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* In Kazan University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

Spin response in HTSC cuprates: generalized RPA approach with projection operators method†

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We derive the dynamical spin susceptibility in the t-J-G model combining the random phase approximation (RPA) and projection operator method, which allows describing the mutual interplay between the local and the itinerant components of susceptibility. Near the antiferromagnetic wave vector the calculated dispersion of the spin excitations reproduces well the so-called hour-glass dispersion, characteristic for several layered cuprates. It is formed as a result of competition between the original spin-gap in magnon-like excitations spectrum and the superconducting gap, which affects the itinerant component of the susceptibility. Furthermore, the calculated collective spin excitations along $(0,0)$-$(0,\pi)$ are in agreement with the positions of the absorption peaks in the inelastic X-ray scattering spectra. They refer to the paramagnon-like modes, characteristic to the itinerant spin system, rather than magnon-like excitations that originate from short range order effect in the system of local spins at Cu sites.

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1. Introduction

The magnetic properties of high-temperature superconductors such as $YBa_2Cu_3O_{6+y}$ are quite unusual. These materials contain charge carriers, distributed mainly over the oxygen positions in CuO_2 plane and localized spins at the copper sites. Correspondingly, two approaches are used for the description of the dynamic spin susceptibility. When one starts from overdoped regime, it is naturally to employ the conventional Fermi liquid type description with effective on-site Coulomb repulsion of the carriers at the same site. If one considers the lightly doped regime, both the tendency towards Mott physics and strong antiferromagnetic correlations have to be taken into account. Here we focus on intermediate doping level, when there are both local and itinerant spins, but the system is still uniform. Possible phase separations in underdoped part of the phase diagram and existence of the spin density waves or charge density waves are not considered.

Previously [1, 2], combining projection Mori method and Green's function technique we derived an analytical formula for the spin susceptibility in superconducting cuprates. It allowed to take self consistently into account both the itinerant and the localized components of magnetic susceptibility. However, the spectrum of collective spin excitations, which is in focus of many experimental investigations, was not investigated in details. A dispersion of the collective spin excitations is needed for the construction of the microscopic theory of high temperature superconductivity, at least, when the spin fluctuations mechanism is assumed. In the present paper we systematize our results. We also discuss the possible improvement of the general expression

†This paper is originally written by authors on the occasion of eightieth birthday of Professor Boris I. Kochelaev.

for the spin susceptibility and will present new numerical results for real and imaginary parts of the dynamic spin susceptibility along symmetry routes of Brillion zone in the normal and superconducting states.

2. Model and general expression for susceptibility

The Hamiltonian of the model is written as [1, 2]

$$H = \sum_{i,j,\sigma} t_{ij}\psi_i^{pd,\sigma}\psi_j^{\sigma,pd} + \frac{1}{2}\sum_{i,j} J_{ij}[\mathbf{S}_i\mathbf{S}_j - \frac{n_i n_j}{4}] + \frac{1}{2}\sum_{i,j} G_{ij}^{\infty}\delta_i\delta_j = H_t + H_J + H_G. \quad (1)$$

Here, $\psi_i^{pd,\sigma}(\psi_j^{\sigma,pd})$ are the creation (annihilation) operators for composite quasiparticles. Symbol pd means that there is a strong coupling between copper and oxygen holes at each Cu-site in Cu-O plane, which is resembled in the formation of the so-called Zhang Rice [3-6] (copper-oxygen) singlet band at strong enough doping level. The second term $H_J = \frac{1}{2}\sum\limits_{i,j} J_{ij}[\mathbf{S}_i\mathbf{S}_j - \frac{n_i n_j}{4}]$ describes the superexchange interaction between Cu-spins at site i and j [7], $n_i = \psi_i^{\uparrow,\uparrow} + \psi_i^{\downarrow,\downarrow}$ is operator of the number of spins at site i. The last term refers to screened Coulomb repulsion between doped oxygen holes, $\delta_i = \psi_i^{pd,pd}$ is the operator of the number of copper-oxygen singlets per one unit cell.

For derivation of the spin susceptibility we employ the Green's function method and projection formalism. It is convenient to start from the equation

$$\omega\langle\langle S_q^+ \,|S_{-q}^-\rangle\rangle = \sum_{k'}(t_{k'+q} - t_{k'})\langle\langle\psi_{k'+q}^{\uparrow,pd}\psi_{k'}^{pd,\downarrow}\,|S_{-q}^-\rangle\rangle + \sum_{j,l} J_{jl}e^{-iqR_j}\langle\langle S_l^+S_j^z - S_l^zS_j^+\,|S_{-q}^-\rangle\rangle. \quad (2)$$

Here it is assumed that $\langle S_i^z\rangle = 0$ i.e. the long range spin order is absent, $t_k = \sum\limits_j t_{ij}\exp(i\mathbf{k}\mathbf{R}_{ij})$ is usual Fourier transform of the hopping integral. On the right-hand side we get two new Green's functions. The first can be naturally referred to itinerant spins, which accompany the motion of copper-oxygen singlet correlations over Cu-O plane, whereas the second term in Eq. (2) is related to localize spins at Cu-sites.

Linearization of the anticommutator

$$\left[\sum_{j,l} J_{jl}e^{-iqR_j}(S_l^+S_j^z - S_l^zS_j^+), H_J\right] \cong \Omega_q^2 S_q^+ \quad (3)$$

was discussed in many papers [8-18], where

$$\Omega_q^2 = 2J_1^2\alpha\,|K_1|\,(2-\gamma_q)(\Delta_{sp} + 2 + \gamma_q)] \quad (4)$$

is the typical expression for collective local spin excitations in layered aniferromagnets, Δ_{sp} is dimensionless spin-gap parameter, $\gamma_q = \cos q_x a + \cos q_y a$, α is decoupling parameter, which is usually calculated self-consistently via the sum rule $\langle S_i^+S_i^-\rangle = \frac{1}{2}(1-\delta)$ which is discussed in Appendix C, δ is a number of carriers per one unit cell, $K_1 = K_{01} = 4\langle S_0^zS_1^z\rangle$ is the spin-spin correlation function of nearest neighbors.

Calculation of the anticommutator $\left[\sum\limits_{i,l} J_{il}e^{-iqR_i}(S_l^+S_i^z - S_l^zS_i^+), H_t\right]$ is given in Appendix A.

It is approximated as follows

$$\left[\sum_{i,l} J_{il} e^{-iqR_i} (S_l^+ S_i^z - S_l^z S_i^+), \sum t_{j,m} \psi_j^{pd,\sigma} \psi_m^{\sigma,pd}\right] \cong$$
$$\cong \overline{J_1} t_1 \left[2 - \cos q_x a - \cos q_y a\right] S_q^+ - \frac{1}{2} \sum_k \left(\overline{J}_{k+q} - \overline{J}_k\right) \left(t_{k+q} - t_k\right) \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow}. \tag{5}$$

Here $\overline{J}_k = \sum\limits_l \overline{J_{il}} \exp(i\mathbf{k}\mathbf{R}_{il})$ and $\overline{J_{il}} = J_{il} \langle \psi_i^{pd,\uparrow} \psi_l^{\uparrow,pd} \rangle$. Angular brackets denote the thermodynamic average.

Using Eqs. (3), (5) we derive the equation for Fourier transform of Green's function as

$$\omega \sum_{i,l} J_{il} e^{-iqR_i} \langle\langle [(S_l^+ S_i^z - S_l^z S_i^+), H_t + H_J] \left| S_{-q}^- \right\rangle\rangle =$$
$$- \frac{i}{\pi} J_1 K_1 (2 - \gamma_q) + \left\{ \Omega_q^2 + \overline{J}_1 t_1 \left[2 - \cos q_x a - \cos q_y a\right] \right\} \langle\langle S_q^+ \left| S_{-q}^- \right\rangle\rangle \tag{6}$$
$$- \frac{1}{2} \sum_k \left(\overline{J}_{k+q} - \overline{J}_k\right) \left(t_{k+q} - t_k\right) \langle\langle \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow} \left| S_{-q}^- \right\rangle\rangle.$$

Appling projection method as it was described in Ref. [1] we write

$$i \frac{\partial \psi_k^{\uparrow,pd}}{\partial t} = \varepsilon_k \psi_k^{\uparrow,pd} + \Delta_k^{\uparrow} \psi_{-k}^{pd,\downarrow} + \frac{1}{N} \sum_q t'_{k-q} \psi_{k-q}^{\downarrow,pd} S_q^+$$
$$- \frac{1}{2N} \sum_q J_q \psi_{k-q}^{\downarrow,pd} S_q^+ + \frac{1}{2N} \sum_q G'_q (\psi_{k-q}^{\uparrow,pd} \psi_q^{pd,pd} + \psi_q^{pd,pd} \psi_{k-q}^{\uparrow,pd}). \tag{7}$$

The expression for the energy of quasiparticales is written as [1, 2]

$$\varepsilon_k = \sum_l \{ t_{lj} [P + (1 + 2F_{jl}^t) \langle S_j^z S_l^z \rangle / P] - \frac{2G_{jl} F_{jl}^G + J_{jl} F_{jl}^J}{1 + \delta} \langle \psi_l^{pd,\uparrow} \psi_j^{\uparrow,pd} \rangle \} e^{ikR_{jl}}. \tag{8}$$

Here, $P = (1+\delta)/2$, F_{jl}^t is projection parameter, which will be calculated later via a number of holes per one unit cell δ and spin-spin correlation function $\langle S_j^z S_l^z \rangle$. It is interesting to compare the quantity in square brackets with Gutzwiller's projection factor $2\delta/(1+\delta)$, which was introduced for the phenomenological description of the doping dependent bandwidth [19]. In contrast to Hubbard 1 approximation for $\delta \to 0$ the bandwidth shrinks to zero. The same result gives expression $P + (1 + 2F_{jl}^t) \langle S_j^z S_l^z \rangle / P$. For this particular case one expects that the spin-spin correlation for nearest neighbors on the square lattice will be given by $\langle S_0^z S_1^z \rangle \cong -1/4$ and $F_1 \to 0$. Note that the role of the last term in the bracket (8) at $\delta \cong 0.2$ is relatively small.

