Influence of strong electron correlations on the spin susceptibility in High-T$_c$ cuprates

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Abstract

A new formula for the dynamic spin susceptibility has been analyzed with taking into account the strong electron correlations. The correlations sufficiently modify the Stoner-like factor and as a consequence change the phase diagram of the instability. It is remarkable to note that the instability area moves to the low doping. The possible approximates (lorentzian and gaussian) of the real part of the spin susceptibility have been considered. The behavior of the correlation length with doping and temperature in both cases is discussed.

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1 Introduction.

It is well known that strong electron correlation effects play the crucial role in High-T$_c$ cuprates [1, 2]. However, up to now there is no clear understanding of how these effects will change the behavior of the electronic system. For example, the $2\Delta_0/k_BT_c$ ratio gives an important information about the nature of the pairing mechanism. But as long as we cannot take into account the strong electron correlations we are not be able to say anything about the correct value of this ratio. The special interest concerns the consideration of the influence of the strong electron correlation effects on the expression for the dynamic spin susceptibility because the susceptibility itself is directly measured by the different experimental technics such as nuclear magnetic resonance (NMR), electron spin resonance (ESR) and inelastic neutron scattering (INS).

Here, the new formula for the dynamic spin susceptibility has been analyzed with taking into account the strong electron correlations. The correlations sufficiently modify the Stoner-like factor and as a consequence change the phase diagram of the instability. It is remarkable to note that the instability area moves to the low doping. Then the possible approximates (lorentzian and gaussian) of the real part of the spin susceptibility have been examined. The behavior of the correlation length with doping and temperature in both cases is discussed. The expression for the uniform spin susceptibility below T$_c$ has been calculated. I compare the calculated curve to the experimental Cu(2) Knight shift and extract the ratio $2\Delta_0/k_BT_c$.

2 Model Hamiltonian.

In the calculation of the spin susceptibility I start from the two bands model proposed by authors [3], [4]:

$$\begin{aligned} H &= \sum \varepsilon_d \Psi_i^{\sigma,\sigma} + \sum E_{pd}\Psi_i^{pd,pd} + \sum t_{ij}^{(11)}\Psi_i^{pd,\sigma}\Psi_j^{\sigma,pd} + \\ &+ \sum t_{ij}^{(22)}\Psi_i^{\sigma,0}\Psi_j^{0,\sigma} + + \sum t_{ij}^{(12)}(-1)^{\frac{1}{2}-\sigma}\left[\Psi_i^{\sigma,0}\Psi_j^{\overline{\sigma},pd} + \Psi_i^{pd,\sigma}\Psi_j^{0,\overline{\sigma}}\right] + \\ &+ \sum J_{ij}\left[(\vec{S}_i\vec{S}_j) - \frac{n_i n_j}{4}\right] \end{aligned} \tag{1}$$

Here, $\Psi_i^{\sigma,0}$ and $\Psi_i^{pd,\sigma}$ are the Hubbard like quasiparticle creation operators, for the lower and upper bands, respectively. $\vec{S}$ are copper spin operators, $t_{ij}^{(11)}$ and $t_{ij}^{(22)}$ are hopping integrals between sites and $t_{ij}^{(12)}$ is a hybridization parameter. ε_d and E_{pd} are the site energies of the copper holes and copper-oxygen singlets. The last term in the Hamiltonian (1) is the superexchange interaction between the nearest copper spins.

The difference of the suggested model in [3], [4] from the standard Hubbard Hamiltonian connects to the following fact. A hole doped into the plane forms a Zhang-Rice singlet and does not go into the upper copper Hubbard band [5]. The standard Hubbard Hamiltonian with a large Coulomb repulsion is replaced by a Hubbard-like Hamiltonian with the upper singlet band and small Coulomb repulsion. The influence of the upper Hubbard bands is taken by superexchange interaction.

