Calculation of the Transverse Nuclear Relaxation Rate for $YBa_2Cu_3O_7$ in the Superconducting State

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The importance of the electronic spin fluctuations in the CuO_2 planes in the theory of the transverse nuclear relaxation for $YBa_2Cu_3O_7$ has been demonstrated by Pennington and Slichter. We present the predictions of an RPA-like theory for the transverse nuclear relaxation time, τ, in the superconducting state. s- and d-wave gap symmetries yield distinctively different results for τ^{-1}; for an s-wave gap τ^{-1} decays rapidly below T_c, while for a d-wave gap it remains nearly constant. Measurements of τ^{-1} below T_c could provide valuable information about the symmetry of the superconducting state. Results for the temperature dependence of τ^{-1} in the normal state are also given.

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Weak-coupling theories [1–4] of the spin fluctuations in high-temperature superconductors have had considerable success explaining the normal-state results for the longitudinal nuclear relaxation rate, T_1^{-1}, of the Cu(2) and O(2,3) nuclei in $YBa_2Cu_3O_7$. Recently, Pennington and Slichter [5] have shown that the indirect nuclear spin-spin coupling mediated by these spin fluctuations, and determined by the static magnetic susceptibility $\chi(\mathbf{q})$, gives a normal-state nuclear transverse relaxation time τ in reasonable agreement with experiment [6]. Here we extend this to the superconducting state using an RPA form for the electronic spin susceptibility $\chi(\mathbf{q})$ in which the irreducible part of the susceptibility, $\chi_0(\mathbf{q})$, is replaced by the BCS expression. Within this framework we examine the temperature dependence of τ^{-1} for superconducting states with s- and d-wave gaps. For an s-wave gap, $\chi(\mathbf{q})$ is suppressed for both $\mathbf{q}\sim 0$ and $\mathbf{q}\sim(\pi,\pi)$. However, for a d-wave gap $\chi(\mathbf{q})$ is suppressed for $\mathbf{q}\sim 0$, but not for $\mathbf{q}\sim(\pi,\pi)$ because of the nodes of the gap on the Fermi surface. Since the dominant contributions to the indirect nuclear spin-spin interaction arise from the antiferromagnetic $\mathbf{q}\sim(\pi,\pi)$ contribution of $\chi(\mathbf{q})$, τ^{-1} decreases rapidly below T_c for an s-wave gap and has little T dependence for a d-wave gap. Thus an experimental determination of τ^{-1} below T_c could help distinguish the symmetry of the superconducting state. We also present results for the T dependence of τ^{-1} in the normal state.

To model the Cu(2) spin fluctuations, we will use an RPA-like form for $\chi(\mathbf{q})$:

$$\chi(\mathbf{q})=\frac{\chi_0(\mathbf{q})}{1-U\chi_0(\mathbf{q})}. \tag{1}$$

Here U is a renormalized Coulomb interaction which is associated with the on-site $Cu(3d_{x^2-y^2})$ Coulomb interaction. In the normal state, we set

$$\chi_0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}})-f(\varepsilon_{\mathbf{p}})}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}+\mathbf{q}}}, \tag{2}$$

where $\varepsilon_{\mathbf{p}}=-2t[\cos(p_x)+\cos(p_y)]-\mu$, $f(\varepsilon_{\mathbf{p}})=[\exp(\varepsilon_{\mathbf{p}}/T)+1]^{-1}$, and μ is the chemical potential. The chemical potential, which sets the filling $\langle n\rangle=\langle n_\uparrow+n_\downarrow\rangle$, and U are chosen to adjust the strength of the antiferromagnetic fluctuations [7]. While this is clearly a phenomenological approach, it has proved useful in fitting the longitudinal nuclear relaxation rate T_1^{-1} for Cu(2) and O(2,3) nuclei in $YBa_2Cu_3O_7$ in the normal state. In addition, it provides a remarkably good fit to $\chi(\mathbf{q},i\omega_m)$ obtained from Monte Carlo simulations of the Hubbard model [8].

