Model of high-T_c superconductivity driven by the intrinsic Kondo-type interaction: Effective phonon scheme

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(Received 17 July 1998; revised manuscript received 9 February 1999)

We have investigated whether electron-hole composite quasiparticles in CuO_2 planes can drive the hole-doped high-T_c superconductivity. Using this quasiparticle concept, we derive a Kondo-type interaction mediated by the effective Gell-Mann and Breuckner-type phonon. It is shown that this interaction opens a superconducting gap near the Fermi level. We explain the resistivities in the *a-b* plane and also along the *c* axis using the same concept of superexchange interactions. We have also found that the measured magnetic susceptibility and nuclear-spin relaxation rates can be explained using the present theoretical scheme in a consistent way.

I. INTRODUCTION

After the discovery of high-T_c superconductivity (HTSC) in the copper-oxide system of La-Ba-Cu-O by Bednorz and Müller,[1] many theoretical models have been proposed to explain this phenomenon: $s=\frac{3}{2}$ hole-composite model,[2,3] ferromagnetic cluster theory,[4,5] spin-fluctuations scheme,[6–8] resonating valence bond view,[9–11] excitonic picture,[12–14] dipolon mechanism,[15–17] etc.

Gap measurements[18–24] were reported to find the gap $2\Delta(0)/k_BT_c \simeq 6\sim 8$ in the plane parallel to the CuO_2 plane but almost equal to the BCS value[25,26] of 3.5 in the direction perpendicular to the CuO_2 plane. These characteristics of gap anisotropy[18,19,22–24] and nonzero $\Delta(T_c)$ values[23] in the HTSC cannot be explained satisfactorily by the BCS theory[25,26] of the low-temperature superconductivity. Inelastic neutron-scattering (INS) experiments[27–32] suggest a pseudospin gap in the spin excitation spectrum, which also cannot be explained by the textbook theories. Resistivity experiments[27,33,34] depicted the *a-b* plane resistance of CuO_2 planes to be proportional to temperature while the *c*-axis resistance in the direction perpendicular to the CuO_2 planes showing the temperature dependence of semiconductors. The INS results of Rossat-Mignod *et al.*[29] and Kasuya[35] show a temperature-independent peak at 41 meV that we want to assign as the effective phonon of Gell-Mann and Breuckner-type elementary excitation.[36] We want to show this effective phonon as responsible for the Cooper pairing in HTSC. On the basis of the effective-phonon theory we attempted to calculate the *a-b* plane and *c*-axis resistivities, nuclear-spin relaxation rates, and magnetic susceptibility, etc.

II. QUASIPARTICLE EXCITATION

We consider a quasiparticle of Fermion-type as composed of an electron-hole pair exciton and a free hole as depicted in Fig. 1. For a triplet state of the core electron-hole part this quasiparticle of $s=\frac{3}{2}$ becomes a Fermion-type electron-hole composite similar to the model of Aharony and co-workers,[2,3] Zhang and Rice,[37] and Emery and Reiter.[38] In our quasiparticle the core hole coupled with the lattice ion is responsible for the Gell-Mann and Breucker-type effective phonon of Fig. 2, the core electron for localized spin flips, and conducting holes and electrons for free carriers.

We now consider the $s=\frac{1}{2}$ electron-hole composite of Fig. 1.

$$H=\frac{p_1^2}{2m_e}+\frac{p_2^2}{2m_h}-\frac{e^2}{\tilde{\epsilon}_1 r_1}-\frac{e^2}{\tilde{\epsilon}_2 r_2}-\frac{e^2}{\tilde{\epsilon}_{12}|\mathbf{r}_2-\mathbf{r}_1|}, \tag{1}$$

$$H^i=\frac{p_i^2}{2m_i}-\frac{e^2}{\tilde{\epsilon}_i r_i}, \tag{2}$$

where m_e and m_h are derived from different bands, and m_e is the mass of the core electron, that is, e_{Cu} the valence electron from the *d* orbitals of copper, and m_{h_c} is the mass of conducting hole, that is, h_c the conducting hole from the *p* orbitals of oxygen, and h_{Cu} represents the valence hole from the *d* orbital of copper. The dielectric constants are defined as $1/\tilde{\epsilon}_1=1/\epsilon_1+1/\epsilon_1^{\mathrm{ph}}$, $1/\tilde{\epsilon}_2=-(1/\epsilon_2)+(1/\epsilon_2^{\mathrm{ph}})$, $1/\tilde{\epsilon}_{12}=(1/\epsilon_{12})+(1/\epsilon_{12}^{\mathrm{ph}})$, where ϵ_i is derived from the direct Coulomb interaction and ϵ_i^{ph} from the indirect Coulomb interaction[39] mediated by the phonon where indirect one is the same as BCS-type electron-electron interaction mediated by the phonon except nongauge invariant coupling-constant product. We thus have $\epsilon_i \gg |\epsilon_i^{\mathrm{ph}}|$ due to the nongauge invariance of ϵ_i^{ph} and a rapid fluctuation[39] of ϵ_i^{ph} between positive and negative leads to the independence between e_{Cu} and h_{Cu} of Fig. 1 with negligible excitonic effect. Strong phonon drag effect also leads to a very large volume of h_{Cu} and thus e_{Cu} is not enough to cancel this but only screening with $m_{h_{\mathrm{Cu}}} \simeq 100 m_{e_{\mathrm{Cu}}}$. This model resembles a Helium atom.[40] Since H^i corresponds to the hydrogen Hamiltonian the energy eigen-

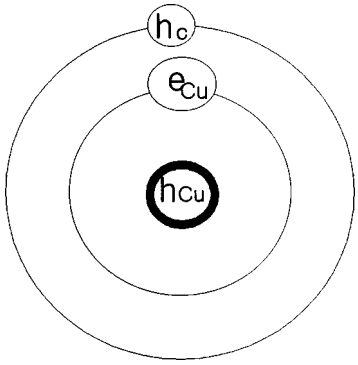

FIG. 1. The core hole h_{Cu} is from the intrinsic copper hole and the electron e_{Cu} from copper and the hole h_c is from a conducting hole in the O($2p$) orbital, where the effective masses are given $m_{h_{\mathrm{Cu}}} \gg m_{e_{\mathrm{Cu}}}$.

values for the case of noninteracting h_c and e_{Cu} of Fig. 1 can be written as

$$E^0_{n_1,n_2} = E_{n_1} + E_{n_2}$$

$$E_{n_1} = -13.6\,\mathrm{eV}/(\tilde{\epsilon}_1^2 n_1^2)$$

$$E_{n_2} = -13.6\,\mathrm{eV}/(\tilde{\epsilon}_2^2 n_2^2), \tag{3}$$

where $\tilde{\epsilon}_1 < \tilde{\epsilon}_2$, $m_{e_{\mathrm{Cu}}} \simeq m_{h_c}$, $m_{h_{\mathrm{Cu}}} \gg m_{e_{\mathrm{Cu}}}$, and $E^0_{n_1,n_2}$ represents the energy eigenvalue of noninteracting $e_{\mathrm{Cu}} - h_c$.

