A model for magnetic relaxation of nuclear spins of Cu(2) in $YBa_2Cu_3O_{7-y}$

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A model for the nuclear spin relaxation of Cu(2) nuclei in $YBa_2Cu_3O_{7-y}$ is proposed. This model explains the experimental NQR data for the temperature dependences $1/T_1$ and $1/T_2$ at $T > T_c$ and $T < T_c$.

The standard BCS theory does not explain several experimental data on high-T_c superconductors, in particular, the temperature dependence of the velocity of the longitudinal relaxation ($1/T_1$) and the transverse relaxation ($1/T_2$) of the nuclear spins of copper.

In the present letter we report the results of measurements of the nuclear-magnetic-relaxation rates of Cu(2) in $YBa_2Cu_3O_{7-y}$ at the NQR frequency of 31.5 MHz and we propose a model which explains the $1/T_1$ and $1/T_2$ behavior in the temperature interval 30–300 K. We will base our discussion on the assumption that $YBa_2Cu_3O_{7-y}$ has two types of current carrier: conduction electrons, which are situated in the copper sites in the upper Hubbard subband, and holes, which are situated in the oxygen sublattice. The conduction electrons of copper are most closely related to the nuclear spins through the anisotropic hyperfine interaction. We assume that only the oxygen holes are paired. Two of these carrier subsystems are related because of the charge transfer from oxygen to copper (hybridization).

The effective Hamiltonian of the upper-subband carriers, which are most closely related to the nuclear spins of copper, can be written as follows after eliminating the terms which are attributable to the hybridization:

$$\mathcal{H} = \Sigma \epsilon_k a^+_{k\sigma} a_{k\sigma} - \Sigma \Delta_\sigma \left(\frac{\epsilon_k}{2\epsilon_k + \epsilon^0_k} \right) (a^+_{k\sigma} a^+_{-k-\sigma} + \text{H.c.}). \tag{1}$$

Here ϵ^0_k is the energy of the lower (oxygen) zone, which is reckoned from the bottom of the upper band ϵ_k, and $\Delta(T) = (\Delta_\uparrow - \Delta_\downarrow)$ is the gap in the spectrum of oxygen holes. This gap determines T_c.

For simplicity, we assume that the density of the energy states in the band is constant. The chemical potential of the electron system can then be described by

$$n = \frac{1}{2W} \int_0^W \left(1 - \frac{\epsilon - \mu}{\sqrt{(\epsilon-\mu)^2 + \alpha^2\epsilon^2}} \tanh \frac{\sqrt{(\epsilon-\mu)^2 + \alpha^2\epsilon^2}}{2T}\right) d\epsilon , \tag{2}$$

where n is the number of electrons per Cu(2) site in the band, W is the width of the energy band, and $\alpha = \Delta/\epsilon^0_k$. It follows from (2) that at moderately large values of W the chemical potential may be both positive and negative.

Let us consider the case in which $\mu < 0$. A calculation of the longitudinal and transverse relaxation rates of the nuclear spins, which are associated with the indicated subsystem of conduction electrons by the hyperfine interaction of the type

$$\mathcal{H}_{\text{HI}} = \frac{1}{2N} I_z A_\parallel \sum_{k,k'} (a^+_{k\uparrow} a_{k'\uparrow} - a^+_{k\downarrow} a_{k'\downarrow}) + \frac{A_\perp}{2N} I_- \sum_{k,k'} a^+_{k\uparrow} a_{k'\downarrow} + \frac{A_\perp}{2N} I_+ \sum_{k,k'} a^+_{k\downarrow} a_{k'\uparrow} , \tag{3}$$

where $A_\parallel$ and $A_\perp$ are the hyperfine interaction constants, and N is the number of Cu(2) sites, gives the result

$$\frac{1}{T_1} = \frac{3\pi T}{2\hbar} \left(\frac{A_\perp \delta}{2T\tilde{W}}\right)^2 \int_{-\mu/2T}^{\sqrt{(\tilde{W}-\tilde{\mu})^2 + \delta^2}/2T} \frac{x^2 dx}{[x^2 - (\delta/2T)^2]\cosh^2 x} , \tag{4}$$

$$\frac{1}{T_2} = \frac{(A^2_\parallel + A^2_\perp)}{2A^2_\perp} \frac{1}{T_1} + \frac{1}{T_{2d}} . \tag{5}$$

