

Spin excitations and pairing gaps in the superconducting state of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$

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We show that it is possible to give a quantitative account of the temperature dependence of the measurements of the Knight shift and the spin-lattice-relaxation times for planar copper and oxygen sites in the superconducting state of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ by assuming that the planar excitations form a strongly coupled antiferromagnetic Fermi liquid. We consider anisotropic singlet and triplet pairing states with an orbital momentum $l \leq 2$ and report on gap parameters and antiferromagnetic enhancement factors that are consistent with experiment. We present as well our calculations for the chain sites, for which an additional relaxation mechanism appears required.

Nuclear magnetic resonance experiments on ^{63}Cu and ^{65}Cu nuclei in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (Refs. 1 and 2) provide an excellent microscopic probe of the static and dynamic field fluctuations in the local surrounding of the nuclei. The recent relaxation time and shift measurements of Pennington *et al.*³ on a single-crystal sample in the normal state, when combined with the measurement of the Knight shift in the superconducting state of the chain Cu(1) and the planar Cu(2) in aligned powder samples of $\text{YBa}_2\text{Cu}_3\text{O}_7$ by Takigawa *et al.*,⁴ who determine the local magnetic field from measurements of bulk demagnetizing factors, and Barrett *et al.*⁵ who determine the local magnetic field by using the ^{91}Y resonance line as a reference probe, make possible a rather complete phenomenological analysis of the possible values of the hyperfine couplings at both the chain Cu(1) and planar Cu(2) sites without referring to any particular model.⁶ As Monien, Pines, and Slichter⁶ and Pennington *et al.*^{3,7} have shown, it is possible to give a consistent account of the normal-state experiments based on a description of the Cu^{2+} spins as local moments, supplemented by the introduction of hole excitations in both the chains and planes. However, such a description runs into difficulties when it is applied to the experimental data for the spin-lattice-relaxation time and the Knight shift in the superconducting state, which show that the spin-relaxation time, $1/T_1$, of the Cu(1) and Cu(2) nuclei drops very rapidly at the transition temperature T_c ,¹ while for the planar sites the spin contribution to the Knight shift likewise decreases, and, at low temperatures, may vanish linearly with temperature.^{4,5}

There are two alternatives to explain the decreasing spin-relaxation time in the superconducting state. One is that the Cu^{2+} local moments are not an essential part of the superconductivity, but that as the system goes superconducting the Cu^{2+} local moments are less effectively scattered by the hole excitations, so that by the time one reaches the ground state at $T=0$ all spins are paired off. In the second picture the Cu^{2+} spins are regarded as an essential part of the normal-state quantum liquid, which then goes superconducting at T_c . In this communication we explore the consequences of this second approach. To

be more specific, we assume that both above T_c and in the superconducting state the Cu^{2+} spins are strongly hybridized with the planar oxygen holes in such a way that the quasiparticles in the resulting Fermi liquid behave in the neighborhood of a Cu nucleus very much like local moments, while maintaining elsewhere an essentially itinerant character. Since local moments at adjacent Cu nuclear sites couple antiferromagnetically, the quasiparticles of the hybridized hole- Cu^{2+} Fermi liquid will consequently interact antiferromagnetically. We show that by treating the Cu^{2+} spins in the superconducting state as an antiferromagnetic Fermi liquid, it is possible to give a quantitative account of the temperature dependence of the planar spin-relaxation rate^{1,2} which is consistent with the temperature dependence of the Knight-shift measurements by Takigawa *et al.*⁴ and Barrett *et al.*⁵

In addition to the usual Bardeen-Cooper-Schrieffer (BCS) isotropic *s*-wave state, we consider in some detail three kinds of anisotropic states: anisotropic *s*-wave states, conventional *d*-wave states, and *d*-wave states with an admixture of higher harmonics.

The gap functions we consider are shown in Fig. 1 as a function of the angle ϕ where ϕ is the angle in the *a, b* plane describing the position on the cylindrical Fermi surface. Our reasons for exploring these anisotropic states are twofold. First, the relaxation rate ($1/T_1$) shows *no* coherence peak just below T_c , as one would expect for a singlet, $l=0$ superconductor, if the quasiparticles are sufficiently well defined. With such anisotropic pairing states one reduces, or eliminates altogether, the BCS coherence peak in T , just below the superconducting transition. Second, Monien and Zawadowski⁸ find that *d*-wave singlet states provide an almost unique explanation of the substantial density of states found below the energy gap in Raman-scattering experiments.⁹ We show that with proper choice of gap parameters and antiferromagnetic enhancement factors, these states also lead to planar spin-lattice-relaxation rates which are in quantitative agreement with experiment.

We first consider the normal state, for which both the magnitude and temperature dependence of the spin relaxation of the Cu(2) nuclei are anomalous. Thus the value

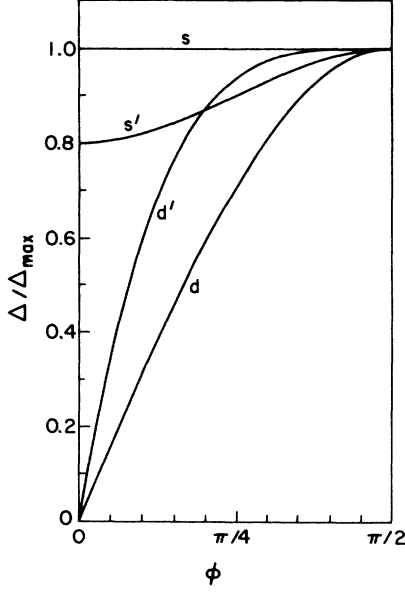


FIG. 1. The gap function for the s -wave and d -wave pairing states considered here are shown as a function of ϕ , the angle on the cylindrical Fermi surface of the CuO_2 planes. For the gap functions on the chain Fermi surface ϕ has to be replaced by position on the chain sheet ak_x , where a is the dimension of the unit cell.

