Impurity effects in d-wave superconductors

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Impurity scattering will provide a crucial test for d-wave superconductor in high T_c copper-oxides. Among other things we calculate the static spin susceptibility and find a simple relation between the susceptibility and superfluid density $\rho_s(T) = \left[\lambda(0)/\lambda(T)\right]^2$ is broken in the presence of impurity scattering. Also we generalize Lee's universal conductivity at $T = 0$ K. In the presence of a finite concentration of impurity, the order parameter Δ_{00} in the conductivity has to be replaced by $\Delta(\Gamma, 0)$ and $\Delta(\Gamma, 0)$ is accessible through the tunneling experiment of the density of states.

I. INTRODUCTION

It is now well documented[1–4] that a small amount (a few percent) of Zn substituted for the Cu in the Cu-O_2 plane of high-T_c copper oxides like $YBa_2Cu_3O_{6+x}$ not only reduces substantially the superconducting transition temperature T_c, but also introduces substantial electronic density of states (i.e., the residual density of states) as seen through the Knight shift and nuclear spin lattice relaxation rate at low temperature. As related analyses[5–7] in heavy fermion superconductors show, this suggests that Zn provides impurity scattering in the unitarity limit common to non-s-wave superconductors. Indeed quite a few analyses have been published along this line recently.[8–13] For example Lee[11] finds a simple universal expression of the real part of the electric conductivity in the $T = \omega = 0$ limit, while Borkowski and Hirschfield[12] and Fehrenfacher and Norman[13] made a comparative study of the effect of impurity scattering on d-wave superconductors and on strongly anisotropic s-wave superconductors. However, none of them has studied the static spin susceptibility which can be measured through the Knight shift and their analysis is not complete. The object of this paper is to study the effect of impurity scattering on thermodynamics as well as some of the transport properties. We find, for example, that the present model reproduces quite well the electron density of states determined by Barbiellini *et al.*,[14] by choosing $\Gamma/\Gamma_c \simeq 0.02$ where Γ_c is the critical scattering rate necessary for the complete suppression of superconductivity.[15] Also in these general circumstances, the static spin susceptibility is no longer related to the superfluid density due to the vertex renormalization associated with impurity scattering. We recall that a similar difference between these two quantities is well known for s-wave superconductors in the presence of magnetic impurities.[16]

II. SELF-CONSISTENT EQUATION

Let us assume that the superconducting order parameter is described by an angle ϕ in the k_1-k_2 plane:

$$\Delta(\mathbf{k}) = \Delta\cos(2\phi), \tag{1}$$

where ϕ is measured from the a axis. Then in the presence of impurity scattering the Green function is given by

$$g^{-1} = i\tilde{\omega} - \xi\rho_3 - \Delta(k)\rho_1, \tag{2}$$

where ρ_1 and ρ_3 are Pauli spin operators operating in the Nambu space and $\tilde{\omega}$ is determined from[8]

$$\tilde{\omega} = \omega + i\,\Gamma \left\langle \frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2 - \Delta^2|f|^2}} \right\rangle^{-1}, \tag{3}$$

where $\Gamma = n_i/\pi N_0$, $f = \cos(2\phi)$, n_i is the impurity concentration, and N_0 is the electron density of states in the normal state on the Fermi surface per spin. Here we assumed that the scattering is in the unitarity limit (i.e., the resonance on the Fermi surface $\omega = 0$), and $\langle \cdots \rangle$ means average over ϕ.

The temperature-dependent order parameter $\Delta(\Gamma, T)$ is determined from the gap equation in the weak-coupling limit:

$$\lambda^{-1} = 4\pi T \sum_n \left\langle \frac{|f|^2}{\sqrt{\tilde{\omega}_n^2 + \Delta^2|f|^2}} \right\rangle, \tag{4}$$

where $\tilde{\omega}_n$ is the renormalized Mastubara frequency and related to ω_n by

$$\tilde{\omega}_n = \omega_n + \Gamma \left\langle \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \Delta^2|f|^2}} \right\rangle^{-1}. \tag{5}$$

