On Magnetic Properties of High T_C Oxides

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It is discussed that typical features of temperature dependences of such magnetic properties as spin susceptibility and nuclear magnetic relaxation rate in various Cu oxides together with the doping dependence of the critical temperatures can be understood by a phase diagram deduced from the mean field theory for the t-J model.

§ 1. Introduction

Various unusual magnetic properties of high T_C Cu-oxides have so far been reported.[1),2)] The temperature dependences of the spin susceptibility and the nuclear magnetic relaxation (NMR) rate appear to have a variety and the systematics of their behavior are not clear at first hand. Those experimental results, however, may be put in a phase diagram on the plane of the doping rate (δ) and temperature (T) as shown in Fig. 1. Here AF indicates antiferromagnetism, which is possible below some critical doping rate, δ_c, and T_S and T_R are characteristic (crossover) temperatures where the spin susceptibility, χ, either has a weak maximum or starts to decrease as T is lowered and the NMR rate $(T_1T)^{-1}\equiv R$ has a maximum, respectively. On the other hand T_C is the true phase transition temperature of superconductivity. In this figure it is clear that there exist two distinct regions of the doping rate, i.e. low and high indicated as L and H, respectively, where the temperature dependences of χ and R are qualitatively different as schematically shown in Fig. 2. The typical examples are YBCO (T_C=60 K)[3)~5)] and YBCO (T_C=90 K);[6)] the former belongs to L while the latter to H. The case of $Tl_2Ba_2CuO_{6+x}$[7),8)] also belongs to H-region.

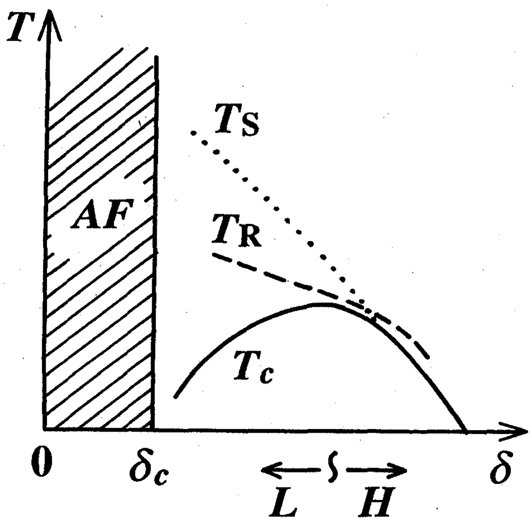


Fig. 1. An experimental phase diagram on the plane of doping (δ) and temperature (T) classifying the temperature dependences of magnetic properties; T_C, critical temperature of superconductivity, T_S, the onset temperature of the suppression of the spin susceptibility, T_R, the temperature at which NMR rate $(T_1T)^{-1}\equiv R$ takes maximum. AF is the antiferromagnetic phase. There are two characteristic regions, L, low doping and H, high doping.