of $(1/T_1)$ just above T_c is strongly enhanced over the band structure value^{10,11} and is weakly temperature dependent, rising by only some 50% between 100 and 300 K.¹² We propose that in the immediate vicinity of T_c the enhancement is produced by an antiferromagnetic coupling between the quasiparticles, leading to a spin-spin correlation function that is strongly peaked at a large q value, say Q . To be more quantitative, we analyze the behavior of a simple random-phase approximation expression for the spin-spin correlation function,

$$\chi(q, \omega, T) = \frac{\chi_0(q, \omega, T)}{1 - N(0)J_{\text{eff}}(q, T)\chi_0(q, \omega, T)}, \quad (1)$$

where χ_0 is the bare spin-spin correlation function, and $N(0)$ is the quasiparticle density of states. The effective antiferromagnetic coupling constant, $J_{\text{eff}}(q, T)$, is assumed to depend on both the wave vector q and the temperature T and to peak at Q . For the spin-relaxation rate, only the imaginary part of χ is needed:¹³

$$\frac{1}{T_1 T} \propto \sum_q \frac{\chi_0''(q, \omega)/\omega}{[1 - N(0)J_{\text{eff}}\chi_0'(q, \omega)]^2 + [\chi_0''(q, \omega)J_{\text{eff}}N(0)]^2}; \quad (2)$$

the prime denotes the real part and the double prime denotes the imaginary part of χ , and ω is the (extremely low) frequency of the nuclear magnetic resonance. The imaginary part of the spin-spin correlation function χ is proportional to energy transfer ω for any type of Fermi liquid; therefore we can neglect the second term in the

denominator, and, in view of the smallness of ω , replace $\chi_0'(q, \omega)$ by its static value, $\chi_0'(q, T)$. The integrand is strongly peaked around the antiferromagnetic wave vector Q . The largest contribution to the integral is therefore proportional to

$$[1 - N(0)J_{\text{eff}}(Q, T)\chi_0'(Q, T)]^{-2},$$

and we can write

$$\frac{1}{T_1} = \frac{1}{(T_1)_{\text{free}}} \frac{1}{[1 - \lambda(T)]^2}. \quad (3)$$

Here we have introduced the average, temperature-dependent, enhancement factor

$$\lambda(T) = \langle N(0)J_{\text{eff}}(Q, T)\chi_0'(Q, T) \rangle \quad (4)$$

to describe the influence of antiferromagnetic correlations on the noninteracting quasiparticle relaxation time, $(T_1)_{\text{free}}$. If we assume that the real part of the spin-spin correlation function at large Q , $\chi_0'(Q, T)$, scales with temperature approximately like $\chi_0'(q=0, T)$, we can write the corresponding expression in the superconducting state in terms of the Yosida function

$$Y(T) = \chi_0(q=0, T)/\chi_0(q=0, T_c)$$

as

$$\frac{1}{T_1} = \frac{1}{(T_1)_{\text{BCS}}} \frac{1}{[1 - \lambda(T)Y(T)]^2}, \quad (5)$$

where $(T_1)_{\text{BCS}}$ is that calculated for a given pairing state in the absence of quasiparticle interaction. On this simple picture, the spin-relaxation rate above T_c is enhanced by a factor $[1 - \lambda(T_c)]^{-2}$, while, as a consequence of the small coherence length the pairing correlations in the superconductivity state reduce the influence of the normal-state enhancement factor, $\lambda(T_c)$. Thus the spin-lattice-relaxation time in the superconducting state is determined by the product of $\lambda(T_c)$ and the Yosida function $Y(T)$. Since for any BCS pairing state, $Y(T)$ decreases with temperature below T_c , to the extent that $\lambda(\leq 1)$ is appreciable, one will get a fall off of $(T_1)^{-1}$ below T_c , which is faster than that predicted by the behavior of $\chi_0''(q, T)$ alone. The magnitude of this enhanced reduction $(T_1)^{-1}$ [which results from a reduction in the normal-state enhancement factor, $(1 - \lambda)^{-2}$] depends of course on $\lambda(T_c)$ and $Y(T)$.

We estimate the possible magnitude of this enhanced reduction by first using the experimental data on the Knight shift to constrain the Yosida function for the four pairing states we consider here. Having obtained the optimal gap function for a specific set of Knight-shift measurements we calculate the resulting spin-relaxation rate and compare it to the actual measurement.

The experimental results on the Knight shift obtained by Takigawa *et al.*⁴ and Barrett *et al.*⁵ possess two remarkable features in common; for a field applied in the c direction, the Knight shift varies little with temperature, while for fields in the a or b directions, it displays a quite considerable temperature variation. Indeed, Barrett *et al.*⁵ find that for the c direction, the Knight shift is,

within experimental error, independent of temperature and nearly equal to zero; for a suitable choice of their demagnetizing factor, a similar result is obtained by Takigawa *et al.*⁴ Since spin-orbit coupling is not expected to play a large role, one possible explanation for these results is that the superconducting pairing state is a triplet such that the spin susceptibility remains constant in one direction, and varies with temperature in the others. To pursue this possibility, we consider a triplet order parameter characterized by a vector \mathbf{d} in spin space, which determines the anisotropy of the spin susceptibility in the superconducting state. At zero temperature the anisotropic spin susceptibility tensor can be written as¹⁴

