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LETTER TO THE EDITOR

The spin-gap in high T_c superconductivity

Je Huan Koo[1] **and Guangsup Cho**

Department of Electrophysics, Kwangwoon University, 447-1 Wallgye-dong, Nowon-gu, Seoul 139-701, Korea

E-mail: koo@kw.ac.kr

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Abstract
We have investigated the spin-gap in high T_c superconductivity. We obtain the effective exchange integral in the presence of conduction in the ab-plane from the interaction U_{sd}, where the electron–electron interaction is mediated by the localized spin flips. We choose the exchange interaction along the c-axis from the superexchange-type interaction, U_{sd}^{c}. We find the spin-gap from the conducting spin-$\frac{1}{2}$ ladder corresponding to the structure of high T_c superconductors.

The provocative proposal that the mechanism of high temperature superconductivity in layered cuprates may be related to the exotic properties of low-dimensional quantum spin systems, such as the RVB (resonating valence bond) state [1], has been a major driving force behind the rapid advance of quantum magnetism. The spin-gap system is a magnetic system having the singlet ground spin liquid state with a finite excitation gap [2]. Recently, the magnetic ordering induced by modifying the gapped ground state by an external field or impurity doping has been energetically investigated. The spin-gap is a gap from the spin excitation spectrum [2–4] shown in various materials. The two-dimensional standard model for a spin-gap is from the anisotropic exchange interaction in the spin-$\frac{1}{2}$ ladder of localized spins. The parent cuprate insulators are now considered the best examples of planar spin-$\frac{1}{2}$ antiferromagnets. The high T_c superconductivity (HTSC) materials can be regarded as a conducting spin-$\frac{1}{2}$ ladder of two legs which are composed of oxygen spins.

In this letter, we obtain the spin-gap by treating HTSC as a conducting spin-ladder, as shown in figure 1.

We consider the Hamiltonian in the ab-plane. We want to explain our basic Hamiltonian with the s–d exchange spin flip interaction [5, 6]. The Hamiltonian for one-band type

[1] Author to whom any correspondence should be addressed.

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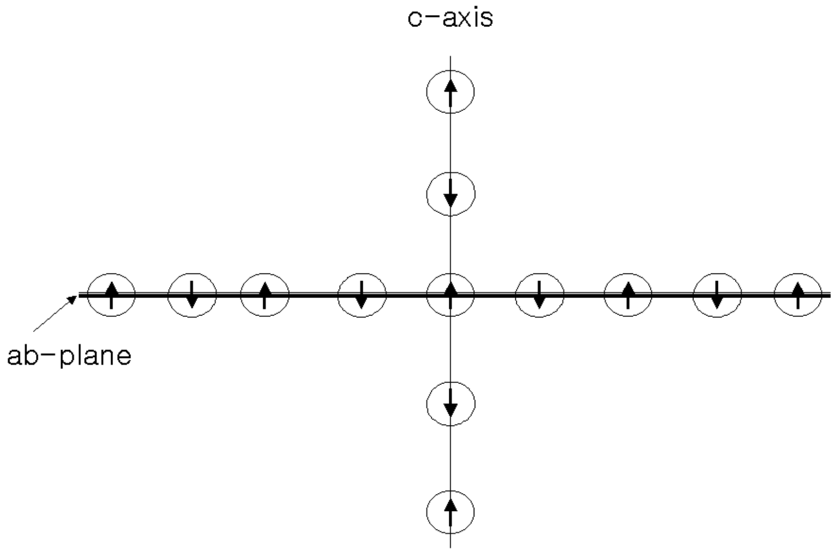

Figure 1. The spin-ladder is from spins of oxygen.

