NMR spectra for a nested Fermi-liquid model

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The anomalous NMR relaxation rate and Knight shift in the $YBa_2Cu_3O_7$ superconducting state contrast notably with conventional BCS theory for s-wave energy gap models. A d-wave energy gap on a nested Fermi surface with a large gap ratio $2\Delta_0 \approx 11T_c$ fits the data and is explained by using a *temperature-dependent* pairing interaction. A spin fluctuation pairing mechanism involves the susceptibility, which develops a T variation from electron collision damping. A superconducting energy gap reduces the damping below T_c, enhances the susceptibility, and therefore strengthens the pairing at low T. [S0163-1829(97)01422-7]

The first indication of d-wave symmetry for high-temperature superconductors came from the NMR relaxation data on cuprates which is much different from the standard BCS theory that explains conventional superconductors. Kitaoka *et al.*[1] noted that the low-temperature relaxation rate $1/T_1$ follows a T^3 variation that is consistent with a d-wave gap, in contrast to the exponential decrease associated with an isotropic BCS state. Near the transition temperature T_c, the cuprates do not show the Hebel-Slichter (HS) peak which is a hallmark of isotropic pairing in ordinary superconductors. Furthermore, a mysterious large energy gap ratio $2\Delta_0 \approx 11T_c$ is evident in various cuprate data, which far exceeds the traditional BCS formula $2\Delta_0 = 3.53T_c$. These primary cuprate features are shown in Fig. 1 by the Cu NMR relaxation in $YBa_2Cu_3O_7$ (YBCO) measured by Martindale *et al.*[2]

The present work explores the above anomalies which also differ from standard d-wave analyses of the NMR spectra of cuprates. We explain the cuprate gap anomaly and the T variation of the NMR relaxation and Knight shift in terms of a spin-fluctuation pairing interaction with a surprising T variation that is attributed to damping by electron collisions on a nested Fermi surface.[3] The susceptibility is reduced above T_c by damping, whereas it is resurrected at low T by a superconducting energy gap that depletes available electron scattering states. We show that realistic collision strengths on a nested Fermi surface yield an enhanced spin susceptibility at low temperature, which increases d-wave pairing at $T=0$ in comparison to the coupling at T_c.

The NMR relaxation rate is related to the spin susceptibility by[4] $(T_1T)^{-1} = (1/N)\Sigma_q |F_q|^2 \chi''(q,\omega_0)/\omega_0$ where F_q contains the hyperfine coupling and $\omega_0 \approx 10$ MHz is a typical low frequency used in NMR experiments. The lowest-order spin susceptibility is[5,6]

$$\chi(q,\omega) = \sum_{k,\sigma_1,\sigma_2} \left(\frac{\sigma_1 A_\sigma}{N}\right) \frac{\text{th}(E_k/2T) - \sigma \text{th}(E_{k+q}/2T)}{\omega + \sigma_1 E_k + \sigma_2 E_{k+q} + i\delta}, \tag{1}$$

where $\sigma = -\sigma_1\sigma_2$, with $\sigma_1, \sigma_2 = \pm 1$, and

$$A_\sigma = \frac{1}{4}\left\{1 + \sigma\left(\frac{\epsilon_k \epsilon_{k+q} + \Delta_k \Delta_{k+q}}{E_k E_{k+q}}\right)\right\}. \tag{2}$$

The energy dispersion ϵ_k is related to the superconducting state energy $E_k = +\sqrt{\epsilon_k^2 + \Delta_k^2}$. The gap is obtained from the BCS gap equation

$$\Delta_p = -\int \frac{d^2k}{(2\pi)^2} V(p-k) \frac{\text{th}(E_k/2T)}{2E_k} \Delta_k, \tag{3}$$

where $V(p-k)$ is the electron pairing interaction. The limiting behavior of the gap as $T \to 0$ and $T \to T_c$ leads to a