$$\frac{\chi_{\alpha\beta}(T)}{\chi_{\alpha\beta}(T_c)} = \delta_{\alpha\beta} - \int \frac{dS_k}{S} \operatorname{Re} \frac{\mathbf{d}_\alpha(\mathbf{k})\mathbf{d}_\beta(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|^2}, \quad (6)$$

where S characterizes the Fermi surface, which has the form of a cylinder for the plane. One p -wave order parameter which has the required properties and is compatible with the orthorhombic symmetry is a so-called planar state with a d -vector $\mathbf{d} = (\psi_x, \psi_y, 0)$, where ψ_x and ψ_y are orbital eigenfunctions which transform like k_x and k_y . For this special pairing state $\chi_{cc}(T)$ stays constant and χ_{aa} and χ_{bb} are reduced at zero temperature by a factor

$$1 - \int \frac{dS_k}{S} \frac{|\psi_{x,y}|^2}{|\psi_x|^2 + |\psi_y|^2},$$

which is $\frac{1}{2}$ for the simplest choice for the orbital eigenfunction $\psi_{x,y} = \hat{k}_{x,y}$. In the superconducting states, both experimental groups find a reduction of the Knight shift in the a, b direction of $\sim 0.3\%$ out of $\sim 0.6\%$ for the total Knight shift, which is possible only if the Knight shift in the a and b direction has a minimal orbital contribution. Since such a result is in sharp contrast with the expected anisotropy (~ 4) of the orbital shift, a planar triplet state can be ruled out.

We next consider the possibility of other triplet pair states. Since the total Knight shift in the c direction is nearly independent of temperature below T_c one is forced to conclude that the measured total Knight shift of 1.2% (Ref. 5) in both the normal and superconducting state is, within experimental error, entirely of orbital origin. Thus $K_c^L = 1.2\%$. Turning next to the a and b directions, Barrett *et al.*⁵ have calculated the orbital susceptibility anisotropy to be, $K_c^L/K_a^L \cong 4.4$, in which case we would expect a orbital Knight shift in the a direction of $K_a^L = 0.29\%$ and a spin Knight shift in the normal state which is $K_a^S = 0.30\%$. Since the measured net change in the total Knight shift is $0.30 \pm 0.02\%$ these results rule out the possibility of a p -wave pairing state inasmuch as the latter requires a minimum residual spin susceptibility of $T=0$, in one direction, of $\frac{1}{3}$ the normal-state value. Put another way, a Balian-Werthamer p -wave state is only consistent with experiment if the orbital susceptibility anisotropy $K_c^L/K_a^L \geq 6$. We therefore turn our attention to *singlet* pair states.

One explanation of the near vanishing of the Knight shift in the c direction is that one has two distinct contri-

butions to the planar Knight shift, one proportional to the spin susceptibility, χ^s , associated with the Cu^{2+} local moments, and a second, proportional to χ^h , an oxygen hole spin susceptibility, and that these respective contributions nearly cancel out for fields applied in the c direction.⁶ If, however, one assumes that the hole contribution to the planar Knight shift is isotropic then one can isolate the Cu^{2+} contribution χ^s , by examining the behavior of the axial Knight shift, $K_{\text{ax}}(T) = K_c(T) - K_a(T)$. The results of Takigawa *et al.*⁴ and of Barrett *et al.*⁵ for the reduced axial Knight shift,

$$\bar{K}_{\text{ax}}(T) = K_{\text{ax}}(T)/K_{\text{ax}}(T_c),$$

which is then identical to $\bar{\chi}^s(T) = \chi^s(T)/\chi^s(T_c)$, are shown in Figs. 2(a) and 2(b). There we see that Takigawa *et al.* find a linear temperature dependence for $\bar{K}_{\text{ax}}(T)$ below 40 K, while Barrett *et al.* find that $\bar{K}_{\text{ax}}(T)$ is flat below ~ 20 K; a measure of the sensitivity of the experimental results to low-temperature values is that within experimental error, a linear temperature dependence, but with a far less pronounced slope, provides a fit to the data of Barrett *et al.*

To compare with experiment we need to calculate the Yosida function $Y(T)$. In a weak coupling BCS superconductor, the Yosida function for an anisotropic singlet superconductor has the form¹⁴

$$Y(T) = \int_{-\infty}^{\infty} dE \left[-\frac{\partial f}{\partial E} \right] N(E), \quad (7)$$

where $N(E)$ denotes the density of states and f is the Fermi distribution function. If, as if the case for the two s -pair states we consider, there is a minimum gap Δ_{min} in the density of states below which $N(E)$ vanishes, $Y(T)$ dies off exponentially like $Y(T) \sim \exp(-\Delta_{\text{min}}/T)$; on the other hand, for a gapless superconductor with a line of nodes on the Fermi surface, such as that proposed by Monien and Zawadowski,⁸ the density of states is proportional to the energy at small energies and the Yosida function is $\sim T$ for temperatures below $0.1 T_c$. More specifically, for a gap with a line of nodes the density of states rises linearly with the energy E ,

$$[N(E/\Delta)/N(0)] \sim A [E/\Delta(0)],$$

where the slope A is determined by the slope with which the gap vanishes in the neighborhood of the node, and the value of the maximum gap. The slope of the gap function in the neighborhood of the node determines therefore how many quasiparticles are available at a given energy.

In contrast to the ordinary s -wave pairing state, the density of states for the anisotropic s -wave state has a much weaker singularity at the maximum gap. We consider here a particular example of such an anisotropic s -wave state, in which the gap modulation that results from coupling to higher angular momentum states is 20%. In considering possible d -wave states, we demonstrate the effect of a large slope of the gap function in the neighborhood of the zero by evaluating the Yosida function for two different d -wave gap functions: one corresponds to a

simple $l=2$ singlet superconductor, while the second contains an admixture of higher l . The gap for pairs in the $l=2$ singlet state is substantial on most parts of the Fermi surface, and therefore the density of states below

the gap is much lower than for the gap function that describes pairs involving higher spherical harmonics.

