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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

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

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

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

where G_k is a superconducting gap function and

$$E_k^{11} = t_k\left(P + \frac{\langle S_iS_j\rangle}{P}\right) - \sum_{k_1}\frac{2J(k_1-k)}{P}\langle\Psi^{pd,1}\Psi^{1,pd}\rangle_{k_1} - \mu, \quad (3)$$

$\langle S_iS_j\rangle$ 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

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

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