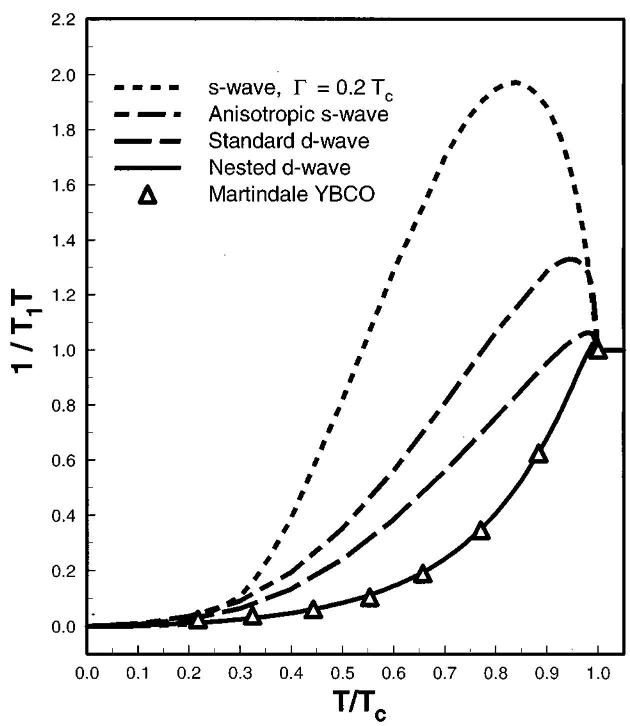

FIG. 1. The Cu NMR relaxation rate of YBCO measured by Martindale *et al.* (triangles) displays the anomalous drop in the superconducting state that is far below conventional BCS theories. An isotropic gap yields a large HS peak shown by the dotted curve even for a density of states smeared by a damping $\Gamma = 0.2T_c$; the anisotropic s-wave gap $\Delta_a \propto |\cos(2\phi)|$ gives the dot-dashed curve and the standard d-wave model for an anisotropic Fermi surface yields the dashed curve. The solid curve is calculated for a d-wave gap on a nested Fermi surface using $\mu = 0.9$, $a_{\text{nd}} = 6.3$, and $b_{\text{nd}} = 1.3$.

phenomenological form for the temperature variation of the gap $\Delta_0(T) = a_i T_c \text{th}(b_i\sqrt{T_c/T-1})$,[7] which gives the standard coefficients for an isotropic s-wave gap, $a_s=1.76$ and $b_s=1.74$, in this weak-coupling limit. The conventional d-wave analysis for an isotropic Fermi surface and a gap $\Delta_d=\Delta_0(T)\cos(2\phi)$, where ϕ is the polar angle in k space, yields $a_d=2.38$ and $b_d=1.65$.

Assuming a constant form factor, the Cu NMR relaxation rate follows from the small-ω approximation of the susceptibility which gives

$$\frac{1}{T_1}=\frac{\pi F^2}{4}\int_{-\infty}^{\infty}dE\{N^2(E)+M^2(E)\}\text{sech}^2\left(\frac{E}{2T}\right), \quad (4)$$

where $N(E)=(1/N)\Sigma_k\delta(E-W_k)$ and $M(E)=(1/N)\Sigma_k\{\delta(E-W_k)(\Delta_k/W_k)\}$. Here $W_k=E_k\{\Theta(\epsilon_k)-\Theta(-\epsilon_k\}$.

The standard BCS isotropic gap Δ creates a square root singularity in the density of states which combines with the coherence factors to generate a prominent HS peak in the NMR rate as shown by the dotted curve in Fig. 1. The conventional d-wave gap $\Delta_d=\Delta_0\cos(2\phi)$ analysis (dot-dashed curve) is also higher than the experimental points, and yields a logarithmic singularity in the density of states (DOS) that produces a small peak below T_c. This peak persists even though the coherence factor $M(E)$ vanishes because of the sign change in the order parameter. An anisotropic s state of the simple form $\Delta_a=\Delta_0|\cos(2\phi)|$ (dashed curve) has a nonvanishing $M(E)$ and consequently pushes the relaxation rate higher than the corresponding d-wave result.

The T^2 variation of the $(T_1T)^{-1}$ data in Fig. 1 at low temperature favors a d-wave gap with a surprisingly large magnitude. At low T, the conventional d-wave analysis yields $T_1(T_c)T_c/(T_1T)\approx(\pi^2/3)(T/\Delta_0)^2$ which can be used to extract Δ_0. Earlier fits to NMR data[8–10,1] also require large energy gap estimates. Evidence for a large d-wave energy gap in cuprates is provided by the break-junction tunneling spectra of Bi2212 (Ref. 11) and Raman spectra.[12]

We consider a model energy band $\epsilon(k)=v_F\{|k_x|+|k_y|\}$, which gives a perfectly nested Fermi surface. This dispersion is defined in the first Brillouin zone and continued periodically to other zones. Nesting yields[3] the anomalous linear frequency variation of the quasiparticle damping which characterizes most of the high-temperature superconductors. Photoemission evidence for nesting in cuprates has been discovered by Shen *et al.*[13]