3 Dynamic Spin Susceptibility.

The dynamic spin susceptibility formula was deduced by the Green function method:

$$\chi(q,\omega) = -\frac{1}{N}\langle\langle S_q^{\sigma}|S_q^{\overline{\sigma}}\rangle\rangle \tag{2}$$

where S_q^{σ} is a Fourier component of the copper spin. Using the standard Hubbard I approximation scheme in the case of $E_{pd} - 2\varepsilon_d >> t^{(12)}$ the general expression for the dynamic spin susceptibility has been got and details are described elsewhere [6]. In high-T_c compounds the copper band is completely filled. Upon doping the carriers go to the singlet band and E_{k1} is filling up. In this case the expression for the static spin susceptibility in the singlet band can be written as follows:

$$\chi'(q) = \frac{\chi_0^{11}(q)}{J_q\chi_0^{11}(q) + \chi_1^{11}(q)} \tag{3}$$

where

$$\chi_0^{11}(q) = \frac{1}{N}\sum\frac{n_{k+q}^{(1)} - n_k^{(1)}}{P_{pd}t_k^{(11)} - P_{pd}t_{k+q}^{(11)}} \tag{4}$$

and

$$\chi_1^{11}(q) = \frac{1}{N}\sum\frac{n_k^{(1)}t_k^{(11)} - n_{k+q}^{(1)}t_{k+q}^{(11)}}{P_{pd}t_k^{(11)} - P_{pd}t_{k+q}^{(11)}} \tag{5}$$

Here, $J_q = J_0(\cos q_x + \cos q_y)$ and $P_{pd} = (1+\delta)/2$ is a thermodynamic average of the anticommutator and δ is a doping level per two copper sites, $n_k^{(1)} =< \Psi^{pd,\sigma}\Psi^{\sigma,pd} >_k$ is a number of the quasiparticles of the copper-oxygen singlet band and

$$\begin{aligned} t_k^{(11)} &= 2t_1^{(11)}(\cos(k_x)+\cos(k_y)) + 4t_2^{(11)}\cos(k_x)\cos(k_y) + \\ &\quad +2t_3^{(11)}(\cos(2k_x)+\cos(2k_y)) \end{aligned} \tag{6}$$

with $t_1^{(11)}$, $t_2^{(11)}$, and $t_3^{(11)}$ referring to hopping to the first, second, and third Cu neighbors, respectively

The obtained formula (3) looks quite different comparing to the ordinary RPA expression due to the strong electron correlations. In particular, those effects can be clear seen on the phase diagram of the instability determined by the condition

$$J_q \chi_0^{11}(q) + \chi_1^{11}(q) = 0 \tag{7}$$

In Fig.1 we present the result of our calculation versus doping level. As one can see, the instability region displaces to the low doping regime on the contrary to the $t-J$ model prediction where at the low doping level there is not any instability [7]. This fact has cast some doubts on the application of the $t-J$ model for the real cuprates. In our case the situation is differed because at low doping there is a large area of the instability. In this connection we could propose the following scenario for the high-T$_c$ cuprates. At low doping, the $t_1^{(11)}/J_0$ ratio is big enough and there is an instability with incommensurate wave vector in the system. Upon doping the $t_1^{(11)}/J_0$ ratio has reached the value (at half-filled band) that satisfies the instability with commensurate wave vector. And in the overdoped regime the $t_1^{(11)}/J_0$ is too small for getting any instability at all. We have to mention that our result will coincide with $t-J$ model phase diagram [7] in the case of the exchanging of the doping level δ on $1-\delta$ and putting zero hopping integrals $t_2^{(11)}$ and $t_3^{(11)}$.