In particular the transition temperature T_c and the order parameter at $T = 0$ in the presence of impurities are given by

$$-\ln\left(\frac{T_c}{T_{c0}}\right) = \psi\left(\frac{1}{2} + \frac{\Gamma}{2\pi T}\right) - \psi\left(\frac{1}{2}\right), \tag{6}$$

and

$$-\ln\left(\frac{\Delta(\Gamma,0)}{\Delta_{00}}\right) = 2\ \langle\ f^2 \ln(C_0 + \sqrt{C_0^2 + f^2})\ \rangle$$
$$-2\ \frac{\Gamma}{\Delta}\int_{C_0}^{\infty} dx\, x^{-2}\left(1 - \frac{E}{K}\right)$$
$$\times\left((1+x^2)\frac{E}{K} - 1\right), \qquad (7)$$

where $\psi(z)$ is the digamma function, $E = E(\frac{1}{\sqrt{1+x^2}})$ and $K = K(\frac{1}{\sqrt{1+x^2}})$ are the complete elliptic integrals, C_0 is determined from

$$C_0^2 = \frac{\pi\Gamma}{2\Delta}\ (1 + C_0{}^2)^{1/2}\left[K\left(\frac{1}{\sqrt{1+C_0^2}}\right)\right]^{-1}, \qquad (8)$$

and T_{c0} and Δ_{00} are the transition temperature and the order parameter at $T = 0$ K in the absence of impurity scattering. Here Eq. (6) is the well-known Abrikosov-Gor'kov formula.[15] Also the critical scattering Γ_c is given by $\Gamma_c = 0.4122\ \Delta_{00} = 0.88T_{c0}$. The same equation as Eq. (8) has been obtained already in Refs. 9 and 10. For small Γ/Δ and large Γ/Δ, Eq. (8) is solved approximately as

$$C_0 \simeq \left(\frac{\pi\Gamma}{2\Delta}\right)^{1/2}\left[\ln\left(4\sqrt{\frac{2\Delta}{\pi\Gamma}}\right)\right]^{-1},$$

and $C_0 = \frac{\Gamma}{\Delta}\ [1 + \frac{1}{4}(\frac{\Gamma}{\Delta})^{-2} + \cdots]$, respectively. Equations (6) and (7) are solved numerically and shown in Fig. 1. It is remarkable that $\Delta(\Gamma,0)/\Delta_{00}$ and T_c/T_{c0} draw almost the same curve. In the same figure we show $N(0)/N_0$ (the residual density of states at $E = 0$ at $T = 0$ K), which is accessible by the Knight shift or the T linear coefficient of the nuclear spin lattice relaxation rate. The residual density of states $N(0)/N_0$ is given by

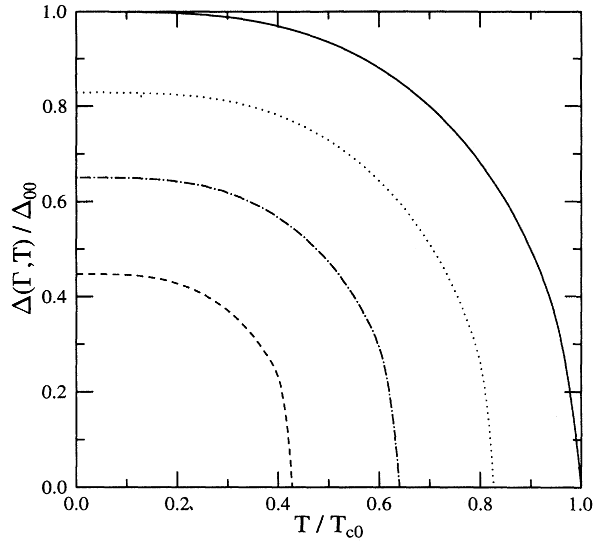

FIG. 2. The temperature-dependent order parameter $\Delta(\Gamma,T)$ for $\Gamma/\Delta_{00} = 0$ (solid line), 0.1 (dotted line), 0.2 (dash-dotted line), and 0.3 (dashed line) is shown as a function of T/T_{c0}.

$$N(0)/N_0 = \frac{2}{\pi}\ \frac{C_0}{\sqrt{1+C_0^2}}\ K\left(\frac{1}{\sqrt{1+C_0^2}}\right)$$
$$= \Gamma\ /\ (\Delta\ C_0). \qquad (9)$$

For derivation of Eq. (9), see Eq. (10) later. The temperature-dependent order parameter $\Delta(\Gamma,T)$ is obtained for a few impurity concentrations and shown in Fig. 2. A very similar result has been already obtained by Hotta.[8] Finally we show the density of states for different Γ/Δ in Fig. 3. Here the density of states is given by

