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NON-FERMI LIQUID CORRECTION TO UNIFORM SPIN SUSCEPTIBILITY OF SINGLET BAND BELOW T_c

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A new expression for the uniform static spin susceptibility below T_c in singlet band model has been deduced. The formula takes into account strong electron correlation effects. The comparison of the theoretical curve with experimental data yields another value of $2\Delta/k_BT_c$ than in the case of the usual Fermi liquid. In particular, for $YBa_2Cu_3O_7$ the extracted ratio $2\Delta/k_BT_c = 4.87$ and can be interpreted in favor of the superexchange pairing mechanism. © 1998 Elsevier Science Ltd

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1. INTRODUCTION

It is well known that the ratio $2\Delta/k_BT_c$ gives important information about the pairing mechanism in high-T_c cuprates. One of the possible way to obtain this value is the analysis of Knight shift data or the uniform static spin susceptibility below T_c. Up to now the analysis was based on the expression for the ordinary Fermi liquid susceptibility [1]. However, as it was pointed out by many authors [2, 3] (and references therein) strong electron correlation effects play a significant role in cuprates. Therefore, the calculation of the non-Fermi liquid correction to the uniform spin susceptibility would be very desirable.

In this communication the new expression for the static spin susceptibility below T_c has been deduced with taking into account strong electron correlation effects or non-Fermi liquid behavior. We compare our result to Pauli susceptibility and find out the essential differences between them. Then we fit the experimental data for $YBa_2Cu_3O_7$ and extract the ratio $2\Delta/k_BT_c$. In conclusion we discuss the possible pairing mechanism which can provide the extracted ratio.

2. MODEL HAMILTONIAN

We start from the standard singlet copper–oxygen band model

$$H_0 = \sum t_{ij}^{pp}\Psi_i^{pd,\sigma}\Psi_j^{\sigma,pd} - \sum J_{ij}\left[(\mathbf{S}_i\mathbf{S}_j) - \frac{n_in_j}{4}\right]. \tag{1}$$

Here $\Psi_i^{pd,\sigma}$, $\Psi_j^{\sigma,pd}$ are quasiparticle Hubbard-like operators for the copper–oxygen singlet band [4, 5], t_{ij}^{pp} is a hopping integral between copper i and j sites of the layer, J_{ij} is the superexchange constant coupling between copper spins, n_i is a number of the copper spins and $\mathbf{S}_i$ is a spin operator.

For simplicity we omit the coupling of the copper–oxygen singlet band with the copper band and restrict ourselves to one band model. Using the decoupling procedure for Green's functions [6] the energy dispersion can be deduced in the following way

$$E_{1k,2k} = \pm [E_k^{11} + |G_k|^2]^{1/2}, \tag{2}$$

where G_k is a superconducting gap function and

$$E_k^{11} = t_k\left(P + \frac{\langle S_iS_j\rangle}{P}\right) - \sum_{k_1}\frac{2J(k_1-k)}{P}\langle\Psi^{pd,\uparrow}\Psi^{\uparrow,pd}\rangle_{k_1} - \mu, \tag{3}$$

$\langle S_iS_j\rangle$ is a spin correlation function for the copper neighbors, μ is a chemical potential, $P = (1+\delta)/2$ is a thermodynamic average of the anticommutator $[\Psi_k^{pd,\sigma}, \Psi_k^{\sigma,pd}]_+$, δ is a doping parameter, t_k are hopping integrals

$$t_k = 2t_1(\cos k_x + \cos k_y) + 4t_2\cos k_x\cos k_y + 2t_3(\cos 2k_x + \cos 2k_y), \tag{4}$$

with t_1, t_2 and t_3 referring to hopping to the first, second and third Cu neighbors, respectively. The largest parameter, t_1, can be estimated as 70 meV from the band width which was measured by photoemission spectroscopy [7]. The choice of t_2 and t_3 is dictated by the agreement with the experimental photoemission data. According to [7] we can expect $t_2 - t_3$ to be 3 to 5 meV at most. For simplicity, we assume $t_2 = 0$ and $t_3 = 5$ meV.

$$J(k) = J_0(\cos k_x + \cos k_y), \tag{5}$$

where J_0 is the parameter of the spin–spin coupling between Cu(2) spins in the plane.

First, let us discuss the last item in equation (3). Substituting the expression for the average $\langle \Psi^{pd,\uparrow} \Psi^{\uparrow,pd} \rangle_k$, this term can be written as $A_k = A_0(\cos k_x + \cos k_y)$ where A_0 is determined by

$$A_0 = \frac{J_0}{N} \sum_k \frac{\cos k_x}{2E_{1k}} [(E_{1k} - E_k^{11}) f(E_{1k}) + (E_{1k} + E_k^{11}) f(-E_{1k})], \tag{6}$$

where $f(E_{1k})$ is Fermi function. According to our numerical calculation we have found that $A_0 = -13$ meV for optimal doping. Thus this correction slightly reduces the hopping integral t_1 only.