The superconducting gap equation is given by [1, 2]

$$\Delta_k = \frac{1}{PN} \sum_{k'} \left(\frac{1}{2} J_{k-k'} \langle \psi_{k'}^{\uparrow,pd} \psi_{-k'}^{\downarrow,pd} \rangle - G'_{k-k'} \langle \psi_{k'}^{\uparrow,pd} \psi_{-k'}^{\downarrow,pd} \rangle \right.$$
$$\left. + t_{k'} \langle \psi_{k'}^{\downarrow,pd} \psi_{-k'}^{\uparrow,pd} \rangle - t'_{k'} \langle \psi_{k'}^{\uparrow,pd} \psi_{-k'}^{\downarrow,pd} \rangle \right), \tag{9}$$

where $t'_k = \sum\limits_l t_{jl} F_{jl}^t \exp(i\mathbf{k}\mathbf{R}_{jl})$ is Fourier transform of the reduced hopping integral and $G_q = G_q^{\infty} - J_1/4$. The analysis of this equation for $J_{k-k'} > 2G_{k-k'}$, which we assume hereafter, reveals $\Delta_k = \Delta(T)(\cos k_x a - \cos k_y a)/2$. Having expression (7) one can construct the equation for functions $\langle\langle\psi^{\uparrow,pd}_{k'+q}\psi^{pd,\downarrow}_{k'}|S^-_{-q}\rangle\rangle$ and $\langle\langle\psi^{pd,\downarrow}_{k'}\psi^{\uparrow,pd}_{k'+q}|S^-_{-q}\rangle\rangle$, which enter in (2) and (5). However, one has to be careful because the rule of differentiation of product composite operators, as it was pointed in Ref. [10], is different from the usual case. Before applying expression (7) we write the following relations

$$\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k} = \frac{1}{N}\sum_{i,j}\psi^{\uparrow,pd}_{i}\psi^{pd,\downarrow}_{j}\left(1-\delta_{ij}\right)e^{-i(k+q)R_i+ikR_j} + \frac{1}{N}S^+_q, \tag{10}$$

$$\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q} = \frac{1}{N}\sum_{i,j}\psi^{\uparrow,pd}_{i}\psi^{pd,\downarrow}_{j}\left(1-\delta_{ij}\right)e^{-i(k+q)R_i+ikR_j}. \tag{11}$$

Then carry out the differentiation of operators with lattices index (site representation) and taking into account (10) and (11) one gets

$$\begin{aligned}
&\omega\langle\langle\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}\left|S^-_{-q}\right\rangle\rangle = \frac{i}{2\pi}\left(\langle\psi^{\uparrow,pd}_{k+q}\psi^{pd,\uparrow}_{k+q}\rangle - \langle\psi^{\downarrow,pd}_{k}\psi^{pd,\downarrow}_{k}\rangle\right)\\
&+\left(\varepsilon_{k+q}-\varepsilon_k\right)\langle\langle\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}\left|S^-_{-q}\right\rangle\\
&-\frac{1}{N}\Bigg([F_J\frac{1}{2}J_q - t_k(1-F_t)]\langle\psi^{\downarrow,pd}_{k}\psi^{pd,\downarrow}_{k}\rangle\\
&-[F_J\frac{1}{2}J_q - t_{k+q}(1-F_t)]\langle\psi^{\uparrow,pd}_{k+q}\psi^{pd,\uparrow}_{k+q}\rangle)]\langle\langle S^+_q\left|S^-_{-q}\right\rangle\rangle\Bigg)\\
&-\frac{1}{N}\sum_{k'}\left(\varepsilon_{k'+q}-\varepsilon_{k'}\right)\langle\langle\psi^{\uparrow,pd}_{k'+q}\psi^{pd,\downarrow}_{k'}\left|S^-_{-q}\right\rangle\rangle + \frac{\omega}{N}\langle\langle S^+_q\left|S^-_{-q}\right\rangle\rangle,
\end{aligned}\tag{12}$$

$$\begin{aligned}
&\omega\langle\langle\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q}\left|S^-_{-q}\right\rangle\rangle = \frac{i}{2\pi}\left(\langle\psi^{pd,\uparrow}_{k+q}\psi^{\uparrow,pd}_{k+q}\rangle - \langle\psi^{pd,\downarrow}_{k}\psi^{\downarrow,pd}_{k}\rangle\right)\\
&+\left(\varepsilon_{k+q}-\varepsilon_k\right)\langle\langle\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q}\left|S^-_{-q}\right\rangle\rangle\\
&-\frac{1}{N}\Bigg([F_J\frac{1}{2}J_q - t_k(1-F_t)]\langle\psi^{pd,\downarrow}_{k}\psi^{\downarrow,pd}_{k}\rangle\\
&-[F_J\frac{1}{2}J_q - t_{k+q}(1-F_t)]\langle\psi^{pd,\uparrow}_{k+q}\psi^{\uparrow,pd}_{k+q}\rangle)]\langle\langle S^+_q\left|S^-_{-q}\right\rangle\rangle\Bigg)\\
&-\frac{1}{N}\sum_{k'}\left(\varepsilon_{k'+q}-\varepsilon_{k'}\right)\langle\langle\psi^{pd,\downarrow}_{k'}\psi^{\uparrow,pd}_{k'+q}\left|S^-_{-q}\right\rangle\rangle.
\end{aligned}\tag{13}$$

These equations are rewritten as follows [2]

$$\langle\langle\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q}\left|S^-_{-q}\right\rangle\rangle = \frac{i}{2\pi}\chi_{k,q} + \frac{1}{N}\eta'_{k,q}\langle\langle S^+_q\left|S^-_{-q}\right\rangle\rangle + \frac{1}{N}\zeta_{k,q}D'(\omega,q), \tag{14}$$

$$\langle\langle\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}\left|S^-_{-q}\right\rangle\rangle = -\frac{i}{2\pi}\chi_{k,q} - \frac{1}{N}\eta''_{k,q}\langle\langle S^+_q\left|S^-_{-q}\right\rangle\rangle - \frac{1}{N}\zeta_{k,q}D''(\omega,q). \tag{15}$$

Here

$$\begin{aligned}
\chi_{k,q} &= \frac{n_{k+q}-n_k}{\omega+\varepsilon_k-\varepsilon_{k+q}}, \quad \eta'_{k,q} = \frac{1}{2}J_q\chi_{k,q} - \frac{t'_{k+q}n_{k+q}-t'_k n_k}{\omega+\varepsilon_k-\varepsilon_{k+q}},\\
\zeta_{k,q} &= \frac{1}{\omega+\varepsilon_k-\varepsilon_{k+q}}, \quad \eta''_{k,q} = \eta'_{k,q} + \frac{P(t'_{k+q}-t'_k)-\omega}{\omega+\varepsilon_k-\varepsilon_{k+q}},
\end{aligned}\tag{16}$$

$n_k = Pf\left(\varepsilon_k\right)$ are occupation numbers, $f\left(\varepsilon_k\right)$ is Fermi function. New Green's functions, which are appeared on right-hand side (14) and (15) are:

$$D'(\omega,q) = -\sum_k\left(\varepsilon_{k+q}-\varepsilon_k\right)\langle\langle\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q}\left|S^-_{-q}\right\rangle\rangle, \tag{17}$$

$$D''(\omega,q)=\sum_k(\varepsilon_{k+q}-\varepsilon_k)\langle\langle\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow}\left|S_{-q}^{-}\right.\rangle\rangle. \tag{18}$$

To compute these functions the following exact relations are used [1, 2]

$$\sum_k\psi_k^{pd,\downarrow}\psi_{k+q}^{\uparrow,pd}=0, \tag{19}$$

$$\sum_k\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow}=\sum_i S_i^{+}e^{-iqR_i}=S_q^{+}. \tag{20}$$

Combining Eqs. (14), (15) and (19), (20) one finds

$$D'(\omega,q)=-\left\{\frac{iN}{2\pi}\chi(\omega,q)+\eta'(\omega,q)\langle\langle S_q^{+}\left|S_{-q}^{-}\right.\rangle\rangle\right\}/\zeta(\omega,q) \tag{21}$$

and

$$D''(\omega,q)=-\left\{\frac{iN}{2\pi}\chi(\omega,q)+\left[1+\eta''(\omega,q)\right]\langle\langle S_q^{+}\left|S_{-q}^{-}\right.\rangle\rangle\right\}/\zeta(\omega,q). \tag{22}$$

Here,

$$\begin{aligned}\chi\left(\omega,q\right)&=\frac{1}{N}\sum_k\chi_{k,q},\;\;\eta'\left(\omega,q\right)=\frac{1}{N}\sum_k{\eta'}_{k,q},\\ \zeta\left(\omega,q\right)&=\frac{1}{N}\sum_k\zeta_{k,q},\;\;\eta''\left(\omega,q\right)=\frac{1}{N}\sum_k{\eta''}_{k,q}.\end{aligned} \tag{23}$$

Taking into account that $\sum\limits_k(\varepsilon_{k+q}-\varepsilon_k)=0$, it is easy to prove that $D'(\omega,q)=D''(\omega,q)$ and derive the relation [2]

$$F_{ij}^t=\frac{|K_{ij}|}{(1+\delta)^2-2\left|K_{ij}\right|}. \tag{24}$$

Substituting $D''(\omega,q)$ functions in (15) we get

$$\begin{aligned}\langle\langle\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow}\left|S_{-q}^{-}\right.\rangle\rangle&=-\frac{i}{2\pi}\left[\chi_{k,q}-\frac{\zeta_{k,q}}{\zeta(\omega,q)}\chi(\omega,q)\right]\\ &+\frac{1}{N}\left([1+\eta''(\omega,q)]\frac{\zeta_{k,q}}{\zeta(\omega,q)}-{\eta''}_{k,q}\right)\langle\langle S_q^{+}\left|S_{-q}^{-}\right.\rangle\rangle.\end{aligned} \tag{25}$$

Then multiplying (2) by frequency and using Eq. (5) we find

$$\begin{aligned}&\left\{\omega^2-\Omega_q^2-\overline{J}_1t_1\left[2-\cos q_xa-\cos q_ya\right]\right\}\langle\langle S_q^{+}\left|S_{-q}^{-}\right.\rangle\rangle=-\frac{i}{2\pi}2J_1K_1\left(2-\gamma_q\right)\\ &-\frac{1}{2}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k\right)\left(t_{k+q}-t_k\right)\langle\langle\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow}\left|S_{-q}^{-}\right.\rangle\rangle\\ &+\omega\sum_{k'}(t_{k'+q}-t_{k'})\langle\langle\psi_{k'+q}^{\uparrow,pd}\psi_{k'}^{pd,\downarrow}\left|S_{-q}^{-}\right.\rangle\rangle\\ &=-\frac{i}{\pi}J_1K_1\left(2-\gamma_q\right)-\frac{1}{2}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k-2\omega\right)\left(t_{k+q}-t_k\right)\langle\langle\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow}\left|S_{-q}^{-}\right.\rangle\rangle.\end{aligned} \tag{26}$$

