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DYNAMICAL MAGNETIC SUSCEPTIBILITY IN THE SPIN-FERMION MODEL FOR CUPRATE SUPERCONDUCTORS

V. V. Val'kov* **and D. M. Dzebisashvili*†**

Using the method of diagram techniques for the spin and Fermi operators in the framework of the $SU(2)$-invariant spin-fermion model of the electron structure of the CuO_2 plane of copper oxides, we obtain an exact representation of the Matsubara Green's function $D_\perp(k, i\omega_m)$ of the subsystem of localized spins. This representation includes the Larkin mass operator $\Sigma_{\mathrm{L}}(k, i\omega_m)$ and the strength and polarization operators $P(k, i\omega_m)$ and $\Pi(k, i\omega_m)$. The calculation in the one-loop approximation of the mass and strength operators for the Heisenberg spin system in the quantum spin-liquid state allows writing the Green's function $D_\perp(k, i\omega_m)$ explicitly and establishing a relation to the result of Shimahara and Takada. An essential point in the developed approach is taking the spin-polaron nature of the Fermi quasiparticles in the spin-fermion model into account in finding the contribution of oxygen holes to the spin response in terms of the polarization operator $\Pi(k, i\omega_m)$.

Keywords: high-temperature conductor, spin-fermion model, magnetic susceptibility, spin polaron

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1. Introduction

The relevance of calculating the magnetic susceptibility of doped cuprate high-temperature superconductors (HTS) is due to the necessity of correctly interpreting a large collection of experimental data on the spin response in cuprates [1]. Parent compounds of HTS based on copper are antiferromagnetic Mott–Hubbard dielectrics. Under doping, current carriers emerge in them, and the long-range magnetic order is simultaneously disrupted. Because electrons are strongly correlated, the problem of calculating the magnetic susceptibility in cuprate compounds is nontrivial.

In [2]–[9], the described problem was solved in the framework of the two-dimensional t–J model and the Hubbard model. But in most cases [3]–[7], the magnetic susceptibility was calculated based on the method of the memory function [10]–[12]. In [13], the problem of the cuprate magnetic susceptibility was studied in the framework of the frustrated Heisenberg model, and a spherically symmetric approach was used to evaluate the spin Green's functions [14].

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

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

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It is assumed that the t–J model is a low-energy effective model obtained from a more general so-called three-band p–d model [15]–[17], which contains all necessary couplings to allow describing the main features of the electron structure of the CuO_2 plane of cuprate HTS. Among all the couplings in the three-band p–d model, the most crucial are (1) the hybridization between p states of the oxygen ions and d states of the copper ions, whose strength is defined by the value $t_{\rm pd}$, (2) the presence of the energy gap $\Delta_{\rm pd} = \varepsilon_{\rm p} - \varepsilon_{\rm d}$ defining the difference of the energies $\varepsilon_{\rm d}$ and $\varepsilon_{\rm p}$ of the holes on the respective copper and oxygen ions, and (3) the Coulomb coupling of two holes on the same copper ion $U_{\rm d}$.

The smallness of the mixing parameter $t_{\rm pd}$ compared with the energy difference $\Delta_{\rm pd}$ and the Coulomb coupling energy $U_{\rm d}$ allows obtaining the $SU(2)$-invariant spin-fermion model [18], [19]. Unlike the t–J model, the spin-fermion model includes (1) the presence of two oxygen ions in the unit cell of the CuO_2 plane and (2) the presence of two hole subsystems, the collective state of holes in the sublattices of the oxygen ions and the holes localized on the copper ions. Obviously, the spin-fermion model is more suitable than the t–J model for describing the low-temperature thermodynamics of cuprate HTS.

In [20] in studying the dynamical magnetic susceptibility of localized spin moments in the framework of the spin-fermion model, a formula was proposed for expressing the spin Green's function of the spin-fermion model in terms of the spin Green's function of the Heisenberg model and the polarization operator with the contribution of the collective holes taken into account. In this case, the Green's function of the Heisenberg model was calculated using the spherically symmetric approach [14], and the polarization operator was evaluated in [20] in the random phase approximation with the Fermi Green's functions that form a fermion loop in the random phase approximation being approximated by the bare Fermi propagators.

Here, in the framework of the spin-fermion model using the diagram method for both spin [21] and Fermi operators [22], we obtain an exact representation of the dynamical magnetic susceptibility of localized spins. We indicate the approximations for which the approximate formula proposed in [20] follows from the obtained exact representation of the response. But in contrast to [20], the Green's function of the Heisenberg model for the spin-liquid phase in the approximate formula is calculated using the diagram method for the spin operators [21]. The Fermi Green's functions defining the fermion loop in the polarization operator are calculated based on the spin-polaron approach [23], which takes the formation of the spin-polaron quasiparticles into account. The latter fact is crucial for describing the cuprate superconductor properties.