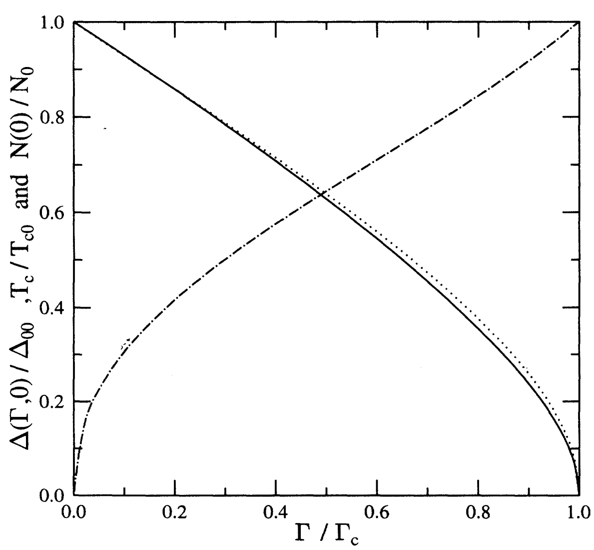

FIG. 1. $\Delta(\Gamma,0)/\Delta_{00}$ (dotted line), T_c/T_{c0} (solid line), and the residual density of states $N(0)/N_0$ (dash-dotted line) are shown as a function of Γ/Γ_c, where $\Gamma_c = 0.4122\Delta_{00}$.

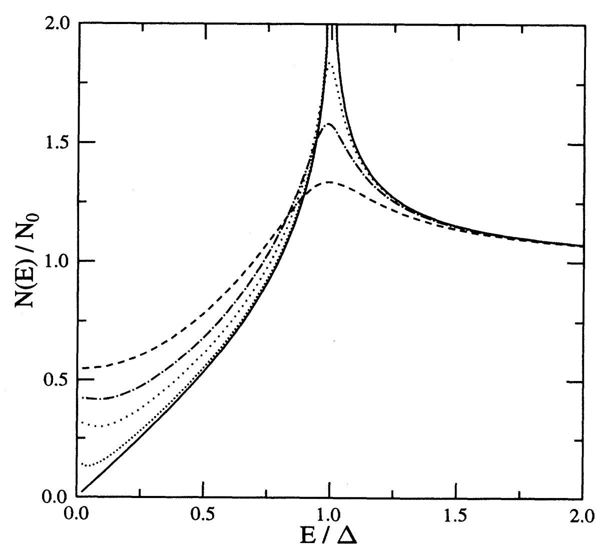

FIG. 3. The density of states for $\Gamma/\Delta = 0$ (solid line), 0.01 (dense-dotted line), 0.05 (dotted line), 0.1 (dash-dotted line), and 0.2 (dashed line) is shown as a function of E/Δ.

$$N(E)/N_0 = \text{Re}\left\langle \frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2 - \Delta^2|f|^2}} \right\rangle. \qquad (10)$$

In the limit of $\omega = E = 0$, Eq. (10) reduces to Eq. (9) where we made use of Eq. (8). The present result is somewhat different from the one obtained by Hotta.[8] For example Hotta appeared to obtain more densities of states at $E = 0$ compared with ours, though we do not know the origin of the discrepancy. But our result not only reproduces quite well the density of states determined by Barbiellini *et al.*,[14] but also appears to satisfy the density of states sum rule more consistently.

III. THERMODYNAMICS AND OTHER PROPERTIES

Making use of $\Delta(\Gamma, T)$ determined from the gap equation (4), the thermodynamics of the system is easily obtained.[17] In Fig. 4 we show $D(T/T_c)$, the derivation from the parabolic law:

$$D\left(\frac{T}{T_c}\right) = \frac{H_c(T)}{H_c(0)} - \left[1 - \left(\frac{T}{T_c}\right)^2\right], \qquad (11)$$

as a function of $(T/T_c)^2$, while in Fig. 5 the specific heat as a function of T/T_{c0} is shown. It is remarkable that the absolute value of $D(T/T_c)$ first increases and becomes largest around $\Gamma/\Delta_{00} \sim 0.15$ and then decreases as Γ increases. Also the specific heat at low temperatures is given by