Substituting here the expression for $\langle\langle\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow}\left|S_{-q}^{-}\right.\rangle\rangle$ function as given by (25), we get the equation

$$\begin{aligned}&\left(\omega^2-\Omega_q^2-\overline{t}_1J_1\left[2-\cos q_xa-\cos q_ya\right]\right)\langle\langle S_q^{+}\left|S_{-q}^{-}\right.\rangle\rangle=\\ &=-\frac{iN}{2\pi}\left[2J_1K_1\left(2-\gamma_q\right)+\frac{\chi}{\zeta}\zeta_{tJ}-\chi_{tJ}\right]-\left[(1+\eta'')\frac{\zeta_{tJ}}{\zeta}-{\eta''}_{tJ}\right]\langle\langle S_q^{+}\left|S_{-q}^{-}\right.\rangle\rangle.\end{aligned} \tag{27}$$

Since $N\chi^{+,-}_{total}(\omega,q) = 2\pi i\langle\langle S^+_q \left| S^-_{-q}\rangle\rangle\right.$ for the dynamical spin susceptibility per one unit cell we get

$$\chi^{+,-}_{total} = \frac{\chi\zeta_{tJ} + \left[2J_1K_1\left(2-\gamma_q\right) - \chi_{tJ}\right]\zeta}{\left[1+\eta''\right]\zeta_{tJ} + \left[\omega^2 - \Omega_q^2 - \overline{J_1}t_1\left(2-\gamma_q\right) - \eta''{}_{tJ}\right]\zeta}. \tag{28}$$

Here the symbol (ω, q), which accompanies the functions χ, ζ, η, is dropped for short. The new functions with index tJ are:

$$\chi_{tJ}(\omega,q) = \frac{1}{2N}\sum_k \left(t_{k+q} - t_k\right)\left[\overline{J}_{k+q} - \overline{J}_k - 2\omega\right]\chi_{kq}, \tag{29}$$

$$\eta''{}_{tJ}(\omega,q) = \frac{1}{2N}\sum_k \left(t_{k+q} - t_k\right)\left[\overline{J}_{k+q} - \overline{J}_k - 2\omega\right]\eta''{}_{kq}, \tag{30}$$

$$\zeta_{tJ}(\omega,q) = \frac{1}{2N}\sum_k \left(t_{k+q} - t_k\right)\left[\overline{J}_{k+q} - \overline{J}_k - 2\omega\right]\zeta_{kq}. \tag{31}$$

The expression (28) can be rewritten also as follows

$$\chi^{+,-}_{total} = \frac{\chi\zeta_{tJ} + \left[2J_1K_1\left(2-\gamma_q\right) - \chi_{tJ}\right]\zeta}{\left[1+\lambda\right]\zeta_{tJ} + \left[\omega^2 - \Omega_q^2 - \overline{J_1}t_1\left(2-\gamma_q\right) - \lambda_{tJ}\right]\zeta}, \tag{32}$$

where $\lambda = \eta'' - \omega\zeta$ (this is a function like defined in [20]):

$$\begin{aligned}
\lambda_{k,q} &= \eta'{}_{k,q} + \frac{P(t'{}_{k+q} - t'{}_k)}{\omega + \varepsilon_k - \varepsilon_{k+q}},\\
\lambda &= \lambda\left(\omega,q\right) = \frac{1}{N}\sum_k \lambda_{k,q},\\
\lambda_{tJ}(\omega,q) &= \frac{1}{2N}\sum_k \left(t_{k+q} - t_k\right)\left[\overline{J}_{k+q} - \overline{J}_k - 2\omega\right]\lambda_{kq}.
\end{aligned}$$

It seems this form is more convenient for numerical calculations. Another form for susceptibility, which has more clear properties under electron-hole transformation, is discussed in Appendix B. Note that in numerical calculations the substitution $\omega \to \omega + i\Gamma$ is assumed in all entering functions. Γ is dumping factor, which can be anisotropic along the Fermi contour. Factor $[1+\lambda]$ in denominator (32) reminds the corresponding Stoner's factor in random phase approximation schema (RPA) for itinerant electron system. On the other hand, the quantity $\left[\Omega_q^2 - \omega^2 + \overline{J_1}t_1\left(2-\gamma_q\right) + \lambda_{tJ}\right]$ is typical for localized spin-subsystem. Collective spin excitations are determined by equation

$$\left[1+\lambda\right]\frac{\zeta_{tJ}}{\zeta}\zeta_{tJ} + \left[\omega^2 - \Omega_q^2 - \overline{J_1}t_1\left(2-\gamma_q\right) - \lambda_{tJ}\right] = 0. \tag{33}$$

Therefore, local spin excitations (magnon-like) and itinerant holes (paramagnon-like) are coupled to each other self-consistently. In other words the total susceptibility (32) can be considered as a possible variant of description magnetic susceptibility compounds with interplay between local and itinerant spin subsystems.

3. Superconducting state

The expression for spin response function (32) retains its form in superconducting state as well. The entering functions, of course, modify due to Bogolyubov transformations in the superconducting state. The method of calculation can be found in Ref. [1]. The $\chi(\omega, q)$ function at $T < T_c$ is written like in BSC theory, except additional factor by $P = (1+\delta)/2$:

$$\begin{aligned}\chi(\omega,q) = \frac{P}{N}\sum S_{xx}\frac{f_{k+q}-f_k}{\omega+i\Gamma+E_k-E_{k+q}} + \frac{P}{N}\sum S_{yy}\frac{f_k-f_{k+q}}{\omega+i\Gamma-E_k+E_{k+q}} \\ +\frac{P}{N}\sum S^{(-)}_{yx}\frac{f_k+f_{k+q}-1}{\omega+i\Gamma-E_k-E_{k+q}} + \frac{P}{N}\sum S^{(+)}_{xy}\frac{1-f_k-f_{k+q}}{\omega+i\Gamma+E_k+E_{k+q}},\end{aligned} \tag{34}$$

$f_k = \{1+\exp[E_k/k_BT]\}^{-1}$ is the usual Fermi function. For the sake of simplicity, we are using the following abbreviation for the coherence factors:

$$\begin{aligned} S_{xx} &= x_k x_{k+q} + z_k z_{k+q}, \quad & S_{yy} &= y_k y_{k+q} + z_k z_{k+q}, \\ S^{(+)}_{xy} &= x_k y_{k+q} - z_k z_{k+q}, \quad & S^{(-)}_{yx} &= y_k x_{k+q} - z_k z_{k+q}, \end{aligned} \tag{35}$$

where

$$\begin{aligned} x_k &= \frac{1}{2}\left[1+\frac{\varepsilon_k-\mu}{E_k}\right], \quad & y_k &= \frac{1}{2}\left[1-\frac{\varepsilon_k-\mu}{E_k}\right], \\ z_k &= \frac{\Delta_k}{2E_k}, & E_k &= \sqrt{(\varepsilon_k-\mu)^2+|\Delta_k|^2}. \end{aligned} \tag{36}$$

The function $\lambda(\omega, q)$ is written as [20]

$$\begin{aligned}\lambda(\omega,q) &= \frac{1}{2}J_qF_J\chi(\omega,q) \\ &-\frac{P}{N}\left(\sum S_{xx}\frac{t'_{k+q}(f_{k+q}-1)-t'_k(f_k-1)}{\omega+i\Gamma+E_k-E_{k+q}} + \sum S_{yy}\frac{t'_kf_k-t'_{k+q}f_{k+q}}{\omega+i\Gamma-E_k+E_{k+q}}\right. \\ &\left.+\sum S^{(-)}_{yx}\frac{t'_kf_k-t'_{k+q}(1-f_{k+q})}{\omega+i\Gamma-E_k-E_{k+q}} + \sum S^{(+)}_{xy}\frac{t'_k(1-f_k)-t'_{k+q}f_{k+q}}{\omega+i\Gamma+E_k+E_{k+q}}\right).\end{aligned} \tag{37}$$

Physically last term in Eq. (37) corresponds to an effective molecular field of kinematic origin. It is strong correlation effect, because in our case the anticommutate relations are different from conventional Fermi liquid.

The function $\zeta(\omega, q)$ is written as follows:

$$\begin{aligned}\zeta(\omega,q) = \frac{1}{N}\sum\frac{S_{xx}}{\omega+i\Gamma+E_k-E_{k+q}} + \frac{1}{N}\sum\frac{S_{yy}}{\omega+i\Gamma-E_k+E_{k+q}} \\ +\frac{1}{N}\sum\frac{S^{(-)}_{yx}}{\omega+i\Gamma-E_k-E_{k+q}} + \frac{1}{N}\sum\frac{S^{(+)}_{xy}}{\omega+i\Gamma+E_k+E_{k+q}}.\end{aligned} \tag{38}$$

Let us now for the moment assume that we do not have any conduction electrons (holes). Substituting zero instead Fermi functions, from expression (26) one gets

$$\chi^{+,-}_{local}(\omega,q) = \frac{-2J_1K_1(2-c_q)}{\Omega_q^2-\omega^2}. \tag{39}$$

This expression is identical to those found by many authors for lightly doped cuprates [8-17]. It is remarkable that magnetism of localized spins at $T < T_c$ is strongly suppressed "or in other words frozen out" due to the superconducting gap, which naturally incorporated in function $\zeta(\omega, q)$. In opposite limit, when spin-spin correlation functions are small, and conducting bandwidth is large enough and correspondently function $\zeta(\omega, q)$ is small the expression (32) corresponds to generalized random phase approximation (GRPA) schema [21-23]. Moreover, in limit $q \to 0$, $\omega \to 0$ the expression (32) converts to static susceptibility expression, which corresponds to those one, which was derived in Ref. [24], beyond Green's function method.