In Eq. (1) the last term of electron-hole Coulomb interaction can be treated as a perturbation to the type-I quasiparticle of noninteracting h_c and e_{Cu} in Fig. 1. Given E^0_{11} for

$$\phi_{100}(r) = \frac{2}{\sqrt{4\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0},$$

where a_0 is the Bohr radius, the perturbation ΔE_{11} can be calculated as

$$\Delta E_{11} \simeq -\int_0^\infty r_2^2\, dr_2 \int d\Omega_2 \int_0^{r_2} dr_1 \int d\Omega_1 r_1^2 \times \frac{1}{\tilde{\epsilon}_{12}^2} \frac{e^2}{|\mathbf{r}_2 - \mathbf{r}_1|} |\phi_{100}(r)|^4,$$

$$= -\frac{11}{8} \frac{13.6\,\mathrm{eV}}{\tilde{\epsilon}_{12}^2}, \tag{4}$$

so that

$$E_{11} = E^0_{11} + \Delta E_{11} = -13.6\,\mathrm{eV}\left(\frac{1}{\tilde{\epsilon}_1^2} + \frac{1}{\tilde{\epsilon}_2^2} + \frac{11}{8}\frac{1}{\tilde{\epsilon}_{12}^2}\right). \tag{5}$$

For the case of Fig. 1 this phonon-mediated interaction between hydrogenlike core electron hole and a conducting electron also makes the Fermion-type quasiparticle. The phonon may be softened at a temperature T_s much higher than the superconducting temperature T_c, where we expect the orthorhombic-tetragonal structural transition.[41] From Eq. (3) we obtain

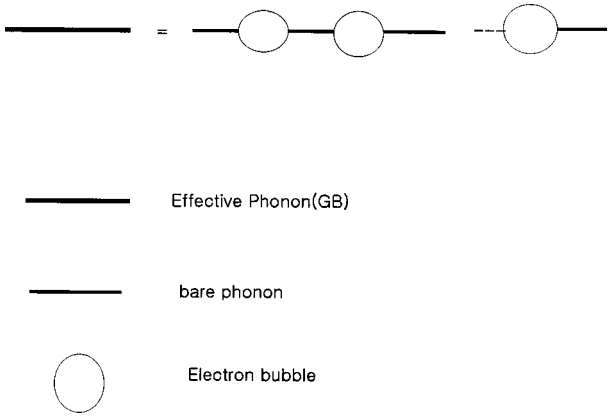

FIG. 2. Our elementary excitation is an effective phonon of Gell-Mann and Breuckner- (GB-) type (Ref. 36) which a bare phonon-h_{Cu} coupled state is called a plasmon-phonon coupled mode.

$$E_{n_1=1,n_2=\infty} \simeq -13.6\,\mathrm{eV}\left(\frac{1}{\tilde{\epsilon}_1^2} + \frac{11}{8}\frac{1}{\tilde{\epsilon}_{12}^2}\right), \tag{6}$$

and from

$$\phi_{200}(r) = \frac{2}{\sqrt{4\pi}} \left(\frac{1}{2a_0}\right)^{3/2} \left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0}$$

the perturbation ΔE_{22} can be calculated as

$$\Delta E_{22} = -0.66 \frac{13.6\,\mathrm{eV}}{\tilde{\epsilon}_{12}^2} \tag{7}$$

to give

$$E_{22} = -\frac{13.6\,\mathrm{eV}}{4}\left(\frac{1}{\tilde{\epsilon}_1^2} + \frac{1}{\tilde{\epsilon}_2^2}\right) - 0.66\frac{13.6\,\mathrm{eV}}{\tilde{\epsilon}_{12}^2}. \tag{8}$$

We can also obtain

$$E_{n_1=2,n_2=\infty} = -13.6\,\mathrm{eV}\left(\frac{1}{4\tilde{\epsilon}_1^2}\right) - 0.66\frac{13.6\,\mathrm{eV}}{\tilde{\epsilon}_{12}^2} \tag{9}$$

and the energy levels of our quasiparticle in Fig. 1 can be represented as in Fig. 3.

III. GAP IN *a-b* PLANE

When the quasiparticle of Fig. 1 is created in the CuO_2 plane we may consider the *s-d* exchange spin-flip interaction[42] of conduction spins with localized spins, where the conduction spin represents h_c of O($2p$) and the localized spin e_{Cu} of Cu($3d$) with spin-flip motion. The original Hamiltonian for the *s-d* exchange interaction is given by

$$H_{sd}=\sum_{k,\sigma}\varepsilon_{k\sigma}a^{+}_{k\sigma,\zeta}a_{k\sigma,\zeta}+\frac{1}{2}U_c\sum_{k\kappa\mu}\sum_{l\nu}a^{+}_{k+\kappa,\mu\zeta}a_{k,\mu\zeta}a^{+}_{l,\nu\zeta}a_{l+\kappa,\nu\zeta}-\frac{1}{N}\sum_{i=1}^{N_0}\sum_{k,\kappa}J_{sd}(\kappa)\exp(i\kappa R_i)\times[S_i^{\zeta}(a^{+}_{k,\uparrow\zeta}a_{k-\kappa,\uparrow\zeta}-a^{+}_{k,\downarrow\zeta}a_{k-\kappa,\downarrow\zeta})+S_i^{+}a^{+}_{k,\downarrow\zeta}a_{k-\kappa,\uparrow\zeta}+S_i^{-}a^{+}_{k,\uparrow\zeta}a_{k-\kappa,\downarrow\zeta}], \tag{10}$$

where $a^{+}_{k\sigma,\zeta}$ is the creation operator of a conduction hole h_c with momentum $\hbar\mathbf{k}$, spin $\sigma=(\uparrow$ or $\downarrow$, the quantization axis being in the direction of the ζ axis) and $\mathbf{S}_i$ the localized spin at site $\mathbf{R}_i$, S_i^{ζ} its ζ component, $J_{sd}(\kappa)$ the Fourier component of the *s-d* or *p-d* exchange integral, U_c the Fourier component of the screened Coulomb interaction, s the magnitude of local spin, N_0 is the number of local spins, and N total number of spins. Using a canonical transformation and as a result to obtain an electron-electron interaction,[42] the effective Hamiltonian can thus be written as

$$H=\sum_{k}\varepsilon_{k,\sigma}a^{+}_{k,\sigma}a_{k,\sigma}+\frac{2J_{sd}^2}{3N^2k_BT}\times N_0s(s+1)\sum_{k,k',q,\sigma}a^{+}_{k,\sigma}a_{k-q,-\sigma}a^{+}_{k',-\sigma}a_{k'+q,\sigma}. \tag{11}$$