$$C_s = \frac{2\pi^2}{3} N(0)\, T = \frac{N(0)}{N_0}\, \gamma_s T, \qquad (12)$$

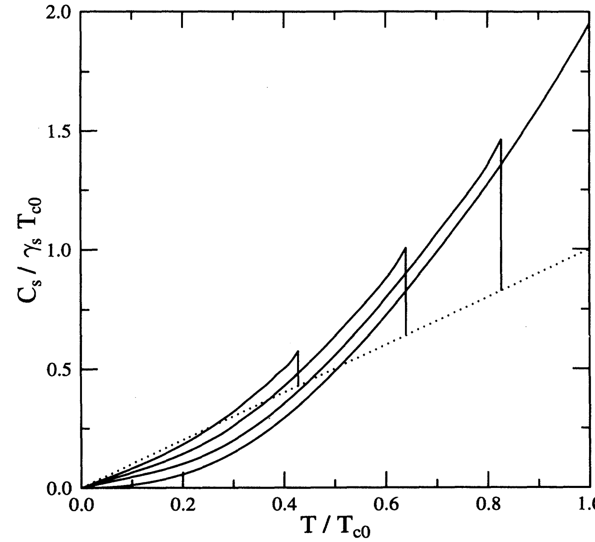

FIG. 5. The specific heat normalized by the normal state one at $T = T_{c0}$ is shown as a function of T/T_{c0} for $\Gamma/\Delta_{00} =$ 0, 0.1, 0.2, 0.3. Here the dotted line is the normal state value.

where $\gamma_s = \frac{2\pi^2}{3} N_0$ is the Sommerfeld constant.

Perhaps of more interest is the static spin susceptibility which is accessible by the Knight shift. In the absence of the Fermi-liquid correction, the susceptibility is given by

$$\chi_{\text{spin}}(0) = 2N_0\, \rho^0_{\text{spin},n}, \qquad (13)$$

with

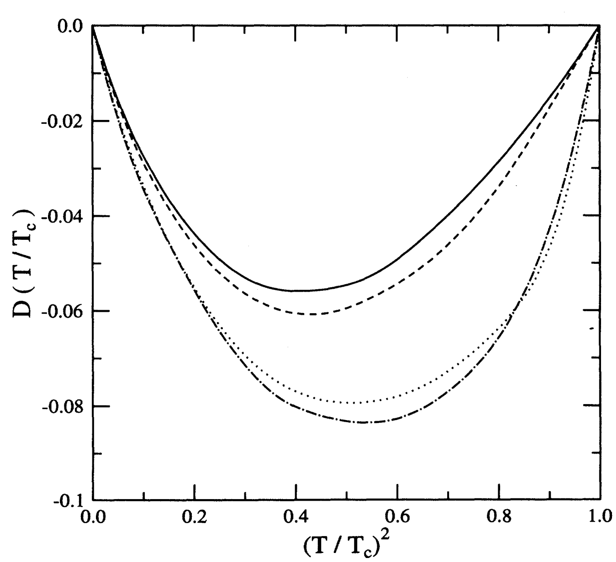

FIG. 4. The deviation $D(T/T_c) = H_c(T)/H_c(0) - [1 - (T/T_c)^2]$ is shown as a function of $(T/T_c)^2$ for $\Gamma/\Delta_{00} = 0$ (solid line), 0.1 (dotted line), 0.2 (dash-dotted line), and 0.3 (dashed line).

