Analysis of NMR Data in the Superconducting State of YBa$_2$Cu$_3$O$_7$

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We have extended a weak-coupling theory of antiferromagnetic fluctuations to the superconducting state and analyzed NMR data for YBa$_2$Cu$_3$O$_7$. Within this framework we find that while an s-wave gap structure with $2\Delta(0)/kT_c=4$ can fit the Knight-shift data for Cu(2) and O(2,3), it does not provide a satisfactory fit to the $T^{-1}$ data. Using a $d_{x^2-y^2}$-wave gap with $2\Delta(0)/kT_c$ of order 6 to 8 provides a reasonable fit to both the Knight-shift and $T^{-1}$ data.

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Measurements of the temperature dependence of the Cu(2) and O(2,3) nuclear relaxation rates in the normal state of YBa$_2$Cu$_3$O$_7$ have been successfully analyzed in terms of a weak-coupling antiferromagnetic Fermi-liquid theory [1,2]. Here we analyze a simple extension of this approach to the superconducting state and compare results for the Cu(2) and O(2,3) Knight shifts and nuclear relaxation times obtained for both s-wave and d-wave gaps [3]. Within this framework, we find for an s-wave gap that the Knight-shift data can be fitted using a $2\Delta(0)/kT_c$ ratio of order 4 but that the $T^{-1}$ results are not well described. A d-wave gap with $2\Delta(0)/kT_c$ of order 6 to 8 provides a reasonable fit to both the Knight shift and the $T^{-1}$ data.

In Ref. [1], we modeled the normal-state susceptibility by an RPA form

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - \tilde{U}\chi_0(q, \omega)},$$

with the irreducible susceptibility $\chi_0(q, \omega)$ replaced by the noninteracting tight-binding susceptibility and $\tilde{U}$ taken as an effective interaction strength [4]. A natural extension of this to the superconducting state [5] involves approximating the irreducible susceptibility by the BCS expression

$$\chi_{\text{BCS}}^{\text{BCS}}(q, \omega) = \frac{1}{N} \sum_p \left\{ \frac{1}{2} \left[ 1 + \frac{\epsilon_{p+q}\epsilon_p + \Delta_p \Delta_{p+q}}{E_{p+q}E_p} \right] \frac{f(E_{p+q}) - f(E_p)}{\omega - (E_{p+q} - E_p) + i\Gamma} \right. \right.$$\[1\]

$$+ \frac{1}{4} \left[ 1 - \frac{\epsilon_{p+q}}{E_{p+q}} + \frac{\epsilon_p}{E_p} \right] \frac{\epsilon_{p+q}\epsilon_p + \Delta_p \Delta_{p+q}}{E_{p+q}E_p} \frac{1 - f(E_{p+q}) - f(E_p)}{\omega + (E_{p+q} + E_p) + i\Gamma} \right.$$\[2\]

$$+ \frac{1}{4} \left[ 1 + \frac{\epsilon_{p+q}}{E_{p+q}} - \frac{\epsilon_p}{E_p} \right] \frac{\epsilon_{p+q}\epsilon_p + \Delta_p \Delta_{p+q}}{E_{p+q}E_p} \frac{f(E_{p+q}) + f(E_p) - 1}{\omega - (E_{p+q} + E_p) + i\Gamma}. \right.$$\[2\]

We will evaluate this expression for both an s-wave gap $\Delta_p = \Delta(T)$ and a d-wave gap $\Delta_p = [\Delta(T)/2](\cos\varphi_p - \cos\varphi_{p+q})$. Here $\Delta(T)$ will be assumed to have a BCS temperature dependence [6] and $2\Delta(0)/kT_c$ will be treated as a parameter. Equation (2) contains the usual coherence factors in the square brackets, and the dispersion relation $E_p = (\epsilon_p^2 + \Delta_p)_{1/2}$ with the tight-binding band structure $\epsilon_p = -2t(\cos\varphi_p + \cos\varphi_{p+q}) - \mu$ and $\mu$ the chemical potential.

Using the Milla-Rice hyperfine form factors [7], the Knight shifts $K_S(T)$ for Cu(2) and O(2,3) both vary as the uniform spin susceptibility

$$\chi(0, 0) = \frac{\chi_{\text{BCS}}^{\text{BCS}}(0, 0)}{1 - \tilde{U}\chi_0^{\text{BCS}}(0, 0)}.$$\[3\]

Here

$$\chi_{\text{BCS}}^{\text{BCS}}(0, 0) = \frac{1}{N} \sum_p f(E_p)$$\[4\]

is the well-known Yosida result for a tight-binding band.