4. Numerical results

Calculated imaginary and real parts of susceptibility along triangle contour in Brillouin zone are displayed in Figs. 1-10. The chosen parameters are: $\Gamma = 4meV$, $\delta = 0.33$. We have neglected J_2 and K_2 as they are small numerically. The energy dispersion was chosen according to photoemission data [25]

$$\varepsilon_k = 2t_1(\cos k_x a + \cos k_y a) + 4t_2 \cos k_x a \cos k_y a - \mu, \tag{40}$$

where (in meV): $t_1 = 139$, $t_2 = -33$, $\mu = 88$. The superconducting gap function was set in agreement with analyzes of the temperature dependencies of nuclear relaxation rate, Knight shift and superfluid density, which were discussed in Ref. [23] and [26];

$$\Delta_k = \frac{\Delta_0}{2}(\cos k_x a - \cos k_y a) \tanh\left(1.76\sqrt{T_c/T - 1}\right). \tag{41}$$

The decoupling parameters α, β and F_J below (except of specific cases in Fig. 9) were set by 1.

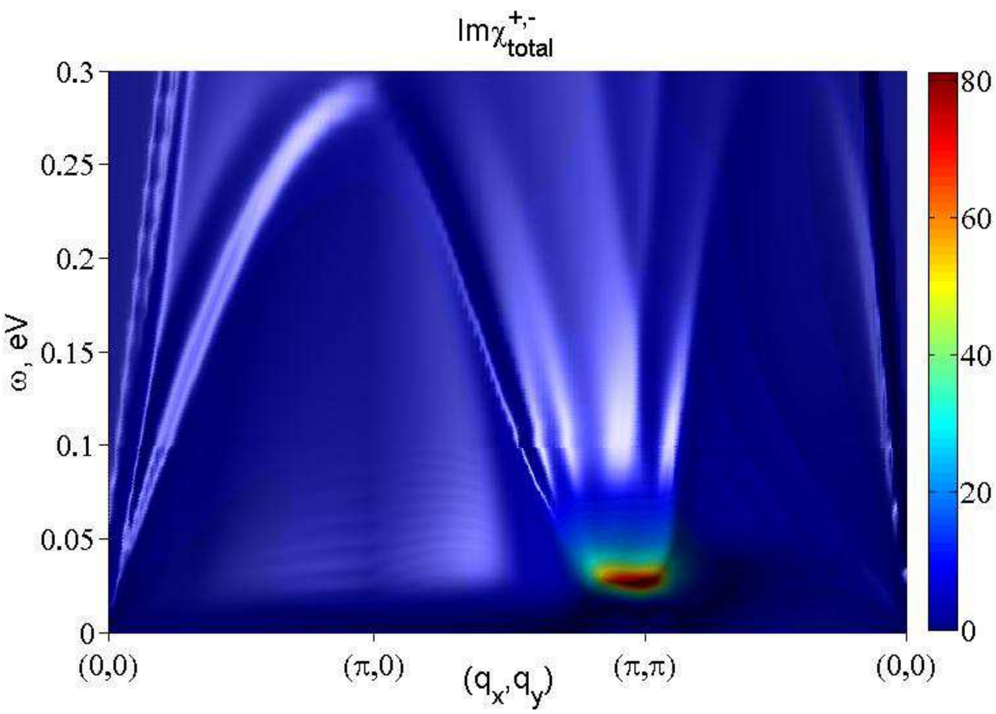

Figure 1. (Color online) Imaginary part of the dynamical susceptibility for the normal state. Input values are: $T = 100\,\mathrm{K}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.1$, $F_t = 0.1$. Upward dispersion can be interpreted as a damped magnon-like collective spin excitations. Vertical scale is in 1/eV.

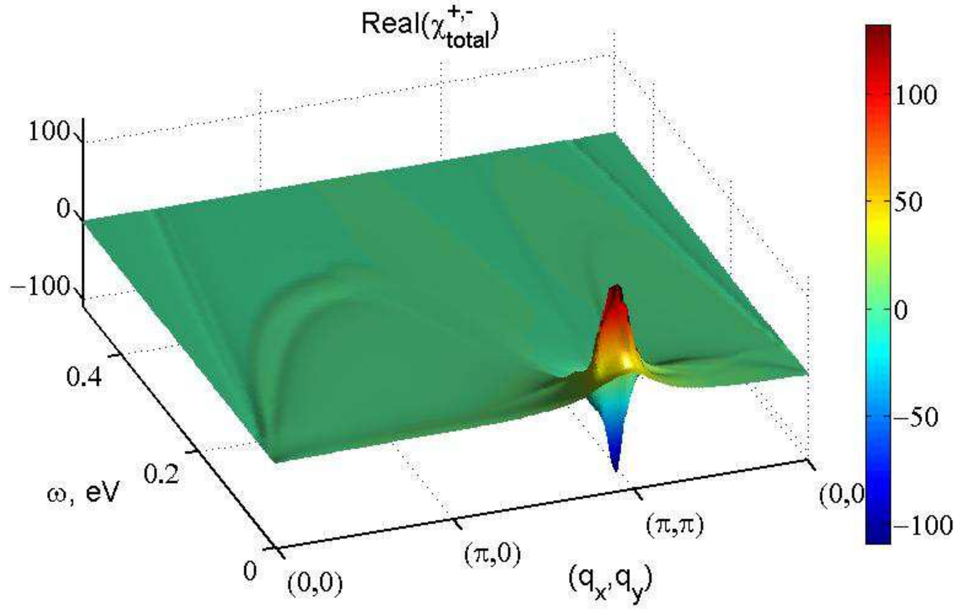

Figure 2. (Color online) The real part of the dynamical spin susceptibility for the superconducting state. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 25\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

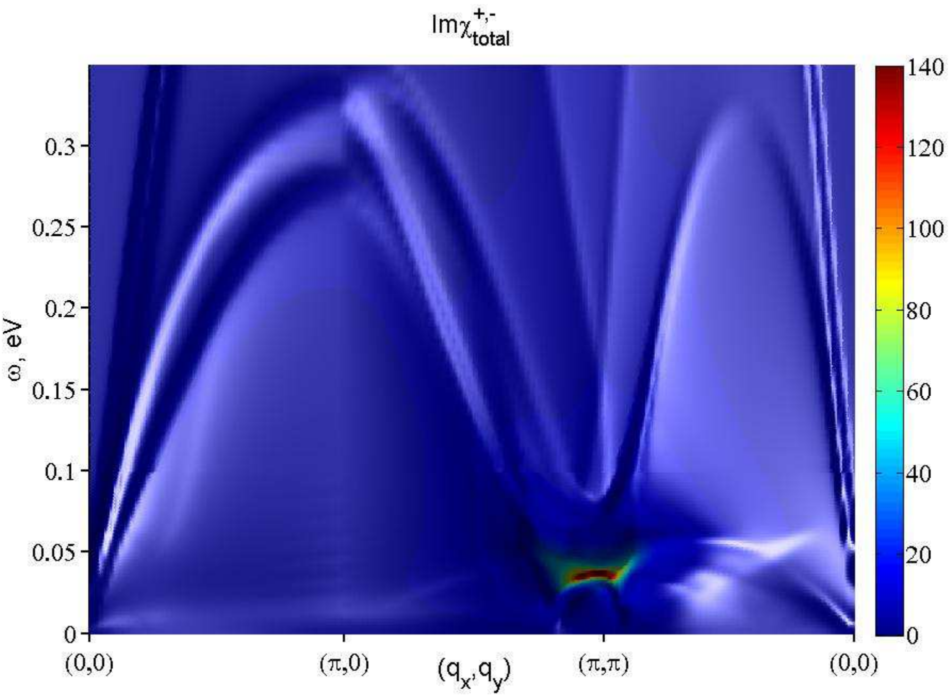

Figure 3. (Color online) The imaginary part of the dynamical spin susceptibility for the superconducting state. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 25\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

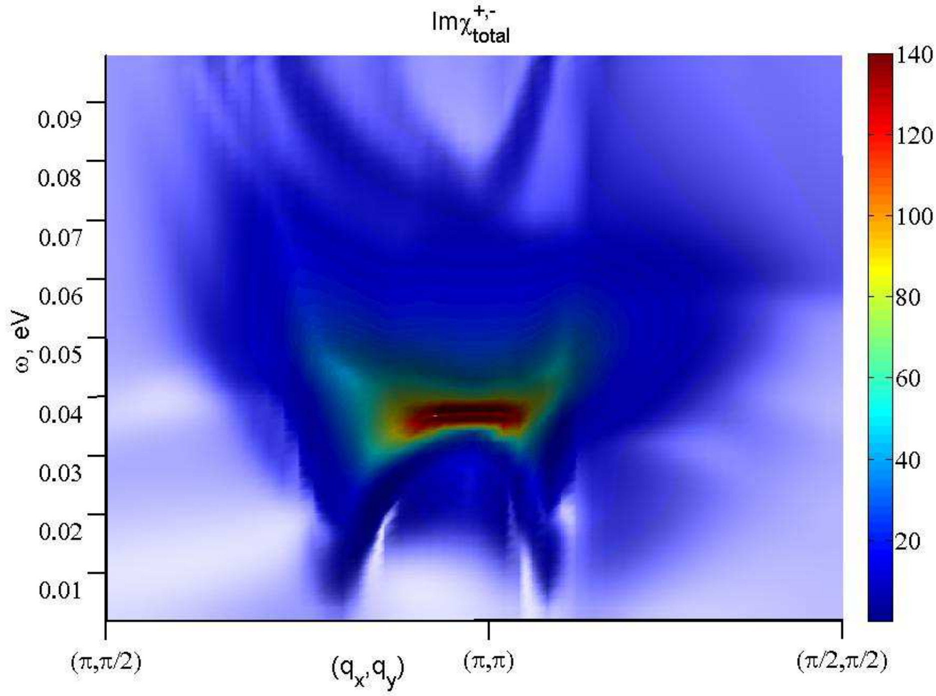

Figure 4. (Color online) Zoomed in region of point the imaginary part of the spin susceptibility for the superconducting state . This aria is usually probed by inelastic neutron scattering [27-33]. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 25\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

