POLARON EFFECTS IN EXTENDED HUBBARD MODEL

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ПОЛЯРОННЫЕ ЭФФЕКТЫ
В РАСШИРЕННОЙ МОДЕЛИ ХАББАРДА

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Starting from the three-band *p-d* Hubbard Hamiltonian we derive the effective *t-J* model Hamiltonian including electron-phonon interaction of quasiparticles with optical phonons and strong electron correlations. We consider two possible cases when the carriers move over the oxygen sites and also if the they move over the copper sublattice. Most importantly, we find that the phonon renormalization of *t* is quite different in both cases. Within an effective Hamiltonian we analyze the influence of phonons on the dynamical spin susceptibility in layered cuprates. For example, we find an isotope effect on resonance peak in the magnetic spin susceptibility, Im $\chi(\mathbf{q}, \omega)$, seen by inelastic neutron scattering. It experimental observation would be a strong argument in favor of polaronic character of the carrier motion in layered cuprates.

Introduction

An understanding of the elementary and the spin excitations in high-T_c cuprates is of central significance. For example, it is known that the Cooper-pairing scenario via the exchange of antiferromagnetic spin fluctuations was quite successful in explaining the various features of superconductivity in hole-doped cuprates such as $d_{x^2-y^2}$-wave symmetry of the superconducting order parameter and its feedback on the elementary and spin excitations [1]. Most importantly, in this scenario the dynamical spin susceptibility, $\chi(\mathbf{q},\omega)$, controls mainly the superconducting and normal state properties of the layered cuprates [1]. One of the key experimental fact in the phenomenology of high-T_c cuprates is the occurrence of a so-called resonance peak in the inelastic neutron scattering (INS) experiments [2,3]. It occurs below T_c in the dynamical spin susceptibility, $\chi(\mathbf{q},\omega)$, at the antiferromagnetic wave vector $\mathbf{Q}=(\pi,\pi)$ and $\omega \approx \omega_{res}$ which is of the order of 40 meV in the optimally doped cuprates. Its feedback in various electronic properties like optical conductivity, Raman response function, and elementary excitations has been observed experimentally by various techniques [1]. Furthermore, its successful explanation within spin-fluctuation-mediated Cooper-pairing together with $d_{x^2-y^2}$-wave symmetry of the superconducting order parameter favors this scenario as a basic one for superconductivity in the cuprates. On the other hand, recent experiments indicate that also electron-phonon interaction influences strongly their behavior [4,5,6,7]. In particular, the observation of the relatively large isotope effect in various characteristics of cuprates like penetration depth [4], 'kink'-structure seen by ARPES [8], and the isotope effect on the EPR linewidth [9] still raises a question: what is the role of phonons in determining the superconducting properties of cuprates?

Here, we derive an effective *t-J* Hamiltonian where the hopping integral, *t*, and the superexchange interaction between neighboring spins, *J*, are renormalized by phonons. We analyze the influence of the electron-phonon interaction on the dynamical spin susceptibility in layered cuprates. In particular, we find an isotope effect on the resonance peak in the magnetic spin susceptibility, Im$\chi(\mathbf{q},\omega)$. It results from both the electron-phonon coupling and the electronic correlation effects taken into account beyond random phase approximation (RPA) scheme. We show that even if the superconductivity is driven by the magnetic exchange the characteristic energy features of cuprates can be significantly renormalized by the strong electron-phonon interaction.

1 Effective Hamiltonian

We start from the atomic limit of the three-center (copper-oxygen-copper) *p-d* Hamiltonian

$$H_0 = \sum \varepsilon_a a_\sigma^+ a_\sigma + \sum \varepsilon_b b_\sigma^+ b_\sigma + \sum \varepsilon_c c_\sigma^+ c_\sigma + $$
$$+ U_a n_\uparrow^a n_\downarrow^a + U_b n_\uparrow^b n_\downarrow^b + U_c n_\uparrow^c n_\downarrow^c + \sum \omega_q p_q^+ p_q \tag{1}$$

where $\varepsilon_{a,b}$ and ε_c are the on-site energies of the copper and the oxygen holes, $n_\sigma^a = a_\sigma^+ a_\sigma$ and $n_\sigma^b = b_\sigma^+ b_\sigma$ are the copper 3*d* and oxygen 2*p* hole densities for site *i*, respectively. $U_a = U_b$ and U_c refer to the on-site copper and oxygen Coulomb repulsion, respectively. $p_\mathbf{q}$ denotes the phonon creation operator and $\omega_\mathbf{q}$ is a phonon energy dispersion. The hopping term between copper and oxygen

$$H_2 = \sum t_{ij} (b_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ b_{i\sigma}) + \sum t_{ij} (a_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ a_{i\sigma}) \tag{2}$$

and the electron-phonon interaction

$$H_1 = F = \sum g_a n^a (p_q + p_{-q}^+) + \sum g_b n^b (p_q + p_{-q}^+) + \sum g_c n^c (p_q + p_{-q}^+), \tag{3}$$

we consider as a perturbation. Here, t_{ij} is a hopping term between copper and oxygen, g_l is a electron-phonon coupling strength at the site *l*. This notation is similar to the simplified Holstein model where the migrating charge interacts locally with breathing phonon modes forming electron-vibrational states.

General remarks on the perturbation theory. To derive an effective *t-J* Hamiltonian we employ the canonical Schrieffer-Wolf-like transformations $e^{-S} H e^{S}$ [10,11]. For determination of the *S*-matrix we perform the following iteration procedure

$$S = S_1 + S_2 + S_3 + S_4 + S_5, \tag{4}$$

where the indexes 1,2,3,4 and 5, correspond to the first, the second, and so on iterations, respectively. For example, the term S_l is determined by the following chain of equations

$$[H_0 S_1] = -H_2, [H_0 S_2] = -[H_1 S_1],$$
$$[H_0 S_3] = -[H_1 S_2] - \frac{1}{3}[[H_2 S_1] S_1],$$
$$[H_0 S_4] = -[H_1 S_3] - \frac{1}{3}[[H_2 S_1] S_2] - \frac{1}{3}[[H_2 S_2] S_1], \tag{5}$$
$$[H_0 S_5] = -[H_1 S_4] - \frac{1}{3}[[H_2 S_1] S_3] - \frac{1}{3}[[H_2 S_3] S_1] -$$
$$- \frac{1}{3}[[H_2 S_2] S_2] + \frac{1}{45}[[[[H_2 S_1] S_1] S_1] S_1]$$

where $[AB] = AB - BA$ are the commutator relation. Then, an effective Hamiltonian for the ground state configuration including sixth order perturbation theory terms can be written

$$H_{eff} = H_0 + H_1 + \frac{1}{2}[H_2 S] - \frac{1}{24}[[[H_2 S]S]S] + \frac{1}{144}[[[[[H_2 S]S]S]S]S] \,. \tag{6}$$