For $T<T_M$ we have $s(s+1)/3k_BT_M\equiv s/g\mu_B\langle H_i\rangle$, where T_M represents the saturation temperature of spin flips, H_i the local field within local spins, g the electron Lande factor, and μ_B the Bohr magneton.

In the Hartree-Fock approximation we have

$$\langle a^{+}_{k,\sigma}a_{k-q,-\sigma}a^{+}_{k',-\sigma}a_{k'+q,\sigma}\rangle\sim-\langle a^{+}_{k,\sigma}a_{k,\sigma}\rangle a^{+}_{k-q,\sigma'}a_{k-q,\sigma'}-\langle a^{+}_{k,\sigma}a_{k+q,\sigma}\rangle a^{+}_{k,\sigma'}a_{k-q,\sigma'}.$$

In the *s-d* exchange integral we use the Pytte approximation[43] for the lattice ionic displacement

$$J_{sd}^2=J_{sd,0}^2+\sum\nabla J_{sd}^2\cdot d\mathbf{u}+\cdots\simeq J_{sd,0}^2+\sum g_{sd}(b_q+b^{+}_{-q}),$$

$$d\mathbf{u}=\mathbf{u}(j)-\mathbf{u}(j+1),$$

$$\mathbf{u}(j)=\frac{1}{\sqrt{m^*N}}\sum_{\mathbf{q}}\mathbf{e}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R}_j}Q(\mathbf{q}),$$

$$Q(\mathbf{q})=\frac{1}{\sqrt{2\omega_0}}(b_q+b^{+}_{-q}), \tag{12}$$

where g_{sd} represents a coupling constant and b_q an annihilation operator for the Gell-Mann and Breuckner-type phonon[36] for copper ions, where

$$g_{sd}(q)=\frac{1}{\sqrt{2\omega_0}}\left[\frac{\mathbf{e}(q)}{\sqrt{m^*N}}\cdot\nabla J_{sd}^2\right](e^{i\mathbf{q}\cdot\mathbf{R}_j}-e^{i\mathbf{q}\cdot\mathbf{R}_{j+1}}),$$

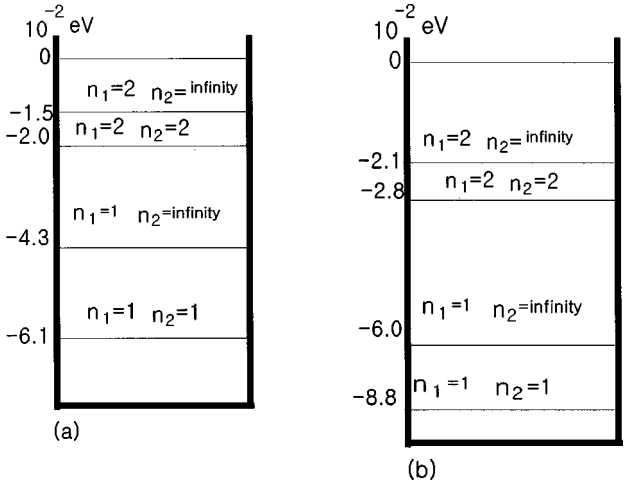

FIG. 3. Energy levels, (a) $\tilde{\varepsilon}_1=25$, $\tilde{\varepsilon}_2=27$, $\tilde{\varepsilon}_{12}=30$; (b) $\tilde{\varepsilon}_1=20$, $\tilde{\varepsilon}_2=22$, $\tilde{\varepsilon}_{12}=27$.

e is a polarization vector, m^* is the effective mass of copper ion, N is the number of lattice-ions, and ω_0 is the wave number of the phonon from copper ions and the order of g_{sd} is $O(g_{sd})\sim O(J_{sd}/\sqrt{\omega_{\rm ph}})$. The resultant Hamiltonian thus becomes

$$H_{\rm eff}\simeq\sum_{k}\varepsilon_k a^{+}_k a_k+\sum_{q}\hbar\omega_q b^{+}_q b_q-\frac{2J_{sd,0}^2N_0s(s+1)}{3k_BT}\sum_{k,k'}\langle a^{+}_{k'}a_{k'}\rangle a^{+}_k a_k+\frac{2N_0s(s+1)}{3k_BT}\sum_{k,k',q}\langle a^{+}_{k'}a_{k'+q}\rangle g_{sd}a^{+}_k a_{k-q}(b_q+b^{+}_{-q}), \tag{13}$$

where $\langle a^{+}_k a_{k+q}\rangle=n(q)$ is the hole momentum distribution, ω_q is from the phonon of copper ions.

We can then apply the Haken's receipe[44] to transform the Hamiltonian to the weak-coupling BCS-type[25,26] for the sake of an estimate:

$$\tilde{H}_{sd}^{\rm BCS}=\sum_{k}(\varepsilon_k-\varepsilon_{sd})a^{+}_k a_k+\sum_{k,k',q}\frac{1}{2}U_c(q)a^{+}_{k+q}a_k a^{+}_{k'}a_{k'+q}+\sum_{k,k',q}\frac{|g_{sd}|^2\hbar\omega_q}{(\varepsilon_{k+q}-\varepsilon_k)^2-(\hbar\omega_q)^2}\times\left(\frac{2N_0s(s+1)}{3k_BT}\right)^2 n(q)n(-q)\times a^{+}_{k+q}a_k a^{+}_{k'}a_{k'+q}, \tag{14}$$

where U_c represents Coulomb interaction and

$$\varepsilon_{sd}=\frac{2J_{sd,0}^2N_0s(s+1)}{3k_BT}\sum_{k}\langle a^{+}_k a_k\rangle. \tag{15}$$

This Hamiltonian is effective during the decoupling only if $\varepsilon_k-\varepsilon_{k+q}\simeq\varepsilon_{k-q}-\varepsilon_k$, $g_{sd}(q)\simeq g_{sd}(-q)$. For $T<T_M$ we can set $T=T_M$ and

TABLE I. We have a phenomenological parameter $\Gamma(T_c)$ due to the finiteness of $\Delta(T_c)$.