For the d -wave states, the Yosida function at low temperatures has the approximate form

$$Y(T) \cong 2 \ln 2 A \frac{T}{\Delta(0)}, \quad (8)$$

where $\Delta(0)$ is the zero-temperature energy gap. The weak-coupling values for the zero-temperature gap $\Delta(T=0)$ and the specific-heat jump associated with the superconductivity in the planes only are given in Table I. We use a common interpolation formula for the temperature dependence of the gap:

$$\Delta(T) = \Delta(0) \tanh \left\{ \left[\left[\frac{\partial \Delta^2}{\partial T} \right]_{T=0} \left(\frac{T_c}{T} - 1 \right) \right]^{1/2} / \Delta(0) \right\}. \quad (9)$$

The fit parameters are the zero-temperature gap and the specific-heat jump that determines the slope of $\Delta^2(T)$ in the neighborhood of T_c . These two parameters take care of the strong-coupling corrections. The resulting Yosida function, $Y(T)$, is compared with the experimental results of Takigawa *et al.*,⁴ for the axial Knight shift, $K_{ax}(T) = K_c(T) - K_a(T)$ in Fig. 2(a). The optimal values of the parameters $\Delta(T=0)$ and the specific-heat jump $\sim \partial \Delta^2 / \partial T$ for the two d -wave states, are given in Table I.

The best fits to the bare $\chi_{a,b}^s(T) / \chi_{a,b}^s(T_c)$ for the Knight-shift data of Barrett *et al.*⁵ with the Yosida function calculated for both anisotropic s states and d states are shown in Fig. 2(b) and 2(c). As may be seen there, for all temperatures except 20 K, equally good fits to their data are obtained with either s -wave pairing or d -wave pairing. The values for the optimal parameters $\Delta(T=0)$ and the specific-heat jump are given in Table I. The gap required for the "best fit" d -wave state appears unphysically large. It is interesting to note that for all investigated pairing states except the d -wave state the specific-heat jump is enhanced by a factor of the order two over the weak-coupling value.

The reasonable agreement of the Knight-shift temperature dependence with our simple fits encourages us to extend our simple analysis to the spin-relaxation rate, and hence to determine $\lambda(T_c)$. A simple formula for the spin-relaxation rate in the superconducting state for an *unconventional* superconductor can be obtained in the following way. For a noninteracting Fermi liquid we may write¹⁵

$$\begin{aligned} (1/T_1 T) &\sim \sum_q \chi_0''(q, \omega) / \omega \\ &= \int_{-\infty}^{\infty} dE \left[-\frac{\partial f}{\partial E} \right] [N^2(E) + M^2(E)], \quad (10) \end{aligned}$$

where $N(E)$ is the density of states

$$N(E) = \langle \text{Re}[E / (E^2 - \Delta_k^2)^{1/2}] \rangle_{\text{FS}}$$

and $M(E)$, defined by

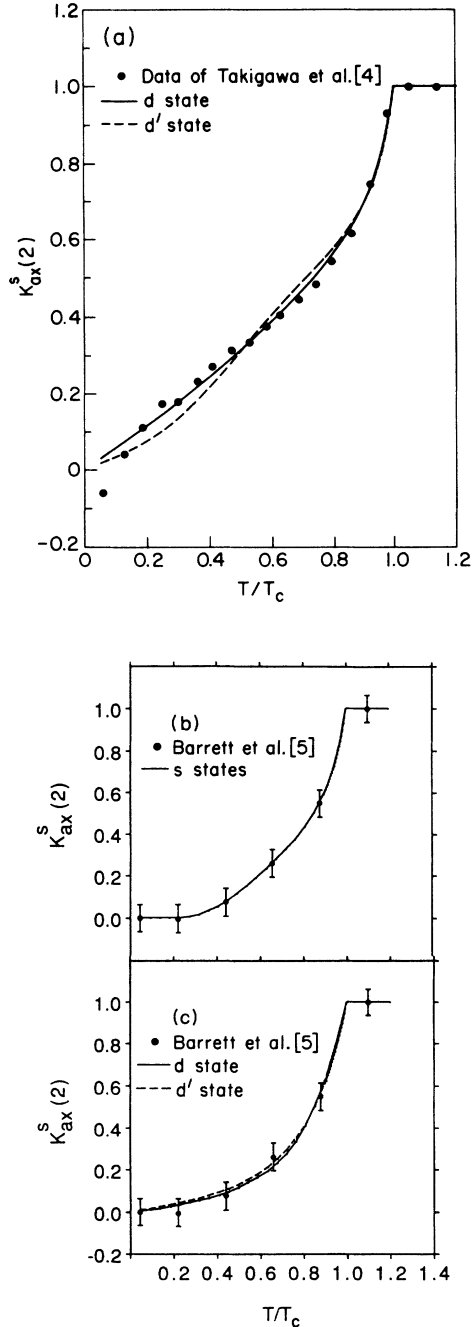


FIG. 2. Fits to the experimental Cu(2) Knight-shift data normalized to the normal-state values in the superconducting state: (a) the data of Takigawa *et al.* (Ref. 4) is compared with the Yosida function calculated for two d -wave states; (b) the data of Barrett *et al.* (Ref. 5) is compared with the Yosida function calculated for two s -wave states, which yield similar results within the accuracy of the plot; (c) the data of Barrett *et al.* is compared with the Yosida function calculated for two d -wave states. Optimal fit parameters are given in Table I.

$$M(E) = \langle \text{Re}[\Delta_k / (E^2 - \Delta_K^2)^{1/2}] \rangle_{\text{FS}},$$

takes into account the coherence factors present for s -wave state. This formula extends the simple Korringa

$$(1/T_1 T) \sim \sum_q \chi''_0(q, \omega) / \omega = \int_{-\infty}^{\infty} dE \left[-\frac{\partial f}{\partial E} \right] [N^2(E) + M^2(E)] / [1 - \lambda(T_c) Y(T)]^2. \quad (11)$$

Since we do not know how much of the enhancement in the normal state comes from band-structure effects, we have plotted, in Figs. 3(a)-3(e), the spin-lattice-relaxation rate, $(1/T_1)$ for the Cu(2) nuclei, for different enhancement factors for the different pairing states normalized to the value at T_c .

