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MICROSCOPIC CALCULATIONS OF THE NMR RELAXATION RATE FOR HIGH TEMPERATURE SUPERCONDUCTORS.

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The calculations of the NMR relaxation rate were carried out using the electronic structure obtained by the LMTO method both for normal and for superconducting states. Some types of superconducting pairing were considered. Values and behavior of the relaxation rate are different on different sites due to the interference between angular dependencies of the energy gap and the matrix elements.

1. INTRODUCTION

The measurements of the nuclear magnetic relaxation rate $1/T_1$ is one of most reliable methods of the investigation of low-energy electronic excitations and can play an important role in understanding of superconductivity in high temperature superconductors. Numerous experiments give us an ambiguous information about the temperature dependencies of the relaxation rate and absence or presence of a hump below T_c. Nevertheless all measurements give large values of $1/T_1$ at $T=T_c$ exceeding simple estimations obtained in ref.7 by a factor ≈40.

In this paper we present the microscopic calculations of $1/T_1$ for the $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$ superconductors based on self-consistent band structure calculations assuming the superconducting pairing with different symmetries (s- and d-pairings). This method give a good agreement with experimental data for transition metals. The band structure,electron wave functions,matrix elements and Fermi surface calculations were carried out by the LMTO method.

2. NORMAL STATE.

The nuclear spin-lattice relaxation rate $1/T_1$ is the sum of several contributions corresponding to following interactions: 1) Fermi-contact one, 2) the interactions with orbital moments, 3) the spin-dipolar interaction. These contributions and total value of $1/T_1$ at T=60 K for different atoms in $La_{2-x}Sr_xCuO_4$ are shown in Tab.1. We can see that the main contribution to total relaxation rate is due to the Fermi-contact interaction.

Table 1 T=60 K

	X	$(\frac{1}{T1})_F$	$(\frac{1}{T1})_D$	$(\frac{1}{T1})_O$	$(\frac{1}{T1})_{FD}$	$(\frac{1}{T1})_{tot}$	$(\frac{1}{T1})_{exp}$
La	0.15	9.18	0.0267	0.0253	−0.1	9.13	4.5 [1]
	0.20	5.40	0.0161	0.0223	−0.584	5.38	6.2 [2]
Cu	0.15	795.0	108.0	1.5	−74.5	830.0	4800 [3]
	0.20	379.0	67.0	1.0	−39.0	408.0	—
O1	0.15	1.33	0.346	0.0478	$<10^{-6}$	1.72	—
	0.20	0.828	0.226	0.0339	$<10^{-6}$	1.088	—

Table 2 T=100 K

	$\left(\frac{1}{T1}\right)_F$	$\left(\frac{1}{T1}\right)_D$	$\left(\frac{1}{T1}\right)_O$	$\left(\frac{1}{T1}\right)_{FD}$	$\left(\frac{1}{T1}\right)_{tot}$	$\left(\frac{1}{T1}\right)_{exp}$
Cu1	309.0	34.5	721.0	−31.5	1033.0	2000 [4]
Cu2	126.0	41.4	121.03	−0.4	288.0	2200 [4]
O1	1.650	0.132	0.239	$<10^{-6}$	2.021	1 [5]
O2	1.270	0.235	0.208	$<10^{-6}$	1.713	6 [6]

For $YBa_2Cu_3O_7$ the differ situation takes place. Tab.2 shows that the main contribution to $1/T_1$ is determined by the orbital terms for Cu1 and Cu2 sites. From Tab.1 and 2 we can conclude that the band structure calculations allows us to obtain the values of the relaxation rate closed to the experimental ones.

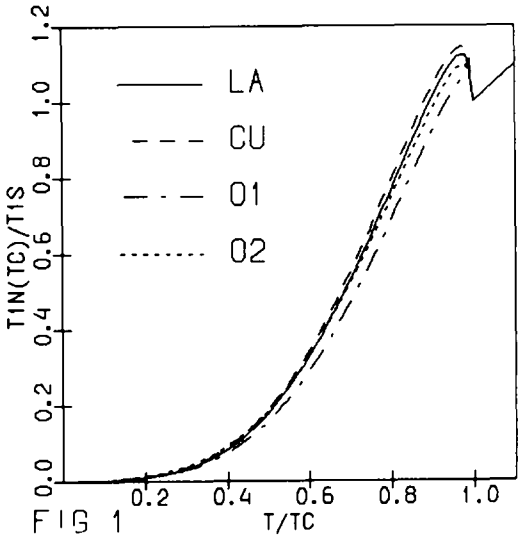

FIG 1

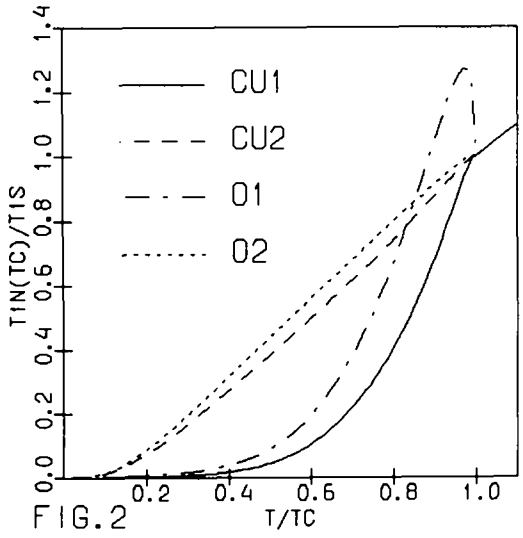

FIG.2

3. SUPERCONDUCTING STATE.

The calculations of $1/T_1$ in superconducting state were carried out by using the following types of pairing: 1) the conventional s-pairing $\Delta(k)$=const, 2) the extended s*-pairing $\Delta(k)=\Delta(\cos k_x+\cos k_y+c)$, 3) d-pairing $\Delta(k)=\Delta(\cos k_x-\cos k_y)$. Fig.1 and 2 show the temperature dependence of $1/T_1$ in the superconducting state for the case of s*-pairing. In this case the energy gap has zeros on the Fermi surface. This leads to reducing of the hump below T_c and to the power dependence at low T. We can see that the height of hump magnitudes are different on the different atoms because of the interference between angular dependencies of the energy gap and the matrix elements on each site.

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