Possible isotope effect on the resonance peak formation in high-$T_c$ cuprates

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(November 12, 2018)

Within effective $t-J$ Hamiltonian we analyze the influence of electronic correlations and electron-phonon interaction on the dynamical spin susceptibility in layered cuprates. We find an isotope effect on the resonance peak in the magnetic spin susceptibility, $\text{Im} \chi(q, \omega)$, seen by inelastic neutron scattering. It results from both the electron-phonon coupling and the electronic correlation effects taken into account beyond random phase approximation (RPA) scheme. We find at optimal doping the isotope coefficient $\alpha_{res} \approx 0.4$ which can be further tested experimentally.

74.72.-h, 74.20.Mn, 74.25.Ha, 74.25.Kc

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, $\chi(q, \omega)$, 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, $\chi(q, \omega)$, at the antiferromagnetic wave vector $Q = (\pi, \pi)$ 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 [4–8]. In particular, the observation of the relatively large isotope effect in various characteristics of cuprates like penetration depth [5], ‘kink’-structure seen by ARPES [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 both 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, $\text{Im} \chi(q, \omega)$. 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.

**Effective Hamiltonian** We start from the atomic limit of the three-band $p-d$ Hamiltonian

$$H_0 = \sum \epsilon_d n_{d\sigma} n_{d\bar{\sigma}} + \sum \epsilon_p n_{p\sigma} n_{p\bar{\sigma}} + \sum U_d n_{d\upsilon} n_{d\bar{\upsilon}} + \sum U_p n_{p\upsilon} n_{p\bar{\upsilon}} + \sum \hbar \omega_q f_q^\dagger f_q$$

(1)

where $\epsilon_d$ and $\epsilon_p$ are the on-site energies of the copper and oxygen holes, $n_{d\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ and $n_{p\sigma} = p_{i\sigma}^\dagger p_{i\sigma}$ are the copper $3d$ and oxygen $2p$ hole densities for site $i$, respectively. $U_d$ and $U_p$ refer to the on-site copper and oxygen Coulomb repulsion, respectively. $f_q^\dagger$ denotes the phonon creation operator and $\hbar \omega_q$ is a phonon energy dispersion. The hopping term between copper and oxygen

$$H_2 = \sum_{\sigma} t_{pd} (d_{i\sigma}^\dagger p_{i\sigma} + h.c.)$$

(2)

and the electron-phonon interaction

$$H_1 = \sum_{l=d,p} g_l n_l (f_q^\dagger + f_q)$$

(3)

we consider as a perturbation. Here, $t_{pd}$ is a hopping term between copper and oxygen, $g_l$ is an 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.

To derive an effective $t-J$ Hamiltonian we employ the canonical Schrieffer-Wolf-like transformations $e^{-S} H e^S$ [10,11]. The matrix of the unitary transformation for the initial Hamiltonian is found by excluding the odd terms with respect to the hopping integral with an accuracy up to the sixth order perturbation theory. Then the $S$-operator consists of the sum of five terms. Each of them is determined by the following iteration procedure.
\[ [H_0S_1] = -H_2, \quad [H_0S_2] = -[H_1S_1], \]
\[ [H_0S_3] = -[H_1S_2] - \frac{1}{3} [[H_2S_1] S_1], \]
\[ [H_0S_4] = -[H_1S_3] - \frac{1}{3} [[H_2S_2] S_2] - \frac{1}{3} [[H_2S_2] S_2], \]
\[ [H_0S_5] = -[H_1S_4] - \frac{1}{3} [[H_2S_3] S_3] - \frac{1}{3} [[H_2S_3] S_3] \]
\[ - \frac{1}{3} [[H_2S_2] S_2] + \frac{1}{45} [[[H_2S_1] S_1] S_1] S_1]. \quad (4) \]

The calculations are straightforward and their details will be given elsewhere. 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. Finally, the relevant effective Hamiltonian is given by

\[ H = \sum_{ij} t_{ij} \Psi_i^{pd,\sigma} \Psi_j^{pd} + \sum_{i>j} J_{ij} \left[ (S_i S_j) - \frac{n_i n_j}{4} \right]. \quad (5) \]

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. In Eq.(5) we use the projecting Hubbard-like operators \( \Psi_i^{\alpha,\beta} = i, \alpha < i, \beta \) in order to satisfy no double occupancy constraint. 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 [12]. Note, \( t_{ij} = t_{ij}^0 e^{-\gamma E_i^{pd}/\hbar \omega_0^p} \) where \( t_{ij}^0 \) is the effective hopping integral without taking into account electron-phonon interaction, \( E_i = (q_i^2)^2/\hbar \omega_0^p \) is the so-called polaron stabilization energy of the copper-oxygen singlet state and \( 0 < \gamma < 1 \). Note, from the experimental data [13] the whole exponential factor was estimated to be \( \gamma E_i^{pd}/\hbar \omega_0^p \approx 0.92 \) around the optimal doping and its value is increasing upon decreasing doping. We further assume that the lifetime of the Zhang-Rice singlet is much larger than the relaxation time of the local deformations.