In this paper it is indicated that the

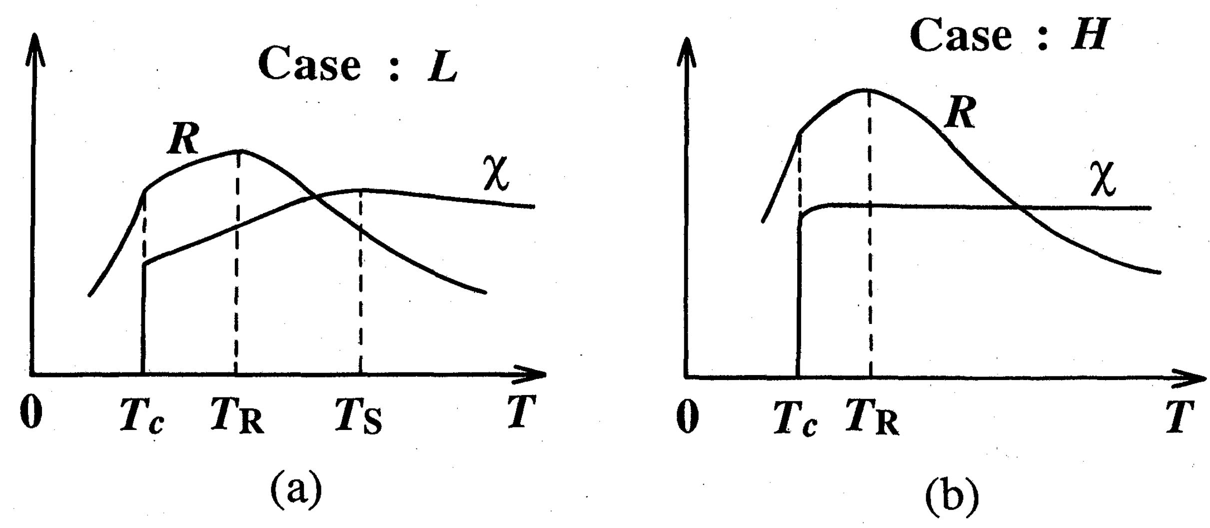


Fig. 2. The schematic representations of temperature dependences of χ and R (a) case L (low doping) (b) case H (high doping).

results of the mean field theory of the t-J model are in qualitative agreement with the overall features of Fig. 1 including the δ-dependence of T_c.

We take in units of $\hbar=k_B=1$.

§ 2. The effective Hamiltonian

Electrons in Cu-oxides are strongly correlated.[2] The difficulties in theoretical study on strong correlations result from the fact that the form of effective Hamiltonian to describe low energy properties is not clear even if the Hamiltonian in the large energy region is well-defined. This is in sharp contrast to electrons in ordinary metals, semimetals and semiconductors, where the knowledge in the high energy region (of the order of 1 eV) can be extended to the low energy region and there exists no crossover phenomenon. A counterexample to such a smoothness is the Kondo lattice, where the state with local moments in high temperatures crossovers into the coherent Fermi liquid state at low temperatures.[9] The case of high T_c oxides shares common features with the latter. It is now widely accepted[10)~18)] that the d-p model with realistic values of parameters for the Cu-O planes results in the t-J model on the square lattice for low energy excitations near the Fermi energy, i.e.

$$H=-t\sum_{\langle ij\rangle\sigma}[\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{j\sigma}+\text{h.c.}]+J\sum_{\langle ij\rangle}\boldsymbol{S}_i\cdot\boldsymbol{S}_j-\mu_e\sum_{i\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}\,, \tag{2·1}$$

where $\langle ij\rangle$ denotes the nearest-neighbor bond, and μ_e is a chemical potential of electrons, and $t\sim(0.4\sim0.5)$ eV and $J\sim0.13$ eV are the transfer integrals and the antiferromagnetic superexchange interactions between nearest-neighbor sites, respectively, and $\tilde{c}_{i\sigma}^{\dagger}\equiv c_{i\sigma}^{\dagger}(1-n_{i,-\sigma})$ creates the electron with spin σ at site i only when the site i is unoccupied, namely, the double occupancy is excluded. In Eq. (2·1) the transfer integral between next nearest neighbors, t', has been ignored for the sake of convenience in the following, though it may play important roles for some physical quantities.

§ 3. Phase diagram derived by mean field theory

Though the t-J model at $t=J$ can been solved exactly in $d=1$,[19] the electronic properties of this model in $d=2$ are far from clear. While there are some progress in the numerical studies of the model,[20] it is not easy to extract the low energy properties from such calculations. There have been, however, proposed several different types of mean field theory based on either slave fermion or slave boson operators.[21] Since the latter operator formalism is believed to be more suited to the description of the doping region without magnetic orderings, which is the region of our main interest in this paper, we employ the slave-boson method where the electron operators, $c_{i\sigma}$, are expressed by those of the spinon, $f_{i\sigma}$, and the holon, b_i; $c_{i\sigma}=b_i{}^\dagger f_{i\sigma}$, under the local constraint, $b_i{}^\dagger b_i+\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}=1$ at each site i. Then the Hamiltonian is written as

$$H=-t\sum_{\langle ij\rangle}[b_j{}^\dagger b_i\chi_{ij}+\text{h.c.}]-\frac{J}{2}\sum_{\langle ij\rangle}\chi_{ij}^\dagger\chi_{ij}-\mu\sum_{i\sigma}f_{i\sigma}^\dagger f_{i\sigma}$$
$$-\sum_i\lambda_i(b_i{}^\dagger b_i+\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}-1)\,, \qquad (3\cdot1)$$

where $\chi_{ij}\equiv\sum_\sigma f_{i\sigma}^\dagger f_{j\sigma}$ is the bond operator for the spinon and the last term represents the local constraint.