The inset of Fig. 3(a) illustrates the way in which a temperature-dependent antiferromagnetic enhancement acts to reduce the coherence peak in the relaxation rate $1/T_1$ for the anisotropic s -wave state. With no temperature-dependent antiferromagnetic enhancement, the coherence peak is so substantial that it appears difficult, if not impossible, to reduce the peak by lifetime broadening without obtaining an unacceptably gradual fall off of $1/T_1$ in the vicinity of T_c . On the other hand, with a temperature-dependent antiferromagnetic enhancement factor, $\lambda \cong 0.7$, the size of the coherence peak is reduced by a factor of 2, and it is possible that the lifetime effects could act to reduce the peak further without producing an unacceptably slow fall off of $(1/T_1)$ in the vicinity of T_c .

Insofar as the coherence peak is concerned, matters are significantly improved by going to pure d -wave pairing states since no coherence peak is found, even in the absence of a temperature-dependent antiferromagnetic enhancement. One can observe clearly that, for states other than the d -wave state, the calculated curve for no temperature-dependent antiferromagnetic enhancement gives a relaxation rate that is too long for all temperatures, while the temperature dependence of the spin-relaxation rate is dramatically changed by a temperature-dependent antiferromagnetic interaction. In Figures 3(a)-3(c), we use the gap parameters deduced from the Knight-shift measurement by Barrett *et al.* to calculate the spin-relaxation rate. We find that for the

law to the superconducting phase for noninteracting fermions with an unconventional gap. Extending this formula to the case of antiferromagnetically interacting fermions we obtain from Eq. (3)

anisotropic s state, Fig. 3(a), an antiferromagnetic enhancement of $\lambda \sim 0.7$ is required for a reasonable fit, whereas for the d -wave state with higher l admixture, Fig. 3(c), a $\lambda \sim 0.3$ is sufficient. The spin-relaxation rate calculated for the pure d -wave state, Fig. 3(b), does not fit the experimental curve. However, if instead of finding a best fit to the Knight shift and then calculating $(1/T_1)$, one inverts the process, choosing gap parameters which fit $(1/T_1)$ and then calculating the Knight shift, matters change significantly. Thus in Fig. 4(a) we show a pure d wave "best fit" to $(1/T_1)$, (the parameters are given in Table II) in which any antiferromagnetic enhancement is assumed to be independent of temperature, and in Fig. 4(b) compare the calculated Knight shift with the experimental results of Barrett *et al.*⁵ The fit to the Knight-shift experiments clearly falls within the experimental error, while our pure d -wave fit to $(1/T_1)$ is comparable to the best fit (with an antiferromagnetic enhancement factor of $\lambda = 0.5$) obtained in Fig. 3(d).

If we use the gap parameters deduced from the Knight-shift experiments by Takigawa *et al.*, we require an antiferromagnetic enhancement of $\lambda \sim 0.5$ [pure d wave, Fig. 3(d)], or $\lambda \sim 0.65$ [d wave with higher λ admixture, Fig. 3(e)], in order to explain the observed Cu(2) relaxation rate. The fact that at temperatures less than $\sim 0.3 T_c$, the experimental values of $(1/T_1)$ lie above the theoretical values may reflect the presence of added mechanisms for spin-lattice relaxation.

We further note that the low-temperature behavior of the calculated spin-relaxation rate depends only very weakly on the antiferromagnetic enhancement factor λ because the enhancement becomes ineffective at low temperatures where the Yosida function is small. For the d wave [Figs. 3(b)-3(e)] states the density of states is proportional to the energy at low energies so that we expect

TABLE I. Upper part: Optimal Parameters for the Cu(2) Knight shift measured by Takigawa *et al.* (Ref. 4). Lower part: Optimal Parameters for the Cu(2) Knight shift measured by Barrett *et al.* (Ref. 5).

Pairing state	Weak coupling		Optimal fit	
	$\Delta(T=0)/k_B T_c$	$\Delta C/C$	$\Delta(T=0)/k_B T_c$	$\Delta C/C$
s	2.13	0.95	2.44	1.97
d'	1.93	1.17	1.74	2.36
s	1.76	1.43	1.90	2.77
s'	2.10	1.27	2.16	2.49
d	2.13	0.95	14.7	1.76
d'	1.93	1.17	3.13	2.14

