PHYSICAL REVIEW B VOLUME 55, NUMBER 18 1 MAY 1997-II

Determining the structure of the superconducting gap in Cu_2O_3 two-leg ladder materials

N. Bulut and D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106-9530

(Received 21 February 1997)

Superconductivity has been recently observed in $Sr_{0.4}Ca_{13.6}Cu_{24}O_{41.84}$ which contains quasi-one-dimensional Cu_2O_3 two-leg ladders. If, as suggested by some theories, the superconductivity arises from these two-leg ladders, it will be important to determine the structure of the superconducting gap. In particular, does the gap on a two-leg ladder change sign when one goes from the bonding to antibonding Fermi surface points? Here we carry out phenomenological calculations of nuclear relaxation rates and inelastic-neutron-scattering intensity in order to provide estimates of the experimental resolution that will be required to determine the structure of the superconducting gap associated with an array of weakly coupled two-leg ladders.
[S0163-1829(97)51218-5]

Recently Uehara *et al.*[1] have reported the observation of superconductivity at 12 K in $Sr_{0.4}Ca_{13.6}Cu_{24}O_{41.84}$ under 3 GPa of pressure. This material consists of alternate planes containing Cu_2O_3 two-leg ladders and single CuO_2 chains separated by Sr-Ca layers. The appearance of superconductivity is consistent with theoretical predictions of pairing in doped two-leg ladders.[2–5] However, further measurements to determine whether pairing in fact occurs on the two-leg ladders and the nature of this pairing will determine to what extent the observed superconductivity is related to the theoretical predictions. In particular, according to the theoretical calculations, the pairing on the two-leg ladders is $d_{x^2-y^2}$-like in that the sign of the gap at the two-bonding band Fermi surface points is opposite to that at the antibonding band Fermi surface points. Alternatively, in a stronger coupling local view, this means that in the real-space superposition of the singlets that makes up the pair, there is a minus sign difference between a singlet across a rung and a near-neighbor singlet along a leg. Now, as opposed to the two-dimensional case in which the node associated with a gap having $d_{x^2-y^2}$-like symmetry gives rise to a linear low-temperature dependence of the Knight shift and the penetration depth, the two-leg ladder is nodeless and, for example, the low-temperature Knight shift will decay exponentially on a scale set by the magnitude of the gap. Knight-shift measurements will thus be unable to distinguish a gap which changes sign on the bonding and antibonding Fermi surfaces from one which does not. However, nuclear relaxation times as well as the inelastic neutron-scattering intensity depend upon coherence factors and thus should in principle allow one to determine the relative sign difference of the gap. Here we present the results of a phenomenological calculation of these quantities in order to estimate what experimental resolution will be required to determine the gap structure on the two-leg ladder. We will compare the results for the $d_{x^2-y^2}$-like gap with those of an s-like gap which has the same sign at the bonding and antibonding Fermi surface points.[6]

Both the nuclear relaxation times and the neutron-scattering intensity depend upon the magnetic susceptibility. Here we use a phenomenological random-phase approximation (RPA)-BCS form for $\chi(\mathbf{q},\omega)$, which we previously introduced to describe the layered cuprates.[7] In this approach, the short-range antiferromagnetic correlations are taken into account by using the RPA form

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

with $\overline{U}$ as a parameter. The superconducting correlations are modeled by using a BCS form for $\chi_0(\mathbf{q},\omega)$:

$$\begin{aligned}\chi_0(\mathbf{q},\omega)=\frac{1}{N}\sum_{\mathbf{p}}&\left\{\frac{1}{2}\left[1+\frac{\varepsilon_{\mathbf{p}}\varepsilon_{\mathbf{p+q}}+\Delta_{\mathbf{p}}\Delta_{\mathbf{p+q}}}{E_{\mathbf{p}}E_{\mathbf{p+q}}}\right]\right.\\ &\times\frac{f(E_{\mathbf{p+q}})-f(E_{\mathbf{p}})}{\omega-(E_{\mathbf{p+q}}-E_{\mathbf{p}})+i\delta}\\ &+\frac{1}{4}\left[1-\frac{\varepsilon_{\mathbf{p}}\varepsilon_{\mathbf{p+q}}+\Delta_{\mathbf{p}}\Delta_{\mathbf{p+q}}}{E_{\mathbf{p}}E_{\mathbf{p+q}}}\right]\frac{1-f(E_{\mathbf{p+q}})-f(E_{\mathbf{p}})}{\omega+(E_{\mathbf{p+q}}+E_{\mathbf{p}})+i\delta}\\ &+\frac{1}{4}\left[1-\frac{\varepsilon_{\mathbf{p}}\varepsilon_{\mathbf{p+q}}+\Delta_{\mathbf{p}}\Delta_{\mathbf{p+q}}}{E_{\mathbf{p}}E_{\mathbf{p+q}}}\right]\\ &\left.\times\frac{f(E_{\mathbf{p+q}})+f(E_{\mathbf{p}})-1}{\omega-(E_{\mathbf{p+q}}+E_{\mathbf{p}})+i\delta}\right\}.\end{aligned} \tag{2}$$

Here $\Delta_{\mathbf{p}}$ is the superconducting gap, $\varepsilon_{\mathbf{p}}$ is the bare quasiparticle dispersion, $E_{\mathbf{p}}=\sqrt{\varepsilon_{\mathbf{p}}^2+\Delta_{\mathbf{p}}^2}$, and f is the usual Fermi factor. The quasiparticle dispersion of the two-chain tight-binding model with the hopping matrix element t along the chains and $t_\perp$ along the rungs is

$$\varepsilon_{\mathbf{p}}=-2t\cos p_x-t_\perp\cos p_y-\mu, \tag{3}$$

where μ is the chemical potential. For simplicity, we will consider the case of isotropic hopping $t_\perp=t$. In order to model a $d_{x^2-y^2}$ superconductor we use the simple form

$$\Delta_{\mathbf{p}}=\frac{\Delta_0}{2}(\cos p_x-\cos p_y). \tag{4}$$

Since we are interested in the low-frequency magnetic response of the system, the only important feature of this gap form is that $\Delta_{\mathbf{p}}$ is finite and has different signs on the bonding ($p_y=0$) and antibonding ($p_y=\pi$) Fermi surface points.

One could have modeled the $d_{x^2-y^2}$ gap just as well by using a form which is $+\Delta_0$ on the bonding band and $-\Delta_0$ on the antibonding band. In order to distinguish the $d_{x^2-y^2}$ gap, we will also make comparisons with results obtained from an s type of gap having the form

$$\Delta_{\mathbf{p}}=\left|\frac{\Delta_0}{2}(\cos p_x-\cos p_y)\right|. \tag{5}$$

In obtaining the following results we have assumed a mean-field superconducting transition temperature $T_c=0.1t$, electronic filling $\langle n\rangle=0.85$, and $\bar{U}=1.5t$. We have also assumed a BCS temperature dependence for the magnitude of the gap with $2\max[\Delta(\mathbf{p}_F)]=7T_c$, where $\max[\Delta(\mathbf{p}_F)]$ is the maximum value of the gap at the Fermi points. Our conclusions will not depend on small variations in these parameters.

We will study the longitudinal relaxation rate T_1^{-1} for ^{63}Cu and ^{17}O nuclei. The nuclear relaxation rate T_1^{-1} is given by

$$\frac{1}{T_1}=\frac{T}{N}\sum_{\mathbf{q}}|A(\mathbf{q})|^2\lim_{\omega\to 0}\frac{\mathrm{Im}\chi(\mathbf{q},\omega)}{\omega}, \tag{6}$$

where $|A(\mathbf{q})|^2$ is the form factor of the corresponding nuclei. For a Cu_2O_3 ladder, the T_1^{-1} response of the oxygen nuclear spins depends on whether they are located on a chain (along the x axis) or on a rung (along the y axis). We will assume that the hyperfine Hamiltonian determining the relaxation of the oxygen nuclear spins is dominated by a transferred hyperfine coupling to the electronic spins centered at the two neighboring Cu sites. The resulting hyperfine form factor of a chain ^{17}O nuclei is given by