Note that using the decomposition (4) one can easily select the different items corresponding to the various orders of the perturbation theory. Quite generally we would like to mention that H_2 is a part of the Hamiltonian which matrix elements are nonzero between the excited and the ground state configurations. It is assumed that the energy distance between the excited and the ground state configurations is large enough with respect to H_2. On the other hand, H_1 is a term which acts within the quasi-degenerate states of the excited and the ground state configurations. We also postulate that the energies associated with H_1 are smaller than the energy distance between the excited and the ground state configurations.
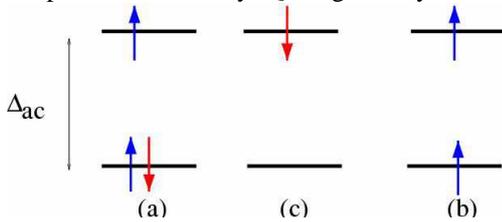

Fig. 1. *Illustration of the effective hopping between the copper sites (**a** and **b**) via the intermediate oxygen position (**c**). In the ground state configuration (Cu^{3+}-O^{2-}-Cu^{2+}) there are two holes on the a site and one hole on the b site. The excited state configuration corresponds to (Cu^{2+}-O^--Cu^{2+}) state*

Polaronic reduction factor of hopping integral between cation sites. Let us consider first the correction to the hopping integral between cation (copper) sites (a and b) via intermediate anion (oxygen) site (c) shown in Fig. 1. In this case the large energy interval is $\Delta_{ac} = \varepsilon_c - \varepsilon_a - U_a$ and it is further assumed that $\omega_a < |\Delta_{ac}|$ and $\Delta_{ac} \simeq \Delta_{bc}$. The first term in the renormalization of the effective hopping integral by electron-phonon interaction appears in the fourth order of the perturbation theory, namely, in the $\frac{1}{2}[H_2 S_3]$ which is quadratic with respect to the electron-phonon coupling operator

$$-\frac{1}{2}\left(\frac{1}{\Delta_{ca}}\right)^3 H_2[F[F\, H_2]] + h.c. = -\frac{1}{2}\left(\frac{1}{\Delta_{ca}}\right)^3 t_{ac}t_{cb}\left[g_c^2 + g_a^2\right]b_\sigma^+ a_\sigma \,, \tag{7}$$

and the effective hopping integral between the (a) and (b) states can be written as:

$$t_{b\to a}(eff) = \frac{t_{ac}t_{cb}}{\Delta_{ab}}\left\{1 - \frac{g_a^2}{\omega_a^2} + \frac{g_a^2 + g_c^2}{\Delta_{ca}^2}\right\} \,. \tag{8}$$

Note, the second term in the brackets has been included according to the usual polaronic theory when the intermediate step of charge transfer process via the oxygen site is ignored [11]. Taking into account the next orders of the perturbation theory one finds $\exp\{-\gamma_{ab}E_a/\omega_a\} \approx 1 - g_a^2/\omega_a^2 + (g_a^2 + g_c^2)/\Delta_{ca}^2$ and thus

$$\gamma_a = \left\{1 - \omega_a\frac{\omega_a + (E_c/E_a)\omega_c}{\Delta_{ca}^2}\right\} \,. \tag{9}$$

Here, we use $g_i^2 = E_i\omega_i$, $i = a, b$. Note, the exponential factor is reduced by the factor γ_a. On the other hand, the dependence of the effective hopping integral on the quasiparticle mass slightly enhances. For example, for the oxygen isotope coefficient determined by $\alpha_m = -d\ln[1/t_{ab}(eff)]/d\ln M$ we obtain

$$\alpha_a = -\frac{E_a}{2\omega_a}\left[\gamma_0 + \left(\frac{\omega_a}{\Delta_{ac}}\right)^2\right] \,, \tag{10}$$

where γ_0 is an empirical factor $0 < \gamma_0 < 1$. According to the recent experiments in $La_{0.8}Ca_{0.2}MnO_3$ the isotope coefficient was found to be $\alpha_m \simeq -1.2$ [12]. In particular, Eq. (10) agrees with the experimental observation, if we assume that the carriers (electrons) move over the manganese positions.

Effective hopping integral between oxygen states. Let us now turn to the discussion of the renormalization of the effective hopping between the oxygen positions. Note, in the cuprates it seems to play the most important role, since the effective carries are supposed to move over the oxygen positions rather on the copper ones. The corresponding process is illustrated in Fig. 2.
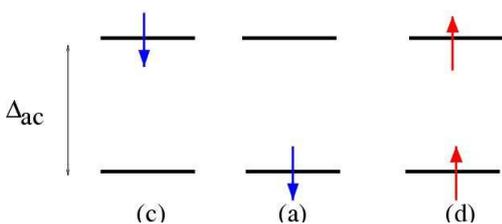
Using the similar procedure as before we find

Fig. 2: *Illustration of the first step in the effective hopping between the oxygen sites (**c** and **d**) via the intermediate copper position (**a**). In the ground state configuration (O^{2-}-Cu^{2+}-O^-) there are two holes on the a and d-sites, respectively. The excited state configuration corresponds to (O^--Cu^+-O^-)*

$$t_{d \to c}(eff) = \frac{t_{da} t_{ac}}{\Delta_{da}} \left\{ 1 - \frac{g_c^2}{\omega_c^2} + \frac{g_a^2 + g_c^2}{2\Delta_{da}^2} \right\}, \tag{11}$$

and

$$\gamma_{cd} = 1 - \frac{g_a^2 + g_c^2}{2\Delta_{da}^2} \frac{\omega_c}{E_c}. \tag{12}$$

Note, the factor 1/2 appears because instead of $\langle c_\sigma^+ c_\sigma \rangle = 1$ we presently have $\langle a_\sigma^+ a_\sigma \rangle = 1/2$. For the oxygen isotope coefficient we also have

$$\alpha_{cd} \simeq -\frac{E_a}{4} \frac{\omega_a}{\Delta_{ca}^2} \tag{13}$$

where $\Delta_{ca} = \varepsilon_c - \varepsilon_a$. Note, the expected isotope effect is quite small. This is in contrast with those expected for the cuprates [16]. We will return to this problem later in the text.