Assuming a model d-wave gap $\Delta_d=\Delta(|k_x|-|k_y|)$ we obtain a superconducting density of states ($v=\pi/a\equiv1,\mu=$ Fermi energy)

$$N_{nd}(E)=\sum_{i=1}^{5}\frac{|E-\mu|}{\Delta\pi^2}\eta_i\Theta(E-E_{i-1})\Theta(E_i-E), \quad (5)$$

where $\eta_1=\arccos(B_+/D)$, $\eta_2=\eta_1+\arcsin(B_-/D)$, $\eta_3=\pi/2$, $\eta_4=\arcsin(\Delta C_1/D)$, $\eta_5=\arcsin(\Delta C_2/D)$, and

$$B_{\pm}=\Delta^2\mu\pm\sqrt{(1+\Delta^2)(E-\mu)^2-\Delta^2\mu^2}, \quad (6)$$

$$C_1=\mu+\sqrt{(1+\Delta^2)(E-\mu)^2-\Delta^2\mu^2}, \quad (7)$$

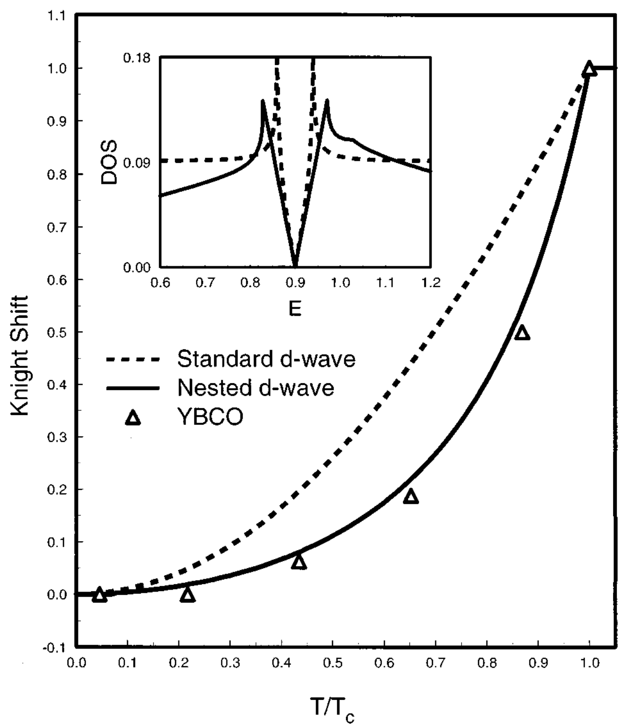

FIG. 2. Knight shift data on YBCO exhibits a decrease below T_c that is lower than conventional d-wave models with isotropic energy bands (dashed curve). The solid curve is calculated for the nesting model using the same a_{nd} and b_{nd} gap parameters that fit the NMR data. The different behavior of the densities of states in the two models is shown in the inset using $\Delta=0.08$ (solid) and $\Delta=0.04$ (dashed) for the nested and isotropic models, respectively. The two curves are scaled so as to give the same normal density of states at the Fermi energy.

$$C_2=(2-\mu)-\sqrt{(1+\Delta^2)(E-\mu)^2-\Delta^2(2-\mu)^2}, \quad (8)$$

$$D=(1+\Delta^2)|E-\mu|. \quad (9)$$

The region limits are $E_0=0$, $E_1=\mu(1-\Delta)$, $E_2=\mu\{1-\sqrt{\Delta^2/(1+\Delta^2)}\}$, $E_3=\mu(1+\Delta)$, $E_4=\mu+\sqrt{(1-\mu)^2+\Delta^2}$, and $E_5=2$. As shown in the inset of Fig. 2, this density of states does not have a singular peak which is important for the HS peak structure. The finite peaks of the DOS are located at $|E-\mu|\approx\mu\Delta$, the effective gap, which is the maximum value of the gap over the Fermi surface, and not at Δ which is the maximum over the whole Brillouin zone. At low T, this model gives $T_1(T_c)T_c/(T_1T)\approx(\pi^4/12)(T/\mu\Delta)^2$ and a fit to the YBCO data in Fig. 1 requires a large gap $\mu\Delta(T=0)=5.7T_c$.

