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SUPERCONDUCTIVITY, INCLUDING HIGH-TEMPERATURE SUPERCONDUCTIVITY

Hierarchy of low-energy models of the electronic structure of cuprate HTSCs: The role of long-range spin-correlated hops

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It is shown that for the three-band Emery p–d-model that reflects the real structure of the CuO_2-plane of high-temperature superconductors in the regime of strong electron correlations, it is possible to carry out a sequence of reductions to the effective models reproducing low-energy features of elementary excitation spectrum and revealing the spin-polaron nature of the Fermi quasiparticles. The first reduction leads to the spin-fermion model in which the subsystem of spin moments, coupled by the exchange interaction and localized on copper ions, strongly interacts with oxygen holes. The second reduction deals with the transformation from the spin-fermion model to the φ–d-exchange model. An important feature of this transformation is the large energy of the φ–d-exchange coupling, which leads to the formation of spin polarons. The use of this fact allows us to carry out the third reduction, resulting in the $\tilde{t} - \tilde{J}^* - I$-model. Its distinctive feature is the importance of spin-correlated hops as compared to the role of such processes in the commonly used t–J*-model derived from the Hubbard model. Based on the comparative analysis of the spectrum of Fermi excitations calculated for the obtained effective models of the CuO_2-plane of high-temperature superconductors, the important role of the usually ignored long-range spin-correlated hops is determined. *Published by AIP Publishing.* https://doi.org/10.1063/1.5020908

1. Introduction

It is known that the three-band p–d-model[1–4] includes interactions that enable describing the main features of the electronic structure of the CuO_2-plane in high-temperature superconductors (HTSs). However, the theoretical complexity that arises in this description due to the presence of three ions in the unit cell with strong electron correlations (SEC), resulted in an effort to reduce the three-band p–d-model to a simple effective model.

To account for the hybridization between the d-states of the copper ions and the p-states of the four nearby oxygen ions, Ref. 5 introduced a symmetric oxygen orbital. The hole, located on this orbital, forms a strongly coupled state with the localized spin moment of the copper ion (Zhang-Rice singlet). Keeping in mind the large energy of this interaction, the descriptions of carrier dynamics in the CuO_2-plane has been carried out by only considering the singlet states. It was assumed that this approach would allow analysis of the cuprate electronic properties in the framework of the single-band t–J-model.[6,7]

The concept of the singlet state formation[5] was also developed in works.[8–12] Analogous to the approach in Ref. 5, they employed a transition from the p_x- and p_y-orbitals of the oxygen ions to Wannier functions (φ- and ψ-orbitals) of the unit cells which host a copper ion in their center. An important property of these orbitals is that only φ was hybridized with the d-state of the copper ions forming the Zhang-Rice singlet, whereas the second ψ orbital remained inactive. As a result, this significantly simplified the problem of finding the energy spectrum and the eigenstates of a single unit cell while accounting for SEC.[12,13]

Introduction of single-cell states allowed to switch over to the atomic representation of the three-band p–d-model Hamiltonian. This approach, termed by the authors in Ref. 12 as generalized tight-binding (GTB) approach, resulted in a complicated and non-transparent structure of the Hamiltonian, since certain types of Coulombic (V_{pd}, V_{pp}, U_p), as well as hybridizational (t_{pd}) interactions became significantly nonlocalized. Therefore, during the actual calculations, the method was limited to a small number of single-cell states corresponding only to the lowest-lying energy states, as well as the intercell interactions between the nearest neighbors. The last point becomes a significant weakness of the method in those cases when the small size of the discarded interactions is compensated by an increase in their number due to an increase in the number of ions in the outer coordination spheres.[14]

Analysis of various interactions arising in the three-band p–d-model effective Hamiltonian was carried out in the

framework of the GTB method.[15] Studies were carried out to justify the legitimacy of using the t–J–V-model for determining the electronic properties of cuprates,[16] as well as the generalization of this method to the multi-band p–d-model, accounting for the state of the topmost oxygen.[4,7,18]

An alternative method for constructing the p–d-model effective Hamiltonian was introduced in Refs. 14, 19, and 20 and was used in studies of HTS cuprates in both normal[21–25] and superconducting phases.[26,27] This method relies on the relatively small value of the hybridization parameter between the p-states of the oxygen ions and the d-states of the copper ions t_{pd} compared to the energy difference between these states ($\Delta_{pd} = \varepsilon_p - \varepsilon_d$) and the Coulombic repulsion parameter between the two holes on the copper ion U_d. These conditions allowed the determination of the three-band p–d-model effective Hamiltonian, using second-order perturbation theory in the t_{pd}/Δ_{pd} and $t_{pd}/(U_d - \Delta_{pd})$ parameters, to assume the form of a SU(2)-invariant spin-fermion model, where the copper ion states were described in the homeopolar state subspace.

It is worth noting that the aforementioned works,[14,19–27] did not use the φ- and ψ-orbitals to study the properties of the spin-fermion model. The switch to the symmetrized orbitals for the spin-fermion model was carried out in Ref. 28. It was shown that the φ-d-exchange model that arises in this case, contains spin-correlated hops between nodes, corresponding to the far-lying cells. However, the calculation of the cuprate spectral properties with this expanded φ–d-exchange model in the works,[28,29] only accounted for the spin-correlated hops between the nearest neighbors.

The current work starts with the three-band p–d-model and proceeds to sequentially construct the three mentioned effective models of the cuprate superconductor electronic structure, while comparing their spectral properties. Section 2 formulates the Hamiltonian for the three-band p–d-model using the second quantization. In Sec. 3, this Hamiltonian is formulated in the atomic representation with the aid of Hubbard operators in order to correctly describe the SEC effect. Section 4, uses the operator formulation of the perturbation theory and derives the Hamiltonian of the spin-fermionic model up to second order in the t_{pd}/Δ_{pd} and $t_{pd}/(U_d - \Delta_{pd})$ parameters. Section 5 switches to the Wannier functions and formulates the φ–d-exchange model. Section 6 introduces the strict reduction of the low-energy $\tilde{t} - \tilde{J}^* - I$-model. An important difference between this model and the regular t–J^*-model that is obtained from the single-band Hubbard model is discussed. Section 7 is dedicated to the calculation of the Fermi spectrum of spin-polaron excitations in the framework of each of the introduced effective models. Comparison of the obtained dispersion curves leads to a conclusion involving the important role of the long-range spin-correlated hops. The main results of the work are summarized in Sec. 8.