Now, we turn our consideration to the possible approximations for the static spin susceptibility expression. Assuming two different formulas we then look for the temperature and doping dependencies of the correlation length and the amplitude in both cases. First, we consider the lorentzian approximation formula:

$$\chi'_L(q) = \frac{A\xi^2}{1+\xi^2(q-Q)^2} \tag{8}$$

where ξ is a correlation length, A is an amplitude and $Q = (\pi, \pi)$. This approximation formula is a currently central topic now in the Nearly Antiferromagnetic Fermi Liquid (NAFL) phenomenological theory for high-T$_c$ cuprates [2]. After fitting we have found that upon doping and temperature the amplitude practically does not change and ξ slightly decreases with increasing temperature and doping from 1.3 till 1.8 constants of a. The use of the second approximation:

$$\chi'_G(q) = 4\pi A\xi^2 \exp\left\{-\xi^2(q-Q)^2\right\} \tag{9}$$

provides another temperature and doping dependencies of the correlation length and amplitude. The amplitude in this case strongly depends on doping and increases with decreasing temperature. Therefore, the correlation length is less sensitive to variations of δ. These results coincides well with experimental results [8] for ^{17}O NMR probe the susceptibility, where assuming a gaussian approximation formula the correlation length was found is nearly T independent albeit the amplitude is T dependent. In this connection we have to remark that the results of approximation are differed depending on the choosing of approximation.

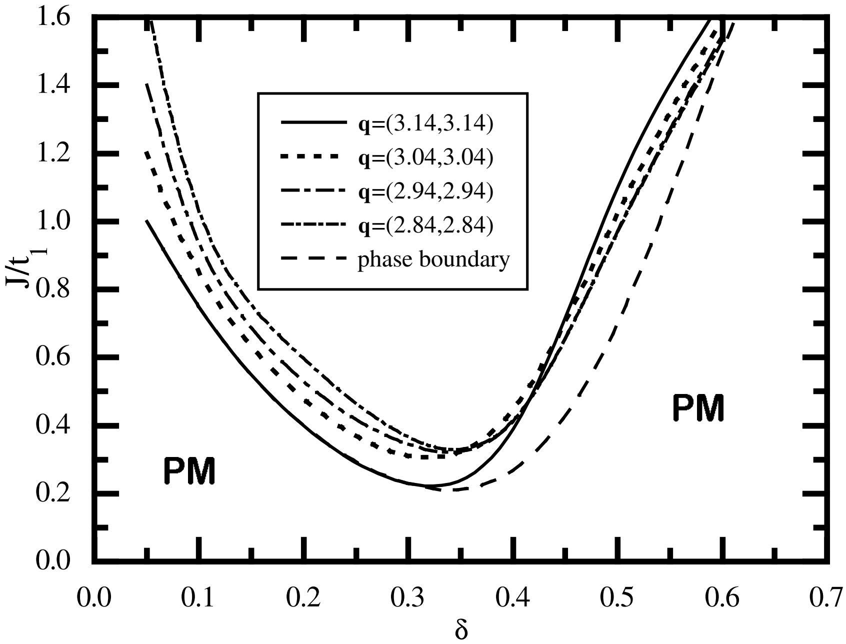

Figure 1: The calculated phase diagram for the copper - oxygen singlet band. The phase boundary line means the appearance of the instability with any wave vector. At low doping the phase boundary corresponds to the wave vector $Q = (\pi, \pi)$ albeit in the overdoped regime it displaces to the incommensurate wave vectors. The perfect nesting does not show up at half-filling because of the non-zero parameter $t_3^{(11)}$.

