Analysis of NMR Data in the Superconducting State of $YBa_2Cu_3O_7$

N. Bulut and D. J. Scalapino
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 11 October 1991)

We have extended a weak-coupling theory of antiferromagnetic fluctuations to the superconducting state and analyzed NMR data for $YBa_2Cu_3O_7$. 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^{-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^{-1} data.

PACS numbers: 74.30.Gn

Measurements of the temperature dependence of the Cu(2) and O(2,3) nuclear relaxation rates in the normal state of $YBa_2Cu_3O_7$ 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^{-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^{-1} data.

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

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

with the irreducible susceptibility $\chi_0(\mathbf{q},\omega)$ replaced by the noninteracting tight-binding susceptibility and $\bar{U}$ 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

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

We will evaluate this expression for both an s-wave gap $\Delta_{\mathbf{p}}=\Delta(T)$ and a d-wave gap $\Delta_{\mathbf{p}}=[\Delta(T)/2](\cos p_x-\cos p_y)$. 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 $E_{\mathbf{p}}=(\varepsilon_{\mathbf{p}}^2+\Delta_{\mathbf{p}})^{1/2}$ with the tight-binding band structure $\varepsilon_{\mathbf{p}}=-2t(\cos p_x+\cos p_y)-\mu$ and μ the chemical potential.

Using the Mila-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

$$\chi(0,0)=\frac{\chi_0^{\mathrm{BCS}}(0,0)}{1-\bar{U}\chi_0^{\mathrm{BCS}}(0,0)}. \tag{3}$$

Here

$$\chi_0^{\mathrm{BCS}}(0,0)=\frac{1}{N}\sum_{\mathbf{p}}f(E_{\mathbf{p}}) \tag{4}$$

is the well-known Yosida result for a tight-binding band. From Eq. (3) it follows that as T decreases below T_c and $\chi_0^{\mathrm{BCS}}(0,0)$ falls, $K_S(T)/K_S(T_c)$ is further reduced by the decrease in the Stoner enhancement factor $[1-\bar{U}\chi_0^{\mathrm{BCS}}(0,0)]^{-1}$. 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 $2\Delta(0)/kT_c\simeq4$. 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

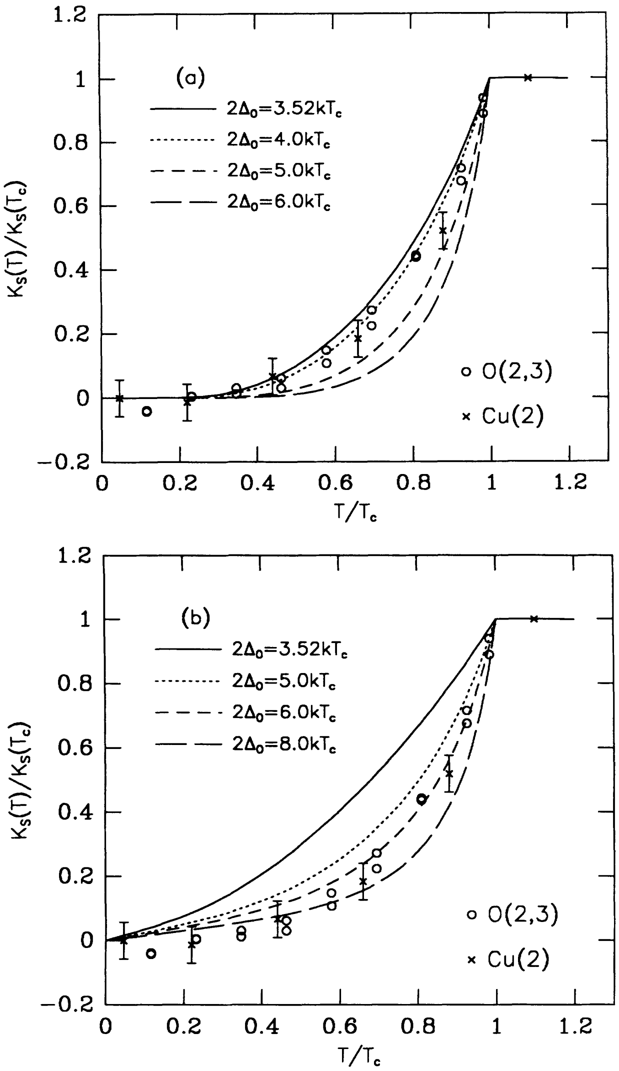

FIG. 1. Knight shift vs reduced temperature obtained from Eq. (3) for various $2\Delta(0)/kT_c$ ratios with (a) an s-wave and (b) a d-wave gap. The points represent experimental data of Barrett *et al.* [15] on Cu(2) and Takigawa and co-workers [16,17] on O(2,3).