2. Emery model Hamiltonian

It is well known that the main features of the electronic structure of the CuO_2-plane in high-temperature superconductors is well described by the Emery model[1–3] that describes the system of holes on the copper and oxygen ions. The Hamiltonian for this model can be represented as

$$\hat{\mathcal{H}} = \varepsilon_d \sum_f \hat{n}_f^d + \varepsilon_p \sum_l \hat{n}_l^p + U_d \sum_f \hat{n}_{f\uparrow}^d \hat{n}_{f\downarrow}^d + U_p \sum_l \hat{n}_{l\uparrow}^p \hat{n}_{l\downarrow}^p + \hat{V}_{pd} + \hat{T}_{pd} + \hat{T}_{pp} + \hat{V}_{pp}, \quad (1)$$

where

$$\hat{V}_{pd} = V_{pd} \sum_{f\delta} \hat{n}_f^d \hat{n}_{f+\delta}^p,$$
$$\hat{T}_{pd} = \sum_{f\delta\sigma} t_{pd} \left[\vartheta(\delta) d_{f\sigma}^+ p_{f+\delta,\sigma} + \text{h.c.} \right],$$
$$\hat{T}_{pp} = \sum_{l\Delta\sigma} t_{pp}(\Delta) p_{l\sigma}^+ pl + \Delta, \sigma,$$
$$\hat{V}_{pp} = \sum_{ll'} V_{pp}(l - l') \hat{n}_l^p \hat{n}_{l'}^p. \quad (2)$$

The first and second terms of the Hamiltonian (1) describe the interaction energy between the hole on the copper and the oxygen ions. The oxygen and copper ion positions are labeled with indices f and l, respectively. When summing over l, one needs to account for the fact that a single unit cell of the CuO_2-plane has two oxygen ions. Number operators for the particles on the copper and oxygen ions are determined by the expressions

$$\hat{n}_f^d = \sum_\sigma \hat{n}_{f\sigma}^d = \sum_\sigma d_{f\sigma}^+ d_{f\sigma}, \quad \hat{n}_l^p = \sum_\sigma \hat{n}_{l\sigma}^p = \sum_\sigma p_{l\sigma}^+ p_{l\sigma},$$

where $d_{f\sigma}^+(d_{f\sigma})$ is the creation (annihilation) operator of the hole on the copper ion in the f position with a spin of $\sigma = \pm 1/2$, and $p_{l\sigma}^+(p_{l\sigma})$ is the creation (annihilation) operator for the hole on the oxygen ions at the l node with a spin of σ. ε_d is the intrinsic hole energy on the copper ion, and ε_p for the oxygen ion.

The third (fourth) term of the Hamiltonian $\hat{\mathcal{H}}$ accounts for the energy of the Hubbard repulsion between two holes with opposing spin projections, located on a single copper (oxygen) ion. The repulsion parameter is denoted by $U_d(U_p)$.

The $\hat{V}_{pd}$ operators in the expression (1), describe the Coulombic interaction between the holes, located on adjacent oxygen and copper ions. The magnitude of this interaction is determined by the V_{pd} parameter. The $\boldsymbol{\delta}$ vector, connecting the copper ion with nearest neighbor oxygen ions, assumes four values $\boldsymbol{\delta} = (\pm a/2, 0), (0, \pm a/2)$.

The term describing the hybridization processes in the p–d-model Hamiltonian, is denoted by $\hat{T}_{pd}$. The t_{pd} parameter determines the intensity of the transition process of the hole from the copper ion to any other nearest oxygen ion and back. The $\vartheta(\delta)$ function accounts for the influence of the relation between the phases of the copper and oxygen orbitals on the hybridization process. For the orbital profiles shown in Fig. 1, the function $\vartheta(\delta)$ assumes the following values: $\vartheta(\delta) = 1$ when $\delta = (-a/2, 0), (0, -a/2)$, and $\vartheta(\delta) = -1$ when $\delta = (a/2, 0), (0, a/2)$.

The $\hat{T}_{pp}$ operator in the Hamiltonian (1) describes the hole hops along the oxygen orbitals. The hole hopping integral between the neighboring oxygen orbitals is denoted as $t_{pp}(\Delta) = t_{pp}\rho(\Delta)$. The sign of the integral is determined by the $\rho(\Delta)$ function, where the Δ vector connects the nearest oxygen ions. For the selected sequence of oxygen orbital phases, $\rho(\Delta) = 1$ when $\Delta = (a/2, a/2), (-a/2, -a/2)$, and $\rho(\Delta) = -1$ when $\Delta = (a/2, -a/2), (-a/2, a/2)$.

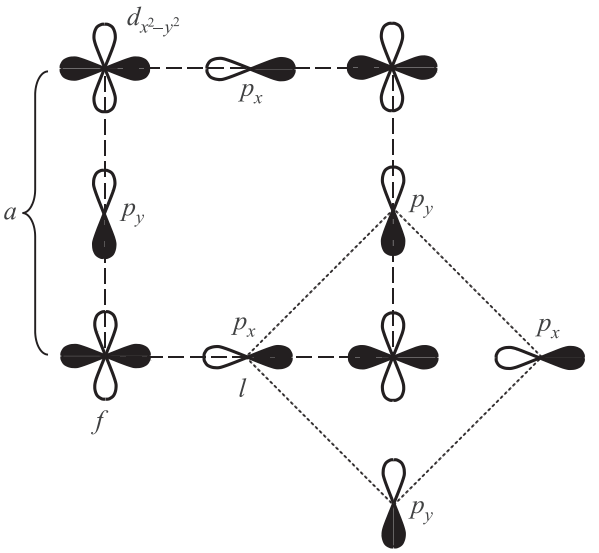

Fig. 1. Orbitals of the copper ($d_{x^2-y^2}$) and the oxygen (p_x, p_y) holes of the CuO_2-plane, in the Emery model. The dashed line represents the unit cell boundary with a parameter a. The dotted line connects the four oxygen orbitals closest to the copper orbital located in the lower right-hand corner of the unit cell.

The last term in (1) is represented with the $\hat{V}_{pp}$ operator, and determines the Coulombic interaction between the holes located on the oxygen nodes l and l'. The strength of this interaction is characterized by the $V_{pp}(l-l')$ function.

3. Emery model in strong correlation regime. Atomic representation

If a single CuO_2-plane unit cell contains only one hole, then according to experimental data, the state of the system can be described as a Mott-Hubbard dielectric. In the Emery model, this ground state occurs in the regime of strong electron correlations when

$$(U_d - \Delta_{pd}),\ \Delta_{pd} \gg t_{pd} > 0. \tag{3}$$

The large gap value with a charge transfer $\Delta_{pd} = \varepsilon_p - \varepsilon_d$ and the difference $U_d - \Delta_{pd}$ requires careful consideration. This is accomplished in two steps. The first step involves introducing the atomic representation with the aid of the Hubbard operators, that enables including the effects of strong electron correlations into the zero-order approximation Hamiltonian. The second step involves construction the effective Hamiltonian, $\hat{\mathcal{H}}_{\text{eff}}$, in the framework of the operator form perturbation theory, for which the Hilbert space does not contain high-energy "double" (with two holes) or "empty" (without holes) states on the copper ion. The processes involving excitations into these states are accounted for by the perturbation theory and are manifested in the $\hat{\mathcal{H}}_{\text{eff}}$ as additional interactions.

The Hubbard operators Z_f^{mn}, corresponding to the copper ion subsystem are determined in the usual fashion: $Z_f^{mn} = |f;m\rangle\langle f;n|$, where $|f;m\rangle$ are the coper ion states on the f node. There are four states such as these: $|f;0\rangle$ is the copper ion state without a hole. $|f;\sigma\rangle = d_{f\sigma}^{+}|f;0\rangle$ are single hole states with a spin projection σ. $|f;2\rangle == d_{f\uparrow}^{+}d_{f\downarrow}^{+}|f;0\rangle$ — is the two-hole state at the f node. The Hilbert subspace for the entire copper subsystem is defined as the linear product of each of the copper ions' subspaces.