In the mean field approximation λ_i is taken to be uniform in space, and as possible order parameters for this model Hamiltonian we can think of $\langle \boldsymbol{S}_i\rangle$, $\langle\chi_{ij}\rangle$, $\langle b_i{}^\dagger b_j\rangle$ and $\langle b_{ij}\rangle$, where $b_{ij}\equiv(f_{i\uparrow}f_{j\downarrow}-f_{i\downarrow}f_{j\uparrow})/\sqrt{2}$. The first one is the familiar magnetic order parameter. The second and the third ones are diagonal order parameters, while the last one, which is off-diagonal and is due to the fact that $\boldsymbol{S}_i\boldsymbol{S}_j$ can also be expressed as $\boldsymbol{S}_i\cdot\boldsymbol{S}_j=-b_{ij}^\dagger b_{ij}+(1/4)n_in_j$, n_i being the number density at the i-th site. This is the singlet RVB order parameter originally introduced by Anderson.[10),22] The complete self-consistent mean field equations without the first magnetic one have been solved some time ago[23] for a slightly different model where $S_iS_j-(1/4)n_in_j$ instead of S_iS_j in the present model in Eq. $(1\cdot1)$. With a corresponding modification the resultant phase diagram is the one schematically given in Fig. 3, where $T_{\rm D}$, $T_{\rm RVB}$ and $T_{\rm B}$ are the onset temperatures of $\langle\chi_{ij}\rangle$ and $\langle b_i{}^\dagger b_i\rangle$, the coherent motions of spinons and holons, $\langle b_{ij}^\dagger\rangle$, the singlet pairing of spinons, and $\langle b_i{}^\dagger\rangle$, the Bose condensation of holons, respectively. In obtain-

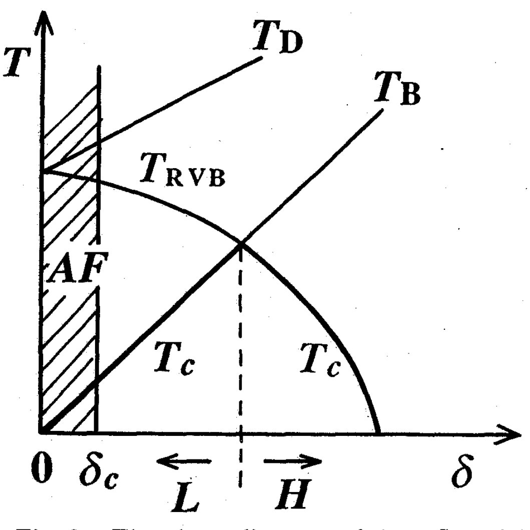


Fig. 3. The phase diagram of the t-J model based on the mean field theory: $T_{\rm D}$, onset temperature of the coherent motions of spinons and holons, $T_{\rm B}$, the Bose condensation temperature, $T_{\rm RVB}$, the onset temperature of the singlet RVB state, T_C, , the critical temperature of superconductivity, $T_C=T_{\rm B}$ in L-region and $T_C=T_{\rm RVB}$ in H-region.

ing finite T_B a finite transfer integral between layers has been assumed implicitly.[23) In this figure T_{RVB} is given by that of the d-wave state and the fact $T_D = T_{RVB}$ at $\delta=0$ is due to the $SU(2)$ symmetry in the undoped case.[24) The critical temperature of the superconducting state in this framework is characterized by the coexistence of $\langle b_{ij}^\dagger \rangle$ and $\langle b_i^\dagger b_j^\dagger \rangle$, the latter of which corresponds to the existence of $\langle b_i^\dagger \rangle$. Hence $T_C = T_B$ and $T_C = T_{RVB}$ if $T_{RVB} > T_B$ and $T_{RVB} < T_B$, respectively. If the magnetic order parameter $\langle \boldsymbol{S}_i \rangle$ is taken into account, the antiferromagnetic state will be stabilized for small doping as shown in Fig. 3.