Superexchange interaction. Let us also consider the charge transfer process suggested by Anderson [13] leading to the appearance of the superexchange interaction illustrated in Fig. 3. In particular, the phonon related correction to superexchange operator

$$H_{ex} = J_0 [(S_a S_b) - \frac{n_a n_b}{4}] \tag{14}$$

appears in the sixth order of the perturbation theory and has the following operator form

$$H_{eff}^{(6)}(1) = \frac{1}{2\Delta_{ca}^3 U_a} \left\{ H_2 H_1 H_1 S^{(3)} + H_2 [F, H_1 H_1 [F, H_2]] + H_2 [F[F, H_1 H_1 H_2]] \right\} + \frac{1}{2\Delta_{ca}^2 U_a^3} H_2 H_1 [F[F, H_1 H_2]] +$$

$$+ \frac{1}{2\Delta_{ca}^3 U_a^2} \left\{ H_2 H_1 H_1 [F, H_1][F, H_2] + H_2 H_1 H_1 [F, [F, H_2]] + H_2 H_1 [F[F, H_1 H_2] + H_2 [FH_1][F, H_1 H_2] \right\} + h.c. \tag{15}$$

In a general case, from $[H_0 S_1] = -H_2$ we deduce that

$$S_1 = C_1 \left(a_\sigma^+ c_\sigma - c_\sigma^+ a_\sigma \right) + C_2 \left(n_\downarrow^a a_\uparrow^+ c_\uparrow + n_\uparrow^a a_\downarrow^+ c_\downarrow - c_\uparrow^+ a_\uparrow n_\downarrow^a - c_\downarrow^+ a_\downarrow n_\uparrow^a \right) +$$
$$+ C_3 \left(a_\uparrow^+ c_\uparrow n_\downarrow^c + a_\downarrow^+ c_\downarrow n_\uparrow^c - n_\downarrow^c c_\uparrow^+ a_\uparrow - n_\uparrow^c c_\downarrow^+ a_\downarrow \right) + C_4 \left(n_\downarrow^a a_\uparrow^+ c_\uparrow n_\downarrow^c + n_\uparrow^a a_\downarrow^+ c_\downarrow n_\uparrow^c - n_\downarrow^c c_\uparrow^+ a_\uparrow n_\downarrow^a - n_\uparrow^c c_\downarrow^+ a_\downarrow n_\uparrow^a \right), \tag{16}$$

where $C_1 = t_{ca} / (\varepsilon_c - \varepsilon_a)$, $C_2 = U_a C_1 / (\varepsilon_c - \varepsilon_a - U_a)$, $C_3 = U_c C_1 / (\varepsilon_a - \varepsilon_c - U_c)$, and $C_4 = -(C_2 U_c - C_3 U_a) / (\varepsilon_c - \varepsilon_a - U_a + U_c)$ Note, the first term describes the hopping of the electron between empty states. On the other hand, the first and second terms together account for hopping between the doubly occupied a and the empty c states. Namely, $C_1 + C_2 = t_{ca} / (\varepsilon_c - \varepsilon_a - U_a)$. Finally, the first and third terms describe the hopping between the doubly occupied c and empty a sites, i.e. $C_1 + C_3 = t_{ca} / (\varepsilon_c - \varepsilon_a + U_c)$.

The solution of the equation $[H_0 S_2] = -[H_1 S_1]$ has the same operator form as for S_1 but with new coefficients C_1', C_2', C_3', C_4' which are determined by

$$C_1' = \frac{C_1}{\varepsilon_c - \varepsilon_a} (\Phi_a - \Phi_c)$$

$$C_2' = \frac{U_a C_1'}{\varepsilon_c - \varepsilon_a - U_a} + \frac{C_2}{\varepsilon_c - \varepsilon_a - U_a} (\Phi_a - \Phi_c) \tag{17}$$

$$C_3' = \frac{U_c C_1'}{\varepsilon_a - \varepsilon_c - U_c} - \frac{C_3}{\varepsilon_a - \varepsilon_c - U_c} (\Phi_a - \Phi_c)$$

$$C_4' = -\frac{C_2' U_c - C_3' U_a}{\varepsilon_c - \varepsilon_a - U_a + U_c} + \frac{C_4}{\varepsilon_c - \varepsilon_a - U_a + U_c} (\Phi_a - \Phi_c)$$

where $\Phi_a - \Phi_c = \sum g_a (p_q + p_{-q}^+) - \sum g_c (p_q + p_{-q}^+)$. Note, one finds here $C_1' + C_2' + C_3' + C_4' = t_{ca}(\Phi_a - \Phi_c) / (\varepsilon_c - \varepsilon_a + U_c - U_a)^2$ Finally, the equation $[H_0 S_3] = -[H_1 S_2] - [[H_2 S_1] S_1]/3$ yields the S_3 in the form of S_1 but also

Fig. 3: *Illustration of the superexchange interaction in the cuprates. The ground state configuration is characterized by the following configuration (Cu^{2+}-O^{2-}-Cu^{2+}) where two holes distributed on the two copper positions (**a** and **b**). In the excited state there are two configurations (Cu^{2+}-O^--Cu^+) and (Cu^{3+}-O^{2-}-Cu^+). The hole is first migrating from site **b** to the oxygen site **c** and then to the copper site **a**. Note, that at $\Delta_{ac} \approx U_a > |t_{ca}|$ the hopping Hamiltonian containing t_{bc} can be included into H_1*
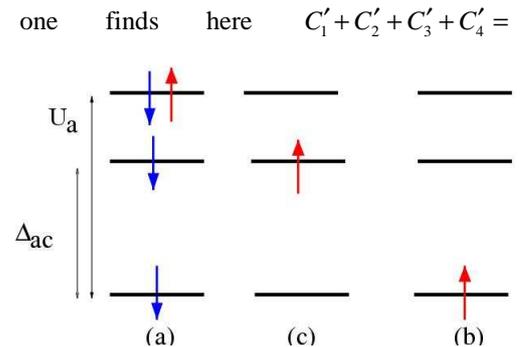
with new coefficients

$$C_1'' = \frac{C_1'}{\varepsilon_c - \varepsilon_a}(\Phi_a - \Phi_c)$$

$$C_2'' = \frac{U_a C_1''}{\varepsilon_c - \varepsilon_a - U_a} + \frac{C_2'}{\varepsilon_c - \varepsilon_a - U_a}(\Phi_a - \Phi_c)$$

$$C_3'' = \frac{U_c C_1''}{\varepsilon_a - \varepsilon_c - U_c} - \frac{C_3'}{\varepsilon_a - \varepsilon_c - U_c}(\Phi_a - \Phi_c) \qquad (18)$$

$$C_4'' = -\frac{U_c C_2'' - U_a C_3''}{\varepsilon_c - \varepsilon_a - U_a + U_c} + \frac{C_4'}{\varepsilon_c - \varepsilon_a - U_a + U_c}(\Phi_a - \Phi_c)$$

It is also useful to point out that

$$C_1'' + C_2'' + C_3'' + C_4'' = -t_{ca}(\Phi_a - \Phi_c)^2 / (\varepsilon_c - \varepsilon_a + U_c - U_a)^3 .$$

