

Diagram Approach to the Problem of the Normal Phase Properties of the Spin-Polaron Ensemble in Cuprate Superconductors

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Abstract

Taking into account the real crystalline structure of the CuO_2 plane within the spinfermion model and using the diagram technique, the spin-polaron concept of the fermionic excitations in cuprate superconductors is implemented. It is shown that an account of the on-site scattering processes leads to considerable binding energy of the spin-polaron quasiparticles. An account of the two-site spin-fermion scattering processes results in the energy spectrum and spectral properties of the spin-polaron quasiparticles which agree well with experimental data on cuprate superconductors.

Keywords Cuprate superconductors · Unconventional superconductivity · Spin-charge correlations

1 Introduction

Nowadays, it is established that the strong interaction between the carriers and the spin subsystem causes the complicated behavior of the spectral and transport properties of the high-temperature superconductors [1-3]. The doping transition from the insulator state to the metal state is accompanied by the appearance of a pseudogap with the modulation of the spectral carrier density and the drastic reduction of the density of states in the vicinity of the chemical potential [4,5]. Despite considerable efforts of

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researchers, the pseudogap behavior is still one of the most exciting and puzzling phenomena in the field of high-temperature superconductivity in the cuprates.

On the other hand, it is also known that the strong spin-fermion correlations underlie the formation of the spin-polaron quasiparticles [6,7]. It was shown that the theory based on the spin-polaron concept within the realistic spin-fermion model (SFM) [8– 14] allows one to describe correctly a number of important features of the spectral properties of the cuprates in the normal phase [15]. An important factor confirming the promise of this concept is the occurrence of the Cooper instability in the ensemble of the spin-polaron quasiparticles for the actual *d*-wave pairing and critical temperatures corresponding to the experimental data [16]. Recently [17,18], the spin-polaron concept acquired special significance, since it allowed one to solve a problem concerning the stability of the superconducting *d*-wave pairing toward the intersite Coulomb repulsion of fermions located at the nearest oxygen ions of the CuO₂ plane.

In view of these circumstances, the problem of description of the pseudogap state under the conditions where this state is formed not for the bare holes but in the subsystem of the spin polarons is of current interest. An elegant method for consideration of this problem is the diagram technique suggesting a particular algorithm for obtaining the exact representation of a single-particle Green's function which involves the self-energy operator

$$\Sigma(\boldsymbol{p}, i\omega_n) = \Sigma^{(1)}(\boldsymbol{p}, i\omega_n) + \Sigma^{(2)}(\boldsymbol{p}, i\omega_n) + \dots$$

Each term $\Sigma^{(m)}(\mathbf{p}, i\omega_n)$ arises as a result of an account for the spin-fermion scattering processes in all the orders of the perturbation theory, which are connected to the *m*-site spin correlations. The diagram technique is considered to be a well-controlled approach and makes it possible to describe adequately the main features of an ensemble of the spin polarons. Thus, the development of the diagram approach to the problem of the properties of the normal phase of the spin-polaron quasiparticles within the SFM is the subject of this work.

2 Hamiltonian of the φ – d Model

It is known that the three-band p - d model or the Emery model [19,20] describes adequately the main features of the electronic structure of the CuO₂ plane in high- T_c cuprate superconductors. In the regime of strong electron correlations, when the on-site Coulomb repulsion energy U_d for holes at one copper ion is large, the Emery model can be reduced to the SFM [8–14] with the Hamiltonian

$$\hat{H}_{h} = \sum_{k\alpha} \left(\xi_{kx} a_{k\alpha}^{\dagger} a_{k\alpha} + \xi_{ky} b_{k\alpha}^{\dagger} b_{k\alpha} + t_{k} (a_{k\alpha}^{\dagger} b_{k\alpha} + b_{k\alpha}^{\dagger} a_{k\alpha}) \right) + \frac{J}{N} \sum_{fkq\alpha\beta} e^{if(q-k)} u_{k\alpha}^{\dagger} (\mathbf{S}_{f} \boldsymbol{\sigma}_{\alpha\beta}) u_{q\beta} + \frac{I}{2} \sum_{f\delta} \mathbf{S}_{f} \mathbf{S}_{f+2\delta}.$$
(1)