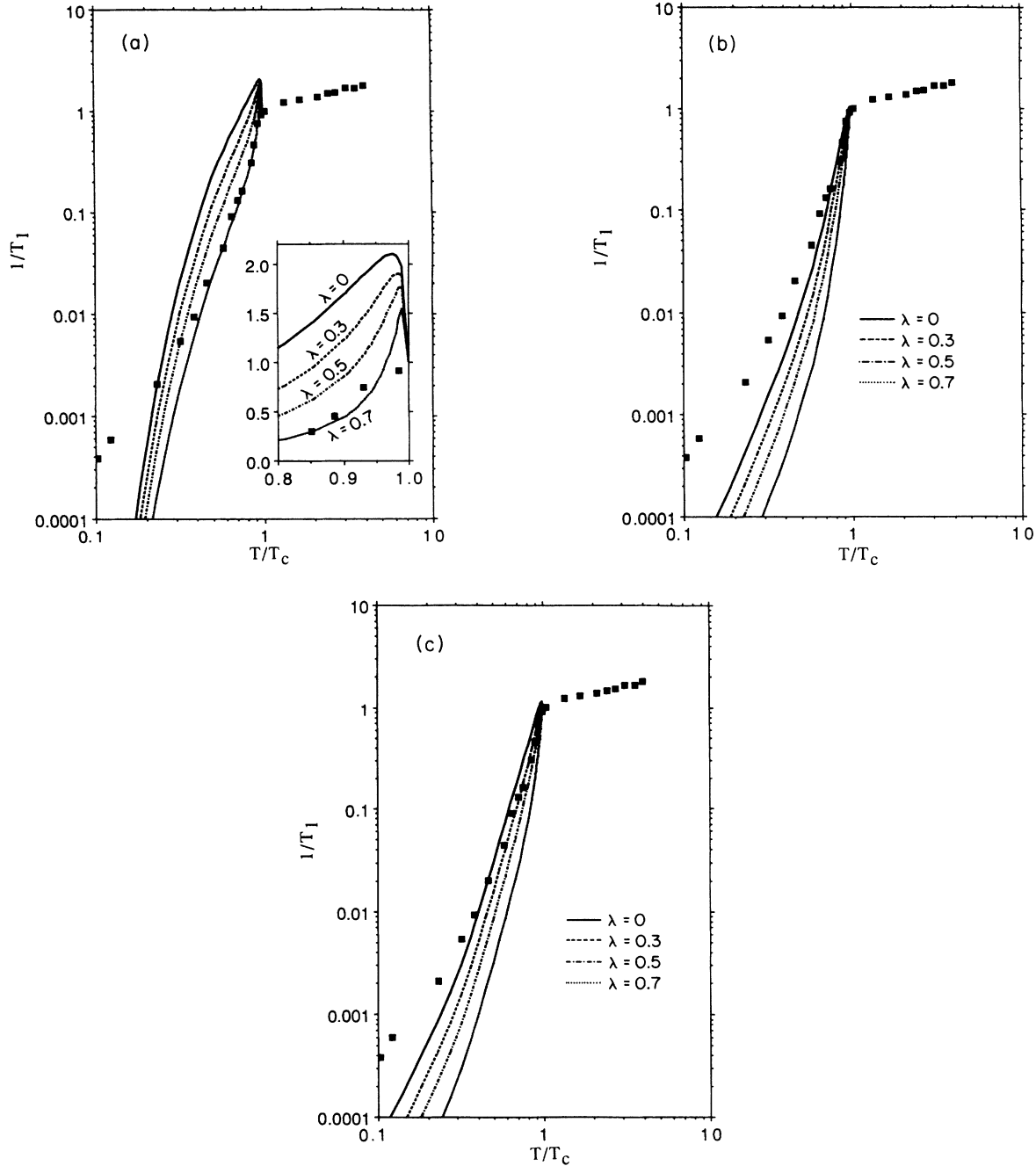


FIG. 3. The spin-relaxation rate for the Cu(2) nuclei normalized to the normal-state value calculated for the anisotropic s -wave state and the two d -wave states are compared as a function of the temperature T with the experimental data of Yasuoka *et al.* in (a), (b), and (c), respectively, for the same parameters as used in the Knight-shift fit to the data of Barrett *et al.* [Fig. 2(b)] and, in (d) and (e) for the parameters used in the Knight-shift fit to the data of Takigawa *et al.* [Fig. 2(a)]. The antiferromagnetic enhancement factor is $\lambda=0.0$ (solid line), $\lambda=0.3$ (dashed line), $\lambda=0.5$ (dashed dotted line), $\lambda=0.7$ (dotted line). The inset shows the calculated spin-relaxation rate for the anisotropic s -wave state as a function of temperature T on a linear scale.

a spin-relaxation rate $1/T_1 \sim T^3$ at temperatures below $0.1 T_c$; for the s -wave states it vanishes exponentially.

It is natural to inquire whether a similar physical picture is applicable for planar excitations in other high-temperature superconductors. For example, Kitaoka¹⁶ has recently reported qualitatively similar results for $(T_1 T)^{-1}$ for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$; while Imai *et al.*¹¹ have re-

cently reported qualitatively similar results in the normal state for the 90 K superconductor $\text{LaBa}_2\text{Cu}_3\text{O}_{7-x}$ and the 60 K superconductor, $\text{YBa}_2\text{Cu}_3\text{O}_{6.52}$. It will be interesting to see whether a quantitative analysis of Knight shift and T_1 data for these and other systems can be carried out along the lines we have suggested here, using similar pairing states.