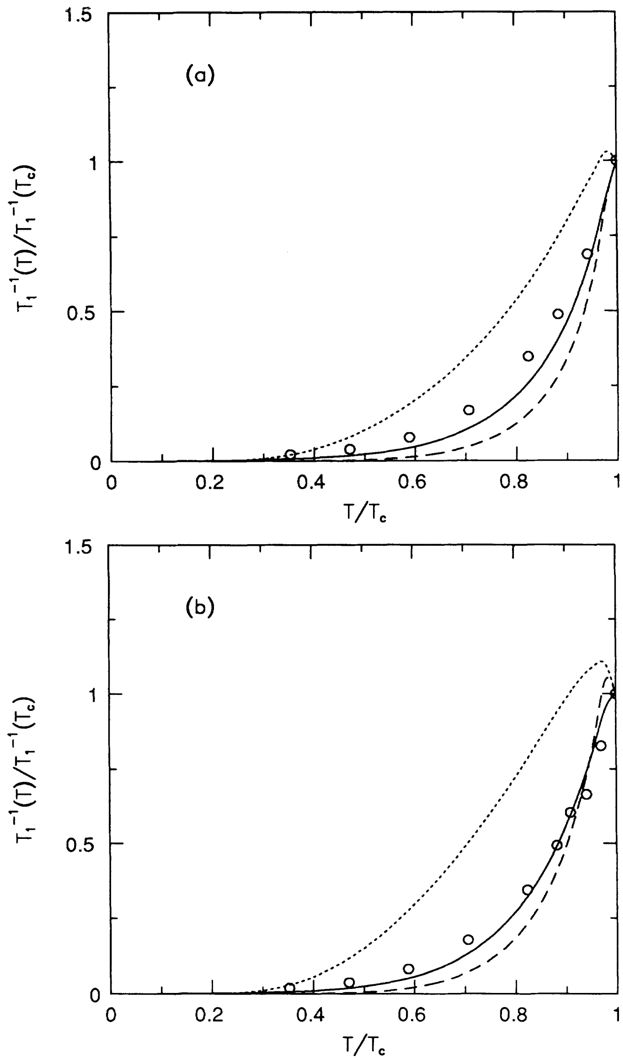

FIG. 2. Temperature dependence of the nuclear relaxation rates below T_c for (a) Cu(2) with **H** along the c axis and (b) O(2,3). The solid curve in this and the following figures is for a d-wave gap, and the dotted and the dashed curves are for an s-wave gap. The d-wave gap amplitude has been taken as $2\Delta(0)/kT_c=8$, and the s-wave gap amplitude as $2\Delta(0)/kT_c=4$ (dotted) and 8 (dashed). The quasiparticle damping rate has been taken as $\Gamma=T_c(T/T_c)^3$. The experimental data are from Hammel *et al.* [18].

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

$$T_1^{-1}=\frac{T}{N}\sum_{\mathbf{q}}|A(\mathbf{q})|^2\frac{\operatorname{Im}\chi(\mathbf{q},\omega)}{\omega}\bigg|_{\omega=0}, \tag{5}$$

where $|A(\mathbf{q})|^2$ is the appropriate Mila-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 $(T_1^{-1})_c$ 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 Γ 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