The switch to the atomic representation for the operators belonging to the copper subsystem is accomplished by connecting the Fermi and the Hubbard operators

$$d_{f\sigma} = Z_f^{0\sigma} + 2\sigma Z_f^{\bar{\sigma}2}, \quad (\sigma = \pm 1/2, \bar{\sigma} \equiv -\sigma). \tag{4}$$

Since the main goal of this work is investigating the role of long-range spin-correlated hops during formation of the spin-polaron spectrum, for simplicity, we discard those interaction terms of the Hamiltonian (1) that do not have a direct relation to the current problem, i.e., let's assume that: $t_{pp} = 0$, $U_p = 0$, $V_{pp} = 0$ and $V_{pd} = 0$. Then the Hamiltonian in the Emery model has the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}, \tag{5}$$

where

$$\hat{\mathcal{H}}_0 = \varepsilon_d \sum_{f\sigma} Z_f^{\sigma\sigma} + (2\varepsilon_d + U_d) \sum_f Z_f^{22} + \varepsilon_p \sum_f \left(\hat{n}_{f+\frac{x}{2}}^p + \hat{n}_{f+\frac{y}{2}}^p \right), \tag{6}$$

$$\hat{\mathcal{H}}_{\text{int}} = \hat{T}_{pd} = \sum_{f\delta\sigma} t_{pd} \left[\vartheta(\delta) \left(Z_f^{\sigma 0} + 2\sigma Z_f^{2\bar{\sigma}} \right) p_{f+\delta,\sigma} + \text{h.c.} \right]. \tag{7}$$

4. Reduction to the spin-fermion model

As was previously mentioned, in the undoped case, when a single unit cell contains only one hole, the ground state of the system can be described as an antiferromagnetic dielectric. In this case, the hole is located on the copper ion. Keeping in mind that the "double" and the "empty" states on the copper ions manifest only virtually, we use the projection operator during construction of the effective Hamiltonian in the perturbation theory operator form

$$\mathcal{P} = \prod_f \left(Z_f^{\uparrow\uparrow} + Z_f^{\downarrow\downarrow} \right). \tag{8}$$

Then the effective Hamiltonian can be represented in the form of an expansion[30]

$$\hat{\mathcal{H}}_{\text{eff}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}^{(2)} + \hat{\mathcal{H}}^{(3)} + \hat{\mathcal{H}}^{(4)} + \cdots, \tag{9}$$

where

$$\hat{\mathcal{H}}_0 = \varepsilon_d \sum_{f\sigma} Z_f^{\sigma\sigma} + \varepsilon_p \sum_f \left(\hat{n}_{f+\frac{x}{2}}^p + \hat{n}_{f+\frac{y}{2}}^p \right), \tag{10}$$

$$\hat{\mathcal{H}}^{(2)} = -\left(\mathcal{P}\hat{\mathcal{H}}_{\text{int}} - \mathcal{P}\hat{\mathcal{H}}_{\text{int}}\mathcal{P} \right) \left(\hat{\mathcal{H}}_0 - E_0 \right)^{-1} \left(\hat{\mathcal{H}}_{\text{int}}\mathcal{P} - \mathcal{P}\hat{\mathcal{H}}_{\text{int}}\mathcal{P} \right). \tag{11}$$

Carrying out simple calculations yields that the contributions of the "double" and the "empty" copper ion states to the effective Hamiltonian in the second-order perturbation theory can be defined by the expression

$$\hat{\mathcal{H}}^{(2)} = -4N \frac{t_{pd}^2}{\Delta_{pd}} + \varepsilon_2 \sum_{f\delta\delta_1\sigma} u\delta\delta_1 p_{f+\delta,\sigma}^{+} p_{f+\delta_1,\sigma} + J \sum_{f\delta\delta_1\sigma\sigma'} u\delta\delta_1 p_{f+\delta,\sigma}^{+} (\mathbf{S}_f \mathbf{s}_{\sigma\sigma'}) p_{f+\delta_1,\sigma'}, \tag{12}$$

where the first term determines the interaction energy contribution of the covalent mixing processes. The second term

leads to a renormalization of the initial spectrum of the hole states on the oxygen ions. The degree of this renormalization depends on the magnitudes of

$$\varepsilon_2 = 2t_{pd}^2\left(\frac{1}{\Delta_{pd}} - \frac{1}{U_d - \Delta_{pd}}\right), \quad u_{\delta\delta_1} = \frac{1}{4}\vartheta(\delta)\vartheta(\delta_1). \quad (13)$$

The third term is due to the exchange interaction between the spins of the Fermi subsystem of oxygen holes with spins of the copper ion subsystem. The parameter J of this interaction is determined by the following expression:

$$J = 8t_{pd}^2\left(\frac{1}{\Delta_{pd}} + \frac{1}{U_d - \Delta_{pd}}\right). \quad (14)$$

In expression (12) $\mathbf{S}_f$ is the vector operator of the spin localized on the f node. $\mathbf{s} = \boldsymbol{\tau}/2$ is an operator where the $\boldsymbol{\tau}$ vector is composed of Pauli matrices: $\boldsymbol{\tau} = (\tau^x, \tau^y, \tau^z)$.

It is known from Ref. 31, that an exchange interaction between the copper ion spin moments arises in the fourth-order with respect to the t_{pd} parameter,

$$\mathcal{H}_{\text{exch}} = \frac{1}{2}\sum_{fm} I_{fm}(\mathbf{S}_f\mathbf{S}_m), \quad (15)$$

with the magnitude of the exchange parameter[32,33]

$$I = \frac{4t_{pd}^4}{\Delta_{pd}^2}\left(\frac{1}{U_d} + \frac{1}{\Delta_{pd}}\right). \quad (16)$$

The terms listed in formulas (10), (12) and (15) determine the Hamiltonian of the spin-fermion model

$$\mathcal{H}_{sp-f} = \varepsilon_p\sum_l \hat{n}_l^p + \hat{\mathcal{H}}^{(2)} + \mathcal{H}_{\text{exch}}, \quad (17)$$

that describes two energy bands of the oxygen holes via exchange interaction with the copper ion spin moments. These spin moments interact between themselves antiferromagnetically.

5. Reduction to the φ-d-exchange model

The split character of the $u_{\delta\delta_1}$ function relative to the δ and δ_1 variables significantly simplifies the energetic structure and physical properties of the cuprate superconductors. Introducing the Fourier transform for the operators $p_{f+\frac{x}{2},\sigma}$ and $p_{f+\frac{y}{2},\sigma}$

$$p_{f+\frac{x}{2},\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{ik(f+x/2)}a_{k\sigma},$$
$$p_{f+\frac{y}{2},\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{ik(f+y/2)}b_{k\sigma}, \quad (18)$$

yields

$$\sum_\delta \vartheta(\delta)p_{f+\delta,\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{ikf}(-2i)(\nu_{kx}a_{k\sigma} + \nu_{ky}b_{k\sigma}),$$

where $\nu_{kx} = \sin(k_x/2), \nu_{ky} = \sin(k_y/2)$.