2. Spin–fermion model Hamiltonian

In the regime of strongly correlated electrons where $U_{\rm d} > \Delta_{\rm pd} \gg t_{\rm pd}$, the spin-fermion model Hamiltonian can be represented in the form [19], [24]

$$\hat{\mathscr{H}} = \hat{\mathscr{H}}_0 + \hat{\mathscr{H}}_J + \hat{\mathscr{H}}_I, \tag{1}$$

where

$$\begin{aligned} &\hat{\mathscr{H}}_0 = \sum_{k,\alpha} [\xi_{k_x} a^+_{k\alpha} a_{k\alpha} + \xi_{k_y} b^+_{k\alpha} b_{k\alpha} + t_k (a^+_{k\alpha} b_{k\alpha} + b^+_{k\alpha} a_{k\alpha})], \\ &\hat{\mathscr{H}}_J = \frac{J}{N} \sum_{k,q,f,\alpha,\beta} e^{if(q-k)} u^+_{k\alpha} (\vec{S}_f \vec{\sigma}_{\alpha\beta}) u_{q\beta}, \qquad \hat{\mathscr{H}}_I = \sum_{f,m} \frac{I_{fm}}{2} \vec{S}_f \vec{S}_m. \end{aligned} \tag{2}$$

The Hamiltonian $\hat{\mathscr{H}}_0$ describes the subsystem of oxygen holes in the momentum representation. The operators $a^\dagger_{k\alpha}$ and $a_{k\alpha}$ create and annihilate holes with the spin projection $\alpha = \pm 1/2$ in the oxygen subsystem with p_x orbitals. The operators $b^\dagger_{k\alpha}$ and $b_{k\alpha}$ act similarly in the oxygen subsystem with p_y orbitals. The functions defining the bare band structure of the oxygen holes are

$$\xi_{k_{x(y)}} = \varepsilon_{\rm p} - \mu + 2\tau\nu^2_{kx(y)}, \qquad t_k = (2\tau - 4t)\nu_{kx}\nu_{ky}, \qquad \nu_{kx} = \sin\frac{k_x}{2}, \qquad \nu_{ky} = \sin\frac{k_y}{2}. \tag{3}$$

Here, $\varepsilon_{\rm p}$ denotes the auxiliary one-site hole energy, μ denotes the system chemical potential, and the rate of the hops of the holes at the oxygen ions is given by the tunneling integrals τ and t. The first integral arises as a result of taking hybridization processes into account in the second order of the perturbation theory and is expressed in terms of the parameters of the initial Emery model:

$$\tau = \frac{t_{\rm pd}^2}{\Delta_{\rm pd}}\left(1 - \frac{\Delta_{\rm pd}}{U_{\rm d} - \Delta_{\rm pd} - 2V_{\rm pd}}\right). \tag{4}$$

The tunneling integral t reflects the presence of direct hops of holes between the nearest-neighbor oxygen ions.

The exchange between the oxygen subsystem and the localized spin subsystem is described by the operator $\hat{\mathscr{H}}_J$, where $\vec{S}_f$ is a vector operator of a spin localized at the f site, $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is a vector composed of Pauli matrices, and the operator

$$u_{k\alpha} = \nu_{kx} a_{k\alpha} + \nu_{ky} b_{k\alpha} \tag{5}$$

is defined as a linear combination of the operators $a_{k\alpha}$ and $b_{k\alpha}$.

The magnitude of the exchange between localized spins and the oxygen holes is defined by the formula

$$J = \frac{4t_{\rm pd}^2}{\Delta_{\rm pd}}\left(1 + \frac{\Delta_{\rm pd}}{U_{\rm d} - \Delta_{\rm pd} - 2V_{\rm pd}}\right). \tag{6}$$

The third term in Hamiltonian (1) takes the superexchange interaction between the localized spins at the sites f and m into account, whose value is determined by the parameter I_{fm}.

The appearance in formulas (3) and (5) of the trigonometric functions of ν_{kx} and ν_{ky} is a consequence of the explicit treatment of the signs of the hole tunneling integrals due to the phase factors of the p and d orbitals.

It follows from expression (1) for the Hamiltonian of the spin-fermion model that if we consider the tunneling integral t for the direct oxygen–oxygen hops small compared with the parameter τ, then the operator structure of Hamiltonian (1) can be substantially simplified. For this, we introduce the unitary transformation

$$\phi_{k\alpha} = \frac{\nu_{kx} a_{k\alpha} + \nu_{ky} b_{k\alpha}}{\nu_k}, \qquad \psi_{k\alpha} = \frac{-\nu_{ky} a_{k\alpha} + \nu_{kx} b_{k\alpha}}{\nu_k}, \tag{7}$$

where $\nu_k^2 = \nu_{kx}^2 + \nu_{ky}^2$. The introduced operators satisfy the usual Fermi commutation relations $\{\varphi_{k\sigma}, \varphi_{p\sigma'}^+\} = \{\psi_{k\sigma}, \psi_{p\sigma'}^+\} = \delta_{kp}\delta_{\sigma\sigma'}$.