Independent evidence for a large gap in YBCO is available from the Knight shift, which is given by

$$\frac{K(T)}{K(T_c)}=\frac{\int_{\infty}^{-\infty}dEN_{\text{nd}}(E,\Delta)\text{sech}^2(E/2T)}{4T_cN_{\text{nd}}(\mu,\Delta=0)}. \quad (10)$$

Using the same gap function as in the previous NMR fit, we compare the theoretical fit with the YBCO Knight shift data of Barrett *et al.*[14] in Fig. 2. The reasonable fit of the nested d-wave model using the same a_{nd} and b_{nd} implies that the gap variation is the dominant contributor to the experimental points, since the Knight shift measures the response

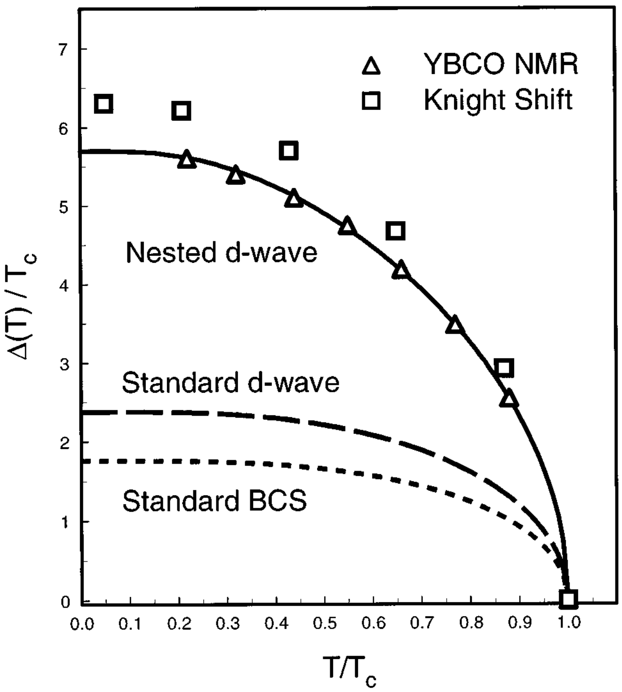

FIG. 3. Using the nesting model the energy gap in YBCO is estimated from the NMR data by triangles and the Knight shift data by squares. Much smaller values of the gap are predicted by a standard BCS isotropic gap (dotted curve) and conventional d-wave theories for isotropic energy bands (dashed curve). The present fit for the NMR data is shown by the solid curve.

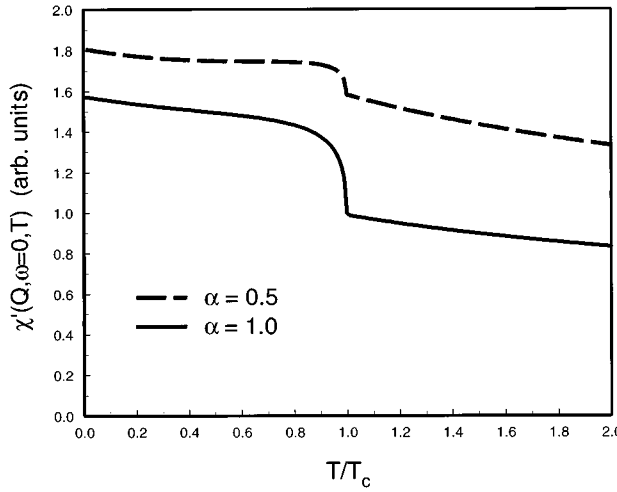

FIG. 4. Real part of the spin susceptibility for a nested Fermi surface shows the surprising increase below T_c that explains the anomalous energy gap ratio estimated for YBCO from the NMR data when the damping coefficient $\alpha=1$ (solid curve). The dashed curve shows the susceptibility for weaker damping with $\alpha=0.5$.

in the limit of long wavelengths and negligible frequency where self-energy and vertex corrections to $K(T)$ cancel.[6] The decrease in $K(T)$ confirms singlet spin pairing in cuprates. The remarkable large gap is compared to the conventional forms derived by Gross *et al.*[7] in Fig. 3: The triangles are extracted from the NMR relaxation data and the squares represent points estimated from the Knight shift.

The solid curve in Fig. 3 is the gap function that we use to fit the NMR data. We propose that the nested topology of the Fermi surface can explain the large gap ratio $\Delta(0)/T_c$ within the weak-coupling spin fluctuation exchange theory. Using a Hubbard model Hamiltonian, with the on-site Coulomb repulsion U, the lowest-order pairing interaction is obtained from the product of two spin susceptibility contributions in the form $V_d(p-k)\propto U^3\{\chi'(p-k)\}^2$. Berk and Schrieffer[15] originally found that this mechanism opposes d-state pairing in metals with a free electron dispersion. Scalapino *et al.*[16] obtained a weak attraction in the d-wave channel for a tight-binding model in lowest-order and they argued that the random phase approximation (RPA) series for the susceptibility will enhance χ, and consequently elevate the pairing strength when the system is close to an antiferromagnetic instability defined by $U\chi'\approx 1$. Nesting of the Fermi surface enhances the d-wave pairing to the point that the leading-order spin-fluctuation terms can give $T_c\approx 100$ K for an orbit topology that resembles the Bi2212 superconductor.[17] Pair breaking due to the quasiparticle scattering lifetime has been argued to suppress the superconducting T_c.[18]