$$|A_O^{\mathrm{chain}}(\mathbf{q})|^2=4|A_O|^2\cos^2(q_x/2), \tag{7}$$

while that of a rung ^{17}O is

$$|A_O^{\mathrm{rung}}(\mathbf{q})|^2=4|A_O|^2\cos^2(q_y/2). \tag{8}$$

We note that for $q_y=\pi$, which corresponds to scatterings between the bonding and antibonding bands, the form factor of the rung ^{17}O nuclei vanishes. Hence the relaxation rate of the rung ^{17}O does not probe the relative phase difference of the gap on the bonding and antibonding Fermi points. Thus for this nuclear spin the $d_{x^2-y^2}$ and s-wave gaps will give the same result. However, T_1^{-1} for the chain ^{17}O are influenced by the relative phase of the superconducting gap. For the ^{63}Cu nuclei, we will assume only an onsite hyperfine coupling and use

$$|A_{\mathrm{Cu}}(\mathbf{q})|^2=|A_{\mathrm{Cu}}|^2. \tag{9}$$

This is a reasonable approximation since in the Cu_2O_3 ladder compounds the magnitude of the transferred hyperfine coupling to the near-neighbor ^{63}Cu sites is small compared to the onsite hyperfine coupling.[8,9]

Figures 1(a)–1(c) show the temperature dependence of the nuclear relaxation rate T_1^{-1} for the chain and rung ^{17}O, and ^{63}Cu nuclei. For the s-wave gap, there is a Hebel-Slichter coherence peak right below T_c for all three of the relaxation rates. As is well known, the Hebel-Slichter peak[10] is due to the nonvanishing of the coherence factor of the first term in Eq. (2) and the singularity in the superconducting density of states. For the $d_{x^2-y^2}$ gap, the T_1^{-1} of the rung ^{17}O is identical to that of the s-wave gap. This is because its form factor vanishes at $q_y=\pi$, and, also, only the magnetic fluctuations with momentum transfer $q_y=\pi$ are sensitive to the relative sign of the $d_{x^2-y^2}$ gap, while the $q_y=0$ fluctua-