Materials	T_c(K)	$\hbar\omega$ (K)	$N(0)V\|_{T_c}$	$N(0)V\|_{T=0}$	$\frac{\hbar\omega}{\Delta(T_c)}\Gamma(T_c)$	$\frac{2\Delta(0)}{k_BT_c}$
La oxide	37	500	0.30	0.51	2.9	7.7
Bi oxide	90	800	0.33	0.56	0.13	6.0

$$U_{sd}\equiv\frac{2|g_{sd}|^2\hbar\omega_q}{(\varepsilon_{k+q}-\varepsilon_k)^2-(\hbar\omega_q)^2}\left(\frac{2N_0s(s+1)}{3k_BT}\right)^2 n(q)n(-q). \tag{16}$$

The order of U_{sd} is

$$U_{sd}\sim\frac{J_{sd}^2}{\omega_{\rm ph}}\frac{1}{\omega_{\rm ph}}\left(\frac{100}{100}\right)^2(0.1)^2\sim 1 \quad \text{if } \frac{J_{sd}}{\omega_{\rm ph}}\sim 10.$$

From the weak-coupling BCS formalism for the sake of an estimate the superconducting gap is expected at T_c given by

$$T_c=1.14\hbar\omega\exp\left[1/\{N(\varepsilon_F^{sd})[U_{sd}+U_c]_{\rm av}|_{T_c}\}\times\left\{\tanh\left(\frac{\hbar\omega}{\Delta(T_c)}\Gamma(T_c)\right)\right\}\right], \tag{17}$$

$\varepsilon_F^{sd}=\varepsilon_F-\varepsilon_{sd}$, and the suffix $[]_{\rm av}$ represents average value. The order of Coulomb interaction U_c between the O($2p$) conduction holes h_c of the Cooper pair in Fig. 1 from the values of Fig. 3 is

$$O(U_c)\simeq O\left(\frac{e^2}{2\epsilon_i r_{h_c-h_{\rm Cu}}}\right)\sim O\left(\frac{13.6\,\text{eV}}{\epsilon_i}\right)\leqslant O(1\text{ eV}),$$

$$U_c\ll U_p\sim 3\text{ eV},$$

where $r_{h_c-h_{\rm Cu}}$ is the distance between h_c and $h_{\rm Cu}$ in Fig. 1 and ϵ_i is given from Eqs. (1)–(9), U_p is the on-site repulsion in p orbital. The largeness of ϵ_i is due to the sufficient screening of $e_{\rm Cu}$ to h_c in Fig. 1 as if h_c and $e_{\rm Cu}$ nearly stick together as a Kondo or s-d bound pair shown in Eqs. (10)–(13). It becomes

$$U_{sd}(q)+U_c(q)\equiv\frac{2\pi e^2N(\varepsilon_F^{sd})}{q\epsilon(0,q)},$$

where ϵ is the longitudinal permittivity. Although for Cu, metallic hydrogen the permittivity becomes $\epsilon>0$ from Ginzburg's work,[64] in the case of O it may be $\epsilon(0,q\neq 0)<0$ where the direct calculations[65,66] will be needed.

Since the pseudogap[27–32,60] can make the superconducting gap at T_c finite (which will be discussed in our later paper) we have $\Delta(T_c)\neq 0$. The additional term of tanh to the BCS form can be derived as follows:

Using the BCS-like formalism, we find

$$k_BT_c\simeq 1.14\hbar\omega\exp\left[\frac{-1}{N(0)V|_{T_c}}\tanh\left(\frac{\hbar\omega}{\Delta(T_c)}\Gamma(T_c)\right)\right], \tag{18}$$

$$2\Delta(0)=2\hbar\omega/\sinh\left[\frac{1}{N(0)V|_{T=0}}\right], \tag{19}$$

where $V=|(U_{sd}+U_c)_{\rm av}|$, $\Gamma(T_c)$ is a phenomenological parameter. Then,

$$\frac{2\Delta(0)}{k_BT_c}\simeq 3.5\exp\left[\frac{1}{N(0)V|_{T_c}}\left(\tanh\left(\frac{\hbar\omega}{\Delta(T_c)}\Gamma(T_c)\right)-\frac{V|_{T_c}}{V_{T=0}}\right)\right], \tag{20}$$

where the ratio is shown in the Table I.

IV. RESISTIVITY IN *a-b* PLANE

Kim's s-d scattering mechanism[45–49] was extended successfully to a general system by Kondo.[50,51] This Kondo-type spin scattering[50] can be shown to be valid also at high temperatures of the magnitude larger than a few kelvins. The main term of the spin scattering of conducting holes is

$$(J_{sd,0})^2\sum_\kappa\frac{[1-f(\varepsilon_{k-\kappa}^{sd})]}{\varepsilon_{k-\kappa}^{sd}-\varepsilon_k^{sd}}, \tag{21}$$

where f represents the Fermi-Dirac distribution function and $\varepsilon_k^{sd}=\varepsilon_k-\varepsilon_{sd}$. At high temperatures of $T\gg T_{\rm Kondo}$, we have

$$T_{\rm Kondo}=\alpha W\exp[-N/(2|J_{sd,0}|N(\varepsilon_F^{sd}))]\sim 0\text{ K},$$

$$1-f(\varepsilon_{k-\kappa}^{sd})\simeq 1-f(\varepsilon_F^{sd})-\left.\frac{\partial f}{\partial\varepsilon}\right|_{\varepsilon_F^{sd}}(\varepsilon_{k-\kappa}^{sd}-\varepsilon_F^{sd}),$$

where the second term becomes important at $\varepsilon_F^{sd}\neq\varepsilon_F$, α a constant related to $J_{sd,0}$ in the range of $0.1\leqslant\alpha\leqslant 0.5$, W the conduction-band width, and αW corresponds to an effective bandwidth and $J_{sd,0}$ is smaller than a normal Kondo exchange interaction, $J_{\rm Kondo}$ in other materials. We thus have

$$\sum_k\frac{[1-f(\varepsilon_{k-\kappa}^{sd})]}{\varepsilon_{k-\kappa}^{sd}-\varepsilon_k^{sd}}\simeq -N(\varepsilon_F^{sd})\{1-f(\varepsilon_F^{sd})\}\ln\left(\frac{k_BT}{\alpha W}\right)+\int_{k_BT}^{\alpha W}\left.\frac{\partial f}{\partial\varepsilon}\right|_{\varepsilon_F^{sd}}N(\varepsilon_F^{sd})d\varepsilon, \tag{22}$$

where $N(\varepsilon)$ is the density of states.