Our analysis considers a temperature-dependent pairing interaction originating from the large self-energy contribution to the renormalization of the spin susceptibility. Consider an effective interaction $V(q)=U(T)\Sigma_j\delta(q-Q_j)$, where $Q_j=\pm(\mu,\pm\mu)$ in the gap equation (4). Assuming the model band dispersion and gap function with d-wave symmetry as presented before, we can obtain an approximate relation $\Delta_c(T=0)/T_c\approx 2U(T=0)/U(T_c)$ if the system is sufficiently removed from half-filling. Δ_c is the magnitude of the d-wave gap at the corners of the Fermi surface. The previous NMR analysis suggests a gap ratio $\Delta_c\approx 6T_c$ which then requires that the pairing coupling at $T=0$ be roughly 3 times greater than its value at T_c. The spin susceptibility therefore needs to increase at low T to reach $\chi'(T=0)\approx\sqrt{3}\chi'(T_c)$. This radical change is unexpected in previous calculations of susceptibilities for tight-binding models.

The nested property of the Fermi surface has been known to generate the anomalous damping $\Gamma=\alpha\omega$ which suppresses the susceptibility in the normal state.[3] Thus elimination of scattering states by a d-wave superconducting energy gap decreases the damping and thereby enhances the susceptibility at $T=0$. We examine this idea for the nesting model which gives the lowest-order susceptibility

$$\chi''_{\rm nd}(Q,\omega)=\frac{\pi}{2}N_{\rm nd}\left(\frac{\omega}{2}\right)\mathrm{th}\left(\frac{\omega}{4T}\right). \qquad (11)$$

We approximate the collision damping within the Born approximation, and obtain a model that represents the physical ingredients caused by a d-wave gap; i.e., we take[19]

$$\Gamma_{\rm nd}(\omega)=\alpha\left\{\frac{|\omega|^3}{9\Delta^2}\Theta(3\Delta-|\omega|)+|\omega|\Theta(|\omega|-3\Delta)\right\}, \qquad (12)$$

where $\alpha\approx 1$ is the magnitude estimated from optical spectra of cuprates. Including the self-energy contributions to the susceptibility gives a renormalized real part

$$\chi'_{\rm nd}(Q,\omega,T)=\mathrm{Re}\int\frac{N_{\rm nd}(\omega')\mathrm{th}(\omega'/2T)d\omega'}{\omega+2\omega'+i\Gamma(\omega,\omega')}, \qquad (13)$$

with $\Gamma(\omega,\omega')=\Gamma_{nd}(\omega')+\Gamma_{nd}(\omega+\omega')$.

A numerical integration yields the susceptibility shown in Fig. 4 for the case $\omega=0$. A value of $\alpha=1$ yields an enhanced susceptibility at $T=0$ whose magnitude is quite suitable for explaining the large gap value in cuprates by this spin fluctuation mechanism. The sensitivity of χ' to the damping strength is illustrated for $\alpha=0.5$ in Fig. 4. Calculations for finite frequency support the general trends shown in Fig. 4. Contributions from the real part of the self-energy, vertex corrections, and the dependence of the response on the Fermi energy will be examined in future work. It should be noted that the RPA series will further enhance the susceptibility at $T=0$ relative to T_c.

Numerical computations for tight-binding models with a Hubbard interaction by Monthoux and Scalapino[20] and Pao and Bickers[21] have generated a large energy gap whose origin is attributed to the pair-breaking terms from their electron self-energy model. These calculations use an effective interaction with a RPA enhancement whose value is fixed very close to a spin density wave (SDW) instability. However, their computed susceptibilities show only a small temperature variation, in contrast to our results.

Several groups have proposed phenomenological forms of the quasiparticle damping as another explanation for the suppressed Hebel-Slichter peak as discussed by Tewari and Ruvalds.[22] Tewari and Ruvalds have found that Fermi-liquid damping with realistic magnitudes cannot remove the HS peak for an s-wave gap, although a significant reduction is possible.

The association of the large gap value at zero temperature with the quasiparticle damping shows how the electron collisions reduce the transition temperature to the 100 K regime found in cuprates. Reduced damping could accordingly be expected to lead to a room-temperature superconductor, providing that the d-wave pairing mechanism remains intact.

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