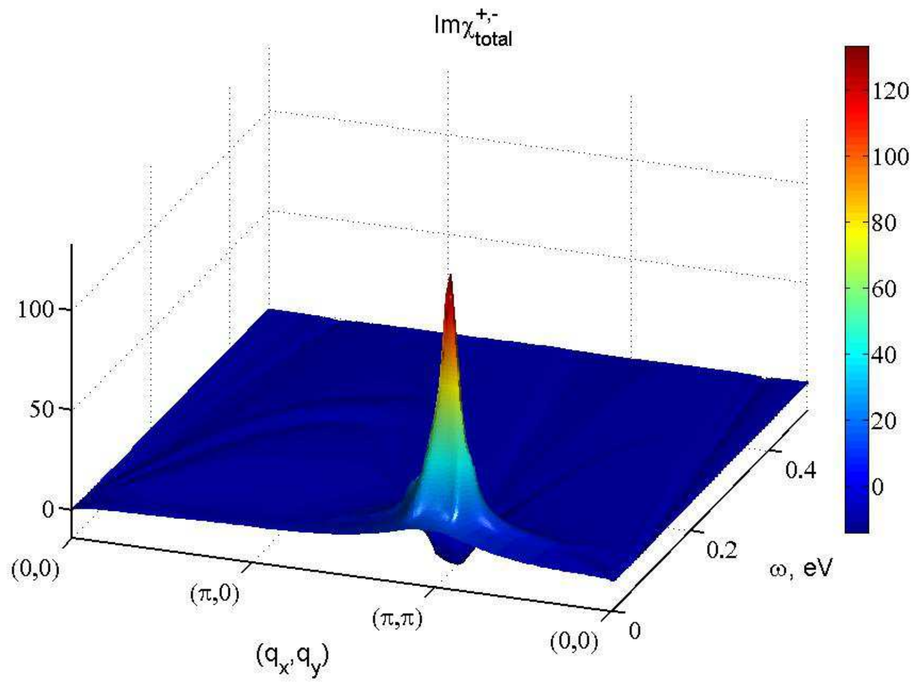

Figure 5. (Color online) Real part of the spin susceptibility for the superconducting state. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 30\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

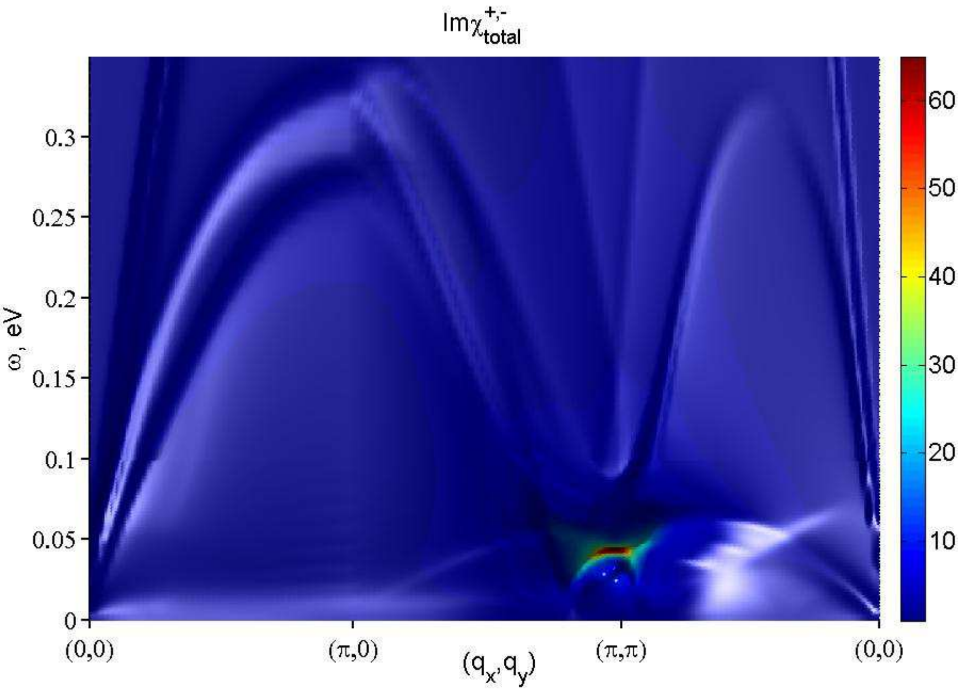

Figure 6. (Color online) Imaginary part of the spin susceptibility for the superconducting state. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 30\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

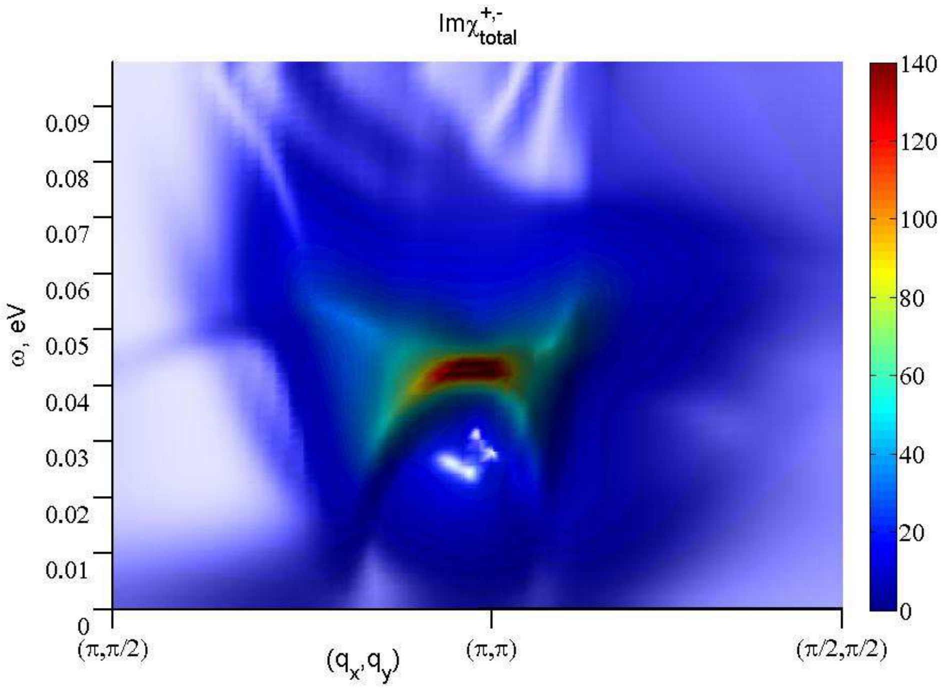

Figure 7. (Color online) The imaginary part of the spin susceptibility for the superconducting state in region of (π, π) point. This region is usually probed by inelastic neutron scattering [27-33]. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 30\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

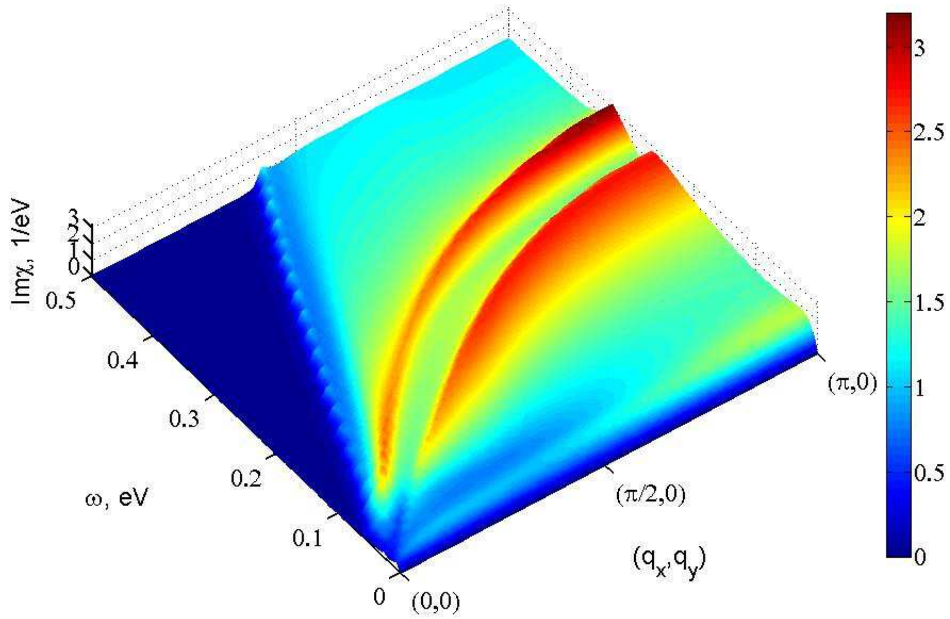

Figure 8. (Color online) Fragment of imaginary part susceptibility in superconducting state along the line in Brillouin zone. This region is studied by resonance inelastic X-ray scattering (RIXS) [34-38]. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 30\,\mathrm{meV}$, $J_1 = 66\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.14$, $F_t = 0.1$. Vertical scale is in 1/eV.

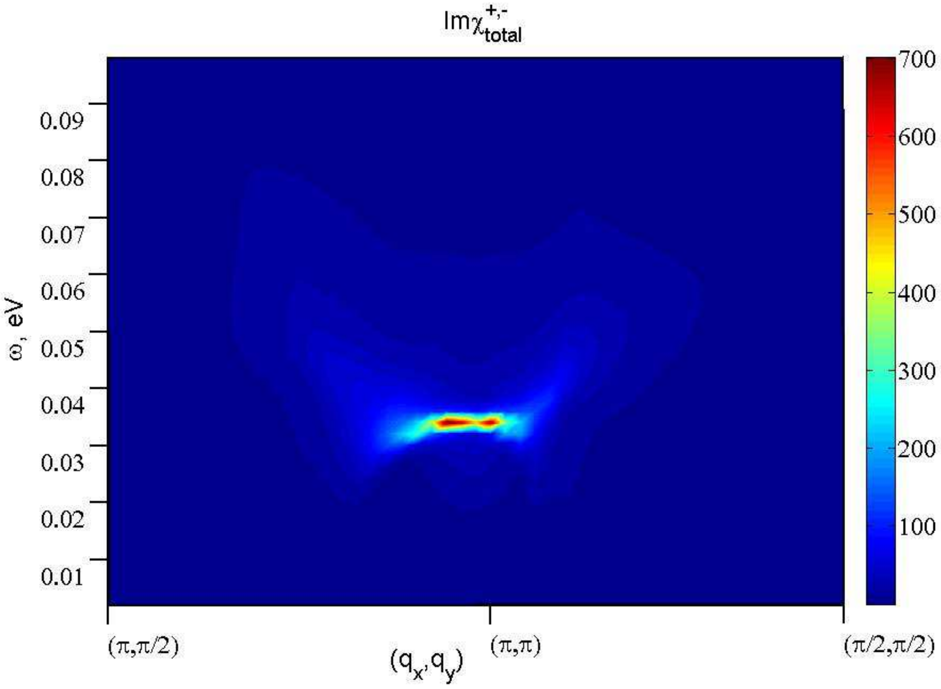

Figure 9. (Color online) Fragment of the imaginary part of the spin susceptibility for the superconducting state near (π,π) point. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 25\,\mathrm{meV}$, $J_1 = 70\,\mathrm{meV}$, $K_1 = -0.2$, $\Delta_{sp} = 0.147$, $F_t = 0.1$, $\beta = 0.6$. Vertical scale is in 1/eV.