We can thus obtain from the Kondo-type formalism the resistance in the a-b plane of the high-T_c superconductors at temperatures higher than T_c as due to the spin scattering as follows:

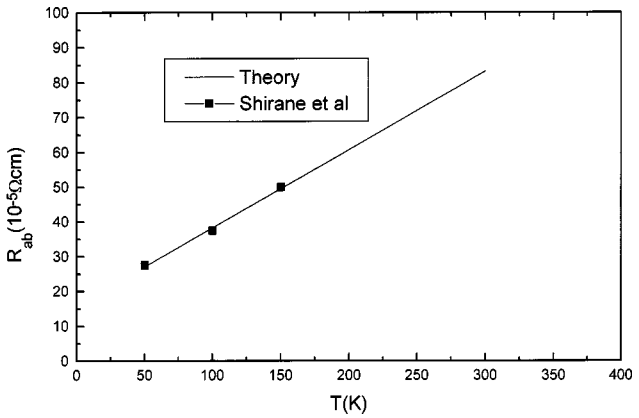

FIG. 4. The in-plane resistivity, R_{ab} from the experiment (Ref. 27) and our theory.

$$R(T)\simeq N_0R_0\left[1+\frac{4J_{sd,0}}{N}N(\varepsilon_F^{sd})\{1-f(\varepsilon_F^{sd})\}\ln\left(\frac{k_BT}{\alpha W}\right)+\frac{4J_{sd,0}}{N}N(\varepsilon_F^{sd})f'(\varepsilon_F^{sd})(k_BT)\right]. \quad (23)$$

At very high temperature of the order, ~100 K when $1-f(\varepsilon_F^{sd})\simeq 0$ can be neglected and $f'(\varepsilon_F^{sd})$ is nearly flat and near to zero for high temperatures, we obtain

$$R(T)\simeq N_0R_0\left[1+\frac{4J_{sd,0}}{N}N(\varepsilon_F^{sd})f'(\varepsilon_F^{sd})(k_BT)\right], \quad (24)$$

with

$$N_0R_0\equiv\frac{2\pi N(\varepsilon_F^{sd})mN_0'}{ze^2\hbar}[(J_{sd,0})^2s(s+1)], \quad (25)$$

where m represents the effective mass of the $2p$ hole, N_0' the total number of $3d$ electrons, and z the average number of the nearest $3d$ electrons. For $z=N_0$ we can obtain the a-b plane resistivity of Fig. 4 as fitted by Table II in agreement with experimental values.

V. c-AXIS RESISTIVITY

Experimental evidences are available[52,53] for a close relation of the hole hopping along the c axis with oxygen atoms of different oxide planes. In our model oxygen, O of the CuO_2 planes and oxygens, $\tilde{O}$ in other oxide planes are contributing to the c-axis resistivity through the superexchange interaction as shown in Fig. 5, for the overlap between $O(2p)$ and the extended $\tilde{O}(3s)$ happens. For $\tilde{\varepsilon}_k-\tilde{\varepsilon}_q\simeq\varepsilon_k-\varepsilon_q$ we have $\langle\tilde{a}_k^+\tilde{a}_k\rangle=\tilde{f}(\tilde{\varepsilon}_k)$, where a refers to oxygens of CuO_2 and $\tilde{a}$ to oxygens of the other oxide planes. The dominating factor from the superexchange interaction of Fig. 5 is

TABLE II. We choose $N(\varepsilon_F^{sd})\sim 1/\text{eV}$ for La-Sr-Cu-O.

N_0R_0	$N(\varepsilon_F^{sd})$	$J_{sd,0}$	$f'(\varepsilon_F^{sd})$
15.8	1/eV	−0.5 eV	−0.0071

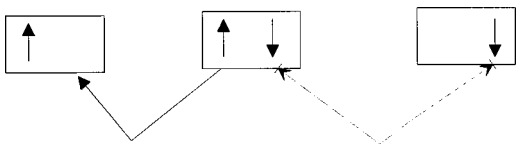

FIG. 5. The left and right orbitals of $O(2p)$ in CuO_2 planes and the middle occupied orbital of $O(3s)$ in other oxide layers.

$$\left[J_O^2\sum_q\frac{\tilde{f}_q}{\tilde{\varepsilon}_k-\tilde{\varepsilon}_q}\right]\left[J_O^2\sum_q\frac{1-f_q}{\varepsilon_k-\varepsilon_q}\right], \quad (26)$$

where J_O represents the exchange interaction between a hole from $O(2p)$ of CuO_2 plane and an electron from $O(3s)$ of other oxide planes. Thus the Kondo formalism[50] of the superexchange interaction through the extended $O(3s)$ orbitals of different oxide planes gives rise to the c-axis resistivity as

$$R_c=R_{\text{const}}\left[1+f(\varepsilon_F)\frac{4J_O}{N}N(\varepsilon_F)\ln\left(\frac{k_BT}{\alpha W}\right)-f'(\varepsilon_F)\frac{4J_O}{N}N(\varepsilon_F)(k_BT)\right]\times\left[1+\{1-f(\tilde{\varepsilon}_F^{sd})\}\frac{4J_O}{N}N(\tilde{\varepsilon}_F^{sd})\ln\left(\frac{k_BT}{\alpha W}\right)+f'(\tilde{\varepsilon}_F^{sd})\frac{4J_O}{N}N(\tilde{\varepsilon}_F^{sd})k_BT\right]+R'_{\text{const}}, \quad (27)$$

where $R_{\text{const}}=N_0R_0'(J_O/Nk_BT_c)^{2\frac{3}{4}}$, $R_0'=R_0(J_{sd,0}\to J_O)$, $\tilde{\varepsilon}_F^{sd}=\varepsilon_F-\varepsilon_{sd}^c=\varepsilon_F^{sd}(J_{sd,0}\to J_O)$, R'_{const} another constant term from nonsuperexchange parts.