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The first term describes the subsystem of oxygen holes in the quasimomentum repre-

sentation, where $\xi_{k_x(y)} = \varepsilon_p - \mu + \tilde{t}(1 - \cos k_{x(y)})$ and $\tilde{t} = \frac{t_{pd}^2}{\Delta_{pd}} \left(1 - \frac{\Delta_{pd}}{U_d - \Delta_{pd}}\right)$ takes into account the dynamics of oxygen holes coupled with the copper subsystem of the localized spins due to the processes of the second order in the hybridization parameter t_{pd} . Here, $\Delta_{pd} = \varepsilon_p - \varepsilon_d$ is the charge transfer gap. The operators $a_{k\alpha}^{\dagger}(a_{k\alpha})$ and $b_{k\alpha}^{\dagger}(b_{k\alpha})$ are the hole creation (annihilation) operators with the p_x - and p_y -orbitals. The bare on-site energy of oxygen holes is ε_p and $\alpha = \pm 1/2$ is the spin projection. The Fourier transform $t_k = (2\tilde{t} - 4t)s_{k,x}s_{k,y}$ describes the hopping processes of holes on oxygen sites, where $s_{k,x(y)} = \sin \frac{k_{x(y)}}{2}$ and t is the hopping parameter. The second term corresponds to the exchange interaction between subsystems of the oxygen holes and the localized copper spins, where \mathbf{S}_f is the operator of a spin localized at the site with index $f, \boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of the Pauli matrices, $u_{k\beta} = s_{k,x}a_{k\beta} + s_{k,y}b_{k\beta}$, and $J = \frac{4t_{pd}^2}{\Delta_{pd}} \left(1 + \frac{\Delta_{pd}}{U_d - \Delta_{pd}}\right)$. The last term corresponds to the superexchange interaction between the neighboring copper spins arising in the fourth order of the perturbation theory.

The analysis of energy structure of the SFM can be simplified with the help of the canonical transformation if one introduces new operators φ_k and ψ_k which are connected with operators $a_{k\alpha}$ and $b_{k\alpha}$ as follows:

$$a_{k\alpha} = \frac{s_{k,x}}{\nu_k} \varphi_{k\alpha} + \frac{s_{k,y}}{\nu_k} \psi_{k\alpha}, \qquad b_{k\alpha} = \frac{s_{k,x}}{\nu_k} \psi_{k\alpha} - \frac{s_{k,y}}{\nu_k} \varphi_{k\alpha}, \tag{2}$$

where $v_k = \sqrt{s_{k,x}^2 + s_{k,y}^2}$. Due to the fact that only φ -fermions interact with the spin subsystem [21] and owing to this interaction their energy band is considerably lower [22], the terms containing inactive ψ -fermions can be omitted, and Hamiltonian (1) of the SFM can be reduced to the Hamiltonian of so-called $\varphi - d$ model [22,23]

$$\hat{H}_{\varphi-d} = \sum_{k\alpha} \xi_k \varphi_{k\alpha}^{\dagger} \varphi_{k\alpha} + \frac{1}{N} \sum_{fkq\alpha\beta} e^{if(q-k)} J_{kq} \varphi_{k\alpha}^{\dagger} \mathbf{S}_f \boldsymbol{\sigma}_{\alpha\beta} \varphi_{q\beta} + \frac{1}{2} \sum_{fm} I_{fm} \mathbf{S}_f \mathbf{S}_m,$$
(3)

where $\xi_k = \varepsilon_p - \mu + 2\tilde{\iota}v_k^2 - 8t\frac{s_{k,x}^2 s_{k,y}^2}{v_k^2}$ and $J_{kq} = Jv_k v_q$.

3 Effective Interaction, Self-Energy Part, and the Spin-Polaron Green's Function

To calculate the fermionic excitations spectrum within the SFM, we introduce the Matsubara Green's function [24,25]

$$G_{\alpha}(k,\tau-\tau') = -\langle T_{\tau}\tilde{\varphi}_{k\alpha}(\tau)\tilde{\varphi}_{k\alpha}^{\dagger}(\tau')\rangle = T\sum_{\omega_n} e^{-i\omega_n(\tau-\tau')}G_{\alpha}(k,i\omega_n), \quad (4)$$

where T_{τ} is the operator of Matsubara time ordering, $\omega_n = (2n + 1)\pi T$, $n = 0, \pm 1, \pm 2, \ldots$ is the Matsubara frequency and T is the temperature. In Eq. (4), the operators φ are written in the Heisenberg representation with Matsubara time τ

$$\tilde{\varphi}_{k\alpha}(\tau) = \exp(\tau \hat{H}_{\varphi-d})\varphi_{k\alpha}\exp(-\tau \hat{H}_{\varphi-d}), \ 0 < \tau < 1/T.$$
(5)