The close similarity between Figs. 1 and 3 is visible; T_S and T_C in L-region may correspond to T_{RVB} and T_B, respectively, while T_C in H-region to T_{RVB}. These correspondences can be considered to a reasonable possibility together with the existence of T_R, as will be further discussed in the following.

§ 4. Magnetic excitations

The magnetic properties are characterized by the generalized spin susceptibility, $\chi(\boldsymbol{q}, \omega)$, which is given as follows in the present mean field theory for t-J model,

$$\chi(\boldsymbol{q}, \omega) = C(\boldsymbol{q}, \omega)\chi_0(\boldsymbol{q}, \omega), \tag{4·1}$$

$$C(\boldsymbol{q}, \omega)^{-1} \equiv 1 + J(\cos q_x + \cos q_y)\chi_0(\boldsymbol{q}, \omega), \tag{4·2}$$

where the lattice spacing is taken as unity and $\chi_0(\boldsymbol{q}, \omega)$ is that in the case without magnetic order parameter $\langle \boldsymbol{S}_i \rangle$, but with possible $\langle b_{ij} \rangle$.

In the temperature range $T_{RVB} < T < T_D$, $\chi(\boldsymbol{q}, \omega)$ is given by that of free spinons and has been investigated recently in great detail.[25) The results of numerical calculations for the choice of $t=4J$, which is considered to be realistic, will be discussed in the following. In Figs. 4(a) and (b) the static spin susceptibility $\chi(\boldsymbol{q}, 0) \equiv \chi(\boldsymbol{q})$ are shown for $\boldsymbol{q}=0$ (a) and $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi, \pi)$ (b). The uniform susceptibility, $\chi(0)$, is hardly dependent on T except for very small δ because of the suppression due to $C(\boldsymbol{q}, 0)$ given by Eq. (4·2), while $\chi(\boldsymbol{Q})$ has an interesting temperature dependence; it obeys the

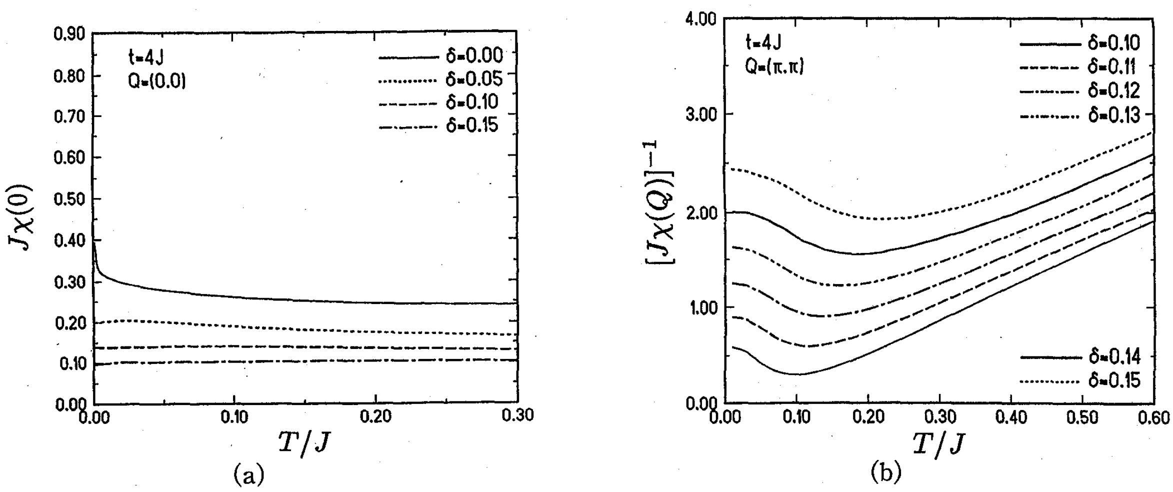


Fig. 4. The temperature dependences of the static susceptibility $\chi(\boldsymbol{q})$ for several choices of the doping rate, δ. (a) $\boldsymbol{q}=0$ and (b) $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi, \pi)$.

