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# Low energy excitation spectrum and Cu(2) spin-lattice relaxation from the singlet correlated band in $YBa_2Cu_4O_8$

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We report the low energy excitation spectrum and the spin-lattice relaxation for the planar Cu of the high $T_c$ superconductor $YBa_2Cu_4O_8$. We use a three band Hubbard model. Its singlet band exhibits a well-established saddle point of strong copper character. The susceptibility is governed by a Fermi-liquid like contribution coming from thermally activated copper holes in this saddle point. By comparing our calculated and experimental results, we can conclude that in $YBa_2Cu_4O_8$ the low energy physics is determined by a high density of charge excitations in the singlet impurity band together with spin excitations in the lower Hubbard band.

## 1. INTRODUCTION

Typical properties of the special quantum fluid in the high-$T_c$ superconductors manifest themselves in low lying excitations which can be investigated via the nuclear magnetic resonance. We have studied intensively the underdoped high-$T_c$ superconductor $YBa_2Cu_4O_8$ in particular the temperature dependence and anisotropy of the spin-lattice relaxation for Cu(2) [1]. These and corresponding data are summarized in a recent review [2].

Our present theoretical interpretation of these data starts from the point, that copper holes are single occupied because of the strong intra-atomic repulsion of two copper holes [3]. When doping, these holes interact via magnetic exchange strongly with doped oxygen extra holes leading to Zhang-Rice singlets [4]. Because of the strong Kondo-like exchange, as compared to the oxygen band width, this exchange gives rise to a new singlet correlated band which separates off from the oxygen band [5]. It corresponds to the motion of singlets through the antiferromagnetic (AF) background of the localized copper spins in the lower Hubbard band. Our experimental NMR data [1,2] are in good agreement with the temperature dependence of the Cu(2) spin-lattice relaxation derived from an idealization of the singlet band. There are two contributions to the susceptibility, namely one from thermally activated copper holes in the van Hove singularity of the singlet band and another from the AF background.

## 2. MODEL HAMILTONIAN FOR THE SINGLET DISPERSION

We start from a Hubbard Hamiltonian for one copper-oxygen plane in the hole picture with the vacuum state given by the electronic occupation $|d^{10}p^6>$. In order to investigate excitations on the transport energy scale we use the smallest possible subspace of low-lying states. Because the largest interaction energy in the system is the Coulomb repulsion $U_{dd}$ between two holes at the same copper site [6] we project out the double occupation of copper states by the Hubbard operators

$$X_i^{\sigma 0} = d_{i\sigma}^{+}(1 - n_{i\bar{\sigma}}), \qquad n_{i\bar{\sigma}} = d_{i\bar{\sigma}}^{+} d_{i\bar{\sigma}}.$$

Here $d_{i\sigma}^{+}$ is a Fermi operator, that creates at the site $i$ a local $d_{x^2-y^2}$ hole with spin $\sigma$ and energy $\varepsilon_d$. The local $p_{x(y)}$ states with energy $\varepsilon_p$ at an oxygen site $j$ are described by usual Fermi operators $p_{j\sigma}^{+}$. Within this subspace the Hubbard-Hamiltonian is given by

$$\begin{aligned} H \;=\; & \varepsilon_d \sum_{i\sigma} X_i^{\sigma\sigma} + \varepsilon_p \sum_{j\sigma} p_{j\sigma}^{+} p_{j\sigma} \\ & + \sum_{ij\sigma} t_{ij}^{pd} (X_i^{\sigma 0} p_{j\sigma} + p_{j\sigma}^{+} X_i^{0\sigma}) \\ & + \sum_{jj'\sigma} t_{jj'}^{pp} p_{j\sigma}^{+} p_{j'\sigma} + J_K \sum_i Z_i^{\psi 0} Z_i^{0\psi}. \end{aligned}$$

The last term in the third line incorporates two-step charge transfers of two holes, causing a Kondo-like exchange $J_K$ between them that fa-


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