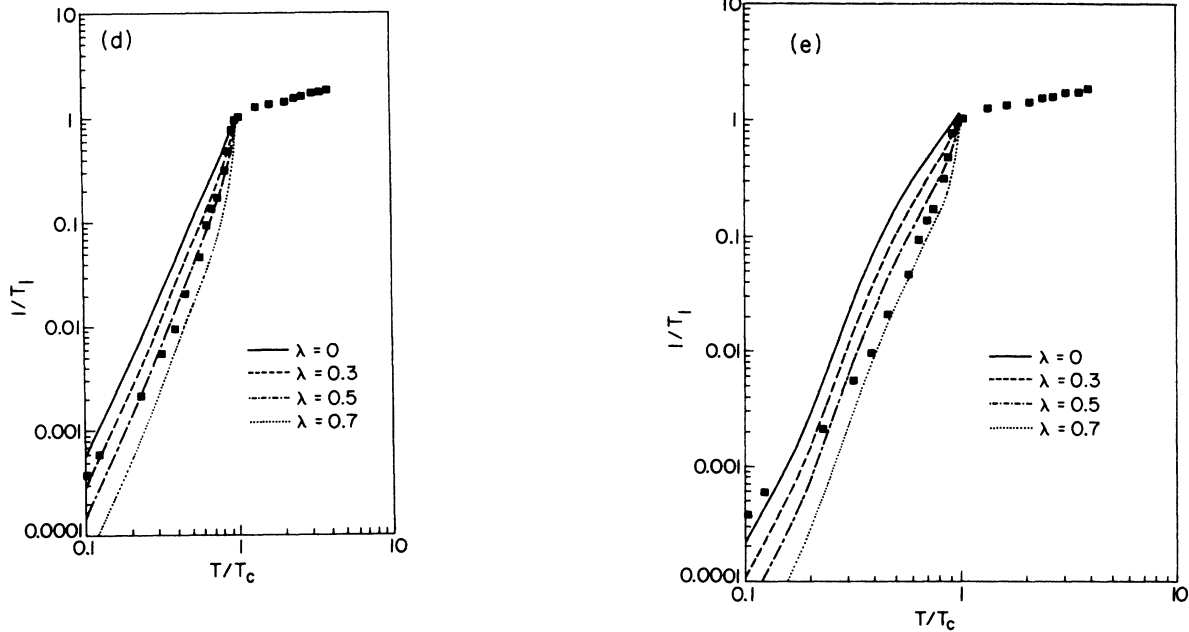


FIG. 3. (Continued).

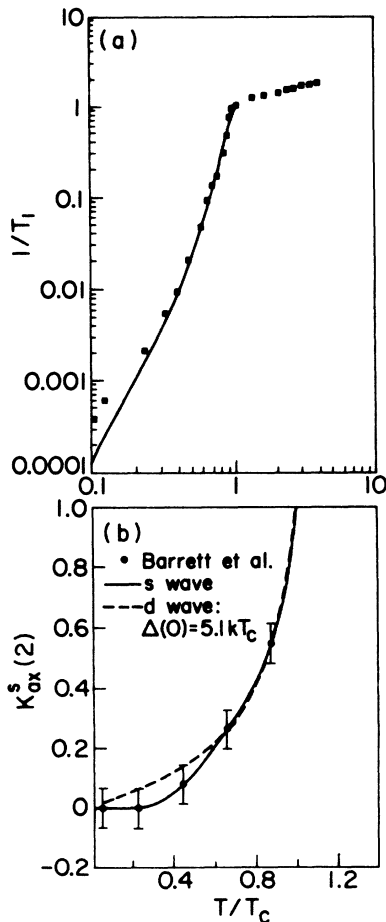


FIG. 4. (a) Fit to the experimental Cu(2) spin-relaxation rate of Imai *et al.* (Ref. 2), with *d*-wave pairing state with $\Delta = 5.12kT_c$, $(\Delta C/C) = 1.89$. (b) Calculated Knight shift for Cu(2) nuclei, using *d*-wave pairing state, with $\Delta = 5.12 kT_c$, $\Delta C/C = 1.89$.

We further note that a Fermi-liquid description (but with a somewhat different quasiparticle interaction) can be used to analyze the T_1 and Knight-shift data for the chain sites in $\text{YBa}_2\text{Cu}_3\text{O}_7$. In Fig. 5 we show the optimal fit to the Cu(1) Knight-shift data of Barrett *et al.*,⁵ with the Yosida function calculated for the two *s*-wave states. We obtain an excellent fit to the Knight shift with the parameter values for the zero-temperature gap and the specific-heat jump given in Table I. We emphasize that the results of Barrett *et al.*⁵ demonstrate that *the pairing states for chain pairs are not identical to those for planar pairs*. As may be seen in Table III, even though it is possible that one can describe both plane and chain Knight shifts with anisotropic *s*-state pairs, the gap parameters and specific-heat jumps for the chain and plane quasiparticles are different.

A second way in which chains and planes differ is in the temperature dependence of the spin-lattice relaxation rate. We are not able to explain the temperature dependence of the Cu(1) relaxation in the superconducting state by using values of the pairing parameters which fit the Knight-shift experiments. As may be seen in Fig. 6, our calculated values do not agree with the experimental values of Yasuoka *et al.*,² with or without antiferromagnetic enhancement.

Hammel *et al.*¹⁷ find that the spin-lattice relaxation of the ^{17}O planar sites below T_c follows the same temperature dependence as that of the Cu(2) nuclei for $T \gtrsim 40 \text{ K}$, while if one calculates the temperature dependence of the

TABLE II. *d*-wave pairing parameters chosen to fit the Cu(2) relaxation rate measured by Imai *et al.* (Ref. 2).

