p + 2\tau(1-\eta)$, $t_g = \tau(1-\eta)/2$, and $s_f = (\sum_k e^{ikf} s_k)/N$.

An important feature of Hamiltonian (10) is the absence of interaction of ψ fermions and holes on the d orbitals of copper ions. The interaction between the states of ϕ fermions and d orbitals of copper ions is described by the last term and describes the processes of scattering of the ϕ current carriers on the localized spin moments with a spin flip or, in other words, the Kondo scattering processes. We note that these processes of the spin-correlated hoppings of ϕ fermions occur between arbitrarily distant cells.

For the parameters $t_{pd} = 1.3\,\text{eV}$, $\varepsilon_{pd} = 3.6\,\text{eV}$, and $U_d = 10.5\,\text{eV}$ of the three-band Emery model characteristic for cuprates [21], [22], we obtain $\tau = 0.47\,\text{eV}$, $\eta = 0.52$, and $t_g = 0.11\,\text{eV}$. The overlapping parameters $(s_n s_m)$ are controlled only by the lattice geometry and decrease rapidly as the numbers n and m of coordination spheres of the lattice of copper ions increase:

$$(s_0 s_0) = 0.920, \qquad (s_1 s_0) = (s_g s_0) = -0.136, \qquad (s_2 s_0) = (s_d s_0) = -0.022,$$
$$(s_3 s_0) = (s_{2g} s_0) = -0.010, \qquad (s_1 s_1) = (s_g s_g) = 0.020, \qquad (s_2 s_1) = 0.003. \tag{11}$$

We show that the Kondo scattering processes lead to the formation of spin-polaron states whose energy is much lower that the energy ε_p. This implies that the low-energy dynamics of fermions in the CuO_2 plane is described only by the spin polarons and the ψ-fermion subsystem can be neglected.

Omitting an insignificant constant, we represent the Hamiltonian as the sum of on-site terms and terms describing hoppings of the ϕ hole:

$$\hat{\mathscr{H}}_{\text{eff}}^\phi = \tilde{\varepsilon}_\phi \sum_{f,\sigma} \phi_{f\sigma}^+ \phi_{f\sigma} + \hat{J}_{\phi-d} + \varepsilon_p \sum_{f,\sigma} \psi_{f\sigma}^+ \psi_{f\sigma} + \hat{t}_g^\phi + \hat{t}^{\text{SC}}, \tag{12}$$

$$\hat{J}_{\phi-d} = \frac{J_{\phi-d}}{2} \sum_{f,\sigma,\sigma_1,\alpha} \phi_{f\sigma}^+ (S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha) \phi_{f\sigma_1} = J_{\phi-d} \sum_f \vec{S}_f \vec{s}_f^\phi,$$

$$J_{\phi-d} = 8\tau(1+\eta)(s_0 s_0), \qquad \hat{t}_g^\phi = -t_g \sum_{f,g,\sigma} \phi_{f\sigma}^+ \phi_{f+g,\sigma},$$

$$\hat{t}^{\text{SC}} = 4\tau(1+\eta) \sum_{f,n,m,\sigma,\sigma_1,\alpha} (1 - \delta_{m0}\delta_{n0})(s_n s_m) \phi_{f-m,\sigma}^+ (S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha) \phi_{f-n,\sigma_1}.$$

In the expression for $\hat{t}^{\text{SC}}$, the factor $1 - \delta_{m0}\delta_{n0}$ (where δ_{mn} is the Kronecker symbol) indicates the absence of the term in the summation with all three sites coinciding. Therefore, the operator $\hat{t}^{\text{SC}}$ describes only spin-correlated hoppings of the hole.

In effective Hamiltonian (12), the maximum term is the on-site $(\phi\text{-}d)$-exchange interaction: $\hat{J}_{\phi-d}$ with the parameter $J_{\phi-d}$. This interaction leads to the formation of two levels at each site. The lower level corresponds to the $(\phi\text{-}d)$-singlet state with the energy $\tilde{\varepsilon}_\varphi^- = \tilde{\varepsilon}_\phi - 3J_{\phi-d}/4$ and wave function $|\varphi_f\rangle = \varphi_f^+ |O\rangle$, where $\varphi_f^+ = (\phi_{f\uparrow}^+ Z_f^{\downarrow 0} + Z_f^{\uparrow 0} \phi_{f\downarrow}^+)/\sqrt{2}$. Here, the localized-spin operator is written using the representation in terms of the Hubbard operators, $Z_f^{\lambda_1 \lambda_2} = |\lambda_1\rangle\langle\lambda_2|$, and the ket vector $|O\rangle$ corresponds to the vacuum of the on-site cluster. The upper triply degenerate level with the energy $\tilde{\varepsilon}_\chi^+ = \tilde{\varepsilon}_\phi + J_{\phi-d}/4$ corresponds to the three $(\phi\text{-}d)$-triplet states with the wave functions