Defining the Fermi operators $\psi_{k\sigma}$ and $\varphi_{k\sigma}$ using the transformation[8]

$$\varphi_{k\sigma} = (\nu_{kx}a_{k\sigma} + \nu_{ky}b_{k\sigma})/\nu_k,$$
$$\psi_{k\sigma} = (\nu_{kx}b_{k\sigma} - \nu_{ky}a_{k\sigma})/\nu_k, \quad \nu_k = \sqrt{\nu_{kx}^2 + \nu_{ky}^2}, \quad (19)$$

yields the following effective Hamiltonian:

$$\hat{\mathcal{H}}_{sp-f} = \sum_{k\sigma}\varepsilon_p\psi_{k\sigma}^+\psi_{k\sigma} + \sum_{k\sigma}\xi_k\varphi_{k\sigma}^+\varphi_{k\sigma}$$
$$+\frac{J}{N}\sum_{fkq\sigma\sigma'} e^{if(q-k)}\nu_k\nu_q\varphi_{k\sigma}^+(\mathbf{S}_f\mathbf{s}_{\sigma\sigma'})\varphi_{q\sigma'}$$
$$+\frac{1}{2}\sum_{fm} I_{fm}(\mathbf{S}_f\mathbf{S}_m), \quad (20)$$

where

$$\xi_k = \varepsilon_p + \varepsilon_2(1 - \gamma_{1k}), \quad \gamma_{1k} = (\cos k_x + \cos k_y)/2. \quad (21)$$

Expression (20) omits constants that are irrelevant to our discussion. The main feature of the presented Hamiltonian is its description of two fermion subsystems that are non-interacting. Only one of these subsystems, corresponding to the φ-fermions, interacts with the localized spin subsystem. The zero-dispersion ε_p state corresponds to the free ψ-fermions. As will be discussed further, these degrees of freedom carry no contribution to the low-temperature thermodynamics of the considered model.

This means that the effective model, describing the spectrum of both fermionic and bosonic elementary excitations of cuprate HTSs, is indeed the φ–d-exchange model

$$\hat{\mathcal{H}}_{\varphi-d} = \sum_{k\sigma}\xi_k\varphi_{k\sigma}^+\varphi_{k\sigma}$$
$$+\frac{J}{N}\sum_{fkq\sigma\sigma'} e^{if(q-k)}\nu_k\nu_q\varphi_{k\sigma}^+(\mathbf{S}_f\mathbf{s}_{\sigma\sigma'})\varphi_{q\sigma'}$$
$$+\frac{1}{2}\sum_{fm} I_{fm}(\mathbf{S}_f\mathbf{S}_m). \quad (22)$$

6. Reduction to the effective $\tilde{t}-\tilde{J}^*-I$-model

One of the most important properties of the φ-d-exchange model (22) is the large value of the interaction parameter J between the copper ion spin moments and the φ-fermion hole subsystem described by the $\varphi_{k\sigma}$ operators. Plugging in the Emery model parameter values corresponding to cuprate HTSs[32,33] (in eV units)

$$U_d = 10,5, \quad \Delta_{pd} = 3,6, \quad t_{pd} = 1,3, \quad (23)$$

yields $J = 5.72$ eV.

The large value of the J constant and its positive sign ensures an energetic favorability of the unit cell singlet state as opposed to the triplet. In line with this result, the work in Ref. 5 proposed to only account for the singlet state $|S\rangle$ and the two states without holes, $|\uparrow\rangle$ and $|\downarrow\rangle$ in the Hilbert space, that account for the degree of freedom of the spin localized on the copper ion. The t–J-model was introduced in Ref. 5 to describe the low-energy hole dynamics in the CuO_2-plane. In this model, the transfer of the Zhang-Rice singlet from one cell to another is treated as a hop of a quasiparticle with an oppositely oriented spin.

The current section presents a strict derivation of the effective Hamiltonian, acting on the specified Hilbert subspace, and shows that it is sufficiently different from the routinely used t–J^*-model Hamiltonian, obtained from the Hubbard model in the SEC regime.

Using the transformations

$$\varphi_{f\sigma} = \frac{1}{\sqrt{N}}\sum_{k} e^{ikf}\varphi_{k\sigma}, \quad \nu_m = \frac{1}{N}\sum_{k} e^{ikm}\nu_k, \qquad (24)$$

we write down the Hamiltonian for the φ–d-exchange model (22) in the Wannier representation[20,28]

$$\hat{\mathcal{H}}_{\varphi-d} = (\varepsilon_p + \varepsilon_2)\sum_{f\sigma}\varphi^{+}_{f\sigma}\varphi_{f\sigma} - \frac{\varepsilon_2}{4}\sum_{f\delta\sigma}\varphi^{+}_{f\sigma}\varphi_{f} + 2\delta,\sigma$$
$$+J\sum_{fnm\sigma\sigma'}\nu_n\nu_m\varphi^{+}_{f+n,\sigma}(\mathbf{S}_f\mathbf{s}_{\sigma\sigma'})\varphi_{f+m,\sigma'} + \frac{1}{2}\sum_{fm} I_{fm}(\mathbf{S}_f\mathbf{S}_m). \qquad (25)$$

This form clearly shows that the φ–d-exchange interactions ($m = n$) and spin-correlated hops of the φ-fermions ($m \neq n$) occur between arbitrarily separated nodes. The strength of interactions is determined by the parameters ν_m and as evidenced from Table 1, decays quickly with distance.

Let's separate the single cell component from the Hamiltonian (25), containing the strongest exchange interaction when $m = n = 0$;

$$\hat{\mathcal{H}}(f) = (\varepsilon_p + \varepsilon_2)\sum_{\sigma}\varphi^{+}_{f\sigma}\varphi_{f\sigma} + J\nu_0^2\sum_{\sigma\sigma'}\varphi^{+}_{f\sigma}(\mathbf{S}_f\mathbf{s}_{\sigma\sigma'})\varphi_{f\sigma'}. \qquad (26)$$

The spectrum of the operator (26) eigenvalues in the single cell sector is determined by the energy of the singlet state $E_S = \varepsilon_p + \varepsilon_2 - (3/4)J\nu_0^2$ and the energy of the triplet states $E_T = \varepsilon_p + \varepsilon_2 + J\nu_0^2/4$. With selected model parameters: $E_T - E_S = J\nu_0^2 = 5.25$ eV. The significant energy separation of the E_S and E_T states indicates that in the single-hole region of the Hilbert space basis, one can ignore the triplet states on a single unit cell. In this case, the cut-down basis of the cell is composed of three, aforementioned states: $|S\rangle$ and $|\sigma\rangle(\sigma = \uparrow, \downarrow)$.