In the superconducting state, we replace $\chi_0(\mathbf{q})$, Eq. (2), with

$$\chi_0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\left\{\frac{1}{2}\left[1+\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}\varepsilon_{\mathbf{p}}+\Delta_{\mathbf{p}+\mathbf{q}}\Delta_{\mathbf{p}}}{E_{\mathbf{p}+\mathbf{q}}E_{\mathbf{p}}}\right]\frac{f(E_{\mathbf{p}+\mathbf{q}})-f(E_{\mathbf{p}})}{E_{\mathbf{p}}-E_{\mathbf{p}+\mathbf{q}}}+\frac{1}{2}\left[1-\frac{\varepsilon_{\mathbf{p}+\mathbf{q}}\varepsilon_{\mathbf{p}}+\Delta_{\mathbf{p}+\mathbf{q}}\Delta_{\mathbf{p}}}{E_{\mathbf{p}+\mathbf{q}}E_{\mathbf{p}}}\right]\frac{1-f(E_{\mathbf{p}+\mathbf{q}})-f(E_{\mathbf{p}})}{E_{\mathbf{p}+\mathbf{q}}+E_{\mathbf{p}}}\right\}. \tag{3}$$

This is just the usual BCS result for the susceptibility, which contains the usual coherence factors, the dispersion relation $E_{\mathbf{p}}=(\varepsilon_{\mathbf{p}}^2+\Delta_{\mathbf{p}}^2)^{1/2}$, and the gap $\Delta_{\mathbf{p}}$. For the gap, we will consider both an s-wave form, $\Delta_{\mathbf{p}}=\Delta_0(T)$, and a d-wave form, $\Delta_{\mathbf{p}}=[\Delta_0(T)/2](\cos p_x-\cos p_y)$. For simplicity we will assume $2\Delta_0(0)=3.52kT_c$ and that $\Delta_0(T)$ has a BCS type of temperature dependence. With $\chi_0(\mathbf{q})$ given by Eq. (3), the $\mathbf{q}\to 0$ limit of Eq. (1) for $\chi(\mathbf{q})$ has the Landau Fermi-liquid form proposed by Leggett [9] for ^3He. We have also used it to discuss the Knight shift and T_1 relaxation times in the superconducting state of $YBa_2Cu_3O_7$ [10].

Given $\chi(\mathbf{q})$, the calculation of the effective coupling between two nuclear spins and the resulting transverse nuclear relaxation time τ proceeds as discussed in Ref. [5]. The hyperfine coupling between a Cu(2) nuclear spin at site $\mathbf{0},\mathbf{I}_0$, and the electronic spins is given by the hyperfine Hamiltonian [11]

$$H_{\mathrm{hf}}=\sum_\alpha A_{\alpha\alpha}I_{0\alpha}S_{0\alpha}+B\sum_{\delta=1}^{4}\mathbf{I}_0\cdot\mathbf{S}_\delta, \tag{4}$$

where $\mathbf{S}_i$ represents the electronic spins. Here $A_{\alpha\alpha}$ is an anisotropic on-site hyperfine coupling and B is an isotropic hyperfine coupling between the nuclear spin and the electronic spins localized on the four neighboring Cu(2)