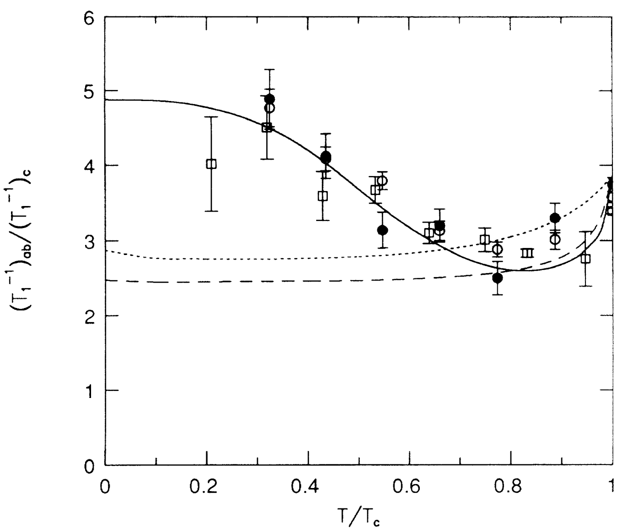

FIG. 3. Temperature dependence of the Cu(2) anisotropy $(T_1^{-1})_{ab}/(T_1^{-1})_c$. The experimental data are from Martindale *et al.* [10] (squares) and Takigawa, Smith, and Hults [19] (solid and open circles). The various curves have the same parameters as in Fig. 2.

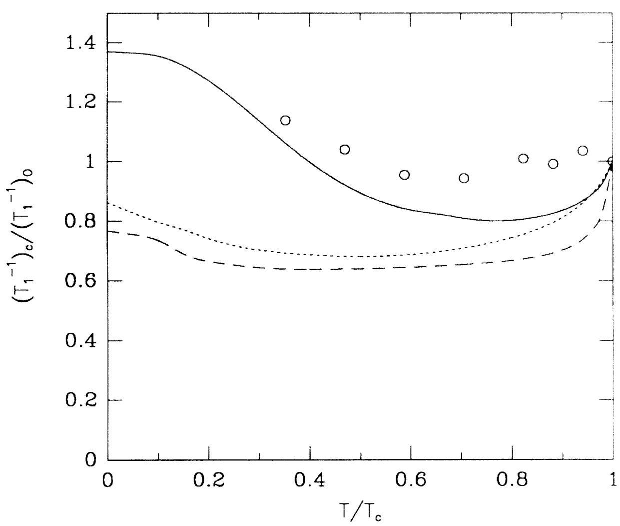

FIG. 4. Temperature dependence of the ratio of the Cu(2) and O(2,3) relaxation rates $(T_1^{-1})_c/(T_1^{-1})_O$. The experimental data are from Hammel *et al.* [18]. The various curves have the same parameters as in Fig. 2.

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_1^{-1} is not as satisfactory as the d-wave fit shown in Fig. 2. In addition, at low temperatures, the T_1^{-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_1^{-1} has significantly decreased, other relaxation processes may become dominant.

As previously discussed [13], the coherence factor $1+(\varepsilon_{\mathbf{p}+\mathbf{q}}\varepsilon_{\mathbf{p}}+\Delta_{\mathbf{p}+\mathbf{q}}\Delta_{\mathbf{p}})/E_{\mathbf{p}+\mathbf{q}}E_{\mathbf{p}}$ determining the low-frequency spin-fluctuation spectral weight of χ_0^{BCS} for $\mathbf{q}\sim(\pi,\pi)$ is finite for an s-wave gap and vanishes for a d-wave gap since $\Delta_{\mathbf{p}+(\pi,\pi)}=-\Delta_{\mathbf{p}}$. Thus the $\mathbf{q}\sim(\pi,\pi)$ spectral weight entering the calculation for T_1^{-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 Δ. 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_1^{-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 $(T_1^{-1})_{ab}/(T_1^{-1})_c$. Here $(T_1^{-1})_{ab}$ 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 $(T_1^{-1})_c/(T_1^{-1})_O$, 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 $(T_1^{-1})_{ab}$ has more weight near $\mathbf{q}\sim(\pi,\pi)$ than does the $(T_1^{-1})_c$ form factor, which in turn has more weight near $\mathbf{q}\sim(\pi,\pi)$ 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 $\mathbf{q}\simeq(0,0)$ 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 $\mathbf{q}\simeq 0$ spectral weight decreases more rapidly than the $\mathbf{q}\simeq(\pi,\pi)$ 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.