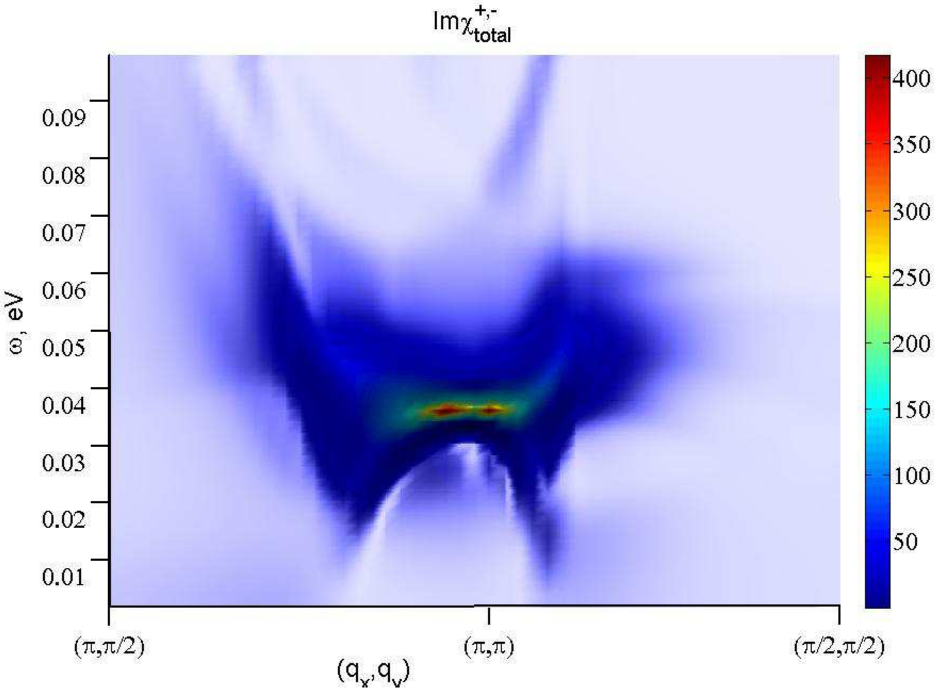

Figure 10. (Color online) Fragment of the imaginary part of the spin susceptibility for the superconducting state near (π, π) point. Input values are: $T = 10\,\mathrm{K}$, $\Delta_0 = 25\,\mathrm{meV}$, $J_1 = 76\,\mathrm{meV}$, $K_1 = -0.152$, $\Delta_{sp} = 0.17$, $F_t = 0.1$, $F_J = 0.89$. Vertical scale is in 1/eV.

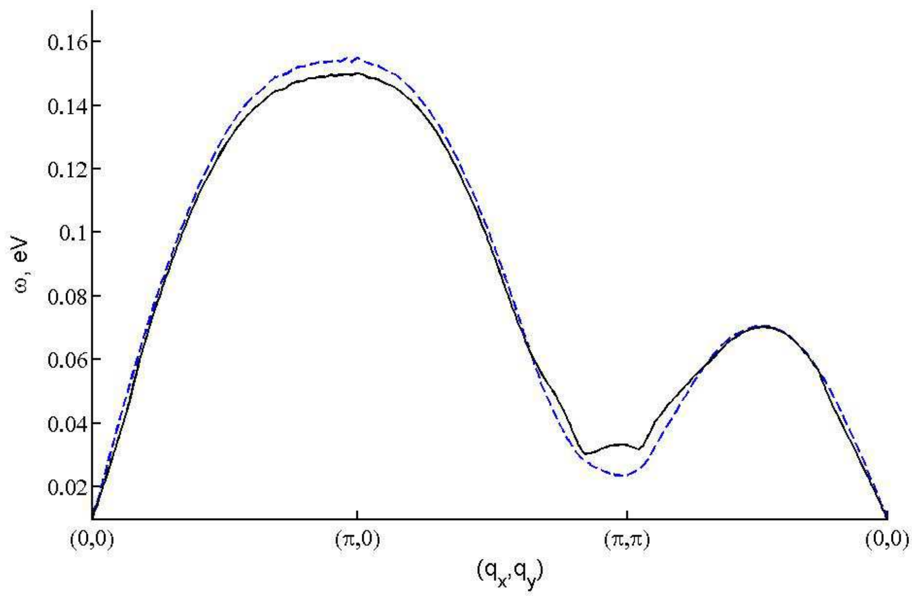

Figure 11. (Color online) Dispersion of the collective spin excitations calculated as a solution to the equation (32) along the route $(0,0) - (0,\pi) - (\pi,\pi) - (0,0)$ in the Brillouin zone for the normal state (dashed line) and superconducting one (solid line). Parameters are the same as in Fig. 3.

5. Conclusions and final remarks

The calculated results, shown in the previous section for the spin response near (π,π) point of the BZ resemble very strongly the experimental results reported by inelastic neutron scattering for hole doped cuprates [27-33]. Both the upward and the downward dispersions are successfully reproduced by our calculations. We have found that the fine features of the dynamical spin susceptibility near (π,π) point around the frequency 40 meV are very sensitive to the possible variation of the spin-gap ($\Delta_{sp} \cong 0.14$ or $\Delta_{sp} \cong 0.16$) and superconducting gap ($\Delta_0 = 25$ meV or $\Delta_0 = 30$ meV) parameters. Relatively small changes of these values lead to quite essential modification in the calculated picture. Under small changes of the input parameters the picture with the intersection of upward and downward dispersions (or in other words X-shape) in Fig. 4 and in Fig. 7 transforms to the so-called hour-glasses picture (Fig. 9).

As for the shape of the imaginary part of the spin susceptibility along the route $(0,0)-(\pi,0)$ is very similar to those which was observed by inelastic resonance X-ray scattering (RIXS) [34-38]. Generally, its dispersion is not so sensitive to the possible variation of the input parameters. Double shape form calculated by us here and in Ref. [20] was not observed experimentally, probably because of the error bars in the current RIXS technique, which is about 300 meV [34-38]. It is interesting to note that the splitting between two mountain chain-like features, found in Fig. 8, is sensitive to the superconducting gap values. This fact clearly demonstrates that these mountain chain-like features are more related to the itinerant part of spin subsystem rather than to the collective spin excitation of the localized spins. Another interesting observation is that the calculated frequency plot of the collective spin excitations (Fig. 11) does not exactly corresponds to the maximum positions of imaginary part, shown in Fig. 3. Especially this can be easily seen for dispersions along the route $(0,0)-(\pi,0)$. This observation strongly supports the idea that peaks in RIXS spectra correspond to the spin excitations, which originate from paramagnon-like features of the itinerant origin rather than magnon-like excitations, which would originate from the short range order of the local spins at Cu sites. The latter explains better the nature of the high-energy spin excitations near (π,π) point with frequencies which are above $2\Delta_0/\hbar$.

Acknowledgments

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Appendix A

Let us consider the commutator:

$$\left[\sum_{i,l} J_{il} e^{-iqR_i} (S_l^+ S_i^z - S_l^z S_i^+), \sum_{j,m} t_{j,m} \psi_j^{pd,\sigma} \psi_m^{\sigma,pd}\right]. \tag{1a}$$

Using relation $[AB, CD] = A[B, C]D + AC[B, D] + [A, C]DB + C[A, D]B$ one has

$$\begin{aligned}
&\left[\sum_{i,l} J_{il} e^{-iqR_i} (S_l^+ S_i^z - S_l^z S_i^+), \sum_{j,m} t_{j,m} \psi_j^{pd,\sigma} \psi_m^{\sigma,pd}\right] = \\
&= -\frac{1}{2} \sum J_{il} e^{-iqR_i} t_{i,m} S_l^+ (\psi_i^{pd,\uparrow} \psi_m^{\uparrow,pd} - \psi_i^{pd,\downarrow} \psi_m^{\downarrow,pd}) \\
&+ \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{j,i} S_l^+ (\psi_j^{pd,\uparrow} \psi_i^{\uparrow,pd} - \psi_j^{pd,\downarrow} \psi_i^{\downarrow,pd}) \\
&- \sum J_{il} e^{-iqR_i} t_{l,m} \psi_l^{pd,\downarrow} \psi_m^{\uparrow,pd} S_i^z + \sum J_{il} e^{-iqR_i} t_{j,l} \psi_j^{pd,\downarrow} \psi_l^{\uparrow,pd} S_i^z \\
&+ \sum J_{il} e^{-iqR_i} t_{i,m} S_l^z \psi_i^{pd,\downarrow} \psi_m^{\uparrow,pd} - \sum J_{il} e^{-iqR_i} t_{j,i} S_l^z \psi_j^{pd,\downarrow} \psi_i^{\uparrow,pd} \\
&+ \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{l,m} (\psi_l^{pd,\uparrow} \psi_m^{\uparrow,pd} - \psi_l^{pd,\downarrow} \psi_m^{\downarrow,pd}) S_i^+ \\
&- \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{j,l} (\psi_j^{pd,\uparrow} \psi_l^{\uparrow,pd} - \psi_j^{pd,\downarrow} \psi_l^{\downarrow,pd}) S_i^+.
\end{aligned} \tag{2a}$$