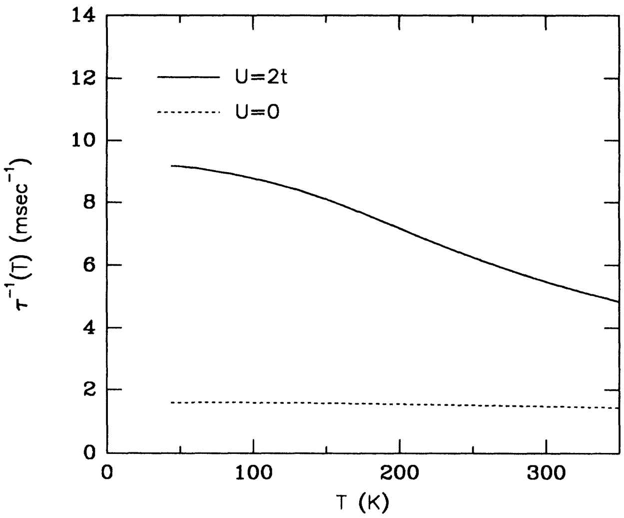

FIG. 1. The temperature dependence of the transverse nuclear relaxation rate for the Cu(2) nuclei with $\mathbf{H}\parallel\mathbf{c}$, τ^{-1}, in the normal state for $U=2t$ (solid line) and for $U=0$ (dotted line).

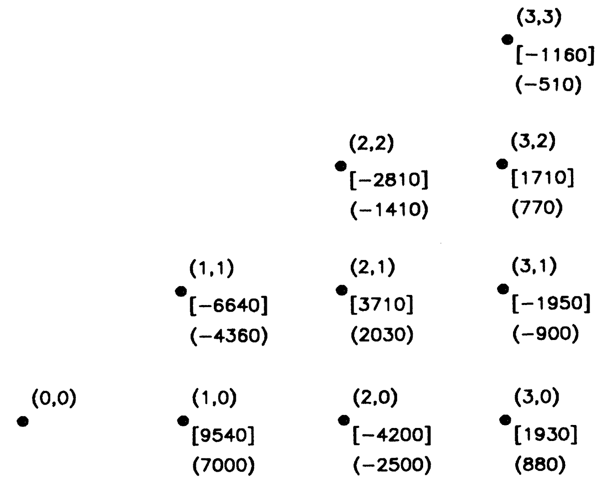

FIG. 2. The z component of the effective coupling, $J_z(\mathbf{x}_i)/\hbar$ (in units of sec^{-1}), between the nuclear spin at the origin (0,0) and the one at site $\mathbf{x}_i=(i_x,i_y)$. Here $J_z(\mathbf{x}_i)$ is shown for $T=100$ K (in square brackets) and $T=300$ K (in parentheses).

atoms. The nuclear spin $\mathbf{I}_0$ polarizes the surrounding electronic spins and, for example, the z component of the induced electronic spin at site $\mathbf{x}_j$ is given by [5]

$$S_z(\mathbf{x}_j) = -\tfrac{1}{2} I_{0z} \left[A_{zz} F(\mathbf{x}_j) + B \sum_{\delta=1}^{4} F(\mathbf{x}_{j+\delta}) \right], \qquad (5)$$

with

$$F(\mathbf{x}_j) = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}_j} \chi(\mathbf{q}). \qquad (6)$$

The polarized spin $\mathbf{S}(\mathbf{x}_j)$ in turn interacts with the nuclear spin $\mathbf{I}_i$ at site $\mathbf{x}_i$, with a hyperfine Hamiltonian similar to that given in Eq. (4). The resulting effective interaction between $\mathbf{I}_0$ and $\mathbf{I}_i$ is $\sum_\alpha J_\alpha(\mathbf{x}_i) I_{0\alpha} I_{i\alpha}$ and the $\alpha=z$ component of $J_\alpha(\mathbf{x}_i)$ is given by

$$J_z(\mathbf{x}_i) = \left[A_{zz} S_z(\mathbf{x}_i) + B \sum_{\delta=1}^{4} S_z(\mathbf{x}_{i+\delta}) \right] \Big/ I_{0z}. \qquad (7)$$