$$|\chi_{fm}\rangle = \chi_{fm}^+ |O\rangle, \quad m = -1, 0, 1, \tag{13}$$

where

$$\chi_{f0}^+ = \frac{1}{\sqrt{2}}(\phi_{f\uparrow}^+ Z_f^{\downarrow 0} - Z_f^{\uparrow 0} \phi_{f\downarrow}^+), \qquad \chi_{f,+1}^+ = \phi_{f\uparrow}^+ Z_f^{\uparrow 0}, \qquad \chi_{f,-1}^+ = \phi_{f\downarrow}^+ Z_f^{\downarrow 0}.$$

This level splitting is qualitatively similar to what arises when considering the Zhang–Rice cluster and polaron [23].

To justify the concept of a spin polaron, we define the distance

$$\Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-} = \varepsilon_p - \tilde{\varepsilon}_\varphi^-$$

between the level $\varepsilon_\psi = \varepsilon_p$ corresponding to the states of the ψ fermions and the singlet level $\tilde{\varepsilon}_\varphi^-$:

$$\Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-} = \varepsilon_p - \tilde{\varepsilon}_\phi + \frac{3}{4}J_{\phi-d} \approx 2\tau[5 + 7\eta]. \tag{14}$$

The low-frequency part of the hole spectrum is formed in the vicinity of the lower single-site level $\tilde{\varepsilon}_\varphi^-$ and is primarily controlled by the motion of the polaron state $|\varphi_f\rangle \to |\varphi_{f+g}\rangle$. If the half-width W of the band of this motion given by the terms $\hat{t}_g^\phi$ and $\hat{t}^{\mathrm{SC}}$ in Eq. (12) is smaller than $\Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$, then the ψ carriers can be neglected.

The width $2W$ of the band provided by the motion of polarons should show the polaron narrowing and in any case should be proportional to the spin–spin correlation function $C_g = \langle \vec{S}_f \vec{S}_{f+g} \rangle \simeq -0.2$ to -0.3 (characteristic values for the two-dimensional AFM in the spin-liquid state). This conclusion follows because the motion $|\varphi_f\rangle \to |\varphi_{f+g}\rangle$ is always associated with the combination of $\varphi_{f+g}^+\varphi_f$, which contains the spin operators on the nearest sites.

The half-width W_g of the band provided by the term $\hat{t}_g^\phi$ in Eq. (12) can be estimated as $W_g = 2t_g|C_g| = \tau(1 - \eta)|C_g|$. Comparing this expression with formula (14), we see that $W_g \ll \Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$.

The half-width W_{SC} of the band provided by $\hat{t}^{\mathrm{SC}}$ in (12) is defined by the term

$$\hat{t}_g^{\mathrm{SC}} = t_g^{\mathrm{SC}} \sum_{f,g,\sigma,\sigma_1,\alpha} [\phi_{f+g,\sigma}^+(S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha)\phi_{f\sigma_1} + \mathrm{H.c.}], \qquad t_g^{\mathrm{SC}} = 4\tau(1+\eta)(s_0 s_g), \tag{15}$$

which contains the maximum overlapping $(s_0 s_g) = -0.136$ in the operator $\hat{t}^{\mathrm{SC}}$ (see Eqs. (11)). The parameter t_g^{SC} is less than the constant of the $(\phi-d)$-exchange coupling $J_{\phi-d}$ by a factor of 13. With the factor C_g taken into account, this leads to the inequality $W_{\mathrm{SC}} \ll \Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$.

The inequalities $W_g \ll \Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$ and $W_{\mathrm{SC}} \ll \Delta_{\varepsilon_p=\varepsilon_\psi;\tilde{\varepsilon}_\varphi^-}$ follow from the inequalities $J_{\phi-d} \gg t_g^{\mathrm{SC}} \gg t_g$ and indicate that the term $\varepsilon_p \sum_{f,\sigma} \psi_{f\sigma}^+\psi_{f\sigma}$ in model (12) can be omitted and the concept of the spin polaron can be introduced.