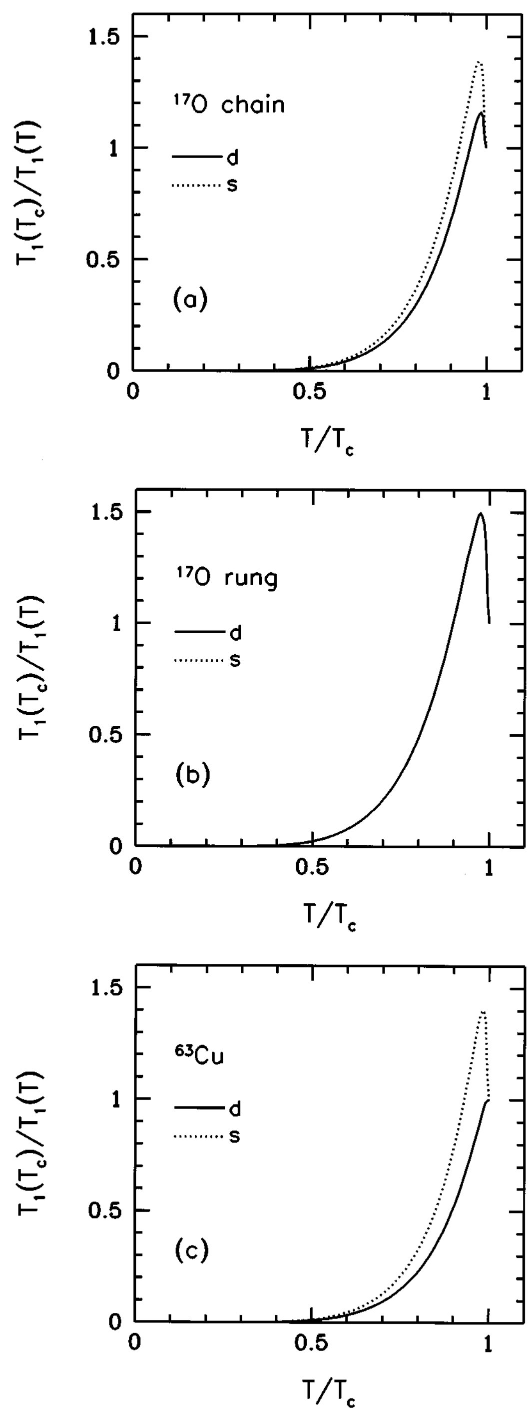

FIG. 1. Temperature dependence of the NMR rate T_1^{-1} for (a) the chain ^{17}O, (b) rung ^{17}O, and (c) ^{63}Cu nuclei obtained using the $d_{x^2-y^2}$ and s type of gaps. For the rung ^{17}O nuclei, these two gap structures yield identical results. The s-wave gap yields a Hebel-Slichter peak in all three of the T_1^{-1} rates. For the $d_{x^2-y^2}$ gap, the T_1^{-1} of the ^{63}Cu nuclei does not have a Hebel-Slichter peak, while the T_1^{-1} of the chain ^{17}O nuclei has a peak which is reduced with respect to that of the rung ^{17}O nuclei.

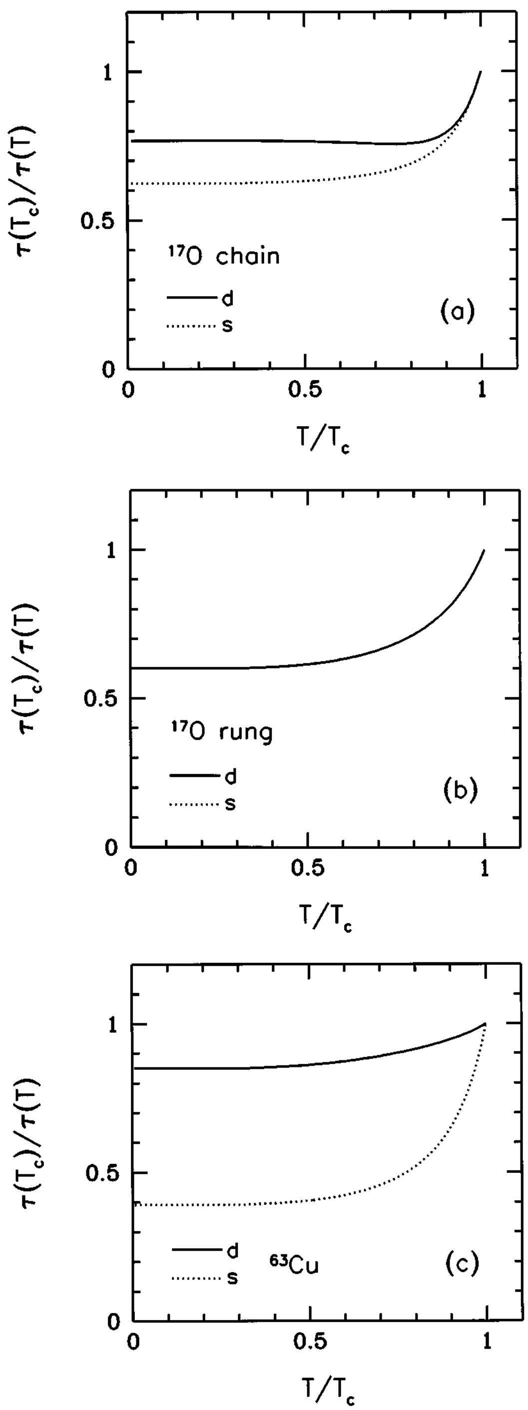

FIG. 2. Temperature dependence of the NMR rate τ^{-1} for (a) the chain ^{17}O, (b) rung ^{17}O, and (c) ^{63}Cu nuclei obtained using the $d_{x^2-y^2}$ and s type of gap structures. For the rung ^{17}O nuclei, the $d_{x^2-y^2}$ and s type of gap structures give identical results for the rung ^{17}O and similar results for the chain ^{17}O. However, measurements of τ^{-1} for ^{63}Cu can be used to make a distinction between the two gap structures.

tions are not. On the other hand, the form factor of the chain ^{17}O nuclei allows comparable contributions to the T_1^{-1} rate from both the $q_y=0$ and $q_y=\pi$ magnetic fluctuations. Consequently, for a $d_{x^2-y^2}$ gap, the T_1^{-1} of the chain ^{17}O has a reduced peak with respect to that of the rung ^{17}O.[11] At $T=T_c$, the T_1^{-1} rate of the ^{63}Cu nuclei is dominated by