Because of the form of the hyperfine coupling, the other components, $J_x(\mathbf{x}_i)$ and $J_y(\mathbf{x}_i)$, are much smaller than $J_z(\mathbf{x}_i)$. Thus the largest deviation from the usual dipole-dipole relaxation will occur for $\mathbf{H}\parallel\mathbf{c}$. Then, as discussed in Ref. [5], the decay of the NMR spin-echo envelope for the $\frac{1}{2} \rightarrow -\frac{1}{2}$ transition of ^{63}Cu(2) can be approximated by a Gaussian $e^{-t^2/2\tau^2}$ with

$$\frac{\hbar^2}{\tau^2} = \frac{0.69}{8} \sum_i J_z^2(\mathbf{x}_i), \qquad (8)$$

where 0.69 is the natural-abundance fraction of the ^{63}Cu isotope. We perform the sum over i in Eq. (8) for sites up to ten lattice spacings away from the origin, where $J_z(\mathbf{x}_i)$ becomes negligible.

In Fig. 1 the T dependence of τ^{-1} is shown for the interacting ($U=2t$) and the noninteracting ($U=0$) systems in the normal state. While τ^{-1} for the $U=0$ system is nearly constant in the temperature regime of interest, for the interacting system it is enhanced through Eq. (1) and has considerable T dependence. Here we have used an effective bandwidth $W=8t$ of 1 eV and $A_{zz}/\hbar\gamma_n = -4B/\hbar\gamma_n = -328$ kG, where γ_n is the gyromagnetic ratio of ^{63}Cu. We find that $\tau=115$ μsec [12] at $T=100$ K, in good agreement with the experimental value of 130 ± 10 μsec [5]. Figure 2 shows the effective coupling $J_z(\mathbf{x}_i)$ between the nuclear spins $\mathbf{I}_0$ and $\mathbf{I}_i$ for a

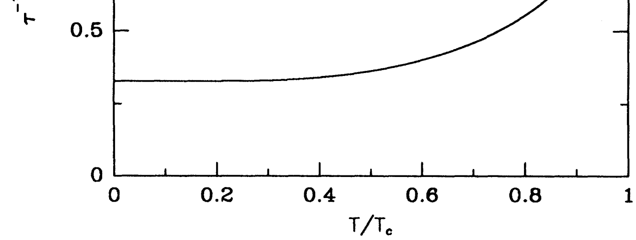

FIG. 3. The temperature dependence of the transverse nuclear relaxation rate, τ^{-1}, in the superconducting state for the s-wave (solid line) and d-wave (dotted line) gap symmetries.

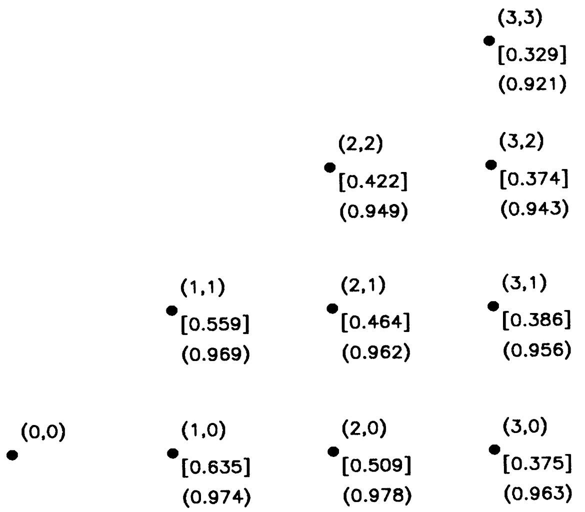

FIG. 4. The z component of the effective coupling, $J_z(\mathbf{x}_i)$ (normalized to its value at $T=T_c$), for $T=0.8T_c$ using s-wave (in square brackets) and d-wave (in parentheses) gap symmetries.