Introducing the Hubbard operators for the cell with index f $X_f^{mn} = |f;m\rangle\langle n;f|(m,n = \uparrow, \downarrow, S)$ and using the completeness condition of the introduced basis set $\sum_m X_f^{mm} = 1$, it is simple to obtain the representation for the φ-operators and spin operators in terms of the Hubbard operators:

$$\varphi_{f\sigma} = \frac{2\bar{\sigma}}{\sqrt{2}}X_f^{\bar{\sigma}S}, \quad S_f^{+} = X_f^{\uparrow\downarrow}, \quad S_f^{-} = X_f^{\downarrow\uparrow}, \quad S_f^{z} = \sum_{\sigma}\sigma X_f^{\sigma\sigma}. \qquad (27)$$

Substituting expression (27) into the φ–d-exchange model Hamiltonian (29), yields the Hamiltonian for the $\tilde{t} - \tilde{J}^* - I$-model

$$\hat{\mathcal{H}}_{t-J-I} = E_S\sum_f X_f^{SS} + \sum_{f\delta\sigma} t_1 X_f^{S\sigma}X_{f+2\delta}^{\sigma S}$$
$$+ \sum_{\substack{fm\sigma \\ m\neq 0,2\delta}} t_m X_f^{S\sigma}X_{f+m}^{\sigma S} + \frac{1}{2}\sum_{fm} I_{fm}\mathbf{S}_f\mathbf{S}_m + \hat{\mathcal{H}}_3, \qquad (28)$$

TABLE 1. ν_m values for the five nearest coordination spheres, m is the coordination sphere number, corresponding to the radius-vector r_m.

m	0	1	2	3	4	5
ν_m	−0.9581	−0.1401	−0.0235	−0.0137	−0.0069	−0.0035

where

$$\hat{\mathcal{H}}_3 = \frac{J}{4}\sum_{fnm\sigma}{}'\nu_n\nu_m\Big[X_{f+n}^{S\sigma}X_f^{\bar{\sigma}\bar{\sigma}}X_{f+m}^{\sigma S}$$
$$-X_{f+n}^{S\bar{\sigma}}X_f^{\bar{\sigma}\sigma}X_{f+m}^{\sigma S} + \frac{1}{2}X_{f+n}^{S\bar{\sigma}}X_f^{SS}X_{f+m}^{\sigma S}\Big],$$
$$E_S = \varepsilon_p + \varepsilon_2 - \frac{3}{4}J\nu_0^2,$$
$$t_1 = -\frac{\varepsilon_2}{8} + \frac{J}{32} - \frac{J}{2}\nu_0\nu_1, \quad t_m = -\frac{1}{2}J\nu_0\nu_m. \qquad (29)$$

In the second term of expression (28), the summation is performed along the nearest neighbors, whereas in the third term along the second and farther-lying coordination spheres.

The prime in the sum of formula (29) indicates that the indices m and n are nonzero and are not equal. The values of J, ε_2 and I are defined in (13)–(16).

The "tilde" on top of t and J symbols in the model name indicates that the model contains hops (t) and three-center interactions (J) between the nodes of the farthest coordination spheres. Presence of the exchange interaction between the copper ions spins is denoted with the I symbol.

The obtained $\tilde{t} - \tilde{J}^* - I$-model (28) is significantly different from the t–J^*-model that is derived from the single-band Hubbard model. The t–J^*-model is simply the usual t–J-model that accounts for the three-center terms that describes spin-correlated jumps of the quasiparticles.[7] The exchange and the three-center interactions in the t–J^*-model have a similar order of magnitude and should be considered on equal footings.[34–36] However, in majority of studies, the three-center interactions are ignored because their strength is proportional to the degree of doping x.[32] Similar arguments are employed when studying the kinetic properties of fermion quasiparticles. However, in those cases when the range of characteristic energies is set by the value of the exchange integral, taking the three-center interactions into the account becomes important. This becomes evident in the description of d-type superconductivity[35] or collective spin oscillations.[37]

The obtained Hamiltonian for the $\tilde{t} - \tilde{J}^* - I$-model drastically changes the current understanding. In Hamiltonian (28), the three-center terms (29) are proportional to the J parameter and are two orders of magnitude smaller relative to the hybridization constant t_{pd}. The exchange interactions, due to the parameter I, are four orders of magnitude smaller than t_{pd}. The $J \gg I$ relation means that in the $\tilde{t} - \tilde{J}^* - I$-model, the role of the three-center interactions is significantly more pronounced than in the t–J^*-model and these interactions need to be accounted for when studying cuprate HTSs in both normal and superconducting phases.

It is also worth noting that the expression for the three-center interactions (29), aside from spin-correlated hops, also contains charge-correlated hops (third term) that is absent in the conventional t–J^*-model.

7. Comparative analysis of the spin-polaron spectra in the effective models of cuprate HTSs: Role of the long-range interactions

The current section presents calculations and comparison of the dispersion curves for the Fermi spin-polaron excitations in the effective low-energy models of cuprate HTSs:

spin-fermion model (17), φ–d-exchange model (22) and the $\tilde{t}-\tilde{J}^{*}-I$-model (28).

The computation of the dispersion curves is carried out using the method of equations of motion with two time-domain delayed Green's functions. The equation chain is completed with the aid of a projection technique of Zwanzig-Mori.[38,39] Carrying out this particular approach (that is equivalent to the method of irreducible Green's functions[40,41]) for the spin-polaron model (17) is discussed in detail in Ref. 23. In the framework of this method, we introduce a minimal basis set of operators A_j ($j = 1, \ldots, n$), sufficient to describe the dynamics of the quasiparticles accounting for the interactions present in the system. The operator of the initial quasiparticle is used for the operator A_1. The right part of the A_1 equation of motion, aside from the starting operator, contains a complicated operator expression that is further used as the next basis operator. It is this complex operator that allows to account for the special physics of the system interactions. As a rule, the basis obtained in this fashion is sufficient. Following this, equations of motion are projected for all basis operators onto this same basis.

The use of the projection method in the framework of delayed Green's function formalism leads to the necessity to calculate the energy matrix $\hat{D}(k)$ with elements $D_{ij}(k) = \langle\{[A_{ik}, \hat{\mathcal{H}}], A_{jk}^{+}\}\rangle$ and the matrix $\hat{K}(k)$ with elements $K_{ij}(k) = \langle\{A_{ik}, A_{jk}^{+}\}\rangle$ where the angled brackets denote a thermodynamic average. Then the matrix form of the time-delayed Green's function $\hat{G}(k,\omega)$ with elements $G_{ij}(k,\omega) = \langle\langle A_{ik}|A_{jk}^{+}\rangle\rangle_{\omega}$ can be determined from the expression

$$\hat{G}(k,\omega) = \left(\omega\hat{I} - \hat{D}(k)\hat{K}^{-1}(k)\right)^{-1}\hat{K}(k), \qquad (30)$$

where $\hat{I}$ is the unity matrix. The spectrum of the Fermi excitations is determined by the poles of the Green's function $\hat{G}(k,\omega)$.