In the representation of $\varphi_{k\alpha}$ and $\psi_{k\alpha}$, the operators $\hat{\mathscr{H}}_0$ and $\hat{\mathscr{H}}_J$ become

$$\begin{aligned} \hat{\mathscr{H}}_0 &= \sum_{k,\alpha} [\xi_k \varphi_{k\alpha}^+ \varphi_{k\alpha} + (\varepsilon_{\rm p} - \mu)\psi_{k\alpha}^+ \psi_{k\alpha}], \\ \hat{\mathscr{H}}_J &= \frac{1}{N} \sum_{k,q,f,\alpha,\beta} e^{if(q-k)} J_{kq} \varphi_{k\alpha}^+ (\vec{S}_f \vec{\sigma}_{\alpha\beta}) \varphi_{q\beta}, \end{aligned} \tag{8}$$

where $\xi_k = \varepsilon_{\rm p} - \mu + 2\tau\nu_k^2$ and $J_{kq} = J\nu_k\nu_q$.

In the obtained expressions, we see that only the quasiparticles described by the operators φ_k interact with the localized spin subsystem on the copper ions. It turns out that the quasiparticles corresponding to the operators ψ_k are not coupled to the localized subsystem and hence do not participate in forming the spin-polaron state. Therefore, the second term in the operator $\hat{\mathscr{H}}_0$ in (8) is hereafter not taken into account.

Moreover, for convenience in constructing the spin diagram technique, we introduce the infinitesimal field $h \to +0$. As a result, we obtain the final version of the effective Hamiltonian [25]:

$$\hat{\mathscr{H}} = \hat{\mathscr{H}}_0 + \hat{\mathscr{H}}_J + \hat{\mathscr{H}}_I, \tag{9}$$

where

$$\hat{\mathscr{H}}_0 = \sum_{k,\alpha} \xi_k \varphi^+_{k\alpha} \varphi_{k\alpha} - h \sum_f S^z_f. \tag{10}$$

3. Matsubara Green's function for the subsystem of localized spins

The dynamical magnetic susceptibility for the subsystem of localized spins, as is known, is related to the Matsubara spin Green's function [21]:

$$D_\perp(f\tau; f'\tau') = -\frac{1}{2}\langle T_\tau \tilde{S}^+_f(\tau)\tilde{S}^-_{f'}(\tau')\rangle = \frac{T}{N}\sum_{k,\omega_n} e^{ik(f-f')-i\omega_n(\tau-\tau')} D_\perp(k, i\omega_n). \tag{11}$$

The dependence of $D_\perp(f\tau; f'\tau')$ on the Matsubara time arguments τ and τ' is due to the evolution of the spin operators in the "Heisenberg" representation

$$\tilde{S}^\pm_f(\tau) = e^{\tau\hat{\mathscr{H}}} S^\pm_f e^{-\tau\hat{\mathscr{H}}}, \tag{12}$$

where $0 < \tau < 1/\beta$, $\beta = 1/T$, and T is the temperature. The circular components of the spin are standardly related to the Cartesian components: $S^\pm_f = S^x_f \pm iS^y_f$. The operator T_τ involved in formula (11) is the operator of chronological ordering with respect to the Matsubara time arguments. The angle brackets in (11) mean that the operator expression inside it is averaged over the density matrix corresponding to the grand canonical ensemble. Taking the Fourier transform of the coordinate–time Green's function, we take into account that because of the quasibosonic commutation relations for the spin operators, the summation over the Matsubara frequencies is only over the even $\omega_m = 2\pi mT$, $m = 0, \pm, 1 \pm 2, \dots$ (see [21]).

To calculate $D_\perp$ using the perturbation theory, we pass to the interaction representation [21]. Then

$$D_\perp(f\tau; f'\tau') = -\frac{1}{2}\langle T_\tau S^+_f(\tau) S^-_{f'}(\tau')\mathfrak{S}(\beta)\rangle_{0c}, \tag{13}$$

where the temperature scattering matrix is defined by the expression

$$\mathfrak{S}(\beta) = T_\tau \exp\left\{-\int_0^\beta d\tau\, (\hat{\mathscr{H}}_J(\tau) + \hat{\mathscr{H}}_I(\tau))\right\} \tag{14}$$

and the dependence on the time operators without the tilde shows that these operators are considered in the interaction representation with a zero Hamiltonian. In particular,

$$S^\pm_f(\tau) = e^{\tau\hat{\mathscr{H}}_0} S^\pm_f e^{-\tau\hat{\mathscr{H}}_0}. \tag{15}$$

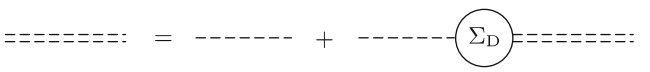
Similar expressions can be written for the operators $\hat{\mathscr{H}}_J(\tau)$ and $\hat{\mathscr{H}}_I(\tau)$. The subscript 0 by the right angle bracket in (13) means that the thermodynamic mean is defined by the statistical operator with the Hamiltonian $\hat{\mathscr{H}}_0$. Expanding $\mathfrak{S}(\beta)$ in a power series and expanding each of the terms by the Wick theorem for the spin operators, we only include contributions corresponding to connected diagrams [21]. This explains the presence of the additional subscript c in (13).