Doing averaging we focus on the quantities $J_{il} \langle \psi_i^{pd,\sigma} \psi_l^{\sigma,pd} \rangle$ and $t_{il} \langle \psi_i^{pd,\sigma} \psi_l^{\sigma,pd} \rangle$ as suggested by Kuz'min [16]. However, assuming that $t_{i,m} \langle \psi_i^{pd,\uparrow} \psi_m^{\uparrow,pd} \rangle = t_{i,m} \langle \psi_i^{pd,\downarrow} \psi_m^{\downarrow,pd} \rangle$, we can see that the first two and the last two amounts in (1a) can be discarded. Further following Kuz'min suggestion for third, fourth, fifth and sixth terms we get following expressions:

$$\begin{aligned}
&- \sum J_{il} e^{-iqR_i} t_{l,m} \psi_l^{pd,\downarrow} \psi_m^{\uparrow,pd} S_i^z \\
&= \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{l,m} \psi_m^{\uparrow,pd} \psi_l^{pd,\downarrow} \left[\psi_i^{\uparrow,pd} \psi_i^{pd,\uparrow} - \psi_i^{\downarrow,pd} \psi_i^{pd,\downarrow}\right] \\
&\cong \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{l,m} \psi_m^{\uparrow,pd} \left[\psi_l^{pd,\downarrow} \psi_i^{\uparrow,pd} \psi_i^{pd,\uparrow} - \langle \psi_l^{pd,\downarrow} \psi_i^{\downarrow,pd} \rangle \psi_i^{pd,\downarrow}\right] \\
&\cong -\frac{1}{2} \sum J_{il} e^{-iqR_i} t_{l,m} \psi_m^{\uparrow,pd} \psi_i^{pd,\downarrow} \langle \psi_l^{pd,\downarrow} \psi_i^{\downarrow,pd} \rangle \\
&+ \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{l,m} \psi_m^{\uparrow,pd} \psi_l^{pd,\downarrow} \psi_i^{\uparrow,\uparrow},
\end{aligned} \tag{3a}$$

$$\begin{aligned}
&\sum J_{il} e^{-iqR_i} t_{j,l} \psi_j^{pd,\downarrow} \psi_l^{\uparrow,pd} S_i^z = \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{j,l} \psi_j^{pd,\downarrow} \psi_l^{\uparrow,pd} \left[\psi_i^{\uparrow,pd} \psi_i^{pd,\uparrow} - \psi_i^{\downarrow,pd} \psi_i^{pd,\downarrow}\right] \\
&= \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{j,l} \psi_j^{pd,\downarrow} \psi_i^{\uparrow,pd} \langle \psi_i^{pd,\uparrow} \psi_l^{\uparrow,pd} \rangle - \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{j,l} \psi_j^{pd,\downarrow} \psi_l^{\uparrow,pd} \psi_i^{\downarrow,\downarrow},
\end{aligned} \tag{4a}$$

$$\begin{aligned}
&\sum J_{il} e^{-iqR_i} t_{i,m} S_l^z \psi_i^{pd,\downarrow} \psi_m^{\uparrow,pd} = \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{i,m} \psi_i^{pd,\downarrow} \left[\psi_l^{\uparrow,pd} \psi_l^{pd,\uparrow} - \psi_l^{\downarrow,pd} \psi_l^{pd,\downarrow}\right] \psi_m^{\uparrow,pd} \\
&= -\frac{1}{2} \sum J_{il} e^{-iqR_i} t_{i,m} \langle \psi_i^{pd,\downarrow} \psi_l^{\downarrow,pd} \rangle \psi_l^{pd,\downarrow} \psi_m^{\uparrow,pd} + \frac{1}{2} \sum J_{il} e^{-iqR_i} t_{i,m} \psi_l^{\uparrow,\uparrow} \psi_i^{pd,\downarrow} \psi_m^{\uparrow,pd},
\end{aligned} \tag{5a}$$

$$-\sum J_{il}e^{-iqR_i}t_{j,i}S_l^z\psi_j^{pd,\downarrow}\psi_i^{\uparrow,pd} = \sum J_{il}e^{-iqR_i}t_{j,i}S_l^z\psi_i^{\uparrow,pd}\psi_j^{pd,\downarrow}$$
$$\cong \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,i}\langle\psi_l^{pd,\uparrow}\psi_i^{\uparrow,pd}\rangle\psi_l^{\uparrow,pd}\psi_j^{pd,\downarrow} - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,i}\psi_l^{\downarrow,\downarrow}\psi_i^{\uparrow,pd}\psi_j^{pd,\downarrow}. \tag{6a}$$

Keeping terms containing $J_{il}\langle\psi_i^{pd,\uparrow}\psi_l^{\uparrow,pd}\rangle = \overline{J_{il}}$ we have

$$\begin{aligned}
&-\frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{l,m}\psi_m^{\uparrow,pd}\psi_i^{pd,\downarrow} + \frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{j,l}\psi_j^{pd,\downarrow}\psi_i^{\uparrow,pd}\\
&-\frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{i,m}\psi_l^{pd,\downarrow}\psi_m^{\uparrow,pd} + \frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{j,i}\psi_l^{\uparrow,pd}\psi_j^{pd,\downarrow}\\
&= -\frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{l,m}\psi_m^{\uparrow,pd}\psi_i^{pd,\downarrow} - \frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{j,l}\psi_i^{\uparrow,pd}\psi_j^{pd,\downarrow}\\
&+\frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{i,m}\psi_m^{\uparrow,pd}\psi_l^{pd,\downarrow} + \frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{j,i}\psi_l^{\uparrow,pd}\psi_j^{pd,\downarrow}\\
&+\frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{i,l}S_i^{+} - \frac{1}{2}\sum \overline{J_{il}}e^{-iqR_i}t_{l,i}S_l^{+}.
\end{aligned} \tag{7a}$$

Next we turn to the Fourier components:

$$S_j^{+} = \frac{1}{N}\sum S_q^{+}e^{iqR_j}, \tag{8a}$$

$$\psi_j^{pd,\uparrow} = \frac{1}{\sqrt{N}}\sum_k \psi_k^{pd,\uparrow}e^{-ikR_j}. \tag{9a}$$

After straightforward calculation the expression (7a) can be rewritten as

$$-\frac{1}{2}(\overline{J_{k+q}} - \overline{J_k})(t_{k+q} - t_k)\psi_{k+q}^{\uparrow,pd}\psi_k^{pd,\downarrow} + \left(\overline{J_1}t_1\right)\left[2 - \cos q_x - \cos q_x\right]S_q^{+}. \tag{10a}$$

Now, consider the remaining in Eqs. (3a)-(6a) four terms:

$$\begin{aligned}
&\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{l,m}\psi_m^{\uparrow,pd}\psi_l^{pd,\downarrow}\psi_i^{\uparrow,\uparrow} - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,l}\psi_j^{pd,\downarrow}\psi_l^{\uparrow,pd}\psi_i^{\downarrow,\downarrow}\\
&+\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{i,m}\psi_l^{\uparrow,\uparrow}\psi_i^{pd,\downarrow}\psi_m^{\uparrow,pd} - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,i}\psi_l^{\downarrow,\downarrow}\psi_i^{\uparrow,pd}\psi_j^{pd,\downarrow}\\
&\cong \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{l,m}\langle\psi_m^{\uparrow,pd}\psi_i^{\uparrow,pd}\rangle\psi_i^{\uparrow,pd}\psi_l^{pd,\downarrow} - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,l}\langle\psi_j^{pd,\downarrow}\psi_i^{\downarrow,pd}\rangle\psi_i^{pd,\downarrow}\psi_l^{\uparrow,pd}\\
&+\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{i,m}\psi_i^{pd,\downarrow}\psi_l^{\uparrow,pd}\langle\psi_l^{pd,\uparrow}\psi_m^{\uparrow,pd}\rangle - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,i}\psi_i^{\uparrow,pd}\psi_l^{\downarrow,pd}\langle\psi_l^{pd,\downarrow}\psi_j^{pd,\downarrow}\rangle.
\end{aligned} \tag{11a}$$

Let us start with the following:

$$\begin{aligned}
&\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{l,m}\langle\psi_i^{pd,\uparrow}\psi_m^{\uparrow,pd}\rangle\psi_i^{\uparrow,pd}\psi_l^{pd,\downarrow} + \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,l}\langle\psi_j^{pd,\downarrow}\psi_i^{\downarrow,pd}\rangle\psi_l^{\uparrow,pd}\psi_i^{pd,\downarrow}\\
&-\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{i,m}\langle\psi_l^{pd,\uparrow}\psi_m^{\uparrow,pd}\rangle\psi_l^{\uparrow,pd}\psi_i^{pd,\downarrow} - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{j,i}\langle\psi_j^{pd,\downarrow}\psi_l^{\downarrow,pd}\rangle\psi_i^{\uparrow,pd}\psi_l^{pd,\downarrow}.
\end{aligned} \tag{12a}$$

The largest terms are:

$$\begin{aligned}
&\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{l,i}\langle\psi_i^{pd,pd}\rangle\psi_i^{\uparrow,pd}\psi_l^{pd,\downarrow} + \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{i,l}\langle\psi_i^{pd,pd}\rangle\psi_l^{\uparrow,pd}\psi_i^{pd,\downarrow}\\
&-\frac{1}{2}\sum J_{il}e^{-iqR_i}t_{i,l}\langle\psi_l^{pd,pd}\rangle\psi_l^{\uparrow,pd}\psi_i^{pd,\downarrow} - \frac{1}{2}\sum J_{il}e^{-iqR_i}t_{l,i}\langle\psi_l^{pd,pd}\rangle\psi_i^{\uparrow,pd}\psi_l^{pd,\downarrow}.
\end{aligned} \tag{13a}$$

In the uniform lattice $\langle \psi_i^{pd,pd} \rangle = \langle \psi_l^{pd,pd} \rangle$. Therefore, the first and fourth (second and third) do cancel each other.

Now let us discuss the role of the three-site correlations. After Fourier transform these terms are written as

$$\begin{aligned} &\frac{1}{2}\sum_{i,m} J_{il} e^{ikR_{il}} t_{lm} \langle \psi_i^{pd,\uparrow} \psi_m^{\uparrow,pd} \rangle \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow} + \frac{1}{2}\sum_{i,j} J_{il} e^{-i(k+q)R_{il}} t_{lj} \langle \psi_j^{pd,\downarrow} \psi_i^{\downarrow,pd} \rangle \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow} \\ -&\frac{1}{2}\sum_{l,m} J_{il} e^{i(k+q)R_{li}} t_{i,m} \langle \psi_l^{pd,\uparrow} \psi_m^{\uparrow,pd} \rangle \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow} - \frac{1}{2}\sum_{l,j} J_{il} e^{-ikR_{li}} t_{j,i} \langle \psi_j^{pd,\downarrow} \psi_l^{\downarrow,pd} \rangle \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow}. \end{aligned} \tag{14a}$$

Performing summation over the square lattice we find

$$\begin{aligned} &\frac{1}{2}\sum_{i,m} J_{il} e^{ikR_{il}} t_{lm} \langle \psi_i^{pd,\uparrow} \psi_m^{\uparrow,pd} \rangle - \frac{1}{2}\sum_{l,j} J_{il} e^{-ikR_{li}} t_{j,i} \langle \psi_j^{pd,\downarrow} \psi_l^{\downarrow,pd} \rangle \\ &\quad \cong J_1 t_1 \left(2\langle \psi_0^{pd,\uparrow} \psi_2^{\uparrow,pd} \rangle + \langle \psi_0^{pd,\uparrow} \psi_3^{\uparrow,pd} \rangle \right) (\cos q_x + \cos q_y) \\ &\quad - J_1 t_1 \left(2\langle \psi_0^{pd,\downarrow} \psi_2^{\downarrow,pd} \rangle + \langle \psi_0^{pd,\downarrow} \psi_3^{\downarrow,pd} \rangle \right) (\cos q_x + \cos q_y) = 0. \end{aligned} \tag{15a}$$

Here $\langle \psi_0^{pd,\downarrow} \psi_2^{\downarrow,pd} \rangle$ refers to the next nearest neighbor correlation. The hopping parameters t2=t02 and t3=t03 are not included into consideration.