As a result, Hamiltonian (12) takes the form of the Kondo lattice Hamiltonian

$$\hat{\mathscr{H}}_{\mathrm{eff}}^{\mathrm{K}} = \tilde{\varepsilon}_\phi \sum_{f,\sigma} \phi_{f\sigma}^+\phi_{f\sigma} + J_{\phi-d} \sum_f \vec{S}_f \vec{s}_f^\phi - t_g \sum_{f,g,\sigma} \phi_{f\sigma}^+\phi_{f+g,\sigma} +$$

$$+ 4\tau(1+\eta) \sum_{f,m,n,\sigma,\sigma_1,\alpha} (1 - \delta_{m0}\delta_{n0})(s_n s_m)\phi_{f-m,\sigma}^+(S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha)\phi_{f-n,\sigma_1}. \tag{16}$$

If we assume that the distant spin-correlated hoppings can be neglected in Eq. (16) in the leading approximation (keeping only terms with $(s_0 s_g)$), then we consequently obtain a Hamiltonian corresponding to the reduced Kondo lattice model:

$$\hat{\mathscr{H}}_{\mathrm{eff}}^{\mathrm{Kr}} = \tilde{\varepsilon}_\phi \sum_{f,\sigma} \phi_{f\sigma}^+\phi_{f\sigma} + J_{\phi-d} \sum_f \vec{S}_f \vec{s}_f^\phi - t_g \sum_{f,g,\sigma} \phi_{f\sigma}^+\phi_{f+g,\sigma} +$$

$$+ t_g^{\mathrm{SC}} \sum_{f,g,\sigma,\sigma_1,\alpha} [\phi_{f+g,\sigma}^+(S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha)\phi_{f\sigma_1} + \mathrm{H.c.}]. \tag{17}$$

In the last summation in this expression, the index f ranges all lattice sites of copper ions, and the index g ranges only the sites that are nearest the site f. The spectral characteristics of the Fermi quasiparticles in the cuprate HTSC were studied based on model (17) in [24], [25].

4. Basis operators and projection method

In the framework of the Zwanzig–Mori projection method [26], [27], we introduce a set of basis operators corresponding to the charge excitations. In our case, it is convenient to choose

$$A_{1f\sigma} = \phi_{f\sigma}, \qquad A_{2f\sigma} = \sum_{\sigma_1,\alpha}(S_f^\alpha \hat\sigma_{\sigma\sigma_1}^\alpha)\phi_{f\sigma_1}, \qquad A_{3f\sigma} = \sum_{\sigma_1,\alpha}(S_f^\alpha \hat\sigma_{\sigma\sigma_1}^\alpha)\phi_{f+g,\sigma_1} \tag{18}$$

as the basis operators. Basis (18) is constructed standardly. In the first step, we choose the "bare" hole operator $\phi_{f\sigma}$ as A_{1f}. The choice of the subsequent operators is dictated by the equation of motion for A_{1f}. The new operators of the type A_{2f} and A_{3f} arise from Eq. (18) as a result of the commutation $[\phi_{f\sigma}, \hat{\mathscr{H}}_{\text{eff}}^{\text{Kr}}]$. These operators are included in the basis, and the equations of motion are also written for them. If there is no need for a further increase in the basis, then the equations of motion for A_{jf} $(j = 1, 2, 3)$ are projected on the same basis.

It is convenient to realize the projection using the formalism of the equations of motion for the retarded Green's functions $(i, j = 1, 2, 3)$: $G_{ij}(k,\omega) = \langle\!\langle A_{ki}|A_{kj}^+ \rangle\!\rangle_\omega$, where $A_{jk\sigma} = \sum_f e^{-ikf} A_{jf\sigma}/\sqrt{N}$ are the Fourier transforms of operators (18).