4. The Dyson equation: The strength and polarization operators

A particular feature of the commutation relations for the spin operators is that the result of commuting two different spin operators corresponding to the same site is again an operator, not a number as for bosonic operators. In the diagram technique, we see this as a result of the appearance of the so-called terminal multipliers [26], [27]. The contributions of the complete collection of the terminal multipliers to all orders of the perturbation theory defines the strength operator $P(k, i\omega_n)$. The Green's function $D_\perp(k, i\omega_n)$ can then be expressed in terms of the complete propagator $G_\perp(k, i\omega_n)$ and the strength operator using the relations [26], [27]

$$D_\perp(k, i\omega_n) = G_\perp(k, i\omega_n)P(k, i\omega_n). \tag{16}$$

For the propagator $G_\perp(k, i\omega_n)$, the Dyson equation, which can be represented graphically as



(17)

holds, where the double dashed line denotes the function $G_\perp(k, i\omega_m)$, the single dashed line corresponds to the bare propagator $g(i\omega_m) = (i\omega_m - h)^{-1}$, and the circle with Σ_D corresponds to the Dyson mass operator, which is the sum of all Dyson-irreducible self-energy parts. Dyson irreducibility means that it is impossible to represent the self-energy part as two disconnected parts by cutting along one single line. Solving (17) with respect to $G_\perp(k, i\omega_m)$, we obtain the Dyson equation for the Green's function $D_\perp(k, i\omega_m)$:

$$D_\perp(k, i\omega_m) = \frac{P(k, i\omega_m)}{i\omega_m - h - \Sigma_D(k, i\omega_m)}. \tag{18}$$

The form of the Heisenberg exchange coupling quadratic in the spin operators allows representing the Dyson mass operator $\Sigma_D(k, i\omega_m)$ as the sum of two terms:

$$\Sigma_D(k, i\omega_m) = \Sigma_L(k, i\omega_m) + P(k, i\omega_m)[I_k + \Pi(k, i\omega_m)], \tag{19}$$

where $\Sigma_L(k, i\omega_m)$ is the Larkin-irreducible self-energy part of the spin Green's function, $P(k, i\omega_m)$ is the strength operator (such a representation of the Heisenberg model was first considered in [28], [29]), I_k is the Fourier transform of the exchange integral, and $\Pi(k, i\omega_m)$ is the polarization operator. Taking all these facts into account, we obtain a convenient representation of the spin Green's function of the spin-fermion model:

$$D_\perp(k, i\omega_m) = \frac{P(k, i\omega_m)}{i\omega_m - h - \Sigma_L(k, i\omega_m) - I_k P(k, i\omega_m) - P(k, i\omega_m)\Pi(k, i\omega_m)}. \tag{20}$$

Introducing the Green's function

$$D_L(k, i\omega_m) = [i\omega_m - h - \Sigma_L(k, i\omega_m) - P(k, i\omega_m)I_k]^{-1}P(k, i\omega_m) \tag{21}$$

allows rewriting Eq. (20) as

$$D_\perp(k, i\omega_m) = \{D_L(k, i\omega_m)^{-1} - \Pi(k, i\omega_m)\}^{-1}. \tag{22}$$

In this formula, the role of the mass operator in $D_\perp(k, i\omega_m)$ is played just by the polarization operator. This is technically convenient in calculating (see the text below). The difference of the diagram series for the Green's function $D_L(k, i\omega_m)$ from the series for $D_\perp(k, i\omega_m)$ is that the first series does not contain contributions to the mass operator that are reducible with respect to the polarization operator. This means

that there are no diagrams in the series for $D_{\mathrm{L}}(k, i\omega_m)$ that can be cut along two Fermi propagation lines into two disconnected parts.

We note that the random phase approximation used in [20] to analyze the magnetic susceptibility in cuprates follows from formula (22) if we take one fermion loop with the bare Fermi Green's functions $G^{(0)}(k, i\omega_n) = (i\omega_n - \varepsilon_k)^{-1}$ ($\omega_n = (2n+1)\pi T$, $n = 0, \pm 1, \dots$) for a polarization operator $\Pi(k, i\omega_m)$ and neglect all the contributions due to the coupling $\hat{\mathscr{H}}_J$ in the diagram expansion of the Green's function $D_{\mathrm{L}}(k, i\omega_m)$. In this case, $D_{\mathrm{L}}(k, i\omega_m)$ describes a purely spin system with the Heisenberg coupling.

It was proposed to use the expression obtained in [14] in the framework of the spherically symmetric theory [30] for the Green's function $D_{\mathrm{L}}(k, i\omega_m)$ for $J = 0$ in [20]. In what follows, we obtain the expression for the spin Green's function of the Heisenberg model in the quantum spin-liquid state using the diagram technique for spin operators.