For the Hamiltonian of the spin-fermion model (17), the starting operators are chosen to be: $a_{k\sigma}$ and $b_{k\sigma}$, that according to (18) are the Fourier images of the $p_{f+\frac{x}{2},\sigma}$ and $p_{f+\frac{y}{2},\sigma}$ operators, respectively. Writing the equation of motion for the specified operators, yields the minimal basis for the model (17) that contains three sets of operators

$$a_{k\sigma}, b_{k\sigma}, L_{k\sigma} = \frac{1}{N}\sum_{qf\alpha} e^{if(q-k)}(\mathbf{S}_f\boldsymbol{\tau}_{\sigma\alpha})(\nu_{qx}a_{q\alpha} + \nu_{qy}b_{q\alpha}). \quad (31)$$

The elements of the $\hat{D}(k)$ and the $\hat{K}(k)$ matrices, calculated using the basis (31) and the Hamiltonian of the spin-fermion model (17) are contained in Ref. 24 and are therefore not listed here. The expressions for these matrix elements contain paired spin correlation functions $C_j = \langle\mathbf{S}_f\mathbf{S}_{f+r_j}\rangle$, where r_j is the radius of the jth coordination sphere. The concentration dependence of the spin correlators C_j in the HTS cuprates has been discussed before in Refs. 21,23, and 24. It was assumed that the magnetic subsystem is in the SU(2)-invariant state of the quantum spin liquid. This in its turn means that $\langle S_f^{x(y,z)}\rangle = 0$ and the expression $\langle S_f^{x(y,z)} S_{f+r_j}^{x(y,z)}\rangle = \frac{1}{3}C_j$ is satisfied for the spin correlators. Following the work of Ref. 24, we pick the following values for the spin correlation with hole concentration $x = 0.07$: $C_1 = -0.255$, $C_2 = 0.075$, $C_3 = 0.064$. Charge and spin-charge correlation functions arising during computation of the $\hat{D}(k)$ and $\hat{K}(k)$ matrix elements are not considered here due to the small degree of doping.

Figure 2 shows the three branches of the energy spectrum for the Fermi excitations in the spin-fermion model (17). The spectra are obtained through a numerical solution of the third-order dispersion equation: $|\omega\hat{I} - \hat{D}(k)\hat{K}^{-1}(k)| = 0$, that determines the poles of the Green's functions (30). The parameter values of $J = 5.72$ eV and $\varepsilon_2 = 0.45$ eV were used during the computation. These values were obtained from (13) and (14) with substitution of the p–d-model parameters (23). The exchange constant I was set to zero for simplicity.

The lower branch in Fig. 2 shows the spectrum of the spin-polaron excitations. A significant decrease in the energy of the spin-polaron states arises due to the contribution of the third operator $L_{k\sigma}$ in the basis (31). An important feature of the obtained spin-polaron spectrum is the presence of a dispersion minimum observed in the ARPES experiments in the (Γ – M) direction of the Brillouin zone. For practical doping ranges of cuprates HTSs, the chemical potential always lies in the lower spin-polaron band, therefore from now on we will only discuss this band.

The computation of the Fermi spectrum for the Hamiltonian of the φ–d-exchange model (22) is also carried out in the framework of the projection technique. In this case, however, the first basis operator must be $\varphi_{k\sigma}$. Accounting for the operator that arises in the equation of motion due to $\varphi_{k\sigma}$, leads to a basis consisting of two operators

$$\varphi_{k\sigma}, L_{k\sigma} = \frac{1}{N}\sum_{qf\alpha} e^{if(q-k)}(\mathbf{S}_f\boldsymbol{\tau}_{\sigma\alpha})\nu_q\varphi_{q\alpha}. \qquad (32)$$

It is evident that the second operator of this basis is the same as the third operator of basis (31).

Calculating the elements of the $\hat{D}(k)$ and $\hat{K}(k)$ matrices in the basis (32) and solving the second-order dispersion equation $|\omega\hat{I} - \hat{D}(k)\hat{K}^{-1}(k)| = 0$, yields the analytical expression for the lower branch of the spin-polaron excitations in the φ–d-exchange model (22):

$$E_{sp}(k) = \frac{\xi_k + D_k/K_k}{2} - \frac{1}{2}\sqrt{(\xi_k - D_k/K_k)^2 + J^2\nu_k^2 K_k}, \quad (33)$$

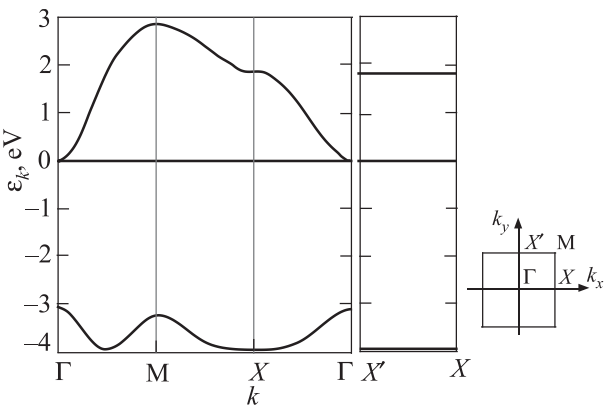

Fig. 2. Spectrum of the Fermi excitation in the spin-fermion model (17). Model parameters, eV: $J = 5.72$, $\varepsilon_2 = 0.45$, $I = 0$. The spin correlators were taken to be: $C_1 = -0.255$, $C_2 = 0.075$, $C_3 = 0.064$.

where

$$D_k = (\varepsilon_p - J + 2\varepsilon_2)K_k + J(3 + C_1)/8 + \varepsilon_2(-9/16 + C_2\gamma_{2k}/2 + C_3\gamma_{3k}/4),$$
$$K_k = 3/4 - C_1\gamma_{1k}, \quad \gamma_{2k} = \cos k_x \cos k_y,$$
$$\gamma_{3k} = (\cos 2k_x + \cos 2k_y)/2. \tag{34}$$

The results of the spin-polaron spectrum computation for the φ–d-exchange model using Eq. (33) are denoted in Fig. 3 with a solid thick line. This line exactly reproduces the lower curve of Fig. 2 that corresponds to the dispersion law for spin polarons in the spin-fermion model (17). The agreement of dispersion curves is not a coincidence and can be explained by the fact the ψ-orbital is inactive in our approximation ($t_{pp} = 0$, $U_p = 0$, $V_{pp} = 0$, $V_{pd} = 0$), and therefore the bases (31) and (32) are equivalent. Including any of the interactions t_{pp}, U_p, V_{pp}, or V_{pd} into the ground state of the system leads to mixing of the ψ-state and the mentioned operator bases are no longer equivalent. Basis (31) remains preferred, since it allows for obtaining a lower ground state energy.

An important question that arises in this theory pertains to the role of the long-range interactions. The correct form of the three-band Emery model using the diagonalizing φ- or ψ-orbitals in the Wannier representation is always accompanied by an appearance of interactions from farthest coordination spheres. An example can be the Hamiltonian for the φ–d-exchange model in the form of (25). Since the strength of the mentioned interactions decreases with distance, practically only nearest neighbor interactions are considered.[29] The adequacy of such simplifications however stems doubt,[14] since the decrease in the long-range interactions can be compensated by an increase in the number of long-range neighbors.