We define

$$\Lambda^c(T)\equiv\left(\frac{J_O}{Nk_BT_c}\right)^2\frac{3}{4}\left[1+f(\varepsilon_F)\frac{4J_O}{N}N(\varepsilon_F)\ln\left(\frac{k_BT}{\alpha W}\right)-f'(\varepsilon_F)\frac{4J_O}{N}N(\varepsilon_F)k_BT\right]. \quad (28)$$

R_c has three type behaviors in agreement with experiments according to αW, the overlap between $O(2p)$ and $O(3s)$. When αW is sufficiently large relative to k_BT, we

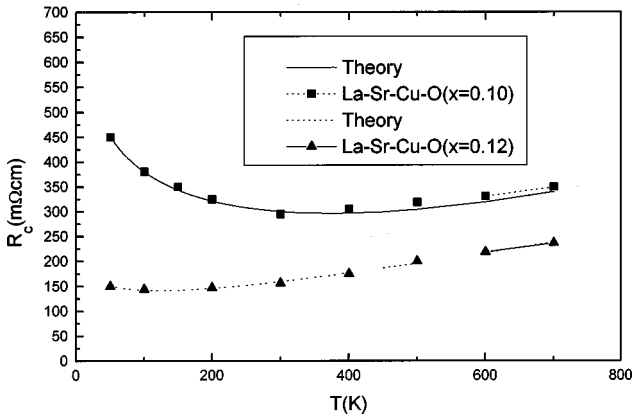

FIG. 6. The resistivity of the c axis, R_c versus temperature for $La_{2-x}Sr_xCuO_4$ materials (Ref. 54) where the special notation from experiment.

TABLE III. We choose the parameters where $J_O \sim -0.5$ eV, $N(\varepsilon_F) \sim 1/\text{eV}$, and $f(\varepsilon_F)=0.6$.

Materials	R_{const}	R'_{const}	$\log(\alpha W)$	$f'(\varepsilon_F^{sd})$	$f'(\varepsilon_F)$
La-Sr-Cu-O ($x=0.12$)	13	193	8.2	-3.0×10^{-2}	-1.0×10^{-3}
La-Sr-Cu-O ($x=0.10$)	57	679	8.0	-4.5×10^{-2}	-3.8×10^{-4}

can neglect $\ln(k_B T/\alpha W)$ for $f(\varepsilon_F)$ is very small relative to $f'(\varepsilon_F)$ so to be $R_c \propto (1+aT+b\log T)$. When αW is extremely large the resistivity becomes $R_c \propto (1+aT)$ because of $f(\tilde{\varepsilon}_F^{sd}) \simeq 1$, where a and b are constants. Our theoretical values are in good agreement with the experimental values of Zha *et al.*[54] as can be seen from Fig. 6 and Table III.

With respect to this superexchange interaction along the c axis in the superconducting state, the energies for $2p$ orbitals in the copper-oxide planes and $3s$ orbitals in the non-copper-oxide planes are given as

$$E_{3s}(\uparrow\downarrow)=E_0+2\epsilon_s,$$

$$E_{2p}(\uparrow\uparrow)=E_0+2\epsilon_p-\tfrac{1}{4}J_O,$$

$$E_{2p}(\uparrow\downarrow)=E_0+2\epsilon_p+\tfrac{1}{4}J_O. \tag{29}$$

The superexchange interaction of Fig. 5 through $(3s)$ orbitals of the non-copper-oxide planes is given by

$$J_O=\left(\frac{2t_0^2}{\epsilon_s}\right)^2\left(-\frac{1}{\epsilon_s}+\frac{2}{\epsilon_p+U_p}\right), \tag{30}$$

where t_0 represents the amplitude of hybridization between $2p$ and $3s$ orbitals, and U_p the on-site repulsion in $2p$ orbitals. If we have $\epsilon_s-\epsilon_p \leqslant U_p \leqslant 2\epsilon_s-\epsilon_p$ and a temporary triplet pair of $2p$ orbitals, the energy difference between $2p$ and $3s$ orbitals should match the onsite repulsion U_p, that is, $2\epsilon_s-\epsilon_p=U_p$, in order to make free hopping between $2p$ and $3s$ orbitals in the superconducting state. This condition of J_O amounts to the *superexchange vacancy* in the oxide plane corresponding to the *Fermi vacancy*.[55] We expect then the c-axis holes to be superconductive through these vacancies over the barriers. The superconducting hole pairs from $O(2p)$ in CuO_2 planes will form two temporary triplet pairs in conjunction with the nonmagnetic electron pairs of $O(3s)$ in the non-copper-oxide planes, where one pair gets an energy gain by $\frac{1}{4}J_O$ and the other pair with an energy loss of $-\frac{1}{4}J_O$. This mechanism of the c-axis superconductivity is equivalent to the violation and recovery of Pauli principle.[56]

In the c-axis resistivity T_c corresponds to the saturation temperature of spin flips, and the global structure of the c-axis formalism follows the BCS theory.[25,26] With appropriate substitutions of J_{sd} by J_{sd}^c, g_{sd} by g_{sd}^c, ε_{sd} by ε_{sd}^c, and U_{sd} by U_{sd}^c, we have

$$(J_{sd,0}^c)^2=J_O^2\Lambda^c(T), \tag{31}$$

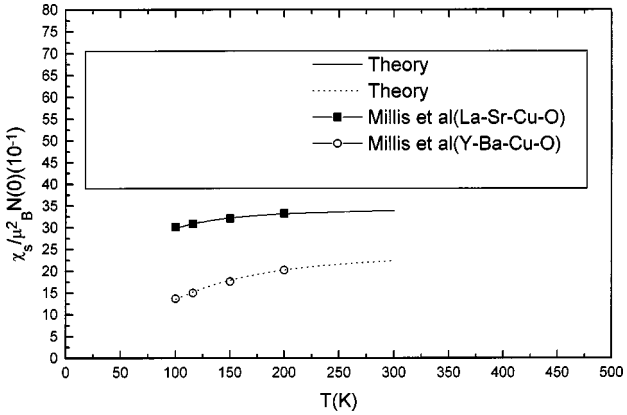

FIG. 7. Spin susceptibilities obtained from the experiment (Ref. 60) and fitted with our theoretical model. The upper graph is for $La_{1.86}Sr_{0.14}CuO_4$ and the lower one is for $YBa_2Cu_3O_{6.6}$, where the diamagnetic correction is added and special notations from experiments.

