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On Correlation between the Magnetic Susceptibilities of Localized and Collective Electrons in Hole High-Temperature Superconductors

M. V. Eremin[a], A. A. Aleev[a], and I. M. Eremin[b]

[a] *Faculty of Physics, Kazan State University, ul. Kremlevskaya 18, Kazan, 420008 Russia*
e-mail: Mikhail.Eremin@ksu.ru
[b] *Max-Planck Institut für Physik Komplexer Systeme, Dresden D-01187, Germany*

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In the framework of the singlet-correlated motion of holes over oxygen sites in CuO_2 layers, a formula for the dynamic spin susceptibility has been derived taking into the strong correlation between the magnetizations of the spins of the collective holes and localized moments on copper sites. The calculated behavior of the imaginary part of the susceptibility as a function of the frequency and wave vector is consistent with the available experimental data on the inelastic neutron scattering. The plot of the dispersion of the collective spin modes over the entire Brillouin zone is proposed.

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There are serious reasons to believe that the magnetism of high-temperature superconductors (HTSCs) based on layered cuprates is double [1]. For weak doping, these are predominantly magnets with localized spins on copper nuclei, and the temperature dependence of their susceptibility in the overdoped region of the phase diagram is similar to the behavior of Pauli paramagnets. The duality of magnetism of $YBa_2Cu_3O_{6+x}$ compounds is clearly manifested in recent experiments on the inelastic neutron scattering [2–5]. Near the wave vector $Q = (\pi, \pi)$, two contours ("modes") of maxima were found in the imaginary part of the susceptibility that cannot coexist in the framework of the theory of simple metals and insulators. Explanation of the mode with arc-like dispersion observed for $T < T_C$ requires the model of collective electrons and this mode is well reproduced by the random-phase approximation (RPA) formula [6–8]. The mode with the U-like dispersion, which is most pronounced in the normal phase, is not explained in the RPA. For its explanation, the model of local magnetic moments on copper sites is more appropriate; however, the problem of describing the superconducting phase appears in this case. In this work, we propose a universal formula for the dynamic spin susceptibility of layered cuprates that provides the simultaneous description of both features observed in the scattering of neutrons by hole HTSCs.

The formula is derived by the Green's function method with the use of the Hamiltonian

$$H = \sum_{ij\sigma} t_{ij}\psi_i^{pd,\sigma}\psi_j^{\sigma,pd} + \frac{1}{2}\sum_{il} J_{il}\left(\mathbf{S}_i\mathbf{S}_l - \frac{n_i n_l}{4}\right) + \frac{1}{2}\sum_{il} G_{il}\delta_i\delta_l. \quad (1)$$

Here, $\psi_i^{pd,\sigma}$ ($\psi_j^{\sigma,pd}$) are the creation (annihilation) operators for composite quasiparticles in the conduction band of hole-doped HTSCs. The superscript *pd* corresponds to singlet formations consisting of copper and oxygen holes [9–11]. The second term describes the superexchange interaction of spins, the last term presents the density–density interaction, and $\delta_i = \psi_i^{pd,pd}$ is the hole number operator per one unit cell. The expression obtained for the dynamic susceptibility has the form

$$\chi^{+,-}(\omega, \mathbf{q}) = \frac{F(\omega, \mathbf{q}) + L_q b(\omega, \mathbf{q})}{D(\omega, \mathbf{q}) + (\Lambda_q^2 - \omega^2) b(\omega, \mathbf{q})}, \quad (2)$$

where

$$F(\omega, \mathbf{q}) = \chi(\omega, \mathbf{q}) - \chi_t(\omega, \mathbf{q}) b(\omega, \mathbf{q}). \quad (3)$$

The function $\chi(\omega, \mathbf{q})$ up to a factor coincides with the spin susceptibility in the BCS theory. For further consideration, it is convenient to represent this function in the form

$$\chi(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\chi_{k,q} = \frac{1}{N}\sum_{\mathbf{k}} S_{xx}\frac{n_p - n_k}{\omega + E_k - E_p} + \frac{1}{N}\sum_{\mathbf{k}} S_{yy}\frac{n_k - n_p}{\omega - E_k + E_p} + \frac{1}{N}\sum_{\mathbf{k}} S_{yx}^{(-)}\frac{n_p + n_k - P}{\omega - E_k - E_p} + \frac{1}{N}\sum_{\mathbf{k}} S_{xy}^{(+)}\frac{P - n_p - n_k}{\omega + E_k + E_p}, \tag{4}$$