carriers [7] with exchange interaction is given by

$$H_{\mathrm{sd}} = \sum_{k,\sigma} \varepsilon_{k,\sigma} a^+_{k\sigma} a_{k\sigma} + \frac{1}{2} \sum_{k\kappa\mu} \sum_{l\nu} U_{\mathrm{c}} a^+_{k+\kappa,\mu} a_{k,\mu} a^+_{l,\nu} a_{l+\kappa,\nu} - \frac{1}{N} \sum_{i=1}^{N_0} \sum_{k,\kappa} J_{\mathrm{sd}}(\kappa) \exp(\mathrm{i}\kappa R_i)$$
$$\times [S^z_i (a^+_{k,\uparrow} a_{k-\kappa,\uparrow} - a^+_{k,\downarrow} a_{k-\kappa,\downarrow}) + S^+_i a^+_{k,\downarrow} a_{k-\kappa,\uparrow} + S^-_i a^+_{k,\uparrow} a_{k-\kappa,\downarrow}], \quad (1)$$

where $a^+_{k\sigma}$ is the creation operator of a conducting hole with momentum $\hbar\vec{k}$ and spin σ. $\vec{S}_i$ is the localized spin at site $\vec{R}_i$ and S^z_i is its z component. $J_{\mathrm{sd}}(\kappa)$ is the Fourier component of the s–d or p–d exchange integral between the conducting hole and localized electron. U_{c} is the Fourier component of the screened Coulomb interaction between holes. s is the magnitude of a localized spin. N_0 is the number of localized spins and N is the total number of conducting carriers. The effective Hamiltonian

$$H = \sum_k \varepsilon_{k,\sigma} a^+_{k,\sigma} a_{k,\sigma} + \frac{2}{3N^2 k_{\mathrm{B}} T} N_0 s(s+1) \sum_{k,k',q,\sigma} (J^2_{\mathrm{sd}}) a^+_{k,\sigma} a_{k-q,-\sigma} a^+_{k',-\sigma} a_{k'+q,\sigma}$$
$$+ \tfrac{1}{2} \sum_{k,k',q,\sigma,\sigma'} U_{\mathrm{c}} a^+_{k,\sigma} a_{k-q,\sigma} a^+_{k',\sigma'} a_{k'+q,\sigma'} \quad (2)$$

can be obtained by use of a canonical transformation [6, 7].

The BCS-like Hamiltonian in ab-planes as shown in figure 1 [7] is given by

$$H^{ab} = \sum_k (\varepsilon_k - \varepsilon_{\mathrm{sd}}) a^+_k a_k + \sum_{k,k',q} \tfrac{1}{2} U_{\mathrm{c}} a^+_{k+q} a_k a^+_{k'} a_{k'+q}$$
$$+ \sum_{k,k',q} \frac{|g_{\mathrm{sd}}|^2 \hbar\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - (\hbar\omega_q)^2} \left(\frac{2N_0 s(s+1)}{3k_{\mathrm{B}} T} \right)^2 n(q) n(-q) a^+_{k+q} a_k a^+_{k'} a_{k'+q}, \quad (3)$$

where g_{sd} is the coupling constant, $\hbar\omega$ the phonon energy of copper ions and

$$n(q) = \langle a^+_k a_{k+q} \rangle$$
$$\varepsilon_{\mathrm{sd}} = \frac{2J^2_{\mathrm{sd},0} N_0 s(s+1)}{3k_{\mathrm{B}} T} \sum_k \langle a^+_k a_k \rangle. \quad (4)$$

Therefore it becomes

$$H^{ab} = \sum_k (\varepsilon_k - \varepsilon_{\mathrm{sd}}) a_k^+ a_k + \sum_{k,k',q} \tfrac{1}{2}(U_{\mathrm{sd}} + U_{\mathrm{c}}) a_{k+q}^+ a_k a_{k'}^+ a_{k'+q}, \tag{5}$$

where

$$U_{\mathrm{sd}} = \frac{2|g_{\mathrm{sd}}|^2 \hbar\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - (\hbar\omega_q)^2} \left(\frac{2N_0 s(s+1)}{3k_{\mathrm{B}}T}\right)^2 n(q)n(-q). \tag{6}$$

Experimental evidences are available 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 $\mathrm{CuO_2}$ planes, and oxygens, $\tilde{\mathrm{O}}$ in other oxide planes, are contributing to the c-axis resistivity through the superexchange interaction, for overlap between O(2p) and the extended $\tilde{\mathrm{O}}$(3s) occurs. 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 $\mathrm{CuO_2}$ and $\tilde{a}$ to oxygens of the other oxide planes.