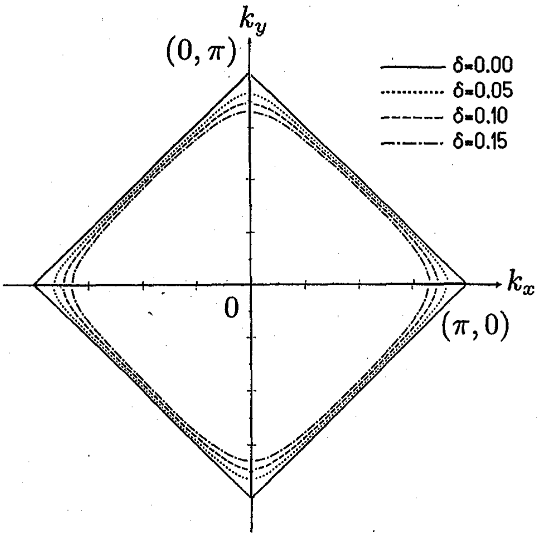


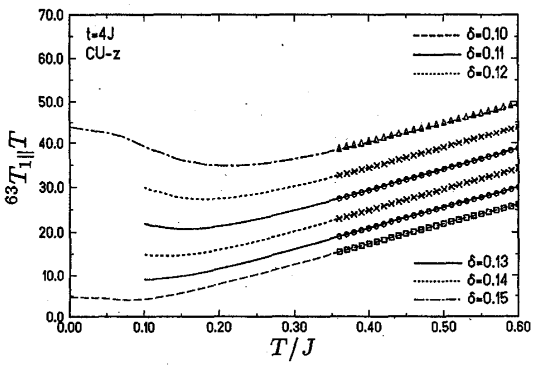
Fig. 5. The spinon Fermi surfaces for several doping rate.

Curie-Weiss law at high temperatures. The reason of the existence of a peak $\chi(\boldsymbol{Q},0)$ as a function of temperature is that $\chi(\boldsymbol{q},0)$ in low temperatures has peaks at incommensurate wave vectors (π, q_M) and (q_M, π),[26] with q_M dependent on the doping rate, but not at $\boldsymbol{q}=\boldsymbol{Q}$. These features are simply due to the band structure of spinons whose Fermi surface is shown in Fig. 5 for several choices of δ.

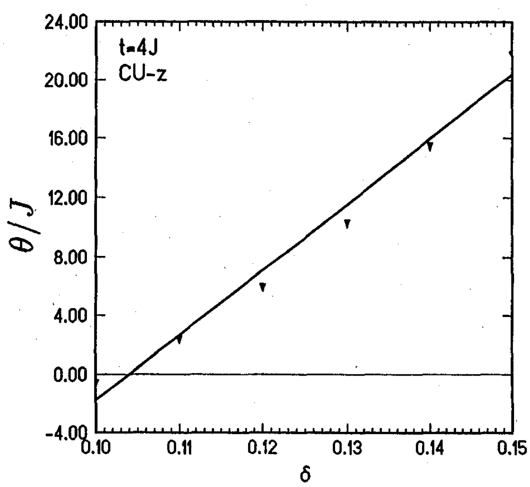
The NMR rate, R, is given as follows,

$$R\equiv\frac{1}{T_1T}=\sum_q F(\boldsymbol{q})\mathrm{Im}\chi(\boldsymbol{q},\omega)/\omega|_{\omega\to 0} \tag{4·3}$$

with a proper form factor $F(\boldsymbol{q})$ for each nucleus. The temperature dependences of R^{-1} at the Cu-site in YBCO with the magnetic field along the c-axis are shown in Fig. 6(a). In accordance with $\chi(\boldsymbol{Q})$, Fig. 4(b), ${}^{63}R$ is seen to obey the Curie-Weiss law, ${}^{63}R=C/(T+\theta)$ with the Wiess temperature, θ, dependent linearly on δ as seen in Fig. 6(b). At the oxygen site, however, R is only weakly dependent on T as seen in Fig. 7. All these features of χ and R are expected for temperatures above superconducting critical temperature in the region of H-doping and are consistent with the experimental observations in YBCO (T_C=90 K) and T1-Ba-Cu-O (overdoped) which can be considered to be in such a region of doping due to the particular δ-dependence of T_C. On the other hand, for $T<T_{\mathrm{RVB}}$ we have to take the effect of finite $\langle b_{ij}\rangle$ in the evaluation of $\chi_0(\boldsymbol{q},\omega)$ in Eqs. (4·1) and (4·2). Such calculations will be necessary to the full understanding of, e.g., $La_{2-x}Sr_xCuO_4$ with $x<0.15$. Though