where $n_k = \langle \alpha_k^{pd,\sigma}, \alpha_k^{\sigma,pd}\rangle = Pf_k$ are the occupation numbers, the coherence factors $S_{xx} = x_k x_p + z_k z_p$, $S_{yy} = y_k y_p + z_k z_p$, $S_{yx}^{(-)} = y_k x_p - z_k z_p$, and $S_{xy}^{(+)} = x_k y_p - z_k z_p$ are expressed in terms of

$$x_k = u_k^2 = \frac{1}{2}\left(1 + \frac{\epsilon_k - \mu}{E_k}\right),$$

$$y_k = v_k^2 = \frac{1}{2}\left(1 - \frac{\epsilon_k - \mu}{E_k}\right), \quad z_k = u_k v_k = \frac{\Delta_k}{2E_k},$$

f_k are the ordinary Fermi functions, $E_k = \sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}$ are the energy of the Bogoliubov quasiparticles, P is the mean values of the anticommutator of the creation and annihilation operators for composite quasiparticles, $\mathbf{p} = \mathbf{k} + \mathbf{q}$, Δ_k is the superconducting gap parameter, and the dispersion law is specified in the form $\epsilon_k = Pt_k - \mu$, where $t_k = 2t_1(\cos(k_x a) + \cos(k_y a)) + 4t_2\cos(k_x a)\cos(k_y a)$. The second term in Eq. (3) is a correction to the susceptibility of collective electrons due to the strong electron correlations. The input functions have the form

$$\chi_t(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\chi_{Ekq}, \tag{5}$$

$$\eta_t(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)(J_q\chi_{Ekq} - \Pi_{Ekq}), \tag{6}$$

$$\zeta_t(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}(t_{k+q} - t_k)\zeta_{Ekq}, \tag{7}$$

where the partial functions in the sums are expressed as

$$\chi_{Ekq} = S_{xx}\frac{(E_p - E_k)(n_p - n_k)}{\omega + E_k - E_p} + S_{yy}\frac{(E_p + E_k)(n_p - n_k)}{\omega - E_k + E_p} + S_{yx}^{(-)}\frac{(E_p + E_k)(n_p + n_k - P)}{\omega - E_k - E_p} - S_{xy}^{(+)}\frac{(E_p + E_k)(P - n_p - n_k)}{\omega + E_k + E_p}, \tag{8}$$

$$\Pi_{Ekq} = S_{xx}\frac{(E_p - E_k)(t_p n_p - t_k n_k)}{\omega + E_k - E_p} + S_{yy}\frac{(E_k - E_p)[t_p(P - n_p) - t_k(P - n_k)]}{\omega - E_k + E_p} + S_{yx}^{(-)}\frac{(E_p + E_k)[t_p n_p + t_k(P - n_k)]}{\omega - E_k - E_p} - S_{xy}^{(+)}\frac{(E_p + E_k)[t_p(P - n_p) - t_k n_k]}{\omega + E_k + E_p}, \tag{9}$$

$$\xi_{Ekq} = S_{xx}(E_p - E_k)\frac{P}{\omega + E_k - E_p} + S_{yy}(E_k - E_p)\frac{P}{\omega - E_k + E_p} + S_{yx}^{(-)}(E_p + E_k)\frac{P}{\omega - E_k - E_p} - S_{xy}^{(+)}(E_p + E_k)\frac{P}{\omega + E_k + E_p}, \tag{10}$$

The function

$$D(\omega, \mathbf{q}) = \eta(\omega, \mathbf{q}) - \eta_t(\omega, \mathbf{q})b(\omega, \mathbf{q}) \tag{11}$$

is expressed in terms of the characteristics of collective electrons and can be compared to the denominator of the spin susceptibility in the RPA. The expression for $\eta(\omega, \mathbf{q})$ contains two terms

$$\eta(\omega, \mathbf{q}) = J_q\chi(\omega, \mathbf{q}) - \Pi(\omega, \mathbf{q}), \tag{12}$$

where $J_q = J_1(\cos(q_x a) + \cos(q_y a))$. The first term is known in the RPA, whereas the origin of the second term in Eq. (12) is attributed to the features of the commutation relations for composite quasiparticles. The commutative relations in this model include the magnetization [10, 11]. The functions $\Pi(\omega, \mathbf{q})$ and $\zeta(\omega, \mathbf{q})$ have the form

$$\Pi(\omega, \mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\Pi_{k,q} = \frac{1}{N}\sum_{\mathbf{k}} S_{xx}\frac{t_p n_p - t_k n_k}{\omega + E_k - E_p} + \frac{1}{N}\sum_{\mathbf{k}} S_{yy}\frac{t_p(P - n_p) - t_k(P - n_k)}{\omega - E_k + E_p} + \frac{1}{N}\sum_{\mathbf{k}} S_{yx}^{(-)}\frac{t_p n_p - t_k(P - n_k)}{\omega - E_k - E_p} \tag{13}$$