The chemical potential is calculated self-consistently by solving the equation

$$\delta = \frac{1}{N} \sum_k \langle \Psi^{pd,\downarrow} \Psi^{\downarrow,pd} \rangle_k, \tag{7}$$

which yields $\mu = -8$ meV for the half-filling ($\delta = 0.33$).

Let us consider now the equation for the gap function:

$$G_k = \frac{1}{N} \sum_{k_1} \frac{2J(k_1 - k) G_{k_1}}{E_{k_1}} \{ f(E_{1k_1}) - f(-E_{1k_1}) \}. \tag{8}$$

The solution of the equation (8) was found as

$$G_k = \Delta(\cos k_x - \cos k_y), \tag{9}$$

where Δ and T_c were calculated self-consistently from the equation

$$1 = \frac{J_0}{N} \sum_k \frac{\cos^2 k_x - \cos k_x \cos k_y}{E_{1k}} \{ f(E_{1k}) - f(-E_{1k}) \}. \tag{10}$$

In fact, our consideration is equivalent to the resonating-valence-bond theory [2]. We do not separate fermionic operators on spinons and holons as in paper [8] due to our restriction to the optimal doping and overdoped regimes only.

The choice of the numerical value for J_0 is based on the following observations. Recent neutron scattering experiments [9] in undoped $YBa_2Cu_3O_{6.15}$ determined $J_0 = 125$ meV. With doping, J_0 decreases due to the ferromagnetic RKKY coupling via carriers. For instance, the inelastic neutron scattering experiments for $YBa_2Cu_3O_{6+x}$, where $0.65 < x < 0.92$, have been successfully explained [10] with $J_0 = 25$ meV. From this broad range of J_0 values, we have chosen $J_0 = 80$ meV in order to get the superconducting transition temperature $T_c = 90$ K for $\delta = 0.33$.

3. UNIFORM SPIN SUSCEPTIBILITY BELOW T_c

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

$$H = H_0 - g\beta H_z \frac{1}{2} \sum (\Psi_i^{\uparrow,\uparrow} - \Psi_i^{\downarrow,\downarrow}). \tag{11}$$

Besides we take into account that anticommutators depend on the magnetization as

$$P^{\uparrow,\downarrow} = P \pm \langle s_z \rangle \tag{12}$$

where $\langle s_z \rangle$ is the thermodynamic expectation value of the copper spin.

Using the equation

$$N\delta = \sum_k \langle \Psi^{pd,\uparrow} \Psi^{\uparrow,pd} \rangle_k = \sum_k \langle \Psi^{pd,\downarrow} \Psi^{\downarrow,pd} \rangle_k \tag{13}$$

in the fast fluctuating regime [11] we have deduced the following expression for the uniform spin susceptibility

$$\chi(\delta, \theta) = \frac{(1+\delta)^2 \chi_{pl}(\delta, \theta)}{4\delta + Z(\delta, \theta)}, \tag{14}$$

where $\chi_{pl}(\delta, \theta)$ is the usual Pauli–Lindhard susceptibility which is given by

$$\chi_{pl}(\delta, \theta) = -\frac{1}{4N}(g\beta)^2 \times \sum_k \left[\frac{E_{1k} - E_k^{11}}{E_{1k}} \frac{\partial f(E_{1k})}{\partial E_{1k}} + \frac{E_{1k} + E_k^{11}}{E_{1k}} \frac{\partial f(-E_{1k})}{\partial(-E_{1k})} \right]. \tag{15}$$

The other terms in equation (14) have appeared due to strong electron correlation effects or non-Fermi liquid behavior of the singlet band. $Z(\delta, \theta)$ function is determined by

$$Z(\delta, \theta) = -\frac{(1+\delta)^2}{4N} \sum_k F_k \times \left[\frac{E_{1k} - E_k^{11}}{E_{1k}} \frac{\partial f(E_{1k})}{\partial E_{1k}} + \frac{E_{1k} + E_k^{11}}{E_{1k}} \frac{\partial f(-E_{1k})}{\partial(-E_{1k})} \right], \tag{16}$$

where

$$F_k = 2t_k \left(1 - \frac{\langle S_i S_j \rangle}{P^2} \right) - \frac{4J_0}{(1+\delta)^2}. \tag{17}$$

As we see from equations (14), (16) and (17) the uniform spin susceptibility expression for the singlet band does