The other commutators are calculated straightforwardly

$$[F, H_2] = (\Phi_a - \Phi_c)\sum t_{ac}(a_\sigma^+ c_\sigma - c_\sigma^+ a_\sigma)$$

$$[F, H_1] = (\Phi_b - \Phi_c)\sum t_{bc}(b_\sigma^+ c_\sigma - c_\sigma^+ b_\sigma)$$

$$[F, H_1 H_2] = (\Phi_a - \Phi_b)\sum t_{ac}t_{cb}(b_\sigma a_\sigma^+ - a_\sigma b_\sigma^+) \qquad (19)$$

$$[F, H_1 H_1 H_2] = (\Phi_a - \Phi_c)\sum t_{bc}t_{ac}t_{cb}(b_\sigma^+ c_\sigma b_\sigma a_\sigma^+ - a_\sigma b_\sigma^+ c_\sigma^+ b_\sigma)$$

and the effective Hamiltonian in the sixth order of the perturbation theory has the form

$$H_{eff}^{(6)}(1) = \frac{t_{ac}^2 t_{cb}^2}{2\Delta_{ca}^2 U_a}\left\{ \frac{3}{\Delta_{ca}^2}\left[\langle\Phi_a^2\rangle + \langle\Phi_c^2\rangle\right] + \right.$$

$$\left. + \frac{2}{\Delta_{ca}U_a}\langle\Phi_a^2\rangle + \frac{1}{U_a^2}\left[\langle\Phi_a^2\rangle + \langle\Phi_b^2\rangle\right]\right\} a_\downarrow b_\downarrow^+ b_\downarrow a_\downarrow^+ + h.c. \qquad (20)$$

where $\langle\Phi_i^2\rangle$ are the usual averaged phonon factors $\langle\Phi_i^2\rangle = g_i^2(2n_q + 1) = = g_i^2 \coth(\omega_i/2k_b T) \approx g_i^2$. Introducing the polaronic energy $E_i = g_i^2/\omega_i$ we arrive to the final formula for the superexchange integral

$$J = J_0\left\{1 + \left[\frac{3}{\Delta_{ca}^2} + \frac{2}{\Delta_{ca}U_a} + \frac{2}{U_a^2}\right]E_a\omega_a + \frac{3E_c}{\Delta_{ca}^2}\omega_c\right\}. \qquad (21)$$

For simplicity we assume a and b centers to be equivalent, J_0 is the superexchange interaction without polaronic effects. Note, the term $2\omega_a/U_a^2$ was found earlier by Kugel and Khomskii [11]. The present result explains well the isotope shift of Neel temperature in undoped compounds [28].

To summarize, the matrix of the unitary transformation for the initial Hamiltonian was found by excluding the odd terms with respect to the hopping integral with an accuracy up to the sixth order perturbation theory. Note, in the second order perturbation the effective hopping integral, t_{ij}, appears.

It is further renormalized by the electron-phonon interaction in the fourth order term where we introduce the average over the phonons. Similarly, the superexchange interaction occurs in the fourth order perturbation theory and its renormalization takes place in the sixth order term.

Singlet-correlated band model. In order to illustrate the effective model we show in Figs.4-5 the simplified energy level scheme for two holes in the elementary unit cell. There are two copper upper and lower Hubbard bands with the energy splitting of about $U_a \sim 6\,\text{eV}$. At half-filling the lower Hubbard band is completely filled which corresponds to $Cu^{2+}(3d^9)$ orbital configuration. Via doping an additional oxygen hole $O^-(2p^5)$ resides on four neighboring oxygen sites (bonding molecular orbitals). The charge transfer gap $\Delta_{ac} \sim 1.5\,\text{eV}$. A kinetic exchange interaction between copper and oxygen holes occurs due to a virtual hopping back and forth of the oxygen hole to the upper copper Hubbard band.
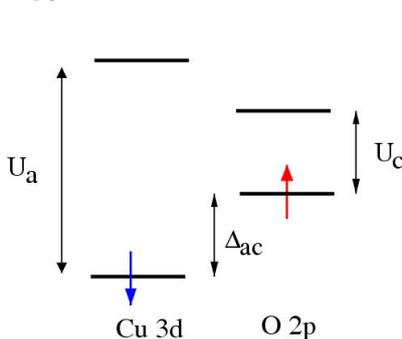
$$H_{ex}^{pd} \simeq t_\sigma^2\left[\frac{6}{U_a - \Delta_{pd}} + \frac{1.5}{\Delta_{ac} + U_c}\right]\left[(\mathbf{s}_p\mathbf{s}_d) - \frac{n_p n_d}{4}\right]. \qquad (22)$$

Since the copper-oxygen transfer integral along σ-bond is large ($t_\sigma \sim 1.2\,\text{eV}$), this exchange coupling is very strong and leads to a copper-oxygen singlet formation [15]. An additional stabilization of the copper-oxygen singlet state takes place (about

Fig. 4:   *Illustration of the copper-oxygen singlet formation on the square lattice. The additional doped hole cannot go to the copper site due to strong on-site Coulomb repulsion and is distributed among four oxygen sites forming together with the copper spin a Zhang-Rice singlet*

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0.5 eV) if one assumes that the lifetime of the singlet at a lattice site i is larger than the relaxation time of the local distortions. Indeed due to a local oxygen contraction around the copper the value of t_σ^2 strongly increases. Thus, one arrives to the copper-oxygen singlet polaron motion with an exponential factor $\gamma^* E_a^* / \omega_a^*$.

Finally, the relevant effective Hamiltonian is given by

$$H = \sum_{ij} t_{ij} \Psi_i^{pd,\sigma} \Psi_j^{\sigma,pd} + \sum_{i>j} J_{ij} \left[(\mathbf{S}_i \mathbf{S}_j) - \frac{n_i n_j}{4} \right].$$ (23)

The index pd corresponds to a Zhang-Rice singlet formation with one hole placed on the copper site whereas the second hole is distributed on the neighboring oxygen sites [15]. Namely, $\Psi_i^{pd,\uparrow} = \left[X_i^{\uparrow,\downarrow} P_i^{\uparrow,0} - X_i^{\uparrow,\uparrow} P_i^{\downarrow,0} \right] / \sqrt{2}$ is the copper-oxygen creation operator in terms of copper (X) and oxygen (P) projecting operators. One can check that copper-oxygen exchange term $J_{pd} \left[(\mathbf{S}_p \mathbf{S}_d) - n_d n_p / 4 \right]$ is diagonal by introducing $\Psi^{pd,\sigma}$ and $\Psi^{\sigma,pd}$ operators, i.e. $i \partial \Psi_i^{pd,\sigma} / \partial t = \left(J_{pd} / 2 \right) \Psi_i^{pd,\sigma}$.