Pairing state	$\Delta(T=0)/k_B T_c$	$\Delta C/C$
<i>d</i>	5.12	1.89

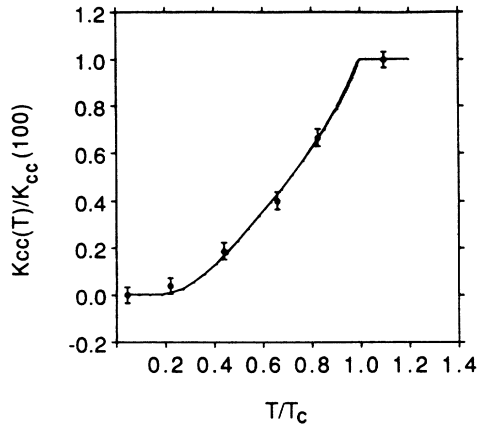


FIG. 5. Fit to the experimental Cu(1) Knight-shift data of Barrett *et al.* (Ref. 5) normalized to the normal-state value in the superconducting state with the Yosida function calculated for the s -wave pairing states.

reduced ^{17}O Knight shift in the superconducting state from the experiment of Horavtić *et al.*,¹⁸ one obtains a result close to that found for the corresponding value for $\chi_s(T)$ from the experimental data of Barrett *et al.*⁵ Thus it is possible that in the superconducting state the same planar excitations are responsible for the Knight shift and T_1 for both the Cu(2) and ^{17}O planar sites.

We would like to emphasize that although the agreement between our calculated values and experiment is quite good it depends only on the energy dependence of the density of states which is quite insensitive to the structure of the gap except for the topology of the zeroes. Although we do not claim that we can determine the structure of the gap, it seems that the interpretation of two experiments, the Knight-shift measurement of Takigawa *et al.*⁴ and the Raman scattering experiment,⁹ require a gap with a line of nodes on the Fermi surface, while the Cu(2) Knight shift of Barrett *et al.*⁵ can be fitted with either s - or d -wave states and the O(2) Knight shift of Horavtić *et al.*¹⁸ require an anisotropic s -wave state with a spatially varying, but everywhere finite, energy gap.

In summary, we find that a simple Fermi-liquid-BCS approach, in which appropriately chosen energy gaps are combined with a moderate antiferromagnetic interaction, is sufficient to explain why the temperature dependence of the Knight shift and the relaxation rate of the Cu(2) nuclei are different from those of the Cu(1) nuclei in the superconducting state. We further note that the departure of the gap function from a constant, combined with

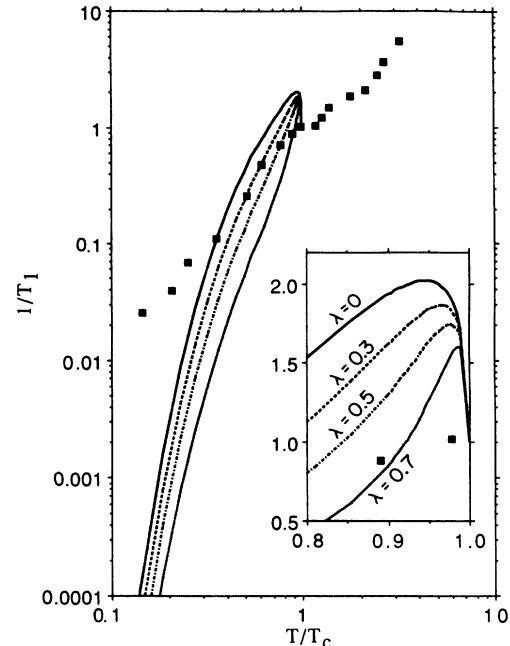


FIG. 6. The spin-relaxation rate calculated normalized to the normal-state value for an anisotropic s -wave state is shown in comparison with experimental data for the Cu(1) spin-relaxation rate of Yasuoka *et al.* (Ref. 2). The notation is the same as in Fig. 4.

the antiferromagnetic interaction, is sufficient to eliminate any sizable coherence peak for spin-lattice relaxation near T_c . On the other hand, measurements of the temperature dependence of the penetration depth at low temperatures¹⁹ are consistent with a finite energy gap everywhere on the Fermi surface, a result which is at first sight in contradiction with the use of d -wave pairing states. Obviously this apparent conflict needs to be resolved; here we would like to point out that the penetration depth for an anisotropic superconductor looks very much like the s -wave case if experimental conditions are such that the current which responds to the external magnetic field involves quasiparticles in a region on the Fermi surface where the gap is large.¹⁹ The gap function (d) shows that even for an anisotropic superconductor the gap can be quite substantial in a large area of the Fermi surface, so that the presence of a line of nodes may not be detectable in a penetration depth experiment.

In carrying out the calculations described here, we examined the role played by a temperature-dependent antiferromagnetic enhancement factor because of the promise it offered to reduce substantially the coherence peak

TABLE III. Optimal Parameters for the Cu(1) Knight shift measured by Barrett *et al.* (Ref. 5).

Pairing state	Weak coupling		Optimal fit	
	$\Delta(T=0)/k_B T_c$	$\Delta C/C$	$\Delta(T=0)/k_B T_c$	$\Delta C/C$
s	1.76	1.43	1.50	1.71
s'	2.10	1.27	1.71	1.55

found for s -state pairing, and to reconcile the best-fit values of the Knight-shift experiments with the experimental results for $(1/T_1)$. However, the experimental results of Hammel *et al.*¹⁷ demonstrate in a one-component model of planar excitations that while considerable antiferromagnetic enhancement is required to explain the magnitude of the measured values of the Cu(2) relaxation rate, in the normal state, *that enhancement must be independent of temperature below T_c* , since only in this way can one understand the measured constant ratio of the O(2) relaxation rate to the Cu(2) relaxation rate over the range rate, $T_c/4 \lesssim T \lesssim T_c$. [For a phenomenological description of the role played by a temperature-dependent antiferromagnetic correlation in the normal state, we refer the interested reader to a forthcoming paper by Millis, Monien, and Pines.²⁰] We conclude therefore that absent temperature-dependent feedback effects (vertex) corrections which, in the superconducting state, mimic our phenomenological temperature-dependent antiferromagnetic enhancement factor, the measured values

of $(1/T_1)$ in the superconducting state would seem to require d -wave pairing, with an energy gap and strong-coupling corrections comparable to those given in Table II.

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