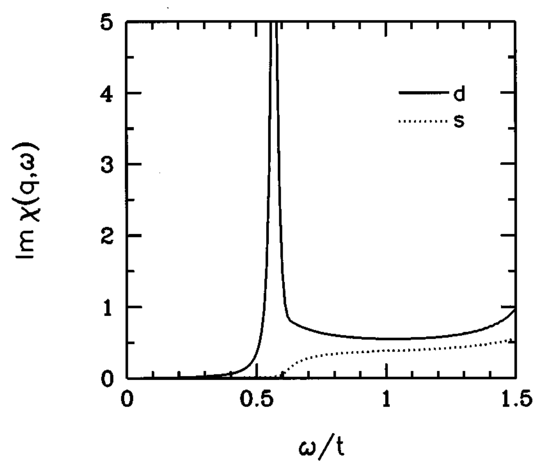

FIG. 3. Inelastic-neutron-scattering spectral weight $\mathrm{Im}\chi(\mathbf{q},\omega)$ versus ω for the $d_{x^2-y^2}$ and s type of gap structures at $T=0.5T_c$. Here, $\mathbf{q}=\mathbf{q}^*=(0.85\pi,\pi)$ is a wave vector that connects the bonding and antibonding Fermi points. For an s-wave gap, the coherence factor of the quasiparticle creation process vanishes and the neutron-scattering intensity at the gap edge $\omega=|\Delta(\mathbf{p}_{\mathrm{Fa}})|+|\Delta(\mathbf{p}_{\mathrm{Fb}})|$ is suppressed. On the other hand, for the $d_{x^2-y^2}$ gap there is a resonance at the gap edge.

antiferromagnetic fluctuations with $q_y=\pi$, and hence it does not have a Hebel-Slichter peak for a $d_{x^2-y^2}$ gap. These results show that the $d_{x^2-y^2}$ and s-wave gaps yield quite different temperature dependences for the ^{17}O and ^{63}Cu T_1^{-1} rates, hence measurements of these relaxation rates can be used to identify the structure of the superconducting gap function.

Another probe of the spin dynamics in the superconducting state is the transverse nuclear relaxation rate τ^{-1} given by[12]

$$\frac{1}{\tau^2}=\frac{1}{N}\sum_{\mathbf{q}}|A(\mathbf{q})|^4\chi^2(\mathbf{q},0)-\left(\frac{1}{N}\sum_{\mathbf{q}}|A(\mathbf{q})|^2\chi(\mathbf{q},0)\right)^2 \tag{10}$$

for a nuclear spin which has a form factor $|A(\mathbf{q})|^2$. Figures 2(a)–2(c) show the temperature dependence of τ^{-1} for the three nuclei in the superconducting state. For the rung ^{17}O, τ^{-1} is identical for the $d_{x^2-y^2}$ and s type of gap structures. It would be difficult to identify the structure of the gap from τ^{-1} of the chain ^{17}O also, since it is similar for both types of gaps. However, the results for the τ^{-1} of the ^{63}Cu nuclei are quite distinct. While there is approximately a 60% decrease in the s-wave result for τ^{-1} as the temperature is lowered in the superconducting state, for a $d_{x^2-y^2}$ gap it drops by only 15%. This reflects the fact that in the superconducting state the antiferromagnetic correlations are more strongly suppressed for an s-wave gap than for a $d_{x^2-y^2}$-wave gap.[13] Hence measurements of τ^{-1} for the ^{63}Cu nuclei would be helpful in determining the structure of the superconducting gap.

Inelastic neutron scattering is a direct probe of the spin fluctuation spectral weight $\mathrm{Im}\chi(\mathbf{q},\omega)$. The wave vectors which connect the bonding and antibonding Fermi surface points, $\mathbf{p}_{\mathrm{Fb}}=(\pm0.6\pi,0)$ and $\mathbf{p}_{\mathrm{Fa}}=(\pm0.25\pi,\pi)$, are particularly helpful in distinguishing between the $d_{x^2-y^2}$ and s type of gap structures. In Fig. 3 we show results for one such wave vector, $\mathbf{q}^*=(0.85\pi,\pi)$. Here we see that for the $d_{x^2-y^2}$ gap there is a resonance at the gap edge $\omega=|\Delta(\mathbf{p}_{Fa})|+|\Delta(\mathbf{p}_{Fb})|$. This resonance is due to the nonvanishing of the coherence factor for a $d_{x^2-y^2}$ gap which is associated with quasiparticle creation, and to the RPA form of Eq. (1). On the other hand, for an s-wave gap this coherence factor vanishes, and the quasiparticle creation process at the gap edge is suppressed.