From Eq. (3) it follows that as $T$ decreases below $T_c$ and $\chi_{\text{BCS}}^{\text{BCS}}(0, 0)$ falls, $K_S(T)/K_S(T_c)$ is further reduced by the decrease in the Stoner enhancement factor $[1 - \tilde{U}\chi_0^{\text{BCS}}(0, 0)]^{-1}$. Keeping the same parameters [8] used in our previous work, the Stoner enhancement is of order 1.7 at $T = T_c$. Results for $K_S(T)/K_S(T_c)$, obtained from Eqs. (2) and (3), for various $2\Delta(0)/kT_c$ ratios are shown in Figs. 1(a) and 1(b) for s- and d-wave gaps, respectively. For an s-wave gap, the best fit is obtained with a gap ratio $2\Delta(0)/kT_c \approx 4$. This relatively small value of $2\Delta(0)/kT_c$ can give the observed rapid drop in $K_S(T)/K_S(T_c)$ because of the additional suppression arising from the Stoner factor. A larger value of $2\Delta(0)/kT_c$, of order 6 to 8, gives the best fit for a d-wave gap. At low temperatures $K_S(T)$ increases linearly with $T$ for a d-wave gap [9], while for an s-wave nodeless gap, $K_S(T)$ varies as $\exp[-\Delta(0)/T]$. As seen in Fig. 1, the experimental data appear to favor the s-wave low-temperature behavior. However, it is important to note

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FIG. 1. Knight shift vs reduced temperature obtained from Eq. (3) for various $2\Delta(0)/kT_c$ ratios with (a) an s-wave and (b) a d-wave gap. The points represent experimental data of Barrett et al. [15] on Cu(2) and Takigawa and co-workers [16,17] on O(2,3).

The error bars and to remember that the lowest-temperature Cu(2) data point has been taken as the zero. In addition, it has been demonstrated [10] for Cu(2) that there is a magnetic field dependence of the data so that the low-field limit is required to obtain intrinsic behavior and at present only 8-T data are available for O(2,3).

The nuclear relaxation times are given by

$$T_{1}^{-1} = T \sum_q |A(q)|^2 \frac{\text{Im} \chi(q,\omega)}{\omega} \bigg|_{\omega = 0}, \quad (5)$$

where $|A(q)|^2$ is the appropriate Mita-Rice hyperfine form factor [7]. We have evaluated this using Eqs. (1) and (2) for the parameters previously used in analyzing the normal state [8]. Results for the temperature dependence of $(T_{1}^{-1})$, for Cu(2) with H along the c axis and that for O(2,3) are compared with experimental data in Figs. 2(a) and 2(b). We have plotted results for $2\Delta(0)/kT_c$ equal to both 4 and 8 for an s-wave gap to show that while a larger $2\Delta(0)/kT_c$ ratio reduces the Hebel-Slichter peak, it does not appear to provide a satisfactory fit to the data. For the d-wave we have taken $2\Delta(0)/kT_c=8$ in these calculations we have used a broadening $\Gamma$ reflecting a quasiparticle lifetime [11] $\tau^{-1}=2kT_c$ at $T=T_c$ and reduced this broadening by $(T/T_c)^3$ as the temperature is lowered. The exact form
of this reduction is not important since the primary effect of the quasiparticle lifetime is to cut off the Hebel-Slichter s-wave logarithmic singularity at $T_c$. While it is possible to suppress the s-wave Hebel-Slichter peak with a sufficiently large damping rate, this would appear to require a lifetime significantly shorter than that estimated from the $\sigma_1(\omega)$, and the overall fit to $T_i^{-1}$ is not as satisfactory as the $d$-wave fit shown in Fig. 2. In addition, at low temperatures, the $T_i^{-1}$ data appear to vary as $T^3$ in agreement with the results for a $d$-wave gap [12]. However, at these low reduced temperatures where $T_i^{-1}$ has significantly decreased, other relaxation processes may become dominant.

As previously discussed [13], the coherence factor $1 + \langle q_0 + q_0 + \Delta_p + q_0 \Delta_p \rangle / E_p + q_0 E_p$ determining the low-frequency spin-fluctuation spectral weight of $g_{BCS}^{\pi \pi}$ for $q \sim (\pi, \pi)$ is finite for an $s$-wave gap and vanishes for a $d$-wave gap since $\Delta_{p_+}(\pi, \pi) = -\Delta_p$. Thus the $q \sim (\pi, \pi)$ spectral weight entering the calculation for $T_i^{-1}$ is suppressed below $T_c$ for a $d$-wave rather than exhibiting a Hebel-Slichter peak as it does for an $s$ wave. In addition, the $d$-wave single-particle density of states has only a logarithmic singularity at $\Delta$. As seen in Fig. 2, these effects along with the decrease in the Stoner enhancement factor and the damping suppress the Hebel-Slichter peak in $T_i^{-1}$ for both Cu(2) and O(2,3), providing a reasonable fit to the experimental data [14].