Note, in general case the effective Hamiltonian contains also the Coulomb interaction between doped holes and the interaction of quasiparticles via the phonon field. We dropped these terms here, because they do not contribute directly to the spin susceptibility. The hopping matrix element is $t_{ij} = t_{ij}^0$ $\exp(-\gamma E_i^* / \omega_i^*) \left[(1+\delta)/2 + 2 \langle S_i S_j \rangle / (1+\delta) \right]$ where t_{ij}^0 is the bare hopping integral. The exponential factor takes into account electron-phonon interaction, $E_i = (g_i^*)^2 / \omega_i^*$ is the so-called polaron stabilization energy of the copper-oxygen singlet state and $0 < \gamma < 1$. From the experimental data [16] the whole exponential factor was estimated to be $\gamma E_i^* / \omega_i^* \approx 0.92$ around the optimal doping. Note, its value is increasing upon decreasing doping. The effect of the copper spin correlations is described by the square brackets. In particular, one sees that for the antiferromagnetic square lattice the hopping between nearest neighbors vanishes. This is illustrated in Fig. 5. As one sees the oxygen hole cannot move between the copper sites with antiparallel spin orientation. Furthermore, there is no more than one oxygen hole per each unit cell. Then, the spectral weight of the singlet-correlated band changes upon doping similar to that of the upper Hubbard band. The half-filling is already reached at $\delta = 1/3$. This doping level we will refer to the optimal doping. We show in Fig. 6 the doping evolution of the spectral weight for the lower Hubbard (copper) band and singlet-correlated (copper-oxygen) band. Note, the latter is completely filled for $\delta = 1$.

In the following section we will discuss the resonance peak seen by Inelastic Neutron Scattering (INS) in high-T_c cuprates. We will show that its position might be sensitive to the renormalization of the hopping integral and could be a good test for the polaronic nature of carrier motion in cuprates.

2. Dynamical spin susceptibility

To derive the dynamical spin susceptibility in the superconducting state we use the method suggested by Hubbard and Jain [18] that allows to take into account strong electronic correlations. First we add the external magnetic field applied along c-axis into the effective Hamiltonian

$$H_i = \mathrm{Re} \sum_{\mathbf{q}} h_{\mathbf{q}} e^{-i(\omega t - \mathbf{q} \mathbf{R}_i)}.$$ (24)

Then we write an equation of motion for the Ψ operators using the Roth-type of the decoupling scheme [19] and expanding the

$$P_{pd}^{\sigma} = \left\{ \Psi_i^{\sigma,pd} \Psi_i^{pd,\sigma} \right\} = (1+\delta_i)/2 + \sigma \, \mathrm{Re} \sum_{\mathbf{q}} \left[S_{\mathbf{q}}^z e^{i(\mathbf{q} \mathbf{R}_i - \omega t)} \right]$$

up to the first order in $S_{\mathbf{q}} = \chi^{zz}(\mathbf{q}, \omega) h_{\mathbf{q}}$. In particular,
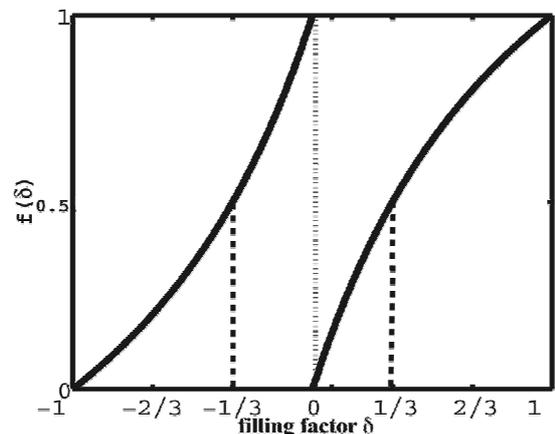

Fig. 6. The spectral weight of the lower Hubbard (copper) band (-
1 < δ < 0) and the singlet-correlated (copper-oxygen) band
(0 < δ < 1). Note, the optimal doping corresponds to the half-
filled copper-oxygen band which is reached for $\delta = 1/3$

$$i\frac{\partial \Psi_{\mathbf{k}}^{-\sigma,pd}}{\partial t} = (\varepsilon_{\mathbf{k}} - \mu)\Psi_{\mathbf{k}}^{-\sigma,pd} + \Delta_{\mathbf{k}}\Psi_{-\mathbf{k}}^{pd,\sigma} +$$

$$+\left[\left(\frac{J_{\mathbf{q}}}{2} - t_{\mathbf{k-q}}\right)S_{\mathbf{q}} - \frac{h_{\mathbf{q}}}{2}\right]\Psi_{\mathbf{k-q}}^{-\sigma,pd}e^{-i\omega t} \tag{25}$$

and the similar expression occurs for $\Psi_{-\mathbf{k}}^{pd,\sigma}$. Here, $\Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x - \cos k_y)$ is the $d_{x^2-y^2}$-wave superconducting gap, $J_{\mathbf{q}} = J(\cos k_x + \cos k_y)$ is the Fourier transform of the superexchange interaction on a square lattice.

Using the Bogolyubov-like transformations to the new quasiparticle states

$$\alpha_{\mathbf{k}}^{-\sigma,pd} = u_{\mathbf{k}}\Psi_{\mathbf{k}}^{-\sigma,pd} + v_{\mathbf{k}}\Psi_{-\mathbf{k}}^{pd,\sigma},$$

$$\alpha_{-\mathbf{k}}^{pd,\sigma} = u_{\mathbf{k}}\Psi_{-\mathbf{k}}^{pd,\sigma} - v_{\mathbf{k}}\Psi_{\mathbf{k}}^{-\sigma,pd}. \tag{26}$$

where $u_{\mathbf{k}}^2 = (1/2)(1 + (\varepsilon_{\mathbf{k}} - \mu)/E_{\mathbf{k}})$ and $v_{\mathbf{k}}^2 = (1/2)(1 - (\varepsilon_{\mathbf{k}} - \mu)/E_{\mathbf{k}})$ are the Bogolyubov coefficients, μ is a chemical potential, and $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}$ is the energy dispersion in the superconducting state, we obtain the new equations of motion for the α operators

$$i\frac{\partial \alpha_{\mathbf{k}}^{\downarrow,pd}}{\partial t} = E_{\mathbf{k}}\alpha_{\mathbf{k}}^{\downarrow,pd} + M_{\mathbf{kq}}(u_{\mathbf{k}}\Psi_{\mathbf{k-q}}^{\downarrow,pd} + v_{\mathbf{k}}\Psi_{-\mathbf{k+q}}^{pd,\uparrow})\exp(-i\omega t)$$

$$i\frac{\partial \alpha_{-\mathbf{k}}^{pd,\uparrow}}{\partial t} = -E_{\mathbf{k}}\alpha_{\mathbf{k}}^{\downarrow,pd} + M_{\mathbf{kq}}(u_{\mathbf{k}}\Psi_{-\mathbf{k+q}}^{pd,\uparrow} - v_{\mathbf{k}}\Psi_{\mathbf{k-q}}^{\downarrow,pd})\exp(-i\omega t). \tag{27}$$