(a)



(b)

Fig. 6. (a) The temperature dependences of the inverse of NMR rate, R, at Cu-sites indicating the Curie-Weiss law, $R^{-1}\propto(T+\theta)$. (b) The doping dependence of the extracted Weiss temperature, θ.

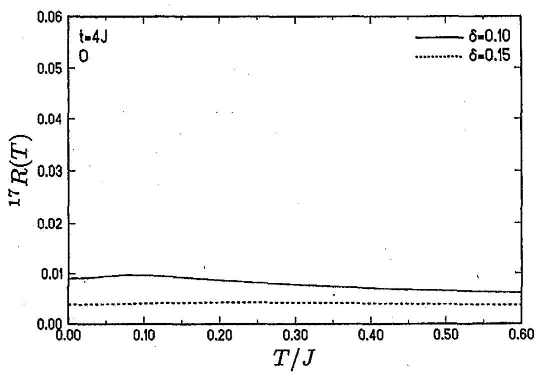


Fig. 7. The temperature dependences of the NMR rate at oxygen sites for two choices of doping rate.

incomplete, a similar study had been performed in Ref. 23) but without the exchange corrections, i.e. $C(\boldsymbol{q}, \omega)$ has been replaced by 1 in Eq. (4·1). In this case it has been shown that χ and R have a maximum at the same temperature T_{RVB}. Admittedly these calculations have to be extended to include $C(\boldsymbol{q}, \omega)$ given by Eq. (4·2), and are actually under way. On the basis of these results, however, together with the recent findings on $\chi(\boldsymbol{q}, \omega)$, Eq. (4·1), for $T_{\mathrm{RVB}} < T < T_{\mathrm{D}}$ it may be argued as follows. As the temperature is lowered χ will be essentially independent of temperature down to T_{RVB} below which it starts to decrease. On the other hand it is expected that R is still increasing for $T < T_{\mathrm{RVB}}$ as T is lowered and then has a maximum at a lowered temperature as in Fig. 2(a). Hence T_S can be understood as T_{RVB}, which is the onset temperature of singlet pairing coinciding with T_C in the H-region but is located above T_C in the L-region.

As was discussed recently by Nagaosa and Lee[27] T_{RVB} in L-doping will be a crossover temperature but not a true transition temperature. It is to be noted that in Figs. 10 and 11 of Ref. 23) that χ and R are hardly affected at T_{B}.

§ 5. Discussion

In this paper the temperature dependences of spin susceptibility, χ, and NMR rate, R, have been analyzed based on the mean field theory of the t-J model. It is indicated that there are two distinct regions of the doping rate, L and H, where χ and R depend on temperature differently. The existence of these two distinct regions has not been noted in our recent analysis of spin excitations.[25] Now it is clear that the results of calculations in Ref. 25) should apply to $T > T_C$ in the H-region and $T > T_{\mathrm{RVB}}$ in L-region since the singlet RVB pairing has not been taken into account in the calculation of $\chi(\boldsymbol{q}, \omega)$. Hence while the temperature dependences in this H-region, Fig. 2(b), have been understood by the results of Ref. 25), we need to extend the calculations to discuss the L-region. This is formally the same as to study the temperature region $T < T_C$ in the H-doping. A brief study of this problem has been made[28] by assuming the same temperature dependence of the singlet RVB order parameter (d-symmetry) as in the BCS theory. The result of $R(T)$ is shown in Fig. 8, where that without the exchange correction, $R_0(T)$, is also shown. The very sharp decrease of $R(T)$ below T_C is noteworthy: this is due to the large enhancement of the rate above T_C by the antiferromagnetic fluctuations and the suppression of this enhancement just below T_C by a finite singlet RVB order parameter. It should be mentioned that irrespective of a nice fit of Fig. 8 to experimental data of temperature dependences in YBCO ($T_C = 90$ K),[29),30] this symmetry of the order parameter does not seem to explain the scaling of the NMR rates at Cu and O sites.[31] This indicates the