$$+\frac{1}{N}\sum_{\mathbf{k}} S_{xy}^{(+)}\frac{t_p(P-n_p)-t_k n_k}{\omega+E_k+E_{k+q}},$$

$$\zeta(\omega,\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{k}}\zeta_{k,q} = \frac{1}{N}\sum_{\mathbf{k}} S_{xx}\frac{P}{\omega+E_k-E_p}$$
$$+\frac{1}{N}\sum_{\mathbf{k}} S_{yy}\frac{P}{\omega-E_k+E_p}$$
$$+\frac{1}{N}\sum_{\mathbf{k}} S_{yx}^{(-)}\frac{P}{\omega-E_k-E_p} \quad (14)$$
$$+\frac{1}{N}\sum_{\mathbf{k}} S_{xy}^{(+)}\frac{P}{\omega+E_k+E_p}.$$

Such functions for describing the normal phase were first introduced in [12, 13]. According to Eq. (7), the factor $b(\omega, \mathbf{q}) = \zeta(\omega, \mathbf{q})/\zeta_t(\omega, \mathbf{q})$ is inverse proportional to the bar bandwidth ($\cong 8t_1$) and thereby the contribution of the magnetization component of local moments in Eq. (2) is suppressed more strongly for a wider conduction band.

The quantity Λ_q^2 in Eq. (2) is the frequency squared of the collective oscillations of the localized spins renormalized due to the presence of band electrons:

$$\Lambda_q^2 = \Omega_q^2 + \frac{1}{N}\sum_{\mathbf{k}}[(t_p-t_k)$$
$$\times(S_{xx}[(J_q-t_k)n_k-(J_q-t_p)n_p]$$
$$+S_{xy}^{(+)}[(J_q-t_k)n_k-(J_q-t_p)(P-n_p)] \quad (15)$$
$$+S_{yx}^{(-)}[(J_q-t_k)(P-n_k)-(J_q-t_p)n_p]$$
$$+S_{yy}[(J_q-t_k)(P-n_k)-(J_q-t_p)(P-n_p)])].$$

The renormalization of such a property was previously discussed in view of the problem of describing the suppression of antiferromagnetism with increasing the doping degree of cuprates [14, 15]. In this respect, our expression is more general, because it is applicable for the superconducting phase. As in [13, 15, 16], the formula for the seed frequency squared Ω_q^2 (in the absence of carriers) coincides with the formula previously obtained for two-dimensional paramagnets with decoupling of the equations of motion for the Green's functions by the Kondo–Yamaji method [14]:

$$\Omega_q^2 = J_1^2(2-c_q)[1+2K_2+K_3-K_1(1+2c_q)], \quad (16)$$

where $c_q = \cos(q_x a) + \cos(q_y a)$ and $K_n = 4\langle S_0^z S_n^z\rangle$ is the spin–spin correlation functions, which are calculated self-consistent. The function L_q in Eq. (2) is given by the expression

$$L_q = -2J_1K_1(2-c_q) - \frac{1}{N}\sum_{\mathbf{k}}(n_p-n_k)(t_p-t_k). \quad (17)$$

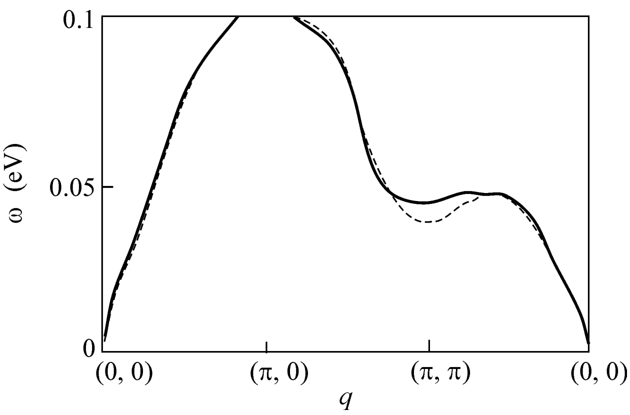

Fig. 1. Plot of collective spin oscillations calculated from the condition of vanishing the real part of the susceptibility denominator in (solid line) the superconducting phase at T = 10 K and (dashed line) the normal phase at T = 90 K. The calculation parameters (in meV) are t_1 = 420, t_2 = –120, μ = 290, Δ_0 = 23, J_1 = 50, and Γ = 2. The correlation functions are K_1 = –0.12, K_2 = 0.009 and K_1 = –0.11, K_2 = 0.007 in the superconducting and normal phases, respectively.