In summary, we have shown how one can obtain information on the structure of the superconducting gap for a Cu_2O_3 ladder system from NMR and magnetic-neutron-scattering experiments. This problem is of interest because of the recent discovery of superconductivity in the ladder material $Sr_{0.4}Ca_{13.6}Cu_{24}O_{41.84}$. It is especially important to know whether the superconducting gap has different signs on the bonding and antibonding Fermi surface points, since this is relevant to our understanding of the nature of the pairing interaction. Here, we have seen that measurements of the NMR rates T_1^{-1} and τ^{-1} and the inelastic-neutron-scattering intensity can provide useful information on the structure of the superconducting gap in this compound. For the $d_{x^2-y^2}$ gap, we expect a Hebel-Slichter peak for the rung ^{17}O nuclei and a reduced peak for the chain ^{17}O, but not for the ^{63}Cu nuclei. An s type of gap structure would yield a Hebel-Slichter peak in all three of these relaxation rates. We have seen that the transverse relaxation rate τ^{-1} of the ^{63}Cu nuclei would have quite different temperature dependences for the $d_{x^2-y^2}$ and s-wave gaps. Magnetic-neutron-scattering experiments can also provide valuable information on the structure of the superconducting gap. For a wave vector that connects the bonding and antibonding Fermi surface points, the scattering intensity at the gap edge is suppressed for an s-wave gap, while we expect to observe a resonance for a $d_{x^2-y^2}$ gap structure.

The authors gratefully acknowledge support from the National Science Foundation under Grant No. DMR95-27304. The numerical computations reported in this paper were performed at the San Diego Supercomputer Center.

[1] M. Uehara, T. Nagata, J. Akimitsu, H. Takahashi, N. Môri, and K. Kinoshita, J. Phys. Soc. Jpn. **65**, 2764 (1996).

[2] E. Dagotto, J. Riera, and D. J. Scalapino, Phys. Rev. B **45**, 5744 (1992).

[3] T. M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. **23**, 445 (1993).

[4] S. Gopalan, T. M. Rice, and M. Sigrist, Phys. Rev. B **49**, 8901 (1994).

[5] R. M. Noack, S. R. White, and D. J. Scalapino, Phys. Rev. Lett. **73**, 882 (1994); Europhys. Lett. **30**, 163 (1995).

[6] In the following we will drop the qualification ''like'' and use $d_{x^2-y^2}$ to denote a gap which has different signs on the bonding and antibonding Fermi surface points and s to denote a gap which has the same sign.

[7] N. Bulut and D. J. Scalapino, Phys. Rev. Lett. **67**, 2898 (1991).

[8] K. Ishida *et al.*, J. Phys. Soc. Jpn. **63**, 3222 (1994); (unpublished).

[9] A. W. Sandvik, E. Dagotto, and D. J. Scalapino, Phys. Rev. B **53**, R2934 (1996).

[10] L. C. Hebel and C. P. Slichter, Phys. Rev. **113**, 1504 (1959).

[11] If the value of $\bar{U}$ is larger, for the $d_{x^2-y^2}$ gap, the peak in the T_1^{-1} of the chain ^{17}O nuclei can be smaller compared to that of the rung ^{17}O because of the faster loss of the low-frequency $q_y=\pi$ magnetic fluctuations as the superconducting gap opens.

[12] C. H. Pennington and C. P. Slichter, Phys. Rev. Lett. **66**, 381 (1991).

[13] The actual value of the drop in τ^{-1} of ^{63}Cu depends on the strength of the antiferromagnetic fluctuations at $T=T_c$. For instance, if one uses $\bar{U}=1.8t$ instead of $1.5t$, then the system has stronger antiferromagnetic correlations at $T=T_c$ and the drop in τ^{-1} for the $d_{x^2-y^2}$ gap is 30%, while for the s-wave gap it is 75%. Measurements of τ^{-1} and T_1^{-1} for ^{63}Cu in the normal state will determine the strength of the antiferromagnetic fluctuations in these materials.