For the closure of the equations of motion of the form

$$\omega \langle\!\langle A_{ki}|A_{kj}^+ \rangle\!\rangle_\omega = K_{ij} + \langle\!\langle [A_{ki}, \hat{\mathscr{H}}_{\text{eff}}^{\text{Kr}}]|A_{kj}^+ \rangle\!\rangle_\omega, \tag{19}$$

we must calculate the energy matrix $D_{ij} = \langle \{[A_{ik}, \hat{\mathscr{H}}_{\text{eff}}^{\text{Kr}}], A_{jk}^+\} \rangle$ and the matrix $K_{ij} = \langle \{A_{ik}, A_{jk}^+\} \rangle$. The Fermi Green's function is derived from a system of equations with the matrix form $\hat{G} = (\omega - \hat{D}\hat{K}^{-1})^{-1}\hat{K}$, and the spectrum of Fermi excitations is defined by the poles of this Green's function:

$$G_{ij}(k,\omega) = \sum_{n=1}^{3} \frac{z_{(i,j)}^n(k)}{\omega - E_n(k)}, \quad i, j = 1, 2, 3.$$

A more detailed description of this method can be found, for example, in [28].

Therefore, the problem of finding the spectrum $E_n(k)$ and the residues of the Green's functions $z_{(i,j)}^n(k)$ reduces to calculating the matrix elements K_{ij} and D_{ij}. These matrix elements calculated in the basis of the three operators (18) with the truncated Hamiltonian of Kondo lattice (17) are presented in the appendix.

A similar procedure for calculating the matrices $\hat{K}(k)$ and $\hat{D}(k)$ in the basis of the three operators (18) can also be performed for the complete Hamiltonian (16). But the matrix elements are cumbersome in this case, and we do not give their explicit form.

The method used for closing the equations of motion for the Green's functions is applicable over a broad temperature region. From the practical standpoint, the properties of cuprate HTSC at temperatures $T \leq 100\,\text{K}$ are most interesting. Taking into account that the characteristic energy parameters controlling the energy structure of the spin-polaron states are of the order of 0.1 to 0.5 eV, we find that in the considered temperature region, the spectrum of Fermi excitations can be studied in the low-temperature approximation.

The problem of the dependence of the energy of Fermi quasiparticles on the concentration of oxygen holes seems more challenging. But the situation is significantly simplified in solving the problem of the spin-polaron states in the normal phase for low temperatures. Indeed, in the narrow concentration region where antiferromagnetism is destroyed but there is still no superconductivity, the concentration of holes can be regarded as unchanged. In this case, the doping parameter is small: $x \simeq 5 \cdot 10^{-2}$.

In the general case, the matrix elements $\hat{K}$ and $\hat{D}$ depend on not only the spin–spin correlators and charge correlators but also the spin–charge correlators. Their concentration dependence was previously

studied in [29]. Not going into the details, we only note that in the considered case with weak doping, the contribution from the charge and spin–charge correlators turns out to be insignificant and negligible. This observation implies that in the considered narrow doping region, the problem of finding the spin-polaron states and the spectrum of Fermi excitations can be solved in the single-hole approximation.

Because we consider the energy structure of the spin-polaron excitations in the case where the localized-spin subsystem exists in the state of a quantum spin liquid, it seems natural that the spin–spin correlators significantly affect the final result. In this case, this theory involves the coupled spin–spin correlators C_j with $j = 1, 2, 3, 4$ and $j = 6$ and the three-site correlators. But the three-site correlators are equal to zero in a spin liquid. Spin correlators with a large number of sites do not arise in the considered approximation.

5. The role of distant spin-correlated hoppings

In this section, we discuss the problem related to the presence of spin-correlated hoppings between the Wanier lattice sites from the distant coordination spheres in the complete effective Hamiltonian. The importance of the spin-correlated hoppings of oxygen holes between sites located at large distances is demonstrated by the example of calculating the spectrum of Fermi excitations. At first sight, it can naturally be expected that because the effective hopping integrals decay relatively rapidly as a result of the multiplicative factors s_n and s_m, hoppings between the sites from distant coordination spheres give a small contribution to the energy spectrum. In fact, as follows from further considerations, this is far from true, primarily because the number of the sites to which a hole can hop also increases as the radius of the coordination sphere increases. These conclusions serve as the basis for the study, and we present the results of this study below.

First, we present the results of calculating the spectrum of Fermi excitations according to generalized Kondo lattice model (16). In Fig. 1, the bold solid line corresponds to the branch of the spin-polaron excitations $E_{\mathrm{sp}}(k)$, which is obtained from the solution of the dispersion equation $|\omega - \hat{D}(k)\hat{K}^{-1}(k)| = 0$. This solution corresponds to the lower of the three branches of the energy spectrum (see the inset in Fig. 1).