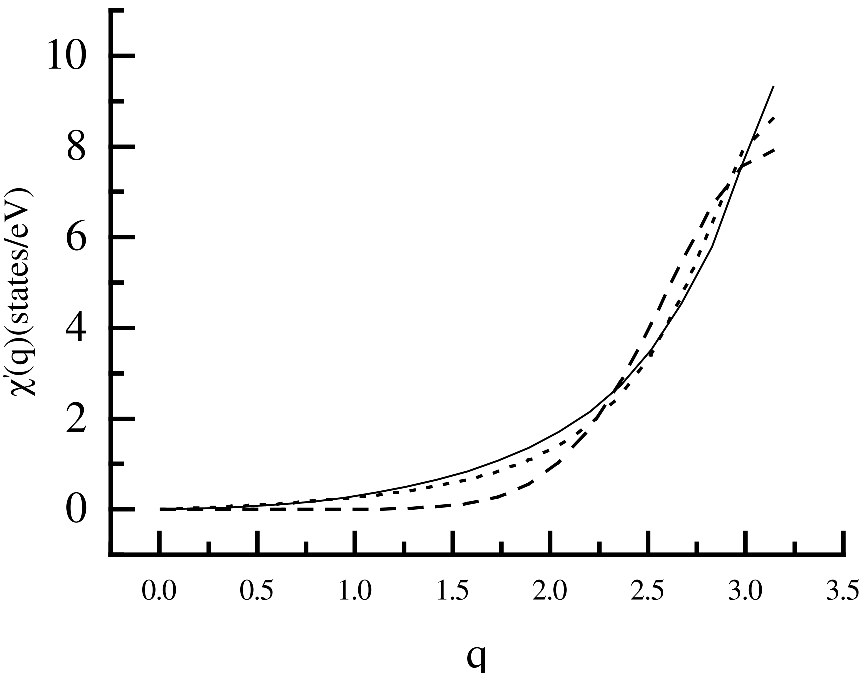

Figure 2: The static spin susceptibility along the diagonal of the Brillouine zone. Black curve - calculated results for the expression (3) with $\delta = 0.33$, $T = 100K$, $J/t_1^{(11)} = 0.2$, dotted curve - the result of the approximation by lorentzian with $\xi = 1.35a$ and $A = 4.9$, dashed - the result of the approximation by gaussian with $\xi = 0.92a$ and $A = 0.75$.

In Fig.2 we present the result of the calculation of the static spin susceptibility for the half-filled band together with approximations As one can see, among both approximations the lorentzian is preferable.

4 Uniform Spin Susceptibility below T$_c$.

In the external magnetic field along z-axis the Hamiltonian can be written:

$$H = H_0 - g\beta H_z \frac{1}{2} \sum \left(\Psi_i^{\uparrow\uparrow} - \Psi_j^{\downarrow\downarrow} \right) \tag{10}$$

The anticommutator in this case has a view:

$$P^{\uparrow,\downarrow} = P \pm < s_z > \tag{11}$$

where $< s_z >$-thermodynamical expectation value of the copper spin.

Using the equation:

$$\sum < \Psi^{pd,\uparrow}\Psi^{\uparrow,pd} >_k = \sum < \Psi^{pd,\downarrow}\Psi^{\downarrow,pd} >_k \tag{12}$$

in the fast fluctuating regime [9] we have deduced the expression for the uniform spin susceptibility [10]:

$$\chi(\delta,\theta) = \frac{(1+\delta)^2\chi_{pl}(\delta,\theta)}{4\delta + Z(\delta,\theta)} \tag{13}$$

where $\chi_{pl}(\delta,\theta)$ is an ordinary Pauli-Lindhard susceptibility below T_c for the ordinary Fermi liquid, $Z(\delta,\theta)$ is a contribution due to strong electron correlation effects:

$$Z(\delta,\theta) = -\frac{(1+\delta)^2}{4}\sum F_k \left\{ \frac{E_{1k} - E_k^{11}}{E_{1k}}\frac{\partial f(E_{1k})}{\partial E_{1k}} + \right.$$
$$\left. + \frac{E_{1k} + E_k^{11}}{E_{1k}}\frac{\partial f(-E_{1k})}{\partial(-E_{1k})} \right\} \tag{14}$$

where

$$F_k = 2\left(t_k - \frac{t_k < S_i S_j >}{P^2}\right) - \frac{4J_0}{(1+\delta)^2} \tag{15}$$

and

$$E_{1k,2k} = \pm\left[(E_k^{11})^2 + \mid \Delta_k \mid^2\right]^{\frac{1}{2}} \tag{16}$$

where $\Delta_k = \Delta_0(\cos k_x - \cos k_y)$ is a superconducting gap function,

$$E_k^{11} = t_k\left(P + \frac{< S_i S_j >}{P}\right) + \sum_{k_1}\frac{2J(k_1 - k)}{P}\left\langle \Psi^{\uparrow pd}\Psi^{pd\uparrow}\right\rangle_{k_1} - \mu \tag{17}$$

$< S_i S_j >$ is a spin correlation function for the copper neighbors, μ is a chemical potential

In the limit case of the zero gap the formulae (13) agrees with the expression for the spin susceptibility in the normal phase [9], [11]. The interested reader I refer to the paper [10].