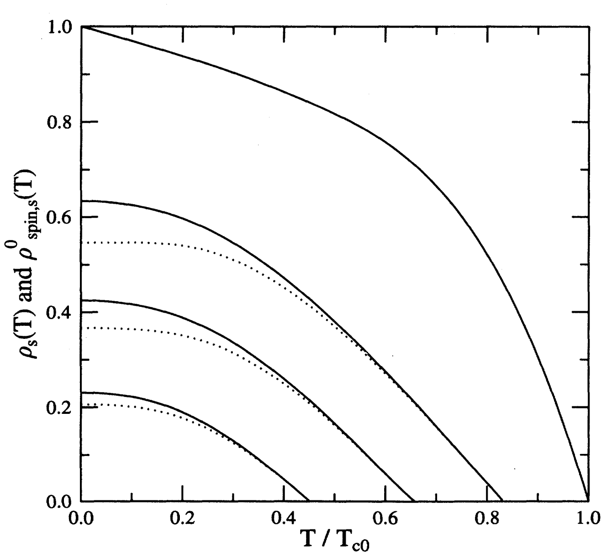

FIG. 6. The superfluid density $\rho_s(T)$ (solid line) and the spin superfluid density $\rho^0_{\text{spin},s}(T)$ (dotted line) are shown as a function of T/T_{c0} for $\Gamma/\Delta_{00} = 0$, 0.1, 0.2, 0.3 from top to bottom. Note that $\rho^0_{\text{spin},n}(T) = 1 - \rho^0_{\text{spin},s}(T)$ is measurable by the Knight shift experiment.

$$\rho^0_{\text{spin},s}(T) = 1 - \rho^0_{\text{spin},n}(T)$$
$$= 2\pi T \sum_{n=0}^{\infty} \left\langle \frac{\Delta^2|f|^2}{(\tilde{\omega}_n^2 + \Delta^2|f|^2)^{3/2}} \right\rangle \left(1 + \Gamma \left\langle \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \Delta^2|f|^2}} \right\rangle^{-2} \left\langle \frac{\Delta^2|f|^2}{(\omega_n^2 + \Delta^2|f|^2)} \right\rangle \right)^{-1}$$
$$= \frac{4T}{\Delta} \sum_{n=0}^{\infty} \frac{1}{\sqrt{\tilde{x}_n^2+1}} (K-E) \times \left(1 + \frac{\Gamma}{\Delta}\tilde{x}_n - 2\sqrt{x_n^2+1}\, K^{-2}(K-E) \right)^{-1}, \tag{14}$$

where $K = K(\frac{1}{\sqrt{\tilde{x}_n^2+1}})$ and $E = E(\frac{1}{\sqrt{\tilde{x}_n^2+1}})$ are the complete elliptic integrals and $\tilde{x}_n = \tilde{\omega}_n/\Delta_0$. At $T = 0$ K, Eq. (14) reduces to

$$\rho^0_{\text{spin},n}(0) = N(0)/N_0 , \tag{15}$$

as expected. In the presence of a Fermi-liquid correction like in the t-J model, $\rho^0_{\text{spin},n}$ has to be replaced by

$$\rho_{\text{spin},n} = \rho^0_{\text{spin},n} \left(1 + 4JN_0\, \rho^0_{\text{spin},n} \right)^{-1} . \tag{16}$$

In Fig. 6 we show $\rho^0_{\text{spin},s}$ for a few impurity concentrations as a function of T/T_{c0}. In the presence of impurity scattering, the Knight shift does not vanish at $T = 0$ K. Making use of data by Ishida *et al.*,[3] we obtain $\Gamma/\Gamma_c = 0.16$ and $\Gamma/\Gamma_c = 0.32$ from the shift in T_c of 1% and 2% Zn-substituted $YBa_2Cu_3O_7$. Then these Γ/Γ_c give the residual density of states $N(0)/N_0 = 0.34$ (0.277) and 0.47 (0.396), respectively, where in the parentheses we include the corresponding ones deduced from the Knight shift data.[3] The observed residual density of states appears to be somewhat smaller than the theory predicts. These small discrepancies ($\sim 20\%$) may be due to the fact that the order parameter in $YBa_2Cu_3O_7$ at $T = 0$ K is somewhat larger than the weak-coupling theory predicts. For example, comparing the slope of a T-linear term in $\rho_s(T)$ of a monocrystal of pure $YBa_2Cu_3O_7$ determined by Hardy *et al.*,[18] we find that the order parameter in the pure $YBa_2Cu_3O_7$ is about 33% larger than the weak-coupling theory predicts.[17] Therefore considering the fact that the residual density of states scales with $(\Gamma/\Delta)^{1/2}$, the above discrepancies are quite consistent with the notion that it is due to the strong-coupling effect.

A closely related topic is the superfluid density which is determined from the temperature dependence of the magnetic penetration depth $\lambda(T)$,

$$\rho_s(T) = [\,\lambda(0)/\lambda(T)\,]^2 = \frac{4T}{\Delta} \sum_{n=0}^{\infty} \frac{1}{\sqrt{\tilde{x}_n^2+1}} (K-E), \tag{17}$$

since we do not have any vertex correction within the present model. This result is essentially obtained already in Ref. 8. We note that in the presence of impurity scattering, the relation

$$\rho_s(T) = \rho^0_{\text{spin},s}(T) \tag{18}$$

no longer holds.