In Fig. 3 we show the temperature dependence of the Cu(2) anisotropy ratio $(T_i^{-1})_{ab} / (T_i^{-1})_c$. Here $(T_i^{-1})_{ab}$ is the Cu(2) nuclear relaxation rate when the magnetic field is in the $a-b$ plane. In Fig. 4, the ratio of the Cu(2) to O(2,3) relaxation rates $(T_i^{-1})_c / (T_i^{-1})_o$, normalized to their ratio at $T_c$, is shown versus the reduced temperature. Within the framework of the simple model we are analyzing, we note that the Mila-Rice hyperfine form factor for $(T_i^{-1})_{ab}$ has more weight near $q \sim (\pi, \pi)$ than does the $(T_i^{-1})_c$ form factor, which in turn has more weight near $q \sim (\pi, \pi)$ than the O(2,3) hyperfine form factor. Thus the decrease in these ratios for an $s$-wave gap reflects the decrease in the antiferromagnetic contribution to the spin-fluctuation spectral weight relative to the $q \approx (0, 0)$ part due to the opening of a gap. A similar initial decrease in this ratio occurs for a $d$-wave gap. However, at lower reduced temperatures, the $q \approx 0$ spectral weight decreases more rapidly than the $q \approx (\pi, \pi)$ spectral weight because of the nodes in the $d$-wave gap. This produces the eventual upturn for the case of a $d$-wave gap shown in Figs. 3 and 4.

From this analysis, it would appear that a gap with $d_{x^2-y^2}$ symmetry and $2\Delta(0)/kT_c$ of order 6 to 8 provides the most reasonable fit to the NMR data below $T_c$. If this is correct, it implies that the pairing interaction is repulsive at large momentum transfers and points directly to the exchange of an antiferromagnetic spin fluctuation as the mechanism responsible for superconductivity in the cuprates. However, it is also possible that the simple form of the susceptibility, Eq. (1) (and perhaps the insulating hyperfine form factors), we have used fails to adequately describe the interplay of superconductivity and spin fluctuations in these materials.

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[4] Since that work, we have found that Eq. (1) at a filling \( \langle n \rangle \approx 0.85 \) with \( \tilde{U} = 2t \) provides an excellent fit to the \( q, i\omega_m \), and \( T \) dependence of the Monte Carlo results for \( \chi(q,i\omega_m) \) obtained on an 8 x 8 lattice with \( U = 4t \) and \( \langle n \rangle \approx 0.85 \). N. Bulut, S. R. White, and D. J. Scalapino (to be published); see also L. Chen, C. Bourbonnais, T. Li, and A.-M. S. Tremblay, Phys. Rev. Lett. 66, 369 (1991).
[5] This form has been used to model the susceptibility of \(^3\text{He}\). A. J. Leggett, Rev. Mod. Phys. 47, 331 (1975); K. Maki and H. Ebisawa, Prog. Theor. Phys. 50, 1452 (1973).
[6] We have solved the BCS gap equation for a separable potential having a \( d \)-wave form, \( V(p'|p) = -|V_0|(|\cos p'_y - \cos p_y|/|\cos p'_y - \cos p_y|)\). We found that \( 1 - \Delta(T)/\Delta(0) \) decays as \( (T/T_c)^4 \) at low temperatures rather than exponentially. The effects of this on the Knight shift and \( T_{1}^{-1} \) are discussed.
[8] We have previously taken hyperfine parameters \( B/|A_{z}| = 0.25 \) and \( A_{xx}/|A_{z}| = 0.4 \), an effective Coulomb interaction \( \tilde{U} = 2t \), and a filling \( \langle n \rangle = 0.86 \). Here we will continue to use these parameters and take \( T_c = 0.10t \).
[9] The leading low-temperature dependence of the \( d_{z^2-r^2} \) gap is \( \Delta(T) = \Delta(0)[1 - a(T/T_c)^4] \) with \( a \) of order 1. However, this only gives higher-order \( (T/T_c)^4 \) corrections to the linear \( T \) dependence of \( K_\psi \). This linear dependence arises from the nodes rather than the temperature dependence of \( \Delta(0) \).
[11] Here we have in mind dynamic lifetime effects arising from spin fluctuation exchange processes rather than broadening due to impurity potential scattering. Experimentally it appears that \( \tau^{-1} = 0.6 \max(\hbar kT,\alpha) \) [R. Collins et al., Phys. Rev. B 39, 6571 (1989)], so that near \( T_c \) we have taken \( \tau^{-1} = 2kT_c \). The nature of scattering vertex corrections and the possibility that the scattering produces a gapless state near \( T_c \) are interesting questions that lie outside the analysis presented here.
[12] For a more detailed discussion see Figs. 15(e) and 18(e) in Ref. [3].
[14] Note that if the quasiparticle damping rate or the gap ratio \( 2\alpha(0)/\hbar T_c \) is reduced a small Hovel-Slichter peak will appear in the \( d \)-wave result for \( T < 1/T_c \) for \( O(2,3) \). It will be interesting to see data for \( O(2,3) \) at low magnetic fields.