To find the Matsubara Green's function, we use a special form of diagram technique which is the combination of the Feynman diagram technique and the diagram technique for the spin operators. For the Fourier transform $G_{\alpha}(k, i\omega_n)$, it is easy to write down the Dyson equation in the graphical form

$$\frac{1}{k\alpha} = \frac{1}{k\alpha} + \frac{1}{k\alpha} \sum_{k\alpha} \frac{1}{k\alpha}$$
(6)

In Eq. (6), the bold line represents the total propagator $G_{\alpha}(k, i\omega_n)$. The circle with inscribed symbol Σ corresponds to the irreducible self-energy operator $\Sigma(k, i\omega_n)$ [26]. The thin line denotes the bare fermionic Green's function for which the explicit expression is

$$G_0(k, i\omega_n) = \frac{1}{i\omega_n - \xi_k}.$$
(7)

In the analytical form, the Dyson equation is given by

$$G_{\alpha}(k, i\omega_n) = \frac{1}{i\omega_m - \xi_k - \Sigma(k, i\omega_n)}.$$
(8)

The calculation of the self-energy part $\Sigma(k, i\omega_n)$ is connected with the calculation of the interaction operator of the Hamiltonian $\hat{H}_{\varphi-d}$. Obviously, an account for $\hat{H}_{\varphi-d}$ cannot be realized using the simple perturbation theory based on the parameter of exchange interaction *J*. Indeed, the value of this interaction is $J \approx 3\text{eV}$ and such a high value results in formation of the spin-polaron quasiparticles [7]. The description of this quasiparticles demands an account for all the contributions of series of the perturbation theory up to infinity corresponding to an account for the processes of on-site scattering. The solution of such a problem is related to the summation of an infinite series for the self-energy part which has the following graphical form



The intersection of the thin solid line and the wavy line forms the bare vertex

$$\frac{\frac{\sqrt{2}}{\sqrt{2}}k - q}{k\alpha \qquad q\alpha}$$
(10)

which corresponds to the amplitude of interaction J_{kq} . It is important that this amplitude is split in indices k and q, namely, $J_{kq} = J v_k v_q$.

The dark circle at the intersection of the interaction lines corresponds to the on-site irreducible cumulant K_n of the *n*-th order. An order of K_n in the graph is determined by the number of convergent lines of interaction and is equal to the order of diagram in parameter J. Cumulant K_n is given by the expression

$$K_n = \sum_{j_1 j_2 \dots j_n} \langle S_f^{j_1} S_f^{j_2} \dots S_f^{j_n} \rangle_{\text{irr}} \, (\sigma^{j_1} \sigma^{j_2} \dots \sigma^{j_n})_{\alpha \alpha}. \tag{11}$$

One can find an exact recurrence relation convenient for the calculation of cumulants K_n

$$K_n = -K_{n-1}. (12)$$

We take into account the fact that the 2D subsystem of spins localized at copper ions at $T \neq 0$ is in the quantum spin-liquid state [27,28]. In this case, spin correlation functions $C_{\delta} = \langle S_f S_{f+\delta} \rangle$ satisfy the relations

$$C_{\delta} = 3\langle S_f^x S_{f+\delta}^x \rangle = 3\langle S_f^y S_{f+\delta}^y \rangle = 3\langle S_f^z S_{f+\delta}^z \rangle, \tag{13}$$

where δ is the distance between the copper ions. Additionally, $\langle S_f^x \rangle = \langle S_f^y \rangle = \langle S_f^z \rangle = 0$. According to Eq. (11), one can obtain that

$$K_2 = \sum_{ij} \langle S_f^i S_f^j \rangle_{\rm irr} \, (\sigma^i \sigma^j)_{\alpha \alpha} = \sum_{ij} \frac{1}{4} \delta_{ij} - \sum_{ijk} \varepsilon_{ijk}^2 \langle S_f^k \rangle \sigma_{\alpha \alpha}^k = \frac{3}{4}, \qquad (14)$$

where ε_{ijk} is the Levi-Civita symbol. Therefore, we obtain

$$K_n = (-1)^n (3/4), \quad n \ge 2.$$
 (15)