5. One-loop approximation of the localized spin Green's function in the quantum spin-liquid state

It is well known that under the doping of a cuprate HTS, destruction of the long-range antiferromagnetic order is initiated by a relatively small number of oxygen holes. This allows using the concept according to which the two-dimensional system of localized spins is in the quantum spin-liquid state at a finite temperature. In this context, in the zeroth approximation with respect to the hole concentration, the collective properties of this ensemble of localized spins are defined by the Heisenberg Hamiltonian

$$\hat{\mathscr{H}}_\Gamma = \hat{\mathscr{H}}_{0\Gamma} + \hat{\mathscr{H}}_I \quad \left(\hat{\mathscr{H}}_{0\Gamma} = -h\sum_f S_f^z\right). \tag{23}$$

We can then assume that after we pass to the limit $h \to +0$, the localized spin ensemble of copper ions is in the state of an $SU(2)$-invariant quantum spin liquid. This means that $\langle S_f^x\rangle = \langle S_f^y\rangle = \langle S_f^z\rangle = 0$, and the spin correlation functions $C_j = \langle \vec{S}_f \vec{S}_{f+r_j}\rangle$ are nonzero (r_j is the radius vector of the jth coordinate sphere). The correlators C_j satisfy the relations

$$C_{r_j} \equiv C_j = 3\langle S_f^x S_{f+r_j}^x\rangle = 3\langle S_f^y S_{f+r_j}^y\rangle = 3\langle S_f^z S_{f+r_j}^z\rangle. \tag{24}$$

The listed conditions lead to the fact that in calculating the Green's function using the diagram technique, we need not take the diagrams whose contribution is proportional to the thermodynamic average $\langle S_f^z\rangle_{0\Gamma}$ into account. The subscript 0Γ in the expression $\langle S_f^z\rangle_{0\Gamma}$ means that we average with the density matrix defined by the "zero" Hamiltonian $\hat{\mathscr{H}}_{0\Gamma}$.

Both the Heisenberg-model spin Green's function $D_{\mathrm{L}}(k, i\omega_m)$ and the Green's function $D_\perp(k, i\omega_m)$ are given by Eq. (11), and the perturbation theory series is generated by the expansion of the temperature scattering matrix in (13) with the only difference that the density matrix used for thermodynamic averaging is now determined by the Hamiltonian $\hat{\mathscr{H}}_I$.

With these facts taken into account, the one-loop contribution to the Dyson mass operator $\Sigma_{\mathrm{D}}(k, i\omega_m)$ is defined by the sum of the six diagrams shown in Fig. 1. A single dashed line, as before, denotes the bare propagator $g(i\omega_m) = (i\omega_m - h)^{-1}$. A double dashed line denotes the Green's function $G_\Gamma(k, i\omega_m)$ satisfying Dyson equation (17). Wavy lines denote the Fourier transform of the exchange coupling integral I_k. In this context, wavy lines with circles denote the longitudinal coupling, and wavy lines with an arrowhead denote the transverse coupling. Striped (or bold in the terminology in [21]) ovals with two circles denote the third part of the Fourier transform of the spin correlator $C_k = \sum_r e^{-ikr} C_r$. The bold ovals are produced by adding diagrams to the bare (open) oval that allow transmitting the quasimomentum but not the Matsubara frequency through the oval. One possible way to produce a bold oval is shown by the diagram equation

(25)

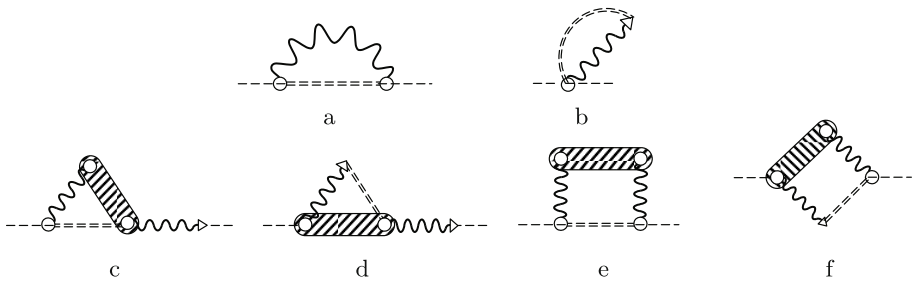


Fig. 1. One-loop diagrams for the Dyson mass operator of the spin Green's function in the Heisenberg model.

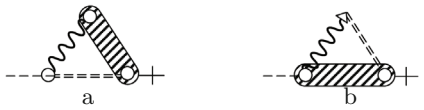


Fig. 2. One-loop diagrams for the strength operator of the spin Green's function in the Heisenberg model.

where the second-order cumulant arising in calculating the pair correlation function $\langle S_f^z S_g^z \rangle_{0\Gamma}$ [21] corresponds to the open oval with two circles.

The sum of the analytic contributions of the diagrams in Figs. 1c–1f containing the bold oval can be represented as

$$\Sigma_{\rm L}^{\rm (c-f)}(k, i\omega_m) = \frac{1}{N}\sum_q \frac{C_q}{3} G_{\rm L}(k-q, i\omega_m)(I_q - I_k)(I_q - I_{k-q}). \tag{26}$$

For the sum of the contributions from the diagrams in Figs. 1a and 1b, we obtain the expression

$$\Sigma_{\rm L}^{\rm (ab)}(k, i\omega_m) = \frac{T}{N}\sum_{q,\omega_n} I_q [G_{\rm L}(q, i\omega_n) - G_{\rm L}(k-q, i\omega_n)]. \tag{27}$$