The thin solid line is constructed for Hamiltonian (17) of the reduced Kondo lattice model; only hoppings between nearest neighbors are taken into account in the Hamiltonian. In each of these two cases, the same basis of the three operators (18) with the corresponding matrix elements K_{ij} and D_{ij} is used. It can be seen that in the direction Γ–M, the thin solid curve has a minimum in the vicinity of the point $(\pi/2, \pi/2)$ of the Brillouin zone, and the width of the band of the spin polarons does not exceed $0.2\,\mathrm{eV}$.

It follows from a comparison of the two mentioned curves that despite the presence of the majorant factors s_n and s_m, taking distant hoppings into account substantially changes the characteristics of the spin-polaron band, leading to five-fold increase (nearly an order of magnitude) in its width. This implies that neglecting distant hoppings leads to a large error in the effective mass of the Fermi carriers, which has a primary importance for the kinetics and low-temperature dynamics of cuprate HTSC.

We note that the spin-polaron spectrum for the complete Kondo lattice model (16) was previously calculated in [28], [30]. In this case, the Hamiltonian is written in form (5), and to calculate the dispersion curves, we used a set of basis operators different from (18):

$$\bar{A}_{1f\sigma} = p_{f+\delta_x,\sigma}, \qquad \bar{A}_{2f\sigma} = p_{f+\delta_y,\sigma}, \qquad \bar{A}_{3f\sigma} = \frac{1}{2} \sum_{\delta,\sigma_1,\alpha} (S_f^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha) p_{f+\delta,\sigma_1}. \qquad (20)$$

The spin-polaron spectrum obtained in [28], [30] is shown in Fig. 1 by the dashed line.

It can be seen that the bold solid curve and the dashed curve, calculated for the same Hamiltonian (16) but using different basis operators (18) and (20), exhibit a good coincidence. The bold solid curve has a minor energy gain because basis (18) takes more spin–charge degrees of freedom into account than basis (20) does. Indeed, the spin–charge correlations are included in two sets, A_{2f} and A_{3f}, of basis operators in
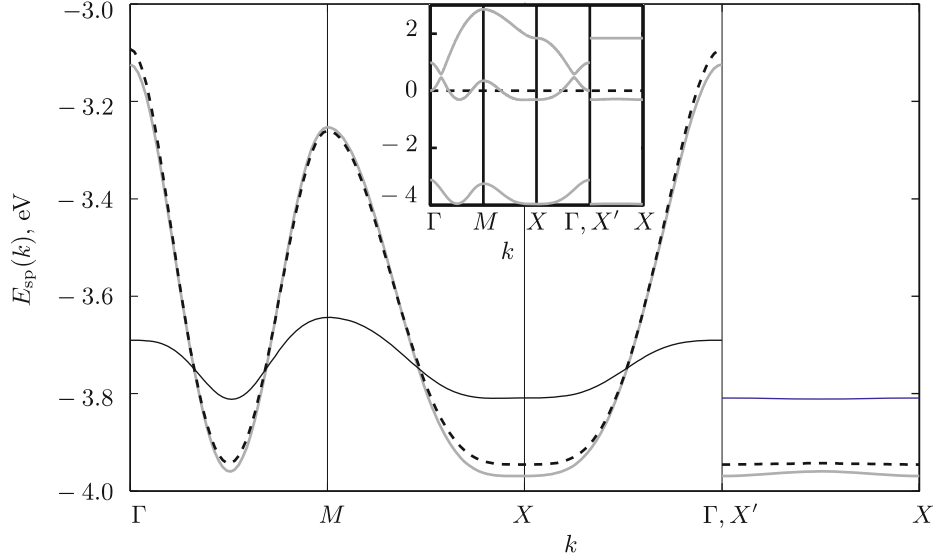
Fig. 1. Dispersion curves of the lower band of spin-polaron excitations for the three effective Hamiltonians of the three-band Emery model: the bold solid curve is calculated for the complete Kondo lattice Hamiltonian (16), the thin solid curve corresponds to Kondo lattice model (17) with distant hoppings omitted, and the dashed curve corresponds to spin–fermion model (5). The calculations were performed with the model parameters $\tau = 0.47$ eV and $\eta = 0.52$. For simplicity, $I = 0$. The values of the pair spin correlation functions were chosen as $C_1 = -0.255$, $C_2 = 0.075$, and $C_3 = 0.064$; all C_j for $j > 3$ are zero. The symmetry points of the Brillouin zone have the coordinates $\Gamma = (0, 0)$, $M = (\pi, \pi)$, $X = (\pi, 0)$, and $X' = (0, \pi)$. The inset shows the dispersion curves describing all three solutions of the cubic dispersion equation $|\omega - \hat{D}\hat{K}^{-1}| = 0$ for Hamiltonian (16) of the Kondo lattice model in basis (18). The lower curve coincides with the bold solid curves in the main plot. The horizontal dashed line in the inset shows the position of the energy level of the inactive ψ orbital.