$$U_{sd}^c=\frac{2|g_{cd}^c|^2\hbar\omega_q}{(\varepsilon_{k+q}-\varepsilon_k)^2-(\hbar\omega_q)^2}\times\left(\frac{2N_0 s(s+1)}{3k_BT}\right)^2 n(q)n(-q), \tag{32}$$

$$\varepsilon_{sd}^c=\frac{2(J_{sd,0}^c)^2N_0 s(s+1)}{3k_BT}\sum_k\langle a_k^+ a_k\rangle, \tag{33}$$

and $T_c^{c\text{-axis}}$ is given as

$$T_c^{c\text{-axis}}=1.14\hbar\omega\exp\left(\frac{1}{N(\varepsilon_F-\varepsilon_{sd}^c)(U_{sd}^c+U_c)_{\text{av}}|_{T_c^{c\text{-axis}}}}\right). \tag{34}$$

VI. MAGNETIC SUSCEPTIBILITY

Considering only Coulomb interactions the magnetic susceptibility becomes[46]

$$(\chi_{zz})_{\text{bare}}=2\mu_B^2\frac{F(q,\omega)}{1-[\tilde{V}_c(q)]F(q,\omega)}, \tag{35}$$

where $F(q,\omega)=\Sigma_k[f(\varepsilon_k)-f(\varepsilon_{k+q})]/(\varepsilon_{k+q}-\varepsilon_k-\hbar\omega)$ is the Lindhard function, $-\tilde{V}_c(q)$ the exchange part of Coulomb interaction. If we denote the exchange part of U_{sd} as $-\tilde{V}_{sd}(q)$ we can write the resultant magnetic susceptibility above T_c for HTSC as

$$\chi_{zz}=2\mu_\beta^2\frac{F^{sd}(q,\omega)}{1-[\tilde{V}_c(q)+\tilde{V}_{sd}(q)]F^{sd}(q,\omega)}, \tag{36}$$

where the modified Lindhard function is given by $F^{sd}(q,w)=\Sigma_k[f(\varepsilon_k^{sd})-f(\varepsilon_{k+q}^{sd})]/(\varepsilon_{k+q}^{sd}-\varepsilon_k^{sd}-\hbar\omega)$, $\varepsilon_k^{sd}=\varepsilon_k-\varepsilon_{sd}$. The susceptibility can be put into a simple form as

$$\chi_{zz}=2\mu_B^2\frac{N(0)}{1-[\tilde{V}_c(q)+\tilde{V}_{sd}(q)]}, \tag{37}$$

TABLE IV. We assume $F_{sd}(q,0)\simeq N(\varepsilon_F)\simeq 0.5$ states/eV.

Materials	$1-V_c(q)$	$-V_{sd}(q)\times T^2\,(K^2)$
$La_{1.86}Sr_{0.14}CuO_4$	0.29	450
$YBa_2Cu_3O_{6.6}$	0.41	3320

where $\overline{V}_{sd}(q)=\tilde{V}_{sd}(q)N(0)$, $N(0)\simeq F_{sd}(q,0)$. Using $\overline{V}_{sd}(q)\propto 1/T^2$ and $N(0)\simeq N(\varepsilon_F)$ we obtain Fig. 7 in agreement with experimental results with parameters given in Table IV.

VII. NUCLEAR-SPIN-RELAXATION RATES

The spin-relaxation rate of Cu from direct *s-d* exchange and indirect superexchange interactions is given by[57]

$$(T_1)^{-1}=(T_1)_D^{-2}+(T_1)_{ID}^{-1}, \tag{38}$$

where the Kondo-type spin-relaxation rate $(T_1)_D^{-1}$ is given by

$$(T_1)_D^{-1}=(T_1)_{\text{Korringa}}^{-1}\left[1+\frac{4J_{sd,0}}{N}f(\varepsilon_F^{sd})N(\varepsilon_F^{sd})\log\left(\frac{k_BT}{\alpha W}\right)-\frac{4J_{sd,0}}{N}f'(\varepsilon_F^{sd})N(\varepsilon_F^{sd})k_BT\right] \tag{39}$$

and

$$(T_1)_{\text{Korringa}}^{-1}=\frac{4\pi}{\hbar}(J_{sd,0})^2N^2(\varepsilon_F^{sd})k_BT. \tag{40}$$

Following Emery and Reiter[57] the superexchange interaction through O sites occupied by holes doubly is given by

$$J'_{sd}=-\left(\frac{2t_0^2}{V}\right)^2\frac{2}{2\varepsilon}+\left(\frac{2t_0^2}{V}\right)^2\frac{1}{U_d}, \tag{41}$$

where t_0 represents the hopping integral between Cu and O, V the interaction between copper-site electrons and oxygen-site holes, U_d the on-site repulsion at copper sites, and ε the energy difference between the copper-site electron and oxygen-site hole. We can put $J'_{sd,d}=(2t_0^2/V)^2(1/U_d)$ to obtain[57] $J'_{sd,d}\simeq 0.12$ eV. The corresponding spin-relaxation rate from the superexchange interaction is given by

$$(T_1)_{ID}^{-1}=\left[\left|\frac{4\pi}{\hbar}(J'_{sd,d})^2\frac{N^2(0)}{N^2}k_BT-\frac{4\pi}{\hbar}(J'_{sd,d})^2\frac{N^2(0)}{N^2}2U_d\int_{\varepsilon_F+k_BT}^{\infty}\times\frac{f(\varepsilon)[1-f(\varepsilon)]}{\varepsilon-\varepsilon_F}d\varepsilon+\frac{4\pi}{\hbar}(J'_{sd,d})^2\frac{N^2(0)}{N^2}\frac{U_d^2}{k_BT}\int_{\varepsilon_F+\gamma U_d}^{\infty}\times\frac{f(\varepsilon)[1-f(\varepsilon)]k_BT}{(\varepsilon-\varepsilon_F)^2}d\varepsilon\right|\right]. \tag{42}$$