Similarly the superexchange interaction between nearest copper spins is given by

\[ J = J_0 \left\{ 1 + \frac{3\hbar}{\Delta_{pd}^2} \left[ E_{pd} \omega_p \coth \left( \frac{\hbar \omega_p}{2k_BT} \right) \right] \right. \]
\[ \left. + E_{pd} \omega_d \coth \left( \frac{\hbar \omega_d}{2k_BT} \right) \right\} \], \quad (6) \]

where \( \Delta_{pd} = \epsilon_p - \epsilon_d + U_p - U_d \) is the energy transfer from copper to oxygen and is known to be of the order of 1.5eV in the cuprates. Here, \( J_0 \) is the superexchange interaction of copper spins via the intermediate oxygen atom in the absence of phonons. We took the phonon frequency of the order of \( \omega_p \approx \omega_d = 50 \text{meV} \) which roughly corresponds to the energy of the longitudinal optical(LO) bond stretching phonon mode in cuprates. According to the recent experiments [6,7] it may play an essential role in the physics of cuprates. The so-called polaronic stabilization energy \( E^* \approx E_p \approx E_d \) was estimated of the order of 0.5eV in accordance with the measurements of the isotope effect in cuprates [14].

**Dynamical spin susceptibility** To derive the dynamical spin susceptibility in the superconducting state we use the method suggested by Hubbard and Jain [15] that allows to take into account strong electronic correlations. First we add the external magnetic field applied along c-axis into the effective Hamiltonian

\[ H_i = Re \sum_{\mathbf{q}} \left[ h_{-\mathbf{q}} e^{i(\omega t - \mathbf{q} \mathbf{R}_i)} + h_{\mathbf{q}} e^{-i(\omega t - \mathbf{q} \mathbf{R}_i)} \right]. \quad (7) \]

Then we write an equation of motion for the \( \Psi \) operators using the Roth-type of the decoupling scheme [16] and expanding the \( F^*_{pd} = \{ \Psi_i^{pd,\sigma}, \Psi_i^{pd,\sigma} \} = \frac{1+\hat{P}}{2} + \sigma Re \sum_{\mathbf{q}} \left[ S_{\mathbf{q}} e^{-i(\mathbf{q} \mathbf{R}_i - \omega t)} + S_{\mathbf{q}} e^{i(\mathbf{q} \mathbf{R}_i - \omega t)} \right] \) up to the first order in \( S_{\mathbf{q}} = \chi^{zz}(z, \omega) \hbar q_z \). In particular, \( i \hbar \frac{\partial \Psi_{k}^{-\sigma, pd}}{\partial t} = (\epsilon_k - \mu) \Psi_{k}^{-\sigma, pd} + \Delta_k \Psi_{pd}^{-\sigma, pd} \)
\[ + \frac{1}{2} \left[ \left( \frac{J_0}{2} - \frac{J_0}{2} S_{-\mathbf{q}} - \frac{\hbar q}{2} \right) \Psi_{k-\mathbf{q}}^{-\sigma, pd} e^{-i\omega t} \right. \]
\[ \left. + \left[ \frac{J_0}{2} - \frac{J_0}{2} S_{\mathbf{q}} - \frac{\hbar q}{2} \right] \Psi_{k+\mathbf{q}}^{-\sigma, pd} e^{i\omega t} \right] \quad \text{up to the first order in } S_{\mathbf{q}} = \chi^{zz}(z, \omega) \hbar q_z. \quad (8) \]

and the similar expression occurs for \( \Psi_{pd, \sigma}^+ \). Here, \( \Delta_k = \Delta_{pd} (\cos k_x - \cos k_y) \) is the superexchange interaction on a square lattice.