Finally the anticommutator (1a) is written as follows:

$$\begin{aligned} &\left[\sum_{i,l} J_{il} e^{-iqR_i} (S_l^+ S_i^z - S_l^z S_i^+), \sum t_{j,m} \psi_j^{pd,\sigma} \psi_m^{\sigma,pd} \right] \\ &\cong \overline{J_1} t_1 \left[2 - \cos q_x a - \cos q_y a \right] S_q^+ - \frac{1}{2} \sum_k \left(\overline{J}_{k+q} - \overline{J}_k \right) (t_{k+q} - t_k)\, \psi_{k+q}^{\uparrow,pd} \psi_k^{pd,\downarrow}. \end{aligned} \tag{16a}$$

Here is, of course, an addition decoupling factor $\beta \cong 1$ is occurred, like factor α in Eq. (4). Therefore here it is logical to change the definition $\overline{J_1}$ as follows

$$\overline{J_1} = J_1 \beta \langle \psi_0^{pd,\uparrow} \psi_1^{\uparrow,pd} \rangle. \tag{17a}$$

It should be noted that our result (16a) is different from those which presented in the original paper [16] by factor 2. Furthermore, we do not approximate additionally the last term in Eq. (16a). The system of self-consistent equations for Green's functions can be obtained (see the main text), using expression for aticommutator, as it is given by (16a). Entering correlation functions in the normal state are calculated as follows

$$\begin{aligned} \langle \psi_j^{pd,\downarrow} \psi_l^{\downarrow,pd} \rangle &= \frac{1}{N} \sum_{k,k'} \langle \psi_k^{pd,\downarrow} \psi_{k'}^{\downarrow,pd} \rangle e^{-ikR_j + ik'R_l} \\ &= P\left(\frac{a}{2\pi}\right)^2 \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \frac{\cos\left(k_x R_{jl}^x + k_y R_{jl}^y\right)}{1 + \exp\left(\frac{\varepsilon_k - \mu}{k_B T}\right)} dk_x dk_y. \end{aligned} \tag{18a}$$

For nearest neighbors it is written as:

$$\langle \psi_0^{pd,\downarrow} \psi_1^{\downarrow,pd} \rangle = 4P\left(\frac{1}{2\pi}\right)^2 \int_0^{\pi} \int_0^{\pi} \frac{\cos q_x}{1 + \exp\left(\frac{\varepsilon_q - \mu}{k_B T}\right)} dq_x dq_y. \tag{19a}$$

Here tetragonal symmetry in Cu-O plane is assumed.

Appendix B

The Green's function of itinerant part in Eq. (2) can be rewritten as follows [2]

$$\begin{aligned}&\sum_k (t_{k+q}-t_k)\langle\langle \psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}\,|S^-_{-q}\rangle\rangle \\ &=\frac{1}{2}\sum_k (t_{k+q}-t_k)\langle\langle \left[\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}-\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}\right]\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}\,|S^-_{-q}\rangle\rangle.\end{aligned}\tag{1b}$$

In equation (16a) the last term can be rewritten as

$$\begin{aligned}-\frac{1}{2}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k\right)(t_{k+q}-t_k)\,\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}&=\frac{1}{2}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k\right)(t_{k+q}-t_k)\,\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q}\\ &-\frac{1}{2N}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k\right)(t_{k+q}-t_k)\,S^+_q.\end{aligned}\tag{2b}$$

In case of square lattice

$$-\frac{1}{2N}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k\right)(t_{k+q}-t_k)\cong -2t_1\overline{J_1}\left(2-\cos q_x a-\cos q_y a\right).\tag{3b}$$

Therefore the equation (16a) becomes

$$\begin{aligned}&\left[\sum_{i,l} J_{il}e^{-iqR_i}(S^+_l S^z_i - S^z_l S^+_i),\sum t_{j,m}\psi^{pd,\sigma}_j\psi^{\sigma,pd}_m\right]\\ &\cong -\overline{J_1}t_1\left[2-\cos q_x a-\cos q_y a\right]S^+_q\\ &-\frac{1}{4}\sum_k\left(\overline{J}_{k+q}-\overline{J}_k\right)(t_{k+q}-t_k)\left[\psi^{\uparrow,pd}_{k+q}\psi^{pd,\downarrow}_{k}-\psi^{pd,\downarrow}_{k}\psi^{\uparrow,pd}_{k+q}\right].\end{aligned}\tag{4b}$$

Using (1b) and (4b) we get the following expression for spin response function

$$\chi^{+,-}_{total}=\frac{\chi\zeta_{tJ}+\left[2J_1K_1\left(2-\gamma_q\right)-\chi_{tJ}\right]\zeta}{\left[\frac{1}{2}+\eta\right]\zeta_{tJ}+\left[\omega^2-\Omega^2_q-\overline{J_1}t_1\left(2-\gamma_q\right)-\eta_{tJ}\right]\zeta},\tag{5b}$$

where

$$\begin{aligned}\eta&=\frac{1}{N}\sum_k\eta_{k,q}=\frac{1}{2}J_qF_J\chi(\omega,q)\\ &-\frac{P}{N}\left(\sum S_{xx}\frac{t'_{k+q}(f_{k+q}-1/2)-t'_k(f_k-1/2)}{\omega+i\Gamma+E_k-E_{k+q}}\right.\\ &+\sum S_{yy}\frac{t'_{k+q}(1/2-f_{k+q})-t'_k(1/2-f_k)}{\omega+i\Gamma-E_k+E_{k+q}}\\ &+\sum S^{(-)}_{yx}\frac{t'_{k+q}(f_{k+q}-1/2)-t'_k(1/2-f_k)}{\omega+i\Gamma-E_k-E_{k+q}}\\ &\left.+\sum S^{(+)}_{xy}\frac{t'_{k+q}(1/2-f_{k+q})-t'_k(f_k-1/2)}{\omega+i\Gamma+E_k+E_{k+q}}\right),\end{aligned}\tag{6b}$$

as it was introduced in [2] and

$$\eta_{tJ}(\omega,q)=\frac{1}{2N}\sum_k(t_{k+q}-t_k)\left[\overline{J}_{k+q}-\overline{J}_k-2\omega\right]\eta_{kq}.\tag{7b}$$

Note the denominator of the dynamical spin susceptibility can be written also via $\eta'(w.q)$ function. Corresponding expression for $\eta'(w.q)$ in superconducting state can be found in Ref. [1]

Appendix C

Spin-spin correlation functions.

The spin-spin correlation functions are calculated self-consistently via expression for the dynamical spin susceptibility. It is useful to start discussion from the Fourier transform:

$$\langle S_i^- S_j^+ \rangle = \frac{1}{N^2} \sum_q \langle S_{-q}^- S_q^+ \rangle e^{iqR_{ij}}. \tag{1c}$$

Then to use Green's function technique

$$\begin{aligned} \langle S_{-q}^- S_q^+ \rangle &= \int \frac{d\omega}{e^{\beta\omega} - 1} [\langle\langle S_q^+ | S_{-q}^- \rangle\rangle_{\omega + i\varepsilon} - \langle\langle S_q^+ | S_{-q}^- \rangle\rangle_{\omega - i\varepsilon}] \\ &= \frac{N}{2\pi i} \int \frac{d\omega}{e^{\beta\omega} - 1} [\chi^{+,-}(q, \omega + i\varepsilon) - \chi^{+,-}(q, \omega - i\varepsilon)] \\ &= \frac{N}{\pi} \int \frac{d\omega}{e^{\beta\omega} - 1} \operatorname{Im} \chi^{+,-}(q, \omega). \end{aligned} \tag{2c}$$

Since

$$\operatorname{Im} \chi^{+,-}(q, \omega) = - \operatorname{Im} \chi^{+,-}(q, -\omega), \tag{3c}$$

integration can be carried out only by positive values ω. Thus, one finds

$$\begin{aligned} \langle S_i^- S_j^+ \rangle &= \frac{1}{N\pi} \sum_q \int \frac{d\omega}{e^{\beta\omega} - 1} \operatorname{Im} \chi^{+,-}(q, \omega) e^{ikR_{ij}} \\ &= \frac{1}{\pi} \left(\frac{a}{2\pi}\right)^2 \iiint [\frac{d\omega}{e^{\beta\omega} - 1} \operatorname{Im} \chi^{+,-}(q, \omega) - \frac{d\omega}{e^{-\beta\omega} - 1} \operatorname{Im} \chi^{+,-}(q, -\omega)] e^{ikR_{ij}} dk_x dk_y \\ &= \frac{1}{\pi} \left(\frac{a}{2\pi}\right)^2 \iiint cth\left(\frac{\beta\omega}{2}\right) \operatorname{Im} \chi^{+,-}(q, \omega) e^{ikR_{ij}} d\omega dk_x dk_y. \end{aligned} \tag{4c}$$

Sum rule.

The case $i = j$ is used for self-consistent control. Since

$$\begin{aligned} \psi_l^{\downarrow,\downarrow} + \psi_l^{\uparrow,\uparrow} + 2\psi_l^{pd,pd} &= 1 + \delta, \\ \psi_l^{\uparrow,\uparrow} - \psi_l^{\downarrow,\downarrow} &= 2S_l^z, \end{aligned} \tag{5c}$$

at $\langle S_i^z \rangle = 0$, and $\langle \psi_l^{pd,pd} \rangle = \delta$ one gets

$$\frac{1-\delta}{2} = \left(\frac{1}{\pi}\right)^3 \int_0^\pi \int_0^\pi \int_0^\infty cth\left(\frac{\beta\omega}{2}\right) \operatorname{Im} \chi^{+,-}(q, \omega) e^{iqR_{ij}} d\omega dq_x dq_y. \tag{6c}$$

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