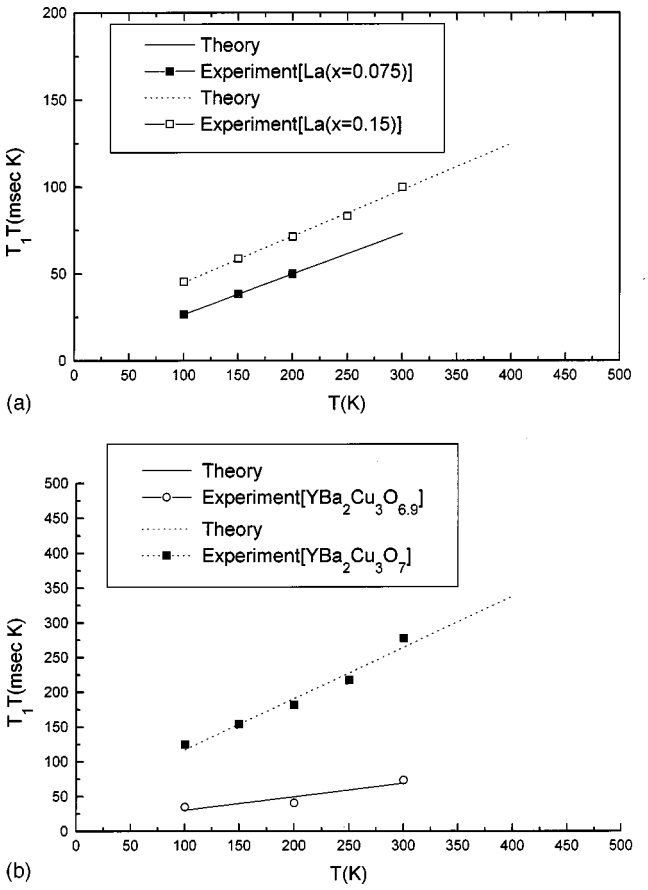

FIG. 8. Spin-relaxation rates obtained from experiments (Refs. 59 and 60) and fitted with our theoretical model. The graph of a line form is for our theoretical model. (a) Graph is for La-Sr-Cu-O; (b) The other one is for Y-Ba-Cu-O.

We can use $\int_1^\infty (e^x dx)/[x(e^x+1)^2]=0.15$, $\gamma=|f'(\varepsilon_F)/f(\varepsilon_F)|k_BT$, and

$$\int_{\frac{\gamma U_d}{k_BT}}^{\infty}\frac{e^x dx}{x^2(e^x+1)^2}\equiv\beta(U_d),$$

where the lower limit of the integral comes from the higher-order expansion of the integrand near Fermi energy, to obtain the resultant spin-relaxation rate above T_c as follows:

$$[T_1T]^{-1}\simeq\frac{4\pi}{\hbar}(J'_{sd,d})^2\frac{N^2(0)}{N^2}(0.3U_d)\frac{1}{T+T_{cw}}-\frac{4\pi}{\hbar}(J'_{sd,d})^2\frac{N^2(0)}{N^2}k_B, \tag{43}$$

where the order of magnitude is estimated to give $O(U_d)\simeq O(10^2)O(k_BT)$ and $O[(T_1)_{ID}^{-1}]\sim O(10)O[(T_1)_D^{-1}]$. The Curie-Weiss–like temperature is given by

TABLE V. The parameters are obtained from fitting values.

Materials	$J'_{sd,d}$(eV)	$N(0)$ (states/eV)	U_d(eV)	T_{CW}(K)	N
$La_{1.85}$	0.12	0.22	7.2	69	10^5
Y-O_7	0.12	0.22	2.6	59	10^5

$$T_{\mathrm{CW}}=\frac{\beta(U_d)}{0.3}\frac{U_d}{k_B}\ll T_c. \tag{44}$$

Figure 8 and Table V show a good agreement between theory and experiment. Below the onset temperature of pseudospin gap, T_{PG} the renormalized spin-relaxation rate is given by[58]

$$[TT_1]^{-1}\simeq\frac{4\pi}{\hbar}(J'_{sd,d})^2\frac{N^2(0)}{N^2}(0.3U_d)\times\frac{1}{T_{\mathrm{PG}}+T_{\mathrm{CW}}}\frac{I(T,\omega)}{I(T_{\mathrm{PG}},\omega)}, \tag{45}$$

where

$$I(T,\omega)=2\int_{\Delta_{\mathrm{PG}}}^{\infty}dE\,\frac{[E(E+\omega)+\Delta_{\mathrm{PG}}^2]\left(-\frac{\partial f}{\partial E}\right)}{(E^2-\Delta_{\mathrm{PG}}^2)^{1/2}[(E+\omega)^2-\Delta_{\mathrm{PG}}^2]^{1/2}}, \tag{46}$$

and ω represents an infinitesimal energy and Δ_{PG} is the pseudospin gap. The spin-relaxation rate below T_c has no Hebel-Slichter peak due to finiteness of $\Delta_{\mathrm{PG}}(T_c)$.[23]

VIII. CONCLUSION

We have constructed a theoretical scheme for high-T_c superconductivity based on the electron-hole composite quasiparticle concept. Using this concept we have investigated the in-plane resistivity R_{ab}. The measured T-linear contribution is satisfactorily explained by the Kondo-type *s-d* spin scatterings as shown in Fig. 4. We have also shown that the resistivity along the c axis, R_c, is dominated by the superexchange interaction between $O(2p)$ in copper planes and $O(3s)$ in non-copper-oxide planes. As shown in Fig. 6, according to the doping rates R_c shows three type behaviors in accordance with experiments. The magnetic susceptibility and nuclear-spin-relaxation rates $[T_1T]^{-1}$ are also explained by the same concept of *s-d* interaction. The transition temperature T_c in *a-b* planes is determined by the Kondo-type *s-d* scatterings U_{sd}. We can predict by our model the anomaly from nonsuperconducting electrons near Kondo temperature, $T_{\mathrm{Kondo}}\sim 0$ K, which will be published elsewhere in more details. U_{sd} is the interaction from local spin flippings mediated by Gell-Mann and Breuckner-type phonons (GB-phonons). In this interaction GB-phonons play a role of *antiferromagnetic attractor*. It means that for a singlet Cooper pair, a hole of a spin-up interacts with the localized spins with spin-down and the other hole of a spin-down interacts with the local spins with spin-up. As shown in Fig. 1, the copper ion is bound up with one core hole at low temperatures below T_c, for intermediately positioned electrons of these quasiparticles seldom overlap with each other. At high temperatures above T_c the copper ion becomes coupled with two core holes of a singlet, which are from overlapped quasiparticles. This is similar to a reverse case of the spin-Peierls transition[43] without lattice instability. The clue of this phenomenon is that the wave number of copper phonon above T_c is $1/\sqrt{2}$ times smaller than that below T_c because of the change of effective mass of core holes coupled to copper ions as shown in Fig. 2. The change of copper phonons is observed in Raman experiments.[61–63] Because the gap is finite at T_c, T_c is modified by tanh term in BCS formulation as shown above. The transition temperature $T_c^{c\text{-axis}}$ along the c axis is completely governed by superexchange interaction between $O(2p)$ in copper planes and $O(3s)$ in non-copper-oxide planes, U_{sd}^c totally different from the properties in *a-b* planes.

ACKNOWLEDGMENT

We are greatly indebted to the late Professor Duk Joo Kim and also to Professor Chul Koo Kim.

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