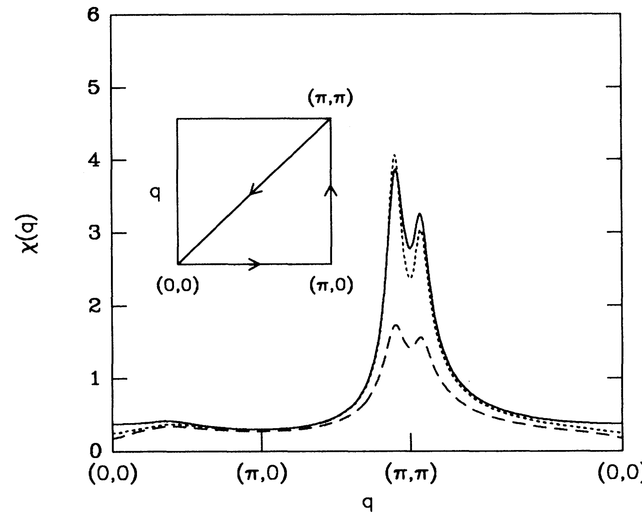

FIG. 5. The static RPA susceptibility $\chi(\mathbf{q})$ vs $\mathbf{q}$ in the Brillouin zone (inset) in the normal state at $T=T_c$ (solid line) and in the superconducting state at $T=0.8T_c$ for the s-wave (dashed line) and the d-wave (dotted line) gap symmetries.

small cluster around site **0** at $T=100$ and 300 K. As T is lowered $J_z(\mathbf{x}_i)$ is enhanced due to the development of antiferromagnetic (AF) correlations.

Results for τ^{-1} in the superconducting state are shown in Fig. 3 for a T_c of $0.10t$. For an s-wave gap, τ^{-1} is rapidly suppressed as the gap opens and then saturates. In contrast, for a d-wave gap, τ^{-1} has little T dependence. Figure 4 shows how $J_z(\mathbf{x}_i)$ changes as T is lowered from T_c to $0.8T_c$. We see that $J_z(\mathbf{x}_i)$ does not change much for a d-wave gap. However, $J_z(\mathbf{x}_i)$ decreases rapidly for an s-wave gap, especially for $|\mathbf{x}_i| \gtrsim \xi_{sc} \simeq 0.18\hbar v_F/\Delta$. For the gap amplitude that we are using, the superconducting coherence length, ξ_{sc}, is of order several lattice spacings at $T=0$ for an s-wave gap.

From Eq. (6), it is clear that the strength and range of the indirect nuclear spin coupling mediated by the spin fluctuations is determined by $\chi(\mathbf{q})$. In Fig. 5 we show $\chi(\mathbf{q})$ vs $\mathbf{q}$ for the normal state at $T=T_c$ and in the superconducting state for s- and d-wave gaps at $T=0.8T_c$. Over a region $0<\mathbf{q}<\xi_{sc}^{-1}$, $\chi(\mathbf{q})$ is suppressed for both types of gap symmetries. As T/T_c goes to zero, we expect that $\chi(0)$ will vanish, reflecting the formation of singlet pairs. In addition, for an s-wave gap, $\chi(\mathbf{q})$ is also suppressed around (π,π) due to the opening of the superconducting gap over the Fermi surface. However, for a d-wave gap, $\chi(\mathbf{q})$ is not suppressed around (π,π), since in this case $\mathbf{q}\sim(\pi,\pi)$ can connect two gapless regions of the Fermi surface. In other words, it is the fact that a d-wave gap has nodes on the Fermi surface that causes τ^{-1} to remain nearly constant below T_c.

We have seen in a simple model how the T dependence of the AF correlations in the CuO_2 layers is reflected in the T dependence of τ^{-1} for the Cu(2) nuclei when $\mathbf{H}\|c$. In the normal state the RPA result for τ^{-1} is enhanced over the $U=0$ result and this enhancement increases with the development of AF correlations. In the superconducting state we have calculated τ^{-1} for s- and d-wave gap symmetries. For an s-wave gap τ^{-1} rapidly decreases due to the suppression of AF fluctuations below T_c. In contrast, for a d-wave gap, τ^{-1} is nearly T independent below T_c, due to the nodes of a d-wave gap on the Fermi surface. Hence we suggest that measurements of τ^{-1} below T_c could give useful information regarding the symmetry of the superconducting wave function.

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