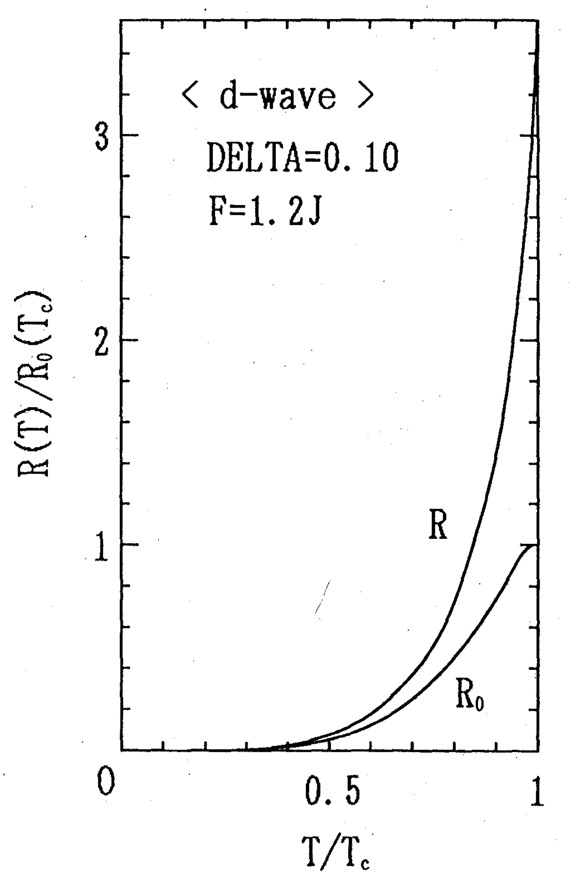


Fig. 8. The temperature dependence of NMR rate, R, at Cu-site in the d-wave singlet RVB state for $T < T_{\rm RVB}$. Plotted is also R_0 estimated without the exchange correction.

necessity of more detailed study about the possible symmetry of the superconducting state.

On the other hand, for the analysis of the temperature region $T_C < T < T_{\rm RVB}$ in the L-doping we need to treat the temperature dependences of $\langle \chi_{ij} \rangle$ and $\langle b_{ij} \rangle$ as well. Though this is the problem to be studied, we have made a rough analysis by combining our former results together with the recent one, and proposed that the overall features of the phase diagram shown in Fig. 1 will be in accordance with the result of mean field theory of the t-J model. In this view the apparent spin gap seen at $T > T_C$ in the neutron scattering[32] in YBCO ($T_C \simeq 60$ K) can be understood as due to the short range order of the singlet RVB pairs, while that in YBCO ($T_C \simeq 90$ K) will be analyzed as due to lattice structure studied in Ref. 25).

The transport properties, such as the resistivity and the Hall effect, have been shown to be understood by taking the fluctuations of the phases (gauge fields) of around the uniform RVB state.[33)~35)] Effects of such gauge fields on χ and R have been also studied[36] by simplifying the Fermi surface of spinons by a circular one as in the study of transport properties and shown to be not crucial in contrast to the transport properties. (If the actual lattice structure is taken into account a singularity is introduced in the propagator of the gauge field along $q_x = q_y$[25] and its effects have to be examined.) According to the present classification these results, however, should apply only to the H-region and the study on the L-region should be made separately. In this framework, as has been shown,[33] two-dimensional electrons described by the t-J model are in Tomonaga-Luttinger liquid state. If this is actually the case, the non-Fermi liquid behavior should be traced in the Hubbard model with strong U, which is the subject of basic importance.[37)~39)]

In summary the uniform and singlet RVB states described by the mean field theory of the t-J model have been shown to be in accordance with the essential features of the magnetic properties of high T_C Cu oxides. It is interesting to make further theoretical exploration of various other quantities to be checked with experiments. At the same time it is necessary to assess the present mean field theory on the other hand.

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