We consider the approximation where the double dashed lines in the diagrams in Fig. 1 are replaced with single dashed lines. This approximation, as is seen below, corresponds to the Shimahara–Takada results. In the analytic form, this approximation corresponds to replacing the Green's functions $G_\Gamma(k-q, i\omega_m)$ in (26) with the propagators $g(i\omega_m)$. It is easy to see that such a replacement leads to the self-energy part $\Sigma_\Gamma^{\rm (ab)}$ vanishing. As a result, the self-energy $\Sigma_\Gamma(k, i\omega_m)$ in this approximation is influenced only by the contributions of $\Sigma_\Gamma^{\rm (c-f)}(k, i\omega_m)$:

$$\Sigma_\Gamma(k, i\omega_m) = \Sigma_\Gamma^{\rm (c-f)}(k, i\omega_m) = g(i\omega_m)\frac{1}{N}\sum_q \frac{C_q}{3}(I_q - I_k)(I_q - I_{k-q}). \tag{28}$$

We present the considered one-loop diagrams for the strength operator $P_\Gamma(k, i\omega_m)$ in Fig. 2.

In the spin-wave approximation, the analytic expression for the strength operator has the form

$$P_\Gamma(k, i\omega_m) = g(i\omega_m)\frac{1}{3N}\sum_q C_q(I_{k-q} - I_q). \tag{29}$$

Taking formulas (28) and (29) into account and passing to the limit $h \to 0$, we obtain the final expression for the spin Green's function D_Γ:

$$D_\Gamma(k, i\omega_m) = \frac{\frac{1}{3N}\sum_q C_q(I_{k-q} - I_q)}{(i\omega_m)^2 - \Omega_k^2}, \tag{30}$$

where Ω_k is the spectrum of the paramagnon excitations given by the equation

$$\Omega_k^2 = \frac{1}{N}\sum_q \frac{C_q}{3}(I_q - I_k)(I_q - I_{k-q}). \tag{31}$$

If the exchange integral I_{fg} is nonzero only for nearest neighbors, then the expression for spectrum (31) in terms of spin correlators (24) has the form

$$\Omega_k^2 = \frac{4}{3}I_1^2(1-\gamma_{1k})\left[\frac{3}{4} + 2C_2 + C_3 - 4C_1\gamma_{1k}\right], \tag{32}$$

where I_1 is an exchange integral for nearest neighbors. The structure of the obtained Green's function agrees with the results of Shimahara and Takada [14].

6. The polarization operator and the dynamical magnetic susceptibility of the localized subsystem in the spin-fermion model

The magnetic susceptibility of the localized subsystem in the spin-fermion model with the oxygen holes taken into account is calculated according to formula (22),

$$D_\perp(k, i\omega_m) = \{D_{\rm L}(k, i\omega_m)^{-1} - \Pi(k, i\omega_m)\}^{-1},$$

using two types of approximation. The first approximation is based on using expression (30) for the Green's function $D_{\rm L}$. Such a substitution, as previously mentioned, means that we neglect all contributions proportional to the parameter J in the diagram expansion of $\Sigma_{\rm L}$. In this case, the contribution of oxygen is contained only in the polarization operator $\Pi(k, i\omega_m)$. The second approximation is based on taking only one-loop diagrams into account for the polarization operator (the random phase approximation). In this approximation for $\Pi(k, i\omega_m)$, we obtain the equality

$$\Pi(k, i\omega_m) = \frac{T}{N}\sum_{q,\omega_n} J_{q,q+k}^2 G(q, i\omega_n)G(q+k, i\omega_m + i\omega_n), \tag{33}$$

where the Fermi Green's functions $G(q, i\omega_n)$ generating the fermion loop are defined by the relation

$$G(q, i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}(-)\langle T_\tau \tilde{\varphi}_{q\sigma}(\tau)\tilde{\varphi}^+_{q\sigma}(0)\rangle. \tag{34}$$

In (34), the operators φ are written in the Heisenberg representation, and ω_n is an odd Matsubara frequency, $\omega_n = (2n+1)\pi T$.

As noted above, using the bare Fermi propagators $G^{(0)}(q, i\omega_n) = (i\omega_n - \varepsilon_q)^{-1}$ instead of the complete Fermi Green's functions $G(q, i\omega_n)$ to calculate $\Pi(k, i\omega_m)$ was proposed in [20]. In this case, the spin-polaron nature of the Fermi quasiparticles is obviously not taken into account.

Here, we use the projection technique of Zwanzig–Mori [10]–[12] to calculate the Green's function $G(q, i\omega_n)$; this allows describing the formation of spin polarons using the spin-fermion model. In the framework of this theory, we introduce a set of basis operators such that they provide an adequate description of the system dynamics. We write the equations of motion for the basis operators, which are then projected onto the chosen basis.

As a first basis operator, we choose φ_k. The equation of motion for φ_k has the form

$$i\,\frac{d\varphi_{k\sigma}}{dt} = [\varphi_{k\sigma}, \hat{\mathscr{H}}] = \xi_k\varphi_{k\sigma} + J\nu_k L_{k\sigma}, \tag{35}$$

where

$$L_{k\sigma} = \frac{1}{N}\sum_{f,q,\beta} e^{if(q-k)}\nu_q(\vec{S}_f\vec{\sigma}_{\sigma\beta})\varphi_{q\beta}. \tag{36}$$

The operator $L_{k\sigma}$ takes the coupling between the spin and charge degrees of freedom into account and is responsible for formation of the spin polaron in the system. As the second basis operator, we take $L_{k\sigma}$ and stop for now.