To answer this question, we compare the spectrum of spin-polaron excitations in the φ–d-exchange model and its reduced variant. The latter is defined according to expression (25), leaving only the φ–d-exchange interactions on a single cell and between neighboring cells

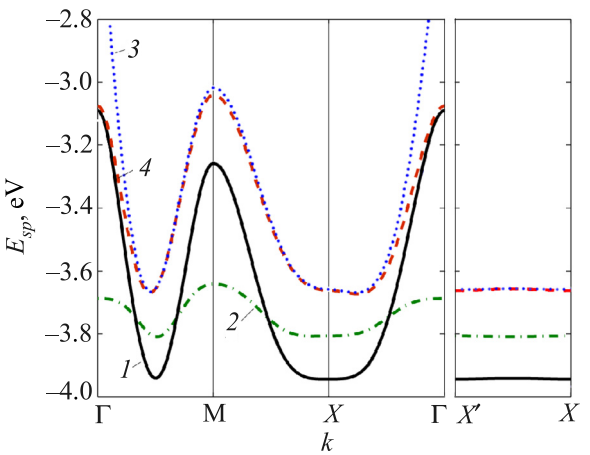

Fig. 3. Comparison of the Fermi excitation spectra for spin-polaron quasiparticles, obtained in the frameworks of various models. Model parameters and the spin correlators are the same as in Fig. 2. *1*—spectrum in the spin-fermion model (17) and the φ–d-exchange model (22), *2*—spin-polaron spectrum in the reduced φ–d-exchange model (35), *3*—spectrum (37) of the $\tilde{t} - \tilde{J}^* - I$-model (28), *4*—spectrum of the spin polarons in the φ–d-exchange model (25), computed by accounting for the basis from two operators $A^{(r)}_{1f\sigma}$ and $A^{(r)}_{2f\sigma}$ (36).

$$\hat{\mathcal{H}}^{(r)}_{\varphi-d} = (\varepsilon_p + \varepsilon_2)\sum_{f\sigma}\varphi^+_{f\sigma}\varphi_{f\sigma} - \frac{\varepsilon_2}{4}\sum_{f\delta\sigma}\varphi^+_{f\sigma}\varphi_{f+2\delta,\sigma} + J\nu_0^2\sum_{f\sigma\sigma'}\varphi^+_{f\sigma}(\mathbf{S}_f\mathbf{s}_{\sigma\sigma'})\varphi_{f\sigma'} + J\nu_0\nu_1\sum_{f\delta\sigma\sigma'}\left[\varphi^+_{f+2\delta,\sigma}(\mathbf{S}_f\mathbf{s}_{\sigma\sigma'})\varphi_{f\sigma'} + \text{h.c.}\right] + \frac{1}{2}\sum_{fm} I_{fm}(\mathbf{S}_f\mathbf{S}_m). \tag{35}$$

The fourth term in (35) describes hole hopping between adjacent cells, that accounts for the correlation with a spin on one of these cells. Similar processes have been considered in Ref. 29.

To compute the spectrum of the Fermi excitation in the system, described by the Hamiltonian of the reduced φ–d-exchange model $\hat{\mathcal{H}}^{(r)}_{\varphi-d}$, let's introduce three sets of basis operators

$$A^{(r)}_{1f\sigma} = \varphi_{f\sigma}, \quad A^{(r)}_{2f\sigma} = \sum_\alpha(\mathbf{S}_f\boldsymbol{\tau}_{\sigma\alpha})\varphi_{f\alpha},$$
$$A^{(r)}_{3f\sigma} = \sum_{\delta\alpha}(\mathbf{S}_f\boldsymbol{\tau}_{\sigma\alpha})\varphi_{f+2\delta,\alpha}. \tag{36}$$

This basis is constructed using the same method as for the bases (31) and (32), but in the Wannier representation. The first operator $\varphi_{f\sigma}$ is the starting and the other two arise in the equation of motion for this operator.

The elements of the $\hat{D}^r(k)$ and $\hat{K}^r(k)$ matrices for the reduced Hamiltonian $\mathcal{H}'^{(r)}_{\varphi-d}$ calculated in the basis (36) are listed in the Appendix, whereas the spectrum of the spin-polaron excitation in the model (35), obtained using the above methodology is shown in Fig. 3 with a dot-dash line.

Ignoring the long-range spin-correlated hops leads to significant repercussions. First of all, the width of the spin-polaron band is almost four times narrower. Secondly, the minimum energy of the quasiparticle that can be reached near the (π/2, π/2) point of the Brillouin zone is significantly higher.

One can suspect that the large difference in the obtained dispersion curves is not only related to omission of the long-range spin-correlated hops in one of the Hamiltonians but also due to the use of different basis operators (32) and (36). However, the computation of spin-polaron excitation spectrum in the full φ–d-exchange model using basis (36) shows that the spectrum of the lower energy band is within a couple percent of the thick solid line in Fig. 3. Therefore, both operator bases (32) and (36), reproduce the behavior of the spin-polarons equally well and the difference between the spectra of the full and reduced φ–d-exchange models can be attributed only to the omission of the long-range spin-correlated hops in the Hamiltonian (35).

We will consider the spectrum of obtained $\tilde{t} - \tilde{J}^* - I$-model in the simplest approximation, only including a single operator $X^{0\sigma}_f$ into the basis. As opposed to the spin-fermion and the φ–d-exchange model, here the starting operator accounts for the single-node correlations due to the strong φ-d exchange interaction. Therefore, the band of the starting quasiparticles in the $\tilde{t} - \tilde{J}^* - I$-model corresponds to the spin-polaron excitations by definition.

In the framework of the projection method, the spin-polaron spectrum for the $\tilde{t} - \tilde{J}^* - I$-model is determined by

the expression $E_{t-J-I}(k) = \langle\{[X_k^{\sigma S}, \hat{\mathcal{H}}_{t-J-I}], X_k^{S\sigma}\}\rangle / \langle\{X_k^{\sigma S}, X_k^{S\sigma}\}\rangle$ where $X_k^{\sigma S} = \frac{1}{\sqrt{N}}\sum_f e^{-ikf} X_f^{\sigma S}$. Carrying out an average computation in the $E_{tJ}(k)$ expression and accounting for the low doping regime, yields

$$E_{t-J-I}(k) = \varepsilon_p + \varepsilon_2 - \varepsilon_2(C_1+1/4)\gamma_{ik} + \frac{J}{2}\left[-\bar{C}_k(\nu_k + 2\nu_0) + \sum_f \nu_f^2 C_f\right], \quad (37)$$

where $\bar{C}_k = \sum_f e^{ikf}\nu_f C_f$ and $\nu_0 \equiv \nu_{f=0}$.

The spin-polaron spectrum calculated according to the formula (37) is shown in Fig. 3 with a dashed line. This spectrum reproduces the main feature characteristic of Fermi excitation spectra in cuprates—presence of a minimum near the (π/2, π/2) point of the Brillouin zone in the $\Gamma - M$ direction. However, the minimum energy of the quasiparticle, compared to the dispersion of the spin-fermion model (solid line in Fig. 3) has increased by approximately 0.3 eV. The noted increase is due to an absence of the $Y_{f\sigma} = \sum_{\delta\alpha}(\mathbf{S}_f \mathbf{s}_{\sigma\alpha}) X_{f+2\delta}^{\alpha S}$ operator in the selected basis for the $\tilde{t} - \tilde{J}^* - I$-model, that allows for accounting for the inter-node φ–d-exchange correlations.

In order to prove this statement, it is necessary to compute the spectrum of the $\tilde{t} - \tilde{J}^* - I$-model in the basis of two operators $X_f^{\sigma S}$, $Y_{f\sigma}$ and become convinced that the low-energy part of this spectrum coincides with the dispersion relations of the spin-fermion excitations in the φ–d-exchange model (25). Due to the algebraic complexity of the Hubbard operators, these calculations are quite difficult, thus instead we will omit the third operator $A_{3f\sigma}^{(r)}$ from the basis (36), that accounts for the inter-node φ–d-exchange correlations. We then calculate the spectrum of spin-polarons in the φ–d-exchange model with the remaining two operators and compare it to the spectrum of the $\tilde{t} - \tilde{J}^* - I$-model.