basis (18) and in the single set $\bar{A}_{3f}$ in basis (20). In this case, in contrast, purely charge degrees of freedom are included in the two sets $\bar{A}_{1f}$ and $\bar{A}_{2f}$ of operators in basis (20) and in the single set A_{1f} in basis (18). But in the absence of direct p–p hoppings and with the condition $\varepsilon_{pd} \gg t_{pd}$ taken into account, the last fact does not provide any benefits in favor of basis (20).

In the inset in Fig. 1, the solid lines shows all three dispersion curves corresponding to the complete Kondo lattice model (16) and calculated with three basis operators (18). The horizontal dashed line corresponds to the energy of the inactive ψ orbital. It can be seen that the lower spin-polaron band is separated from the bare energy ε_p of the oxygen p orbitals (here, assumed to be zero) downward by a value of about 3 eV.

6. The role of direct oxygen–oxygen hoppings

An important feature of the hole spectrum for cuprate HTSC is the existence of the absolute minimum in the vicinity of the point $(\pi/2, \pi/2)$ of the Brillouin zone. The dispersion curves in Fig. 1 show the minimum only in the direction Γ—M, but not in the direction M–M'. This "incorrect" behavior is related to our neglect of the direct p–p hoppings in constructing effective Hamiltonian (16). Taking these hoppings into account is likely to lead to renormalizing the tunneling integral t_g between nearest neighbors and also to initiating new hoppings between distant cells with a rate rapidly decaying with distance.

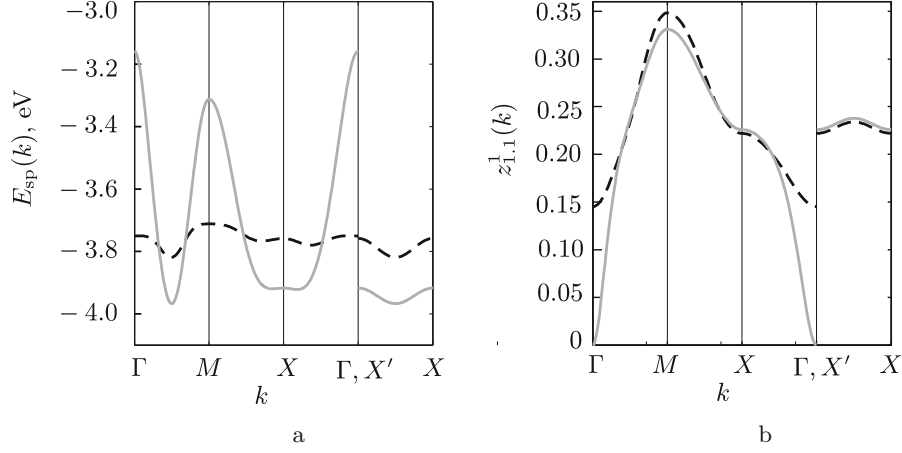As an example, we consider the hopping between the next-nearest cells with the tunneling integral t_d,

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Fig. 2. (a) Spectrum and (b) spectral intensity of the lower band of the spin-polaron states calculated with hopping of quasiparticles between the next-nearest cells taken into account (see (21)): solid lines correspond to complete Kondo lattice model (16), and dashed lines correspond to reduced Kondo lattice model (17). In both cases, three basis operators (18) are used. The tunneling integral is $t_d = 0.05\,\text{eV}$. The other model parameters have the same values as in Fig. 1.

which is the largest of the initiated hoppings. The corresponding kinetic-energy operator

$$\hat{t}^d = -t_d \sum_{f,d,\sigma} \phi_{f\sigma}^+ \phi_{f+d,\sigma} \tag{21}$$

should be added to Hamiltonians (16) and (17). In this case, each matrix element D_{ij} of the energy matrix is additionally renormalized by

$$t_{ij}^d = \langle\{[A_{ik\sigma}, \hat{t}^d], A_{jk\sigma}^+\}\rangle, \quad i,j = 1,2,3.$$