It is seen that Eq. (2) has the correct limiting expressions. For the zero filling numbers, it transforms into the expression for the dynamic susceptibility of the localized spins of two-dimensional antiferromagnets with the spin $s = 1/2$ [13, 15, 16]. If the function $F(\omega, \mathbf{q})$ and all expressions with the coherence factor are rejected in Eq. (2), the remaining part is similar to the expression obtained for the spin susceptibility by the memory function method proposed in [17, 18] for the *t–J* model, where the main attention was focused on the renormalization of the susceptibility of the localized spins due to the effect of conduction electrons. The detailed comparison with [17, 18] is complicated, because some functions were not calculated in those works; they were instead specified phenomenologically involving experimental data. When the spin correlation functions vanish, Eq. (2) corresponds to the susceptibility of collective electrons. We also emphasize that the denominator of the susceptibility for localized and band spins in Eq. (2) is common, which is natural for coupled subsystems. According to our calculations some of which are presented below, the correlation between localized and collective electrons in layered cuprates is so strong that the simple two-component model (local moments + collective electrons), which is applied in a number of works, becomes senseless. In particular, this is seen in the dispersion law of collective spin modes that is shown in Fig. 1. There is one common mode of the collective oscillations in the spin system of the hole-activated CuO_2 layer. The frequency

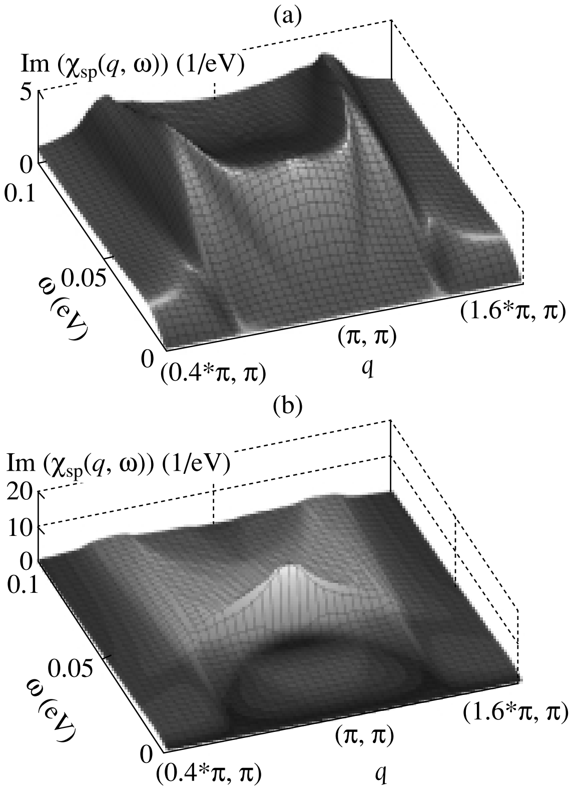

Fig. 2. Imaginary part of the total susceptibility near the wave vector $Q = (\pi, \pi)$ in the (a) normal and (b) superconducting phases for the calculation parameters given in Fig. 1.

minimum near the antiferromagnetic wave vector is similar to the behavior of the localized-spin mode. This minimum is shifted towards to higher frequencies in the transition to the superconducting state. This behavior is direct evidence of the effect of the susceptibility of collective holes.

Figure 2 shows the imaginary part of the susceptibility calculated by Eq. (2) for the (a) normal and (b) superconducting phases for the typical parameters for hole HTSCs. It is seen that all basic features of the inelastic scattering of neutrons (the most complete data for $YBa_2Cu_3O_{6+x}$ were presented in [19]) are well reproduced. The U-like mode exists in the normal phase. In the superconducting phase, the relief of the imaginary part of the susceptibility exhibits simultaneously two “ridges”: U-like with the valley (silence zone, according to experimenters) and arc-like with the common peak at $Q = (\pi, \pi)$. The parameter P is taken to be equal to 0.665, which corresponds to the Fermi surface shape of the $YBa_2Cu_3O_{6+x}$ compound, and $\Delta_k = \Delta_0\cos((k_xa) - \cos(k_ya))/2$. Damping is taken into account in the calculations by means of the usual change of ω to $\omega + i\Gamma$. In this paper, we do not discuss the form of the pseudopotential of the Coulomb interaction G, because the spin operator commutates with the last term of Hamiltonian (1).

In conclusion, we note that Eq. (2) can be applied not only to the analysis of the inelastic scattering of the neutrons by the HTSCs. Moreover, the result gives hope that a similar formula can be obtained for other compounds with localized and collective electrons.

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