Here, we have introduced the notation $M_{\mathbf{kq}} = (J_{\mathbf{q}}/2 - t_{\mathbf{k-q}})S_{\mathbf{q}} - h_{\mathbf{q}}/2$. It is further useful to re-write these equations in the form.

$$i\frac{\partial \alpha_{\mathbf{k}}^{\downarrow,pd}}{\partial t} - E_{\mathbf{k}}\alpha_{\mathbf{k}}^{\downarrow,pd} =$$

$$= M_{\mathbf{kq}}\left[(u_{\mathbf{k}}u_{\mathbf{k-q}} + v_{\mathbf{k}}v_{\mathbf{k-q}})\alpha_{\mathbf{k-q}}^{\downarrow,pd} + (u_{\mathbf{k-q}}v_{\mathbf{k}} - u_{\mathbf{k}}v_{\mathbf{k-q}})\alpha_{-\mathbf{k+q}}^{pd,\uparrow}\right]\exp(-i\omega t) \tag{28}$$

and

$$i\frac{\partial \alpha_{-\mathbf{k}}^{pd,\uparrow}}{\partial t} + E_{\mathbf{k}}\alpha_{-\mathbf{k}}^{pd,\uparrow} =$$

$$= M_{\mathbf{kq}}\left[(u_{\mathbf{k}}v_{\mathbf{k-q}} - v_{\mathbf{k}}u_{\mathbf{k-q}})\alpha_{\mathbf{k-q}}^{\downarrow,pd} + (u_{\mathbf{k}}u_{\mathbf{k-q}} + v_{\mathbf{k}}v_{\mathbf{k-q}})\alpha_{-\mathbf{k+q}}^{pd,\uparrow}\right]\exp(-i\omega t) \tag{29}$$

which could be solved by the iteration procedure. Because the quantities $M_{\mathbf{kq}}$ are assumed to be small one can put into the right hand sides of Eqs. (28)-(29) the time dependence of the quasiparticle operators in the absence of the external magnetic field, *i.e.* $\alpha_{\mathbf{k-q}}^{\downarrow,pd} = \alpha_{\mathbf{k-q}}^{\downarrow,pd}(0)\exp(-iE_{\mathbf{k-q}}t)$, $\alpha_{-\mathbf{k+q}}^{pd,\uparrow} = \alpha_{-\mathbf{k+q}}^{pd,\uparrow}(0)\exp(iE_{\mathbf{k-q}}t)$. Then the solution can be written as

$$\alpha_{\mathbf{k}}^{\downarrow,pd} = \alpha_{\mathbf{k}}^{\downarrow,pd}(0)\exp(-iE_{\mathbf{k}}t) + B_1\alpha_{\mathbf{k-q}}^{\downarrow,pd}(0)\exp[-i(E_{\mathbf{k-q}} + \omega)t] +$$

$$+B_2\alpha_{-\mathbf{k+q}}^{pd,\uparrow}(0)\exp[i(E_{\mathbf{k-q}} - \omega)t] \tag{30}$$

where the coefficients are:

$$B_1 = \frac{M_{\mathbf{kq}}(u_{\mathbf{k}}u_{\mathbf{k-q}} + v_{\mathbf{k}}v_{\mathbf{k-q}})}{-E_{\mathbf{k}} + E_{\mathbf{k-q}} + \omega}$$

$$B_2 = \frac{M_{\mathbf{kq}}(u_{\mathbf{k-q}}v_{\mathbf{k}} - u_{\mathbf{k}}v_{\mathbf{k-q}})}{-E_{\mathbf{k}} - E_{\mathbf{k-q}} + \omega}. \tag{31}$$

Similarly, the solution of the next equation can be found:

$$\alpha_{-\mathbf{k}}^{pd,\uparrow} = \alpha_{-\mathbf{k}}^{pd,\uparrow}(0)\exp(iE_{\mathbf{k}}t) + A_1\alpha_{\mathbf{k-q}}^{\downarrow,pd}(0)\exp[-i(E_{\mathbf{k-q}} + \omega)t] +$$

$$+A_2\alpha_{-\mathbf{k+q}}^{pd,\uparrow}(0)exp[i(E_{\mathbf{k-q}} - \omega)t] \tag{32}$$

with coefficients

$$A_1 = \frac{M_{\mathbf{kq}}(u_{\mathbf{k}}v_{\mathbf{k-q}} - u_{\mathbf{k-q}}v_{\mathbf{k}})}{E_{\mathbf{k}} + E_{\mathbf{k-q}} + \omega}, \quad A_2 = \frac{M_{\mathbf{kq}}(u_{\mathbf{k}}u_{\mathbf{k-q}} + v_{\mathbf{k}}v_{\mathbf{k-q}})}{E_{\mathbf{k}} - E_{\mathbf{k-q}} + \omega}. \tag{33}$$

The expression for the longitudinal component of the dynamical spin susceptibility can be obtained from the relation

$$\left\langle \Psi_i^{pd,\uparrow}\Psi_i^{\uparrow,pd} \right\rangle - \left\langle \Psi_i^{pd,\downarrow}\Psi_i^{\downarrow,pd} \right\rangle = 0. \tag{34}$$

For example, for the spin 'up' we have

$$\left\langle \Psi_i^{pd,\uparrow}\Psi_i^{\uparrow,pd} \right\rangle = \frac{1}{N}\sum \left\langle \Psi_{\mathbf{k}}^{pd,\uparrow}\Psi_{\mathbf{k'}}^{\uparrow,pd} \right\rangle e^{i(\mathbf{k-k'})\mathbf{R}_i} = \delta_i + \frac{1}{N}\sum \left\langle \Psi_{\mathbf{k}}^{pd,\uparrow}\Psi_{\mathbf{k+q}}^{\uparrow,pd} \right\rangle e^{i\mathbf{qR}_i}. \tag{35}$$