After summation of infinite series with regard to Eq. (15), we find an expression for the self-energy operator which takes into account the processes of the on-site scattering in all the orders of the perturbation theory

$$\Sigma^{(1)}(k, i\omega_n) = \frac{3}{4} J v_k^2 \frac{X(i\omega_n)}{1 + X(i\omega_n)},$$
(16)

where

$$X(i\omega_n) = \frac{1}{N} \sum_{q} J v_q^2 G_0(q, i\omega_n) = \frac{1}{N} \sum_{q} \frac{J v_q^2}{i\omega_n - \xi_q}.$$
 (17)

Using the Dyson equation, we arrive at the expression for the spin-polaron Green's function

$$G_{\alpha}^{(1)}(k, i\omega_n) = \frac{1 + X(i\omega_n)}{(i\omega_n - \xi_k)(1 + X(i\omega_n)) - (3/4)J\nu_k^2 X(i\omega_n)}.$$
 (18)

Note that Eq. (18) in the limiting case, when one can neglect the intraband hopping of fermions, leads to the right result for the energies corresponding to the singlet and triplet states. Indeed, in this limit $v_k^2 \rightarrow 1$, $\varepsilon_k \rightarrow \varepsilon$ and $X(i\omega_n) = J/(i\omega_n - \varepsilon + \mu)$. As a result, the energies of the singlet and triplet states are

$$\omega = \varepsilon - \mu - \frac{3J}{2}, \qquad \omega = \varepsilon - \mu + \frac{J}{2}.$$
 (19)

4 Two-Site Processes of the Spin-Fluctuation Scattering

The approximation used in Sect. 3 takes into account the on-site spin-fluctuation scattering processes in all the orders of perturbation theory and allows us to obtain the self-energy operator and the Green's function describing the main effect which is the formation of a strongly coupled spin-polaron state. However, to describe the correct quasimomentum dependence of the spin-polaron quasiparticle energy, the used approximation is not enough. In this Section, we go beyond the first order approximation by taking into account the contributions determined by the multisite spin-fluctuation scattering processes in the self-energy part.

To calculate these contributions, we take into account two circumstances. The first one is connected with the fact that the subsystem of localized copper ions is in the spin-liquid state as it was mentioned in Sect. 3. This state is characterized by nonzero values of the two-site correlation functions C_{δ} . The second circumstance is related to the fact that the multisite correlation functions $C_{f_1 f_2 \dots f_{2n}} = \langle S_{f_1}^{i_1} S_{f_2}^{i_2} \dots S_{f_{2n}}^{i_{2n}} \rangle$ are reduced rapidly with an increase in an even number of sites (the correlation functions with an odd number of sites are equal to zero). Correspondingly, we can restrict ourselves to the contributions induced by only the two-site scattering processes. The contributions of these processes to the self-energy operator are described by the following two classes of diagrams

$$-\sum_{1}^{(2)} = \frac{1}{k\alpha} + \frac{1}{$$



The analysis shows that the other diagrams give zero or insignificant contributions to the self-energy operator. In graphs (20) and (21), the ovals, which include two points at the ends of the lines of interaction, correspond to the two-site correlator

$$C_{\delta} = \langle \mathbf{S}_f \mathbf{S}_{f+\delta} \rangle, \quad \delta \neq 0.$$
⁽²²⁾

The values of these correlators for the spin-liquid phase of the 2D system of localized spins coupled by the antiferromagnetic Heisenberg interaction are well established [29].

The bold wavy line stands for an effective interaction

$$\tilde{J}_{kq}(i\omega_n) = \frac{J_{kq}}{1 + X(i\omega_n)}.$$
(23)