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

\[ \langle \Psi_i^{pd,\uparrow} \Psi_i^{pd,\uparrow} \rangle - \langle \Psi_i^{pd,\downarrow} \Psi_i^{pd,\downarrow} \rangle = 0 \quad , \quad (9) \]

and using the Bogolyubov-like transformations to the new quasiparticle states

\[ X_{pd, \sigma}^{-\delta} = u_k \Psi_{pd, \sigma}^\dagger - v_k \Psi_{pd, \sigma}^\dagger, \quad X_{pd, \sigma}^{+\delta} = u_k \Psi_{pd, \sigma}^\dagger - v_k \Psi_{pd, \sigma}^\dagger \quad , \quad (10) \]

Here, \( u_k^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k - \mu}{\epsilon_k} \right) \) and \( v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k - \mu}{\epsilon_k} \right) \) are the Bogolyubov coefficients, \( \mu \) is a chemical potential, and \( E_k = \sqrt{\left( \epsilon_k - \mu \right)^2 + \Delta_k^2} \) in the superconducting state. Substituting Eq.(10) in Eq.(9) and using the equations of motion (8) one obtains the expression for the dynamical spin susceptibility in the form

\[ \chi(q, \omega) = \chi_0(q, \omega) \frac{\chi_0(q, \omega)}{J_0 \chi_0(q, \omega) + \Pi(q, \omega) + Z(q, \omega)}. \quad (11) \]
This is a central result of our paper. Here, $\chi_0(q,\omega)$ is the usual BCS-like Lindhard response function, $\Pi(q,\omega)$ and $Z(q,\omega)$ result from the strong electronic correlation effects. In the normal state the expression for $\Pi(q,\omega)$ has been obtained by Hubbard and Jain [15]. In the superconducting state it is given by

$$\Pi(q,\omega) = \frac{P_{pd}}{N} \sum_k u_k u_{k+q} (u_k u_{k+q} + v_k v_{k+q}) \frac{f_k f_{k+q} - f_k - f_{k+q} (1 - f_k + f_{k+q})}{\omega + i\Omega - E_k - E_{k+q}} + v_k v_{k+q} (v_k v_{k+q} + u_k u_{k+q}) \frac{t_k (1 - f_k) - t_k f_{k+q} (1 - t_k + f_{k+q})}{\omega + i\Omega - E_k - E_{k+q}} + u_k u_{k+q} (u_k u_{k+q} - u_k v_{k+q} + v_k v_{k+q}) \frac{t_k f_k - t_k f_{k+q} (1 - f_k + f_{k+q})}{\omega + i\Omega - E_k - E_{k+q}} + u_k + v_k v_{k+q} (v_k u_{k+q} - u_k v_{k+q}) \frac{t_k (1 - t_k) - t_k f_{k+q} (1 - t_k + f_{k+q})}{\omega + i\Omega - E_k - E_{k+q}} (12)$$

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

$$Z(q,\omega) = \frac{1}{N} \sum_k \frac{\omega + i\Omega}{\omega + i\Omega + \epsilon_k^{(1)} - \epsilon_k^{(1)}} . \quad (13)$$

Here, $f_k$ is the Fermi distribution function, $\epsilon_k^{(1)} = \frac{1}{2} t_k$, $\epsilon_k = P_{pd} t_k$ 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-nearest neighbor hopping, respectively. The origin of the terms $\Pi(q,\omega)$ and $Z(q,\omega)$ 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 [17]. For the $\Delta_k = 0$ Eq.(11) agrees with the normal state result for the dynamical spin susceptibility [15,18,19].

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 on the ‘resonance’ peak formation seen by INS [3]. Using various approaches this feature was well understood mainly as a result of the spin density wave (SDW) collective mode formation at $\omega = \omega_{res}$, i.e. when the denominator of the spin susceptibility at the antiferromagnetic wave vector $Q$ is close to zero [20,21].

In Fig. 1 we show the results of our calculations for the $\text{Im} \chi(Q,\omega)$ as a function of frequency in the normal and the superconducting state. Here, we use $t = 200\text{meV}$, $t' = -0.1t$, and $t'' = 0.02t$ at optimal doping. Clearly in the normal state the spin fluctuation spectrum is characterized by a broad feature which starts around $10\text{meV}$ and extends up to a higher frequencies. In the superconducting state it strongly renormalizes due to a presence of the $d_{x^2-y^2}$-wave gap ($\Delta_k \propto (\cos k_x - \cos k_y)$) that leads to a resonance peak formation similar to the RPA result [20,21]. However, due to a strong frequency dependence of $Z(Q,\omega)$ and $\Pi(Q,\omega)$ the spectral weight of the resonance peak is redistributed away from $(\pi,\pi)$ (see the dashed curve for comparison) leading to a well-pronounced dispersion of the latter. This is illustrated in Fig.2(a) where we show the calculated frequency and momentum dependence of $\text{Im} \chi(Q,\omega)$ away from the antiferromagnetic wave vector $Q = (\pi,\pi)$. The dispersion of the resonance excitations is clearly visible and is shown in Fig.2(b) as a function of $q_x$ ($q_y = \pi$). As one sees there are well-pronounced dispersion curves $\propto q^2$ in good agreement with experiment [23,24]. Note, that in the RPA the dispersion of the resonance is much weaker (in particular the upper branch of the dispersion) due to a $\delta$-function character of the resonance condition [21] while $Z$– and II-terms, in particular, lead to a redistribution of the spectral weight away from $Q = (\pi,\pi)$. Note, due to the tetragonal symmetry the same dispersion takes place for $q_y$ ($q_x = \pi$).