On the Fig. 3 ESR experimental results for Gd:$YBa_2Cu_3O_7$ [12] are compared to our numerical calculations. The chemical potential was chosen on 10 meV below Van-Hove singularity (we employ the "hole" picture) in according to the experimental observation [13]. The results fit well the experimental data and yields $2\Delta_0/k_BT_c = 4.87$.

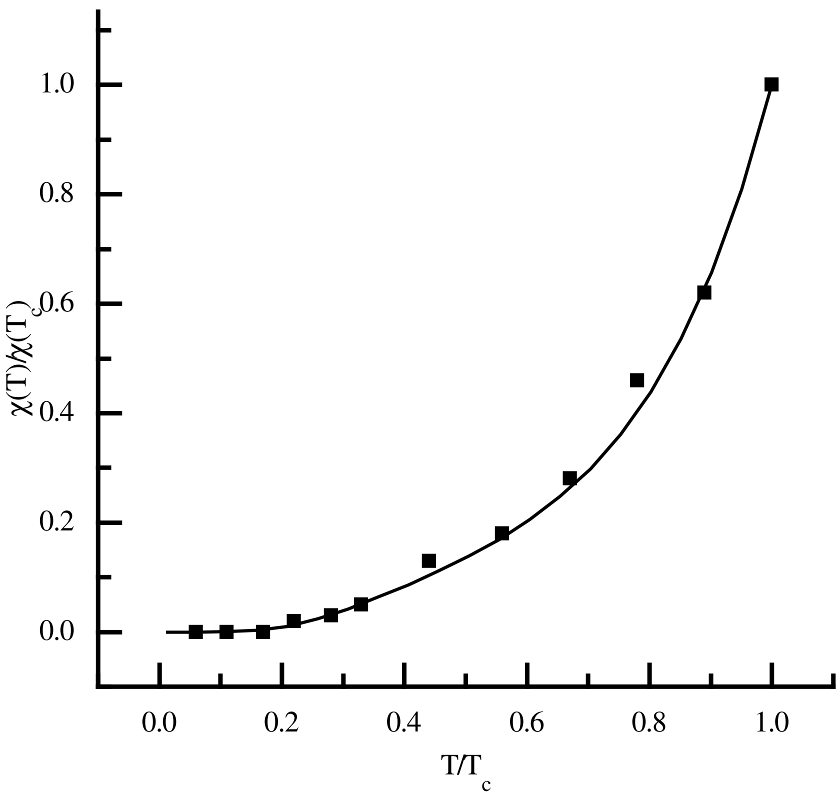

Figure 3: Temperature dependence of the normalized Knight shift for Cu(2) in the plane (magnetic field $\perp$ c axis): experiment, black squares (taken from [12]); theory, straight line.

5 Conclusion.

In this paper, the new expression for the dynamic spin susceptibility for the singlet copper-oxygen band has been analyzed.

i. After calculating the phase diagram we have found that the instability region moves to the low doping regime comparing to pure Fermi-liquid regime.

ii. The behavior of the correlation length and amplitude of the possible approximations of static spin susceptibility is differed. For the gaussian the correlation length practically does not depend on doping but amplitude changes significantly. For the lorentzian the situation is upside down - correlation length slightly decrease with increasing doping albeit amplitude is not altered. A comparison between both approximations leads to conclusion that lorentzian is more favorable for further calculations.

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