$\rho_s(T)$ is calculated numerically and also shown in Fig. 6. As noted already by Hirschfield and Goldenfeld,[9] $\rho_s(T)$ first decreases like T^2 and then this decrease changes into a T-linear law. Indeed a recent experiment by Liang *et al.*[19] confirmed this. We note also in the presence of impurity scattering $\rho_s(T) \geq \rho^0_{\text{spin},s}(T)$. Only in the vicinity of $T = T_c$ would they become equal.

Finally we comment on the electric conductivity and the nuclear spin lattice relaxation rate at the low-temperature limit. At higher temperatures the relaxation time in the electric conductivity and the nuclear spin lattice relaxation rate are determined by antiparamagnon[20–23] (or antiferromagnetic) spin fluctuation. The real part of the electric conductivity at $\omega = 0$ is given within the present model:

$$\sigma_1 = \frac{e^2 n}{m} \int_0^\infty \frac{dz}{2T} \operatorname{sech}^2\!\left(\frac{z}{2T}\right) \left\langle \frac{(\text{Re}\frac{\tilde{x}}{\sqrt{\tilde{x}^2-f^2}})^2 + (\text{Re}\frac{f}{\sqrt{\tilde{x}^2-f^2}})^2}{2\Delta\, \text{Im}\sqrt{\tilde{x}^2-f^2}} \right\rangle$$
$$= \frac{e^2 n}{2m\Delta} \int_0^\infty \frac{dz}{2T} \operatorname{sech}^2\!\left(\frac{z}{2T}\right) \left\langle \left(\text{Im}\sqrt{\tilde{x}^2-f^2}\right)^{-1} \left(1 + 2f^2 \text{Re}\frac{1}{\tilde{x}^2-f^2} + \frac{|\tilde{x}|^2+f^2}{|\tilde{x}^2-f^2|} \right) \right\rangle, \tag{19}$$

and $\tilde{x} = \tilde{\omega}/\Delta$. At $T = 0$ K, Eq. (19) reduces to

$$\sigma_1 = \frac{e^2 n}{m\Delta} \left\langle \frac{C_0^2}{(C_0^2+f^2)^{3/2}} \right\rangle = \frac{2}{\pi} \frac{e^2 n}{m\, \Delta(\Gamma,0)}, \tag{20}$$

which is essentially the universal conductivity found by Lee.[11] Of course in the present, more general circumstance $\Delta(\Gamma,0)$ depends also on Γ. Also though in the derivation we used the relation (5) for unitarity limit scattering, it is easy to show that the final result does

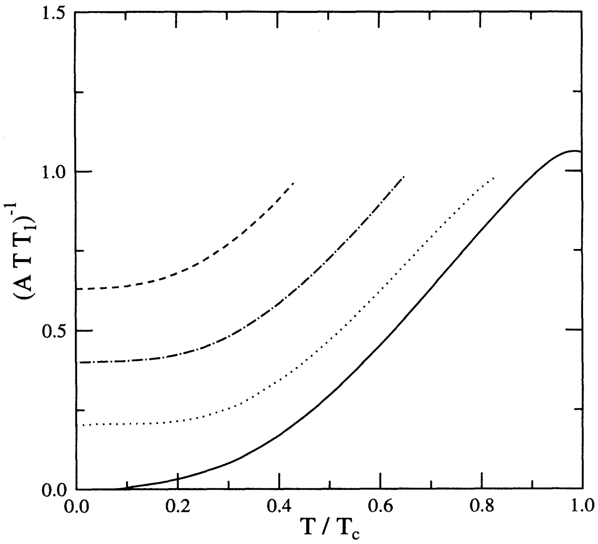

FIG. 7. The spin lattice relaxation rate due to normal electrons (excluding the antiparamagnon contribution) is shown as function of T/T_{c0} for $\Gamma/\Delta_{00} = 0$ (solid line), 0.1 (dotted line), 0.2 (dash-dotted line), and 0.3 (dashed line). $(ATT_1)^{-1}$ goes to unity in the normal state at $T = 0$ K.

not depend on the scattering phase shift at $\omega = 0$ but only on $\Delta(\Gamma, 0)$ consistent with Ref. 11. Note that we introduced Δ which is twice the one used by Lee,[11] since the present $\Delta(\Gamma, 0)$ corresponds to the peak in the density of states and is readily accessible experimentally.

