63Cu and 17O NMR Studies on the Magnetic and Superconducting Properties of YBa2Cu3O7−y

M. Takigawa

IBM T. J. Watson Research Center, Yorktown Heights, NY, USA

Received April 21, 1992

Abstract. Results of 63Cu and 17O NMR experiments in YBa2Cu3O7 and YBa2Cu3O6.63 are reviewed. The normal state data revealed two important aspects of the magnetic properties of these materials, namely, the temperature dependent antiferromagnetic Cu spin correlations and the spin gap behavior, the latter being observed in the reduced oxygen material. These features appear to be the general properties of many high-Tc cuprates. Anomalous temperature dependence of the anisotropy of the Cu relaxation rate was found in the superconducting state of YBa2Cu3O7, which can be explained by a d-wave pairing model.

1. Introduction

Nuclear Magnetic Resonance (NMR) experiments have provided valuable microscopic information on the magnetic and superconducting properties of high temperature superconductors [1]. In this note, we briefly summarize our NMR results on the planar Cu and O sites in YBa2Cu3O7−y [2] and the current understanding of the magnetic properties of cuprates. The paper is organized as follows. In Section 2, we will describe the one component ionic model of the hyperfine interaction at the planar Cu and O sites. In Section 3, results of the nuclear relaxation rates in the normal state are discussed, which indicate the persistence of the short range antiferromagnetic (AF) correlations into the superconducting materials and the formation of spin gap above Tc in the reduced oxygen material. Some anomalous features of the nuclear relaxation rate in the superconducting state of YBa2Cu3O7 are discussed in Section 4, followed by a few remarks.
2. Hyperfine Interaction and Knight Shift

It is important to have detailed knowledge of the hyperfine interaction for unambiguous interpretation of NMR results. Fortunately, in YBa$_2$Cu$_3$O$_{7-y}$, Knight shift measurements by many groups at various atomic sites allowed us to understand the hyperfine interaction in detail. Although the atomic states relevant to the low energy excitations in CuO$_2$ planes are Cu-3$d_x^2$-$y^2$ and O-2$p_o$ states, Cu-4$s$ and O-2$s$ states contribute significantly to the hyperfine interaction as demonstrated by the large positive isotropic Knight shift at the planar Cu and O sites [3–5]. Since the spin density on these s-states results from weak hybridization with the Cu-d or O-p states on the neighboring sites, the Knight shift results imply the hyperfine coupling between Cu or O nuclei and the electronic spin degrees of freedom on adjacent sites, which is called the transferred hyperfine interaction.

Soon after the discovery of the high-$T_c$ superconductors, it was indicated from high energy spectroscopic experiments that holes doped into the antiferromagnetic insulator go mainly into the O-2$p$ states. It has been a controversial issue whether the Cu-d holes and doped holes have distinct spin degrees of freedom (two spin fluid) or they are strongly hybridized to form a single spin liquid in the superconducting materials (single spin fluid).

All the NMR data obtained so far are consistent with the single spin fluid model [6–8]. In particular, the Knight shift results in the $T_c = 60$ K YBa$_2$Cu$_3$O$_{6.63}$ material support this picture. Fig. 1 shows the temperature dependence of various Knight shift components at Cu($^{63}K$) and O($^{17}K$) sites [7]. The Knight shift is strongly temperature dependent above $T_c$. This is in contrast to the $T_c = 90$ K YBa$_2$Cu$_3$O$_{6}$ material, where the Knight shift is temperature independent [3–5]. However, all shift components show the identical temperature dependence after a constant orbital shift is subtracted. It should be noted that the anisotropic (axial) part of the O Knight shift, $^{17}K_{ax} = (^{17}K_a - ^{17}K_b)/3$, exclusively probes the spin density on O-p states, since the s-electrons contribute only to the isotropic Knight shift. Likewise anisotropic part of the Cu Knight shift, $^{63}K_{ax} = (^{63}K_{ab} - ^{63}K_c)/3$, probes the spin on the Cu-d states. Since $^{63}K_c$ is temperature independent, implying that the spin part of $^{63}K_c$ is zero, the proportionality of $^{63}K_{ab}$ and $^{17}K_{ax}$ demonstrates the identical temperature dependence of the spin susceptibilities of Cu-d and O-p holes.

It was shown by Mila and Rice [9] that a simple ionic model of the hyperfine interaction explains the anisotropy of the Knight shift and the relaxation rate at Cu sites in YBa$_2$Cu$_3$O$_y$. This model includes the coupling of Cu nuclei to the electronic spins both on the same sites and on the nearest neighbor Cu sites. It is straightforward to extend the model to include the O sites,

$$\mathcal{H} = ^{63}I \cdot (A \cdot S_0 + B \sum_{i=1}^4 S_i) + ^{17}I \cdot C \cdot \sum_{j=1}^2 S_j,$$

(1)