For convenience, we introduce the notation $A_{1k} = \varphi_k$ and $A_{2k} = L_k$. The expansion of the equations in terms of the operator basis $\{A_{1k}; A_{2k}\}$ is then written in the form $i\,dA_{jk\sigma}/dt = [A_{jk\sigma}, \hat{\mathscr{H}}] = \sum_l R_{jl}A_{lk\sigma}$. But for the matrix $\widehat{R}$, we can write the equality $\widehat{R} = \widehat{F}\widehat{K}^{-1}$, where the matrix entries $\widehat{F}$ and $\widehat{K}$ are defined by the relations

$$F_{ij} = \langle\{[A_{ik\sigma}, \hat{\mathscr{H}}], A^+_{jk\sigma}\}\rangle, \qquad K_{ij} = \langle\{A_{ik\sigma}, A^+_{jk\sigma}\}\rangle.$$

Taking the introduced notation into account, the system of equations for the retarded Green's functions $\mathcal{G}_{ij}(k,\omega) = \langle\langle A_{ik}|A^+_{jk}\rangle\rangle_\omega$ can be represented in the form

$$\hat{\mathcal{G}} = (\omega - \widehat{F}\widehat{K}^{-1})^{-1}\widehat{K}. \tag{37}$$

Calculating the matrix entries K_{ij} and F_{ij}, we obtain the formulas

$$\begin{aligned}
&K_{11} = 1, \qquad K_{12} = K_{21} = 0, \qquad K_{22} \equiv K = \frac{3}{4} - C_1\gamma_{1k},\\
&F_{11} = \xi_k, \qquad F_{12} = F_{21} = J\nu_k K,\\
&F_{22} \equiv \xi_{\text{L}}K = (\varepsilon_{\text{p}} - \mu + 4\tau)K + \tau\left(-\frac{9}{8} + C_2\gamma_{2k} + \frac{C_3\gamma_{3k}}{2}\right) -\\
&\qquad\qquad - \frac{3J}{4} + JC_1\left(2\gamma_{1k} + \frac{1}{4}\right) - IC_1(4 + \gamma_{1k}),
\end{aligned} \tag{38}$$

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

The expressions for the two branches $\varepsilon^{\pm}_k$ of the polaron spectrum are determined from the condition that the determinant $\det|\omega - \widehat{F}\widehat{K}^{-1}|$ is zero. They have the form

$$\varepsilon^{\pm}_k = \frac{\xi_k + \xi_{\text{L}}(k)}{2} \pm \frac{1}{2}\sqrt{(\xi_k - \xi_{\text{L}}(k))^2 + 4J^2\nu_k^2 K(k)}. \tag{39}$$

We note that the lower branch ε^-_k of this spectrum coincides with the spin-polaron spectrum of Hamiltonian (1) calculated in the basis $\{c_{f+a_x}; c_{f+a_y}; 1/2\sum_\delta(\vec{S}_f\vec{\sigma})c_{f+\delta}\}$ of three operators in [31].

Solving system of equations (37) for the Green's function $\mathcal{G}_{11}(k,\omega)$, we obtain

$$\mathcal{G}_{11}(k,\omega) = \frac{\omega - \xi_{\text{L}}(k)}{(\omega - \varepsilon^+_k)(\omega - \varepsilon^-_k)}. \tag{40}$$

Replacing the frequency ω with the odd Matsubara frequency $i\omega_n$ transforms the retarded Green's function $\mathcal{G}_{11}(k,\omega)$ into the Matsubara Green's function $G_\varphi(k, i\omega_n)$. Substituting the function $G_\varphi(k, i\omega_n)$ thus obtained in the expression for polarization operator (33), we obtain the expression

$$\Pi(k, i\omega_m) = \frac{T}{N}\sum_{q,\omega_n} J^2_{q,q+k}\frac{i\omega_n - \xi_{\text{L}}(q)}{(i\omega_n - \varepsilon^-_q)(i\omega_n - \varepsilon^+_q)} \times \frac{i\omega_{n+m} - \xi_{\text{L}}(q+k)}{(i\omega_{n+m} - \varepsilon^-_{q+k})(i\omega_{n+m} - \varepsilon^+_{q+k})}. \tag{41}$$

After the sum over the Matsubara frequency ω_n is calculated, the polarization operator becomes

$$\Pi(k,i\omega_m)=\frac{T}{N}\sum_q J^2_{q,q+k}\biggl\{f(\varepsilon^-_q)\frac{\varepsilon^-_q-\xi_{\rm L}(q)}{(\varepsilon^-_q-\varepsilon^+_q)}\times\frac{\varepsilon^-_q+i\omega_m-\xi_{\rm L}(q+k)}{(\varepsilon^-_q-\varepsilon^-_{q+k}+i\omega_m)(\varepsilon^-_q-\varepsilon^+_{q+k}+i\omega_m)}+$$

$$+f(\varepsilon^-_{q+k})\frac{\varepsilon^-_{q+k}-\xi_{\rm L}(q+k)}{(\varepsilon^-_{q+k}-\varepsilon^+_{q+k})}\times\frac{\varepsilon^-_{q+k}-i\omega_m-\xi_{\rm L}(k)}{(\varepsilon^-_{q+k}-\varepsilon^-_q-i\omega_m)(\varepsilon^-_{q+k}-\varepsilon^+_q-i\omega_m)}\biggr\},\qquad(42)$$

where $f(\varepsilon)=(e^{\varepsilon/T}+1)^{-1}$ is the Fermi–Dirac distribution function. In calculating this expression, we neglected the summands containing the distribution functions of the quasiparticles in the upper band with the dispersion ε^+_q because in the region of low current-carrier density that interests us, the chemical potential μ always belongs to the lower spin-polaron band.