Similarly the low-temperature nuclear spin lattice relaxation rate is determined by the Fermi-liquid term

$$\left(T_1T\right)^{-1} = A \int_0^\infty \frac{dz}{2T}\,\mathrm{sech}^2\left(\frac{z}{2T}\right)\left\langle \mathrm{Re}\frac{\tilde{x}}{\sqrt{\tilde{x}^2 - f^2}}\right\rangle^2$$
$$= A[N(0)/N_0]^2 \quad (\text{at } T = 0 \text{ K}) \,. \tag{21}$$

The temperature dependence of $(T_1T)^{-1}$ is evaluated and shown in Fig. 7. Unfortunately the present result at high temperatures (say, $T \geq \frac{1}{3}T_c$) cannot describe the observed T_1 as we neglected the antiparamagnon effect.[20–23]

IV. CONCLUDING REMARKS

We examine a variety of aspects of impurity scattering in d-wave superconductors. The rapid appearance of the residual density of states, $N(0)/N_0$, due to an impurity is taken as another signature of d-wave superconductors. In particular, the appearance of the residual density of states as deduced from Knight shift measurements and the nuclear spin lattice relaxation rate in Zn-doped $YBa_2Cu_3O_7$ is clearly correlated with the decrease in the transition temperature T_c. Also the change in the temperature dependence of the penetration depth is consistent with a recent experiment on the superfluid density by Liang *et al.*[19]

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[1] K. Ishida *et al.*, Physica C **179**, 29 (1991).
[2] K. Ishida *et al.*, Physica C **185-189**, 1115 (1991).
[3] K. Ishida *et al.*, J. Phys. Soc. Jpn. **62**, 2803 (1993).
[4] Y. Kitaoka, K. Ishida, and K. Asayama, J. Phys. Soc. Jpn. **63**, 2053 (1994).
[5] C. J. Pethick and D. Pines, Phys. Rev. Lett. **57**, 118 (1986).
[6] P. J. Hirschfield, D. Vollhardt, and P. Wolfle, Solid State Commun. **59**, 111 (1986); P. J. Hirschfield, P. Wolfle, and D. Einzel, Phys. Rev. B **37**, 83 (1988).
[7] S. Schmitt-Rink, K. Miyake, and C. M. Varma, Phys. Rev. Lett. **57**, 2575 (1986).
[8] T. Hotta, J. Phys. Soc. Jpn. **62**, 274 (1993).
[9] P. J. Hirschfield and N. Goldenfeld, Phys. Rev. B **48**, 4219 (1993).
[10] P. J. Hirschfield, W. O. Putikka, and D. J. Scalapino, Phys. Rev. Lett. **71**, 3705 (1993).
[11] P. A. Lee, Phys. Rev. Lett. **71**, 1887 (1993).
[12] L. S. Borkowski and P. J. Hirschfield, Phys. Rev. B **49**, 15404 (1994).
[13] R. Fehrenfacher and M. R. Norman, Phys. Rev. B **50**, 3445 (1994).
[14] B. Barbiellini *et al.*, Physica C **220**, 55 (1994).
[15] A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys. JETP **12**, 1243 (1961)].
[16] K. Maki, in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), p. 1066.
[17] See, for a parallel analysis for $\Gamma = 0$, H. Won and K. Maki, Phys. Rev. B **49**, 1397 (1994).
[18] W. N. Hardy *et al.*, Phys. Rev. Lett. **20**, 3999 (1993).
[19] R. Liang *et al.*, Phys. Rev. B **50**, 4212 (1994); W. N. Hardy *et al.*, Physica B **197**, 609 (1994).
[20] N. Bulut and D. J. Scalapino, Phys. Rev. Lett. **67**, 2898 (1991).
[21] J. P. Lu, Mod. Phys. Lett. B **2**, 547 (1992); D. Thelen, D. Pines, and J. P. Lu, Phys. Rev. B **47**, 9151 (1993).
[22] B. W. Statt and A. Griffin, Phys. Rev. B **46**, 3199 (1992); **48**, 619 (1993).
[23] H. Won and K. Maki (unpublished).