Calculating the matrix elements $t_{ij}^d = t_{ji}^d$ gives the relations

$$t_{11}^d = -4t_d\gamma_{2k}, \qquad t_{12}^d = t_{13}^d = 0, \qquad t_{22}^d = -4t_dC_2\gamma_{2k}, \qquad t_{23}^d = -8t_d(C_1\gamma_{1k} + C_4\gamma_{4k}),$$

$$t_{33}^d = -8t_d\left(\frac{3}{4} + 3C_2\gamma_{2k} + 2C_3\gamma_{3k} + C_5\gamma_{5k} + C_7\gamma_{7k}\right), \tag{22}$$

where $\gamma_{5k} = \cos 2k_x \cos 2k_y$ and $\gamma_{7k} = (\cos k_x \cos 3k_y + \cos 3k_x \cos k_y)/2$.

    In Fig. 2a, the solid line depicts the spectrum of spin polarons calculated with three basis operators (18) based on complete Hamiltonian (16) of the Kondo lattice extended by adding the operator $\hat{t}^d$, which takes hoppings to the next-nearest cells into account. The dashed line shows the spin-polaron spectrum of reduced Kondo model (17) obtained with the same basis (18) with the hopping operator $\hat{t}^d$ taken into account.

    Comparing these curves with the similar dependences in Fig. 1 shows that taking the p–p hoppings into account leads to a minimum in the spectrum of Fermi spin-polaron excitations developing in the vicinity of the points $(\pm\pi/2, \pm\pi/2)$ of the Brillouin zone in the directions Γ–M and X–X'. This is important and is responsible for the existence of small hole pockets at these points that are observed in the angle-resolved photoemission (ARPES) experiments with weakly hole-doped copper-based HTSC. This evolution

of the Fermi surface with doping of the compound $\mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4$ in terms of the projection method was studied in [30]. The resulting Fermi surfaces and the dependences of the Fermi momentum on x show a fair agreement with the results of ARPES measurements [31].

Figure 2b shows the dependence of the residues $z_{(1,1)}^{(1)}(k)$ of the Green's function $G_{11}(k,\omega)$ on the wave vector k. These residues determine the contribution of "bare" hole states to the lower spin-polaron state for each k. It can be seen that in the case of complete Kondo lattice Hamiltonian (16), the contribution of "bare" holes to the spin-polaron state becomes zero at the Γ point of the Brillouin zone. This behavior fully agrees with the results of calculating $z_{(1,1)}^{(1)}(k)$ using spin–fermion model (5) with basis operators (20) in [32], [33]. But this behavior is not reproduced for reduced Hamiltonian (17). In this case, as follows from Fig. 2b, the residue of the Green's function $z_{(1,1)}^{(1)}(k)$ does not vanish at the Γ point of the Brillouin zone. This also demonstrates the importance of taking the distant spin-correlated hoppings into account.

7. Conclusion

We have demonstrated a regular way to obtain an effective low-energy Hamiltonian for the three-band Emery model. The main conclusion form the presented consideration is related to the statement that the effective low-energy model of the electron structure of the CuO_2 plane is a generalized model of the regular Kondo lattice. Its most important feature is the presence of effective spin-correlated hoppings of fermions between sites of the Wanier lattice from distant coordination spheres.

For the obtained generalized Kondo lattice model, we analyzed the role of distant spin-correlated hoppings. Based on a comparison of the dispersion curves of the spin-polaron spectrum and the spectral density of "bare" holes calculated for complete generalized Kondo lattice model (16) and its reduced version (17), we clearly demonstrated the essential role of distant spin-correlated hoppings. In particular, we showed that taking these interactions into account leads to a significant (five-fold) increase in the width of the spin-polaron band and also an additional decrease in the minimum energy of the spin-polaron quasiparticle.

We analyzed the role of the direct oxygen p–p hoppings and showed that these hoppings must be taken into account to reproduce the experimentally observed minimum of the dispersion law for spin-polaron excitations at the points $(\pm\pi/2, \pm\pi/2)$ of the Brillouin zone.