Note, the last term has the same exponential factor ($e^{i\mathbf{qR}_i}$) as for external magnetic field. Then the correlation function can be found

$$\frac{1}{N}\sum \left\langle \Psi_{\mathbf{k}}^{pd,\uparrow}\Psi_{\mathbf{k+q}}^{\uparrow,pd} \right\rangle e^{i\mathbf{qR}_i} = \frac{1}{N}\sum \left\{ u_{\mathbf{k}}u_{\mathbf{k+q}}\left\langle \alpha_{\mathbf{k}}^{pd,\uparrow}\alpha_{\mathbf{k+q}}^{\uparrow,pd} \right\rangle + v_{\mathbf{k}}v_{\mathbf{k+q}}\left\langle \alpha_{-\mathbf{k}}^{pd,\downarrow}\alpha_{-\mathbf{k-q}}^{\downarrow,pd} \right\rangle + \right. $$
$$\left. + u_{\mathbf{k}}v_{\mathbf{k+q}}\left\langle \alpha_{\mathbf{k}}^{pd,\uparrow}\alpha_{-\mathbf{k-q}}^{pd,\downarrow} \right\rangle + v_{\mathbf{k}}u_{\mathbf{k+q}}\left\langle \alpha_{-\mathbf{k}}^{\downarrow,pd}\alpha_{\mathbf{k+q}}^{\uparrow,pd} \right\rangle \right\} e^{i\mathbf{qR}_i} \tag{36}$$

Substituting in the *rhs* the solution for the quasiparticle operators (30) and (32) one can see that each correlation function gives two terms which are proportional to $M_{\mathbf{kq}}$. For example, in the function $\left\langle \alpha_{\mathbf{k}}^{pd,\uparrow}\alpha_{\mathbf{k+q}}^{\uparrow,pd} \right\rangle$ one obtains the first term after substitution $\alpha_{\mathbf{k}}^{pd,\uparrow}$ and taking the linear correction with respect to the magnetic field into account. Similarly, the second item arises from the substitution of operator $\alpha_{\mathbf{k+q}}^{\uparrow,pd}$. Note, we use $\left\langle \alpha_{\mathbf{k}}^{pd,\downarrow}(0)\alpha_{\mathbf{k}}^{\downarrow,pd}(0) \right\rangle = P_{pd}f_{\mathbf{k}}$ and $\left\langle \alpha_{\mathbf{k}}^{\downarrow,pd}(0)\alpha_{\mathbf{k}}^{pd,\downarrow}(0) \right\rangle = P_{pd}(1-f_{\mathbf{k}})$, where $f_{\mathbf{k}} = 1/\left[1+\exp(E_{\mathbf{k}}/k_BT)\right]$ is the usual Fermi function.

Finally, after straightforward calculations and using the following definition

$$S_{\mathbf{q}}^z = \chi^{zz}(\mathbf{q},\omega)h_{\mathbf{q}} \tag{37}$$

one obtains the expression for the dynamical spin susceptibility in the form

$$\chi(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{J_{\mathbf{q}}\chi_0(\mathbf{q},\omega) + \Pi(\mathbf{q},\omega) + Z(\mathbf{q},\omega)} \tag{38}$$

This is a central result of our paper. Here, $\chi_0(\mathbf{q},\omega)$ is the usual BCS-like Lindhard response function, $\Pi(\mathbf{q},\omega)$ and $Z(\mathbf{q},\omega)$ result from the strong electronic correlation effects. In the normal state the expression for $\Pi(\mathbf{q},\omega)$ has been obtained by Hubbard and Jain [18]. In the superconducting state it is given by

$$\Pi(\mathbf{q},\omega) = \frac{P_{pd}}{N}\sum_{\mathbf{k}} \left\{ u_{\mathbf{k}}u_{\mathbf{k+q}}\left(u_{\mathbf{k}}u_{\mathbf{k+q}} + v_{\mathbf{k}}v_{\mathbf{k+q}}\right)\frac{t_{\mathbf{k}}f_{\mathbf{k}} - t_{\mathbf{k+q}}f_{\mathbf{k+q}}}{\omega + i0^+ + E_{\mathbf{k}} - E_{\mathbf{k+q}}} + \right.$$
$$+ v_{\mathbf{k}}v_{\mathbf{k+q}}\left(v_{\mathbf{k}}v_{\mathbf{k+q}} + u_{\mathbf{k}}u_{\mathbf{k+q}}\right)\frac{t_{\mathbf{k}}(1-f_{\mathbf{k}}) - t_{\mathbf{k+q}}(1-f_{\mathbf{k+q}})}{\omega + i0^+ - E_{\mathbf{k}} + E_{\mathbf{k+q}}} +$$
$$+ u_{\mathbf{k}}v_{\mathbf{k+q}}\left(u_{\mathbf{k}}v_{\mathbf{k+q}} - u_{\mathbf{k+q}}v_{\mathbf{k}}\right)\frac{t_{\mathbf{k}}f_{\mathbf{k}} - t_{\mathbf{k+q}}(1-f_{\mathbf{k+q}})}{\omega + i0^+ + E_{\mathbf{k}} + E_{\mathbf{k+q}}} +$$
$$\left. + u_{\mathbf{k+q}}v_{\mathbf{k}}\left(v_{\mathbf{k}}u_{\mathbf{k+q}} - u_{\mathbf{k}}v_{\mathbf{k+q}}\right)\frac{t_{\mathbf{k}}(1-f_{\mathbf{k}}) - t_{\mathbf{k+q}}f_{\mathbf{k+q}}}{\omega + i0^+ - E_{\mathbf{k}} - E_{\mathbf{k+q}}} \right\} \tag{39}$$

The function $Z(\mathbf{q},\omega)$ is written as follows

$$Z(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{k}}\frac{\omega + i0^+}{\omega + i0^+ + \varepsilon_{\mathbf{k}}^{(1)} - \varepsilon_{\mathbf{k+q}}^{(1)}}. \tag{40}$$

Here, $f_{\mathbf{k}}$ is the Fermi distribution function, $\varepsilon_{\mathbf{k}}^{(1)} = (1-\delta)t_{\mathbf{k}}/2$, $\varepsilon_{\mathbf{k}} = P_{pd}t_{\mathbf{k}}$ is the energy dispersion in the normal state, and

$$t_k = 2t(\cos k_x + \cos k_y) + 4t'\cos k_x \cos k_y + 2t''(\cos 2k_x + \cos 2k_y)$$

is the Fourier transform of the hopping integral on a square lattice including nearest, next- and next-next-nearest neighbor hopping, respectively. The origin of the terms $\Pi(\mathbf{q},\omega)$ and $Z(\mathbf{q},\omega)$ relates to the no double occupancy constraint. In particular, for the Coulomb repulsion $U = \infty$ and $J = 0$ the dynamical spin susceptibility does not reduce to the

standard Lindhard response function but is renormalized by the electronic correlation effects [20]. For the $\Delta_k = 0$ Eq. (37) agrees with the normal state result for the dynamical spin susceptibility [18,21,22].

Results and Discussion

Inelastic neutron scattering (INS) measurements probe directly the imaginary part of the dynamical spin susceptibility. Therefore, it is of interest to analyze the role played by the electronic correlations in connection with the 'resonance' peak seen by INS [3]. This feature is well understood using various approaches [23,24] as a result of the spin density wave (SDW) collective mode formation at $\omega = \omega_{res}$, *i.e.* when the denominator of the RPA spin susceptibility at the antiferromagnetic wave vector **Q** is close to zero.