The position of the resonance peak is determined mainly by the magnitude of the $d_{x^2-y^2}$-wave superconducting gap, $\Delta_0$, the superexchange coupling constant, $J$, and by the proximity of the Fermi energy to the extended saddle point (the so-called van-Hove singularity) in the density of states determined by the ratio of $t'/t$. In order to illustrate this dependence we show in Fig. 3 the resonance peak position as a function of $J/t$ and $\Delta_0/t$ at optimal doping. One can clearly see that it depends almost linearly on $2\Delta_0$. This follows from our Eq. (11). In particular, the superconducting gap determines mainly the position of the continuum of the spin excitations from $\text{Im} \chi_0$ and which is around $2\Delta_0$ [20]. Thus,
values of remain the same [20]. On the other hand, for the fixed
lective mode) and the continuum of the states has to
between the position of the resonance peak (SDW col-
gularity influences also the resonance peak. Its influence
addition, the ratio of lower frequency enhances its intensity and visa versa. In
values. We note that the shift of the resonance peak to the
J/t
is somewhat similar to J with one important difference. In
particular, an increase of t’/t rather weakens the in-
tensity of the resonance peak than changes the position
itself (not shown). Note, that our analysis agrees qual-
itatively with the previous ones [20]. Most importantly
we find that by the slight variation of all parameters one
could find another realistic set of Δ0/t, J/t, and t’/t
which would also correctly explain the position of the
resonance peak at optimal doping [25]. This means that
at present stage we could make only a qualitative analysis
of the experimental data. Further factors like orthorhom-
bigic distortions may influence the difference between
the resonance peak intensity in BiSr2CaCu2Oy (BSCCO)
and YBa2Cu3O7(YBCO).

Finally, we discuss the influence of the electron-phonon
interaction on the resonance peak formation by chang-
ing the isotope mass of 16O by 18O. This shifts the
average frequency of the LO phonon mode and conse-
quently renormalizes the hopping integral t and the su-
perexchange coupling constant, J. Most importantly,
the electron-phonon interaction changes most dramatically
the hopping integral t rather than the superexchange
coupling J. In particular, as can be seen from Eq.(6)
the superexchange coupling constant J changes less than
1% upon substituting the isotopes [26] which agrees well
with experimental data [27]. 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 ωres value upon
changing the isotopes. In the case of Eq.(11) the most
important contribution to the isotope effect on the reso-
ence peak appears due to Π(q, ω) ∝ tk. In particular,
using our estimation given above we find that at opti-
mal doping the hopping integral changes by 6% upon
replacing 16O by 18O. This results in the lowering of the
resonance frequency at (π, π) from 41meV for the 16O
isotope towards 39meV for the 18O sample. This leads
to αres = −d ln ωres
d ln M ≈ 0.4 for optimally-doped cuprates.

\[\Delta_0(t, \omega) = \frac{\pi}{2t} \ln \left(\frac{\omega}{\omega_0}\right)\]

\[\Delta_0(t, \omega) = \frac{\pi}{2t} \ln \left(\frac{\omega}{\omega_0}\right)\]
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 $\gamma E^*_c/\hbar \omega^*_c$ [13]. At the same time the superconducting transition temperature which is determined by $J$ shows much weaker isotope effect and is around $\alpha_T \approx 0.05$ [26]. 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.

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 $(\pi, \pi)$ leading to the pronounced dispersion. This is in good agreement with recent INS data [23,24]. 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.

It’s pleasure to thank P. Bourges, A. Lanzara, T. Timusk, D. Manske for useful discussions and M. Mali for critical reading of the manuscript. The work of I.E. is supported by INTAS grant No. 01-0654. M.V.E. and O.K. are supported by the RFBR Grant No. 03-02-16550 and RSP "Superconductivity" 98014-3.

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