Combining formulas (22) and (30) and continuing ($i\omega_m\to\omega+i\delta$) analytically, we obtain the final expression for the dynamical magnetic susceptibility:

$$\chi(k,\omega)=\frac{(1/3N)\sum_q C_q(I_q-I_{k-q})}{\omega^2-\Omega^2_k+(1/3N)\sum_q C_q(I_q-I_{k-q})\Pi(k,i\omega_m\to\omega+i\delta)},\qquad(43)$$

where the paramagnon excitation spectrum Ω_k is given by formula (31) and the polarization operator $\Pi(k,i\omega_m)$ is given by formula (42).

It can be seen that the polarization operator is zero in the absence of doping, and expression (43) describes the response of the localized spin subsystem. This response corresponds to the spherically symmetric Shimahara–Takada theory [14]. The addition of current carriers to the system leads to damping controlled by the imaginary part of the polarization operator $\Pi(k,\omega)$. As the concentration of current carriers increases, the damping should obviously increase, which finally completely destroys the short-range magnetic order.

Expression (43) for the dynamical magnetic susceptibility in the spin-fermion model taking the collectivized subsystem in the random phase approximation into account corresponds in structure to expressions for the response obtained by other authors [2]–[9], [13]. Although the used models and the applied theoretic approaches differ, the final formula for the dynamical magnetic susceptibility in all cited works can be represented in the unified form $\chi(k,\omega)=P(k,\omega)/(\omega^2-\omega^2_k-\Sigma(k,\omega))$. Formula (43) obtained here has the same form, but the new feature is that the polarization operator is calculated with the spin-polaron nature of the quasiparticles taken into account.

7. Conclusion

Applying the diagram technique to spin operators and the usual Feynman technique has turned out to be effective for studying systems with a strong coupling between localized spins and collectivized fermions. This has been demonstrated here for the spin-fermion model where the spacing between the Wannier centers of the spin and Fermi subsystems and the presence of p_x- and p_y-orbital oxygen holes in the same unit cell plays a crucial role in forming the nontrivial properties of the normal and superconducting phases of copper oxides.

The obtained exact representation for the transverse spin Green's function $D_\perp(k,i\omega_m)$ in terms of the Larkin mass operator $\Sigma_{\rm L}(k,i\omega_m)$ and the strength and polarization operators $P(k,i\omega_m)$ and $\Pi(k,i\omega_m)$ allows convenient calculations using perturbation theory and its diagram form.

Using the obtained representation with the subsequent calculation of $\Sigma_{\rm L}(k,i\omega_m)$ and $P(k,i\omega_m)$ in the one-loop approximation for the Heisenberg spin system in the quantum spin-liquid state allowed easily obtaining the spin function $D_{\rm L}(k,i\omega_m)$ and establishing the correspondence with the known results. Because the long-range magnetic order is not present in the spin-liquid state and only the short-range order is

preserved, the spin correlators must be defined self-consistently. In this regard, it is important that the obtained expression for $D_{\mathrm{L}}(k, i\omega_m)$ is more general, allows developing the self-consistent Born approximation, and takes the retardation effects into account.

The appearance of oxygen holes under doping opens an additional channel for influencing the spin-liquid state via the spin-fermion coupling mechanism. It induces the appearance of new diagrams for the Larkin mass operator $\Sigma_{\mathrm{L}}(k, i\omega_m)$ and the strength operator $P(k, i\omega_m)$. But the strongest effect is connected with the appearance of the polarization operator $\Pi(k, i\omega_m)$. As is known, the simplest approximation for it leads to an expression involving quantities that depend on the fermion energy spectrum.

Currently, it is established [32], [33] that the spin-polaron band of Fermi quasiparticles splits off in the spin-fermion model because of the large value of the coupling constant between localized spins and oxygen holes. The ensemble of these quasiparticles leads to unusual properties of the normal phase and also induces peculiarities of the Cooper instability of the copper oxides [31], [34]. Therefore, a correct solution of the problem of the influence of oxygen holes on the properties of the spin-liquid phase of the localized-spin subsystem presupposes that the polarization operator must be expressed in terms of the characteristics of the spin-polaron quasiparticles. The solution of this problem is one of our results here. Together with the obtained expression for the spin Green's function $D_{\mathrm{L}}(k, i\omega_m)$ of the Heisenberg system, it solves the posed problem of finding the transverse spin Green's function $D_{\perp}(k, i\omega_m)$ and the dynamical magnetic susceptibility of the localized subsystem in the one-loop approximation.

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