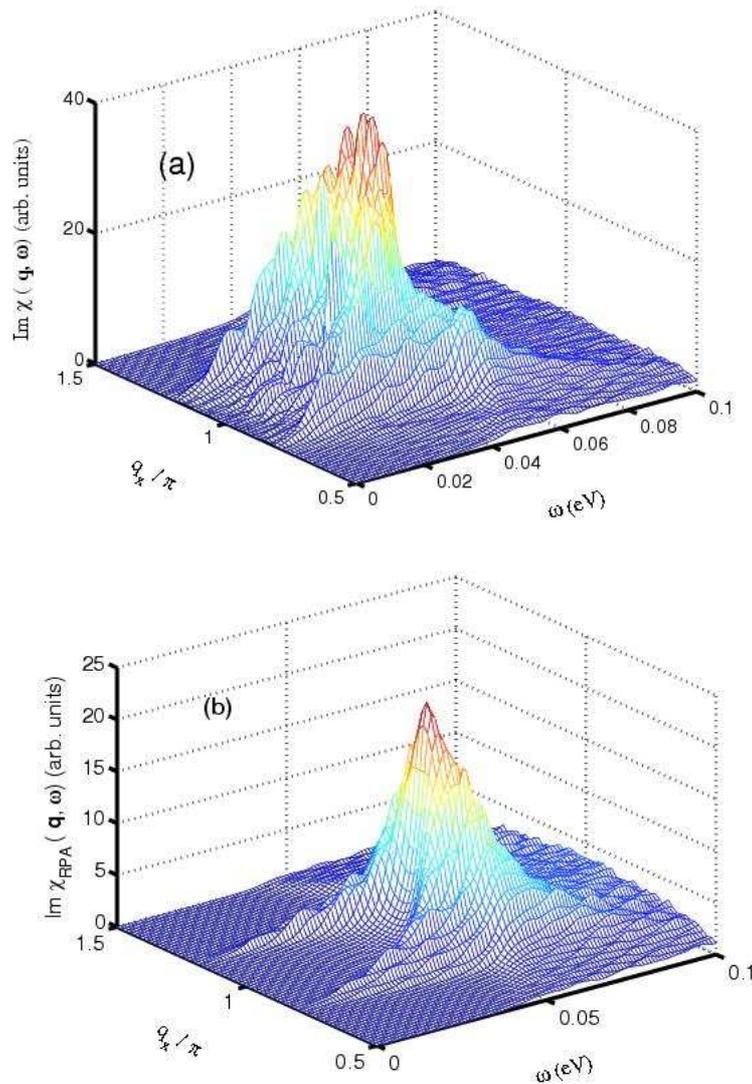*Fig. 7. Dispersion of the resonance peak calculated from Eq. (37) **(a)** as a function of frequency and q_x away from (π,π). Two branches of the dispersion curves are in good agreement with recent experimental data [26]. For comparison we also put the RPA results **(b)** using the same parameters*

Let us first concentrate on the influence of the electronic correlations beyond RPA on the resonance peak formation at $\mathbf{Q} = (\pi,\pi)$ In Fig. 7(a) we show results of our calculations for the Im $\chi(\mathbf{Q},\omega)$ from Eq. (37) as a function of frequency and q_x ($q_y = \pi$) in the superconducting state. Here, we use $t = 200$, $t' = -20$, and $t'' = 4$ (in meV) at optimal doping. For comparison we also put RPA results using the same parameters in Fig. 7 (b). Clearly, additional electronic correlations beyond RPA (Π and Z terms) affect significantly the Imχ behavior in the superconducting state. First, in contrast to the RPA the position of the resonance peak obtained from Eq. (37) is shifted to a lower frequencies. The main reason is that due to Π and Z-terms the resonance condition can be satisfied easily in a more wide range of parameters. Furthermore, its intensity is also much higher than in the RPA case. In addition, the upper branch of the resonance peak dispersion away from ω_{res} and $\mathbf{Q}_{AF}$ is much more pronounced. Note, these dispersion curves $\propto \mathbf{q}^2$ are in good agreement with experiment [25,26]. Finally, we discuss the influence of the electron-phonon interaction on the resonance peak formation by changing the isotope mass of ^{16}O by ^{18}O. This

shifts the average frequency of the LO phonon mode and consequently renormalizes the hopping integral t and the superexchange coupling constant, J. Most importantly, the electron-phonon interaction changes most dramatically the hopping integral t rather than the superexchange coupling J. In particular, the superexchange coupling constant J changes less than 1% upon substituting the isotopes [27] which agrees well with experimental data [28]. Therefore, there is almost no influence of the isotope substitution on the resonance peak determined from RPA, since in this approximation its formation is determined mainly by J. In particular, we find *within RPA* no change in the ω_{res} value upon changing the isotopes. In the case of Eq. (37) the most important contribution to the isotope effect on the resonance peak appears due to $\Pi(\mathbf{q}, \omega) \propto t_k$. In particular, using our estimation given above we find that at optimal doping the hopping integral changes by 6% upon replacing ^{16}O by ^{18}O. This results in the lowering of the resonance frequency at (π, π) from 41 meV for the ^{16}O isotope towards 39 meV for the ^{18}O sample. This leads to $\alpha_{res} = -d\ln\omega_{res}/d\ln M \approx 0.4$ for optimally-doped cuprates. This effect is beyond the experimental error and can be further tested experimentally. Furthermore, in the underdoped cuprates one may expect larger isotope effect due to a larger value of $\gamma E_i^*/\omega_i^*$ [16]. At the same time the superconducting transition temperature which is determined by J shows much weaker isotope effect and is around $\alpha_{T_c} \approx 0.05$ [27]. Therefore, even if the superconductivity is driven by the magnetic exchange the resonance peak formation can be significantly renormalized by the strong electron-phonon interaction.

Summary

To summarize, we analyze the influence of the electronic correlations and the electron-phonon interaction on the dynamical spin susceptibility in layered cuprates. The electronic correlations taken beyond RPA redistribute the spectral weight of the resonance peak away from (π, π) leading to the pronounced dispersion. This is in good agreement with recent INS data [25,26]. Furthermore, we find the isotope effect on the resonance peak due to strong coupling of the carriers to LO phonon mode. It results from both electron-phonon coupling and electronic correlation effects. In contrast to the small isotope effect on the superconducting transition temperature we find larger isotope coefficient on the resonance peak $\alpha_{res} \approx 0.4$ in optimally-doped cuprates. We also would like to note that the value of the isotope coefficient depends strongly on the value of the exponential factor. Therefore, the experimental verification of our prediction is desirable. In particular, it would put a strong constraint on the ingredients the theory of cuprates must contain.

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