The dashed line in Fig. 3 shows in the spin-polaron spectrum of the φ–d-exchange model calculated with only two ($A_{1f\sigma}^{(r)}$ and $A_{2f\sigma}^{(r)}$) operators and demonstrates its equivalence with the spectrum from the $\tilde{t} - \tilde{J}^* - I$-model in the low-energy region. The differences in the high-energy parts of the spectra are due to the lack of the contributions from single-cell triplet states to the $\tilde{t} - \tilde{J}^* - I$-model Hamiltonian, that are accounted for during construction of the φ–d-exchange model spectrum.

To conclude the current section, we note that in the investigated low doping regime, construction of the Fermi excitation spectra did not require the use of the chemical potential. Nevertheless, description of thermodynamics or superconducting properties of spin-polaronic quasiparticles should be conducted in the framework of the large canonical ensemble. In this case, the Hamiltonians of the spin-fermion and the φ–d-exchange model should contain and additional term $-\mu\sum_l \hat{n}_l^p$, and the Hamiltonian of the $\tilde{t} - \tilde{J}^* - I$-model—the term $-\mu\sum_f X_f^{SS}$.

8. Conclusion

This work sequentially derives three low-energy models of the cuprate high-temperature superconductor electronic structure. The first step involves taking the realistic three-band Emery model with parameters corresponding to the regime of strong electron correlations and the spin-fermion model[14,19] is derived in the framework of the operator perturbation theory. One of the main features of this effective model is that the copper ion states become homeopolar and are characterized by a spin moment of $S = 1/2$. A second important model property is the presence of spin-correlated hops of oxygen holes. As a result, the hole movement along the oxygen ions is accompanied by correlated dynamics with spin degrees of freedom in the copper ion spin moment subsystem. These processes determine the characteristic features of the Fermi state energy spectrum due to, for example, the minimum near the (π/2, π/2) point of the Brillouin zone.

The second step in the Emery model reduction involves introduction of the φ and ψ functions[8,10,15,17] constructed using the p_x- and the p_y-orbitals of oxygen. This allows for a transition from the spin-fermion model to the φ–d-exchange model, that is characterized by a presence of exchange interactions and spin-correlated hops from long-range coordination spheres.

The final step in the Emery model reduction is based on the introduction of the atomic representation for the description of local strongly interacting spin polarons. This approach leads to the $\tilde{t} - \tilde{J}^* - I$-model. The tilde in $\tilde{t}$ underscores the fact that the hops between the nodes located on the far-lying coordination spheres are manifested directly in the model. The $\tilde{J}^*$ symbol denotes the presence of three-center terms, that describe correlated hops of oxygen holes while accounting for the hops from the farthest coordination spheres. The model also contains both spin and charge correlations. The presence of an exchange interaction between copper ion spins is denoted with the I symbol.

By comparing the spectra of the spin-polaron quasiparticles from the first two models with a corresponding spectrum of the reduced φ–d-exchange model (where only interactions between adjacent cells are considered), the importance of the long-range spin-correlated hops that are usually ignored is further asserted. In particular, it is shown that accounting for the long-range interactions leads to a significant widening of the spin-polaron band as well as an additional lowering of the spin-polaron quasiparticle energy (see Fig. 3).

It is shown that the obtained $\tilde{t} - \tilde{J}^* - I$-model differs significantly from the conventional t–J^*-model that follows from the Hubbard model in the regime of strong electron correlations.[42] The main difference lies in that the three-center interactions in the $\tilde{t} - \tilde{J}^* - I$-model, that describe the spin-correlated quasiparticle hops, significantly exceed the exchange interactions. This marks a new view on the role of three-center interactions in the HTS theory of cuprates. As mentioned before, accounting for three-center interactions causes an appearance of a minimum in the dispersion relation of the spin-polaron excitations near the (π/2, π/2) point of the Brillouin zone in the Γ – M direction. This minimum is characteristic of all spectral curves shown in Fig. 3.

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APPENDIX

For a system described by the reduced Hamiltonian of the φ–d-exchange model (35), the elements of the $\hat{D}^r(k)$ and $\hat{K}^r(k)$ matrices calculated in the basis of three operators (36) have the following form ($D^r_{ij} = D^r_{ij}, K^r_{ij} = K^r_{ij}$):

$$
\begin{aligned}
&K^r_{11} = 1; \quad K^r_{12} = K^r_{13} = 0, \quad K^r_{22} = 3/4;\\
&K^r_{23} = 4C_1\gamma_{1k}; \quad K^r_{33} = 3 + 8C_2\gamma_{2k} + 4C_3\gamma_{3k},\\
&D^r_{11} = \varepsilon_p + \varepsilon_2(1-\gamma_{1k}),\\
&D^r_{12} = J\nu_0^2 3/8 + J\nu_1\nu_0(3/2 + 2C_1)\gamma_{ik},\\
&D^r_{13} = 2J\nu_0^2 C_1\gamma_{1k} + J\nu_1\nu_0\left(3/2 + 8C_1\gamma_{1k}^2 + 4C_2\gamma_{2k} + 2C_3\gamma_{3k}\right),\\
&D^r_{22} = (\varepsilon_p + \varepsilon_2)3/4 - \varepsilon_2 C_1\gamma_{1k} - J\nu_0^2 3/8 - 4J\nu_1\nu_0 C_1\gamma_{1k},\\
&D^r_{23} = (\varepsilon_p + \varepsilon_2)4c_1\gamma_{1k} - \varepsilon_2(3/4 + 2C_2\gamma_{2k} + C_3\gamma_{3k})\\
&\quad -2J\nu_0^2 C_1\gamma_{1k} - 2J\nu_1\nu_0(3/4 - C_1 + 2C_2\gamma_{2k} + C_3\gamma_{3k}),\\
&D^r_{33} = (\varepsilon_p + \varepsilon_2)(3 + 8C_2\gamma_{2k} + 4C_3\gamma_{3k})\\
&\quad -\varepsilon_2(9C_1\gamma_{1k} + 6C_4\gamma_{4k} + C_6\gamma_{6k})\\
&\quad +2J\nu_0^2 C_1 + 16J\nu_1\nu_0 C_1(1-\gamma_{1k}),
\end{aligned}
\tag{S1}
$$

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

$$
\begin{aligned}
\gamma_{1k} &= (\cos k_x + \cos k_y)/2, \quad \gamma_{2k} = \cos k_x \cos k_y,\\
\gamma_{3k} &= (\cos 2k_x + \cos 2k_y)/2,\\
\gamma_{4k} &= (\cos 2k_x \cos k_y + \cos 2k_y \cos k_x)/2,\\
\gamma_{6k} &= (\cos 3k_x + \cos 3k_y)/2.
\end{aligned}
$$

When obtaining expressions (S1), the ($\tilde{S}_m = \mathbf{S}_m\boldsymbol{\tau}$) relations were taken into account

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

that are valid in the SU(2)-invariant spin-liquid phase.

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