We note that in the framework of the ordinary Kondo lattice model for doped two-dimensional AFM, the pseudo-gap behavior of the spectral function of current carriers and the anomalous temperature behavior of the kinetic coefficients was previously considered in [34], [35]. But those studies contained an essential deficiency related to ignoring the processes of the motion of holes with a spin flip. As a result, to achieve a satisfactory agreement of the theory and experiment, it was necessary to artificially introduce additional hoppings on the first three nearest neighbors for the bottom of the bare band (i.e., without spin interactions) to be located near the boundary of the magnetic Brillouin zone. This problem does not arise if Kondo lattice model (16) obtained here is used to describe the spectral characteristics of the cuprate HTSC.

Appendix

The matrix elements $\hat{D}(k)$ and $\hat{K}(k)$ calculated using reduced Hamiltonian (17) of the Kondo lattice with three basis operators (18) have the forms ($D_{ij} = D_{ji}$, $K_{ij} = K_{ji}$)

$$K_{11} = 1, \qquad K_{12} = K_{13} = 0, \qquad K_{22} = \frac{3}{4}, \qquad K_{23} = 4C_1\gamma_{1k},$$

$$K_{33} = 3 + 8C_2\gamma_{2k} + 4C_3\gamma_{3k};$$

$$D_{11} = \varepsilon_p + 4t_g(1 - \gamma_{1k}), \qquad D_{12} = \frac{3}{8}J_{\phi-d} + t_g^{\mathrm{sc}}(3 + 4C_1)\gamma_{1k},$$

$$D_{13} = 2J_{\phi-d}C_1\gamma_{1k} + 4t_g^{\mathrm{sc}}\left(\frac{3}{4} + 4C_1\gamma_{1k}^2 + 2C_2\gamma_{2k} + C_3\gamma_{3k}\right),$$

$$D_{22} = \frac{3}{4}(\varepsilon_p + 4t_g) - 4t_g C_1\gamma_{1k} - \frac{3}{8}J_{\phi-d} - 8t_g^{\mathrm{sc}}C_1\gamma_{1k},$$

$$D_{23} = (\varepsilon_p + 4t_g)4C_1\gamma_{1k} - t_g(3 + 8C_2\gamma_{2k} + 4C_3\gamma_{3k}) -$$
$$- 2J_{\phi-d}C_1\gamma_{1k} - 4t_g^{\mathrm{sc}}\left(\frac{3}{4} - C_1 + 2C_2\gamma_{2k} + C_3\gamma_{3k}\right),$$

$$D_{33} = (\varepsilon_p + 4t_g)(3 + 8C_2\gamma_{2k} + 4C_3\gamma_{3k}) - 4t_g(9C_1\gamma_{1k} + 6C_4\gamma_{4k} + C_6\gamma_{6k}) +$$
$$+ 2J_{\phi-d}C_1 - 32t_g^{\mathrm{sc}}C_1\gamma_{1k},$$

(A.1)

where the functions γ_{jk} $(j = 1, 2, 3, 4, 6)$ are the invariants of the square lattice,

$$\gamma_{1k} = \frac{\cos k_x + \cos k_y}{2}, \qquad \gamma_{2k} = \cos k_x \cos k_y, \qquad \gamma_{3k} = \frac{\cos 2k_x + \cos 2k_y}{2},$$
$$\gamma_{4k} = \frac{\cos 2k_x \cos k_y + \cos 2k_y \cos k_x}{2}, \qquad \gamma_{6k} = \frac{\cos 3k_x + \cos 3k_y}{2}.$$

To derive expressions (A.1), we use the relations $(\tilde{S}_m = \sum_\alpha S_m^\alpha \hat{\sigma}^\alpha)$

$$\langle \tilde{S}_m \tilde{S}_n \rangle = C_{m-n}, \qquad \langle \tilde{S}_f \tilde{S}_m \tilde{S}_n \rangle = -\delta_{f,m}C_{f-n} - \delta_{m,n}C_{f-m} + \delta_{f,n}C_{f-m},$$

which hold in the $SU(2)$-invariant spin-liquid phase, and also the identity

$$\sum_f s_{f-n}s_{f-m} = \delta_{m,n} - \frac{1}{4}\sum_g \delta(m - n - g),$$

(A.2)

where the vectors f, n, and m range all the sites of the sublattice of copper ions and the vector g takes the four values $(\pm a, 0)$ and $(0, \pm a)$.

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