Here $\tilde{\mu} = \mu/\sqrt{1+\alpha^2}$, $\delta = \alpha\tilde{\mu}$, $\tilde{W} = W\sqrt{1+\alpha^2}$, and $1/T_{2d}$ is the transverse relaxation rate which is governed by the dipole-dipole interaction of nuclei.[1] The asymmetry parameter of the electric field gradient of the Cu(2) nuclei is assumed to be zero. As can be seen from (4) and (5), the temperature dependence of the relaxation rate differs considerably from that predicted by the BCS model.[2] In contrast with the BCS

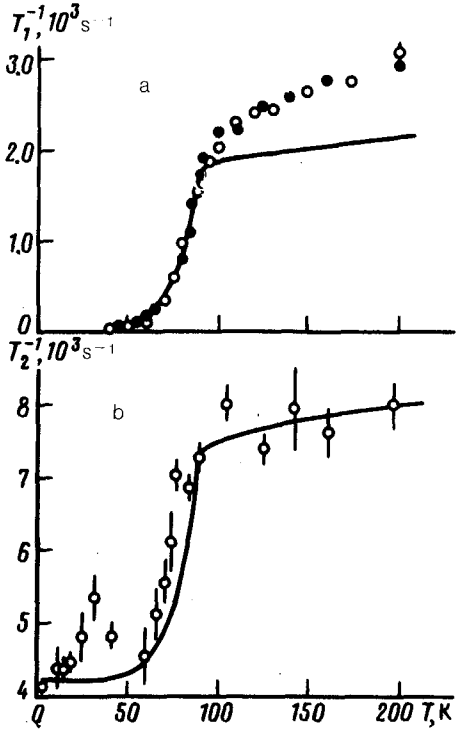

FIG. 1. Temperature dependence of the magnetic relaxation rates of ^{63}Cu(2) nuclei in $YBa_2Cu_3O_{7-y}$ at the frequency 31.5 MHz. a—$1/T_1$, ●—data taken from Ref. 4, $y = 0$; ○—our data, $y = 0.05 \pm 0.05$; b—$1/T_2$, ○—data taken from Ref. 1, $y \approx 0.1$; solid lines—calculation based on Eqs. (5) and (6) with $1/T_{2d} = 4.2 \times 10^3$ s^{-1} (Ref. 1).

model, the relaxation rate in it does not accelerate at $T \sim T_c$. In our model of this type, acceleration can in principle occur at $\mu > 0$.

Another distinguishing feature of our model is the manner in which the relaxation rates behave at high temperatures; in particular, at $T > T_c$ we have

$$\frac{1}{T_1} = \frac{3\pi A_\perp^2 T}{2\hbar W^2} \cdot \frac{\left[\exp\left(\frac{nW}{T}\right) - 1\right]\left[\exp\left(\frac{(1-n)W}{T}\right) - 1\right]}{\exp\left(\frac{W}{T}\right) - 1}. \qquad (6)$$

The transverse relaxation rate is determined by expression like (5). As can be seen from (6), at high temperature ($T \gg nW$) the relaxation rates do not obey the Corringa law and depend only weakly on the temperature. The solid lines in Fig. 1 represent the results of numerical calculations of $1/T_1$ and $1/T_2$ for the following parameter values: $|A_\perp| = 63 \times 10^{-4}$ cm^{-1}, $|A_\parallel| = 100 \times 10^{-4}$ cm^{-1} (Refs. 3 and 4), $2\Delta(0) = 3.9T_c$, $\epsilon^0 = 300$ K, $W = 1580$ K, and $n = 0.039$. We see that the results of the calculations are in agreement with the experimental data. A slight difference at high temperatures can be attributed to thermal contraction of W.

We can see from the proposed model that the measurements of the temperature dependence of the time T_1 for copper nuclei, which were carried out specially to

determine the size of the gap Δ, should be treated with caution, because at low temperatures ($T < 40$ K) the relaxation rate [cf. Eq. (4)]

$$1/T_1 \approx (3A_\perp^2 \pi / \hbar W^2)\, T \exp(-|\mu| / T)$$

depends on the chemical potential μ, rather than on Δ.

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