We would like to acknowledge useful discussions with J. R. Schrieffer, C. P. Slichter, and M. Takigawa. We also thank the latter two authors for providing us with the data shown in the figures. This work was partially supported by the National Science Foundation under Grants

No. DMR90-02492 and No. PHY89-04035, and the Electric Power Research Institute. The numerical calculations reported in this paper were performed at the San Diego Supercomputer Center.

[1] N. Bulut, D. Hone, D. J. Scalapino, and N. E. Bickers, Phys. Rev. B **41**, 1797 (1990); Phys. Rev. Lett. **64**, 2723 (1990).

[2] A. J. Millis, H. Monien, and D. Pines, Phys. Rev. B **42**, 167 (1990).

[3] For a more extensive analysis, see N. Bulut and D. J. Scalapino, Phys. Rev. B (to be published).

[4] Since that work, we have found that Eq. (1) at a filling $\langle n\rangle \simeq 0.85$ with $\bar{U}=2t$ provides an excellent fit to the **q**, $i\omega_m$, and T dependence of the Monte Carlo results for $\chi(\mathbf{q},i\omega_m)$ obtained on an 8×8 lattice with $U=4t$ and $\langle n\rangle \simeq 0.85$. 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}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, $V(\mathbf{p}'|\mathbf{p})=-|V_0|(\cos p_x' - \cos p_y')(\cos p_x - \cos p_y)$. We found that $1-\Delta(T)/\Delta(0)$ decays as $(T/T_c)^3$ at low temperatures rather than exponentially. The effects of this on the Knight shift and T_1^{-1} are discussed.

[7] F. Mila and T. M. Rice, Physica (Amsterdam) **157C**, 561 (1989).

[8] We have previously taken hyperfine parameters $B/|A_{zz}|=0.25$ and $A_{xx}/|A_{zz}|=0.4$, an effective Coulomb interaction $\bar{U}=2t$, 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 $d_{x^2-y^2}$ gap is $\Delta_d(T)=\Delta_d(0)[1-a(T/T_c)^3]$ with a of order 1. However, this only gives higher-order $(T/T_c)^4$ corrections to the linear T dependence of K_S. This linear dependence arises from the nodes rather than the temperature dependence of $\Delta_d(T)$.

[10] J. A. Martindale, S. E. Barrett, C. A. Klug, K. E. O'Hara, S. M. DeSoto, C. P. Slichter, T. A. Friedmann, and D. M. Ginsberg, this issue, Phys. Rev. Lett. **68**, 702 (1992).

[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 $\tau^{-1} \simeq 0.6\max(\pi kT,\omega)$ [R. Collins *et al.*, Phys. Rev. B **39**, 6571 (1989)], so that near T_c we have taken $2\Gamma=2kT_c$. 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].

[13] D. J. Scalapino, *High Temperature Superconductivity*, edited by K. S. Bedell, D. Coffey, D. Meltzer, D. Pines, and J. R. Schrieffer (Addison-Wesley, Reading, MA, 1990); J. P. Lu (to be published) has recently discussed the same feature of a d-wave gap.

[14] Note that if the quasiparticle damping rate or the gap ratio $2\Delta(0)/kT_c$ is reduced a small Hebel-Slichter peak will appear in the d-wave result for T_1^{-1} for O(2,3). It will be interesting to see data for O(2,3) at low magnetic fields.

[15] S. E. Barrett *et al.*, Phys. Rev. B **41**, 6283 (1990).

[16] M. Takigawa, P. C. Hammel, R. H. Heffner, and Z. Fisk, Phys. Rev. B **39**, 7371 (1989).

[17] M. Takigawa, P. C. Hammel, R. H. Heffner, Z. Fisk, K. C. Ott, and J. D. Thompson, Physica (Amsterdam) **162-164C**, 853 (1989).

[18] P. C. Hammel, M. Takigawa, R. H. Heffner, Z. Fisk, and K. C. Ott, Phys. Rev. Lett. **63**, 1992 (1989).

[19] M. Takigawa, J. L. Smith, and W. L. Hults, Phys. Rev. B **44**, 7764 (1991).