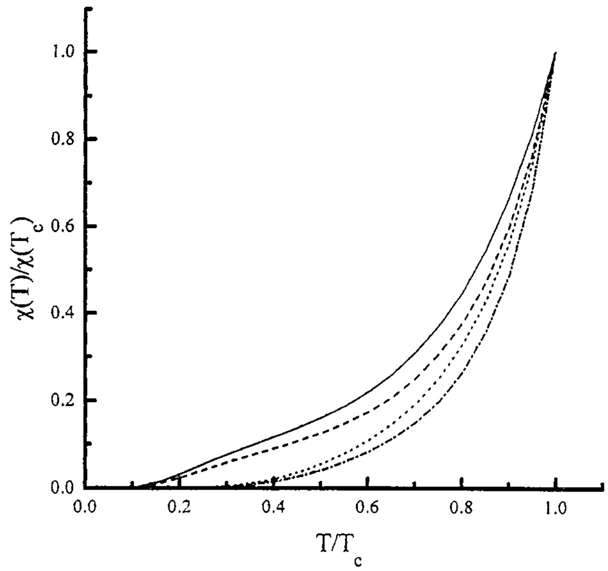

Fig. 1. Temperature dependence of the normalized uniform static spin susceptibility (14) and Pauli susceptibility (15) below T_c for the optimal doping regime $\delta = 0.33$, $2\Delta/k_BT_c = 4.87$ [straight line, (14); dashed line, (15)] and overdoped regime $\delta = 0.46$, $2\Delta/k_BT_c = 5.93$ [dotted line, (14); dashed–dotted, (15)].

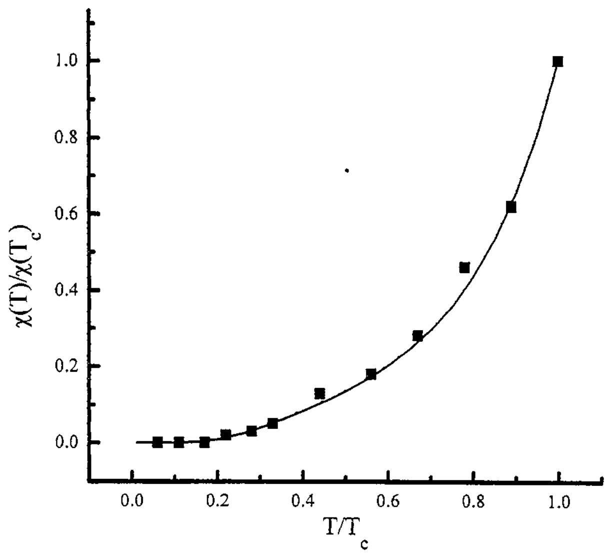

Fig. 2. Temperature dependence of the normalized Knight shift for Cu(2) in the plane (magnetic field $\perp$**c**): experiment, black squares (taken from [15]); theory, straight line.

not look like the usual Fermi liquid variant as it was widely believed [1]. The denominator in equation (14) is not reduced to Stoner like factor. We note that F_k can not be factored out from the sum. $Z(\delta, \theta)$ function strongly depends on doping level because of F_k at the Fermi level is mainly important.

In the limit case of zero gap the formula (14) agrees with the expression for the spin susceptibility in the normal phase which was obtained before [11, 12]. In Fig. 1 we present our calculated curves of the normalized spin susceptibility (14) and Pauli-Lindhard susceptibility for the optimal doping and the overdoped regimes. The values of the gap and T_c were calculated self-consistently from the equations (7) and (10). In order to make clear the role of the strong correlation effect we have drawn the Pauli susceptibility for comparison. The most important point is that this effect changes the extracted ratio $2\Delta/k_BT_c$ (where k_B is a Boltzmann constant) significantly with respect to the value which can be obtained by using Pauli-Lindhard susceptibility.

The first measurements of the static spin susceptibility below T_c for $YBa_2Cu_3O_7$ were carried out by authors [13, 14] using NMR method. Recently in [15] it has been measured with great accuracy using ESR method. In Fig. 2 we compare the result of our numerical calculation with the experimental data for $YBa_2Cu_3O_7$ [15]. The chemical potential was chosen 10 meV below Van-Hove singularity (we employ the "hole" picture) according to the experimental observation [7]. As one can see the results coincide well with the experimental data. $2\Delta/k_BT_c = 4.87$ and $T_c = 92$ K calculated from equation (8) really fit the experimental data and therefore our model used for the gap and the susceptibility is mutually self-consistent.

4. CONCLUSIVE REMARKS

In this communication, we have obtained the new expression for the static spin susceptibility for the singlet band model below superconducting transition temperature T_c. For the first time we were taking into account the strong electron correlation effect or non-Fermi liquid behavior of the uniform susceptibility. We have shown that this effect is important for extracting the effective ratio $2\Delta/k_BT_c$ from the experimental data. Assuming the superexchange pairing mechanism our numerical calculations for $YBa_2Cu_3O_7$ fit well the experimental Knight shift data.

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