The analytical expression for the contributions determined by the two-site spinfluctuation scattering processes (20) and (21) in the self-energy part has the form

$$\begin{split} \Sigma^{(2)}(k, i\omega_n) &= \Sigma_1^{(2)}(k, i\omega_n) + \Sigma_2^{(2)}(k, i\omega_n), \\ \Sigma_1^{(2)}(k, i\omega_n) &= J v_k^2 \sum_{\delta} C_{\delta} \frac{e^{-ik\delta} X_{\delta}(i\omega_n)}{(1 + X(i\omega_n))^2}, \\ \Sigma_2^{(2)}(k, i\omega_n) &= J v_k^2 \sum_{\delta} C_{\delta} \frac{X_{\delta}^2(i\omega_n)}{(1 + X(i\omega_n))^3}, \end{split}$$
(24)

where

$$X_{\delta}(i\omega_n) = \frac{1}{N} \sum_{q} \frac{J v_q^2 e^{-iq\delta}}{i\omega_n - \xi_q}.$$
(25)

5 Results and Discussion

Using Eqs. (8), (16), (26), and taking into account that $\Sigma(k, i\omega_n) = \Sigma^{(1)}(k, i\omega_n) + \Sigma^{(2)}(k, i\omega_n)$, one can calculate the energy spectrum of the system. The Fermi excitation spectrum in the $\varphi - d$ model is determined by the solutions of the dispersion equation



$$\omega - \xi_k - \frac{1}{4} J v_k^2 \frac{1}{1 + X(\omega)} - J v_k^2 \sum_{\delta} C_{\delta} \left(\frac{1}{(1 + X(\omega))^2} + \frac{1}{(1 + X(\omega))^3} \right) = 0.$$
(26)

The calculations show that the main mechanism for the formation of the spinpolaron coupling consists in the strong spin-fermion interaction provided that on-site correlations are taken into account in all the orders of the perturbation theory in the exchange parameter J. However, this spin-polaron quasiparticle has a minimum energy at the point (π, π) of the Brillouin zone, since the effective spin-fermion coupling constant Jv_k^2 at this point has the greatest value.

The energy structure of the spin-polaron quasiparticles is changed qualitatively as soon as two-site spin-fermion scattering processes are taken into account. The most important result of such a change manifests itself in the displacement of the minimum of the spin-polaron band from point (π, π) to point $(\pi/2, \pi/2)$ of the Brillouin zone. Figure 1 shows the lower energy band of the $\varphi - d$ model obtained for the set of parameters J = 2.86, $\tilde{t} = 0.22$, t = 0.1 [23] and the values of the two-site correlation functions $C_1 = -0.27$, $C_2 = 0.1$, $C_3 = 0.1$ [29]. The energy spectrum of the spin-polaron quasiparticles agrees quantitatively well with the energy structure of quasiparticles in the normal phase of cuprate superconductors. It should be emphasized that the shift of the minimum of the bottom of the spin-polaron band due to the twosite spin-fluctuation scattering processes occurred without introducing any additional fitting parameters.

Another important result of the developed theory is connected with the nonmonotonic dependence of the spectral intensity

$$A(k,\omega) = -\frac{1}{\pi} \operatorname{Im} G(k,\omega+i\delta), \qquad (27)$$

when moving along the Brillouin zone (Fig. 2). This suggests the pseudogap behavior of the normal phase of cuprate superconductors.



Fig. 2 Spectral intensity $A(k, \omega)$ (**a**) and the residue of the Green's function $Z(k) = \int_{\omega} A(k, \omega) d\omega$ (**b**) calculated for the same parameters as those in Fig. 1 (Color figure online)

Conclusion

The proposed method for calculating the Fermi excitation spectrum in the normal phase of cuprate superconductors takes into account the main features of the real structure of these materials. First of all, this is due to the special features of the CuO_2 plane containing two oxygen ions in the unit cell. The second important feature is that the hole motion over oxygen ions is strongly correlated with the spin dynamics of the copper ions. This circumstance demands rigorous account for the on-site correlations. This problem is solved by the method based on the combination of the Feynman diagram technique and cumulant expansion for the spin operators.

It is essential that we managed to obtain an exact analytical expression for the part of the self-energy operator which is associated with the one- and two-site scattering processes in all the orders of perturbation theory. This allows us to derive the Green's function describing the spin-polaron quasiparticle possessing the energy which is smaller than the energy of the bare hole by the value $\sim J$.

The calculations of the energy structure result in the spin-polaron band with the minimum of the bottom at the point $(\pi/2, \pi/2)$ of the Brillouin zone, which is in a good agreement with experimental data on cuprate superconductors. The calculation of the spectral intensity when moving along the Brillouin zone demonstrates the modulation, which can lead to the formation of the pseudogap.

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