The dominating factor from the superexchange interaction is

$$\left[J_{\mathrm{O}}^2 \sum_q \frac{\tilde{f}_q}{\tilde{\varepsilon}_k - \tilde{\varepsilon}_q}\right]\left[J_{\mathrm{O}}^2 \sum_q \frac{1 - f_q}{\varepsilon_k - \varepsilon_q}\right], \tag{7}$$

where J_{O} represents the exchange interaction between a hole from O(2p) of the $\mathrm{CuO_2}$ plane and an electron from O(3s) of other oxide planes. Thus the Kondo formalism [7] of the superexchange interaction through the extended O(3s) orbitals of different oxide planes gives rise to the c-axis resistivity as

$$R_{\mathrm{c}} = R_{\mathrm{const}}\left[1 + f(\varepsilon_{\mathrm{F}})\frac{4J_{\mathrm{O}}}{N}N(\varepsilon_{\mathrm{F}})\ln\left(\frac{k_{\mathrm{B}}T}{\alpha W}\right) - f'(\varepsilon_{\mathrm{F}})\frac{4J_{\mathrm{O}}}{N}N(\varepsilon_{\mathrm{F}})(k_{\mathrm{B}}T)\right] \times \left[1 + \{1 - f(\tilde{\varepsilon}_{\mathrm{F}}^{\mathrm{sd}})\}\frac{4J_{\mathrm{O}}}{N}N(\tilde{\varepsilon}_{\mathrm{F}}^{\mathrm{sd}})\ln\left(\frac{k_{\mathrm{B}}T}{\alpha W}\right) + f'(\tilde{\varepsilon}_{\mathrm{F}}^{\mathrm{sd}})\frac{4J_{\mathrm{O}}}{N}N(\tilde{\varepsilon}_{\mathrm{F}}^{\mathrm{sd}})k_{\mathrm{B}}T\right] + R'_{\mathrm{const}} \tag{8}$$

where $R_{\mathrm{const}} = N_0 R'_0 (\frac{J_{\mathrm{O}}}{Nk_{\mathrm{B}}T_{\mathrm{c}}})^2 \frac{1}{4}$, $R'_0 = R_0(J_{\mathrm{sd},0} \to J_{\mathrm{O}})$, $\tilde{\varepsilon}_{\mathrm{F}}^{\mathrm{sd}} = \varepsilon_{\mathrm{F}} - \varepsilon_{\mathrm{sd}}^c = \varepsilon_{\mathrm{F}}^{\mathrm{sd}}(J_{\mathrm{sd},0} \to J_{\mathrm{O}})$, and R'_{const} is another constant term from non-superexchange parts.

We define

$$\Lambda^c(T) \equiv \left(\frac{J_{\mathrm{O}}}{Nk_{\mathrm{B}}T_{\mathrm{c}}}\right)^2 \frac{1}{4}\left[1 + f(\varepsilon_{\mathrm{F}})\frac{4J_{\mathrm{O}}}{N}N(\varepsilon_{\mathrm{F}})\ln\left(\frac{k_{\mathrm{B}}T}{\alpha W}\right) - f'(\varepsilon_{\mathrm{F}})\frac{4J_{\mathrm{O}}}{N}N(\varepsilon_{\mathrm{F}})k_{\mathrm{B}}T\right]. \tag{9}$$

Using the same method as obtaining Hamiltonian in ab-planes, by substituting J_{sd}^c for J_{sd} [7], the Hamiltonian along the c-axis as shown in figure 1 is given by

$$H^c = \sum_k (\varepsilon_k - \varepsilon_{\mathrm{sd}}^c) a_k^+ a_k + \sum_{k,k',q} \tfrac{1}{2}(U_{\mathrm{sd}}^c + U_{\mathrm{c}}) a_{k+q}^+ a_k a_{k'}^+ a_{k'+q}, \tag{10}$$

where

$$\varepsilon_{\mathrm{sd}}^c = \frac{2(J_{\mathrm{sd},0}^c)^2 N_0 s(s+1)}{3k_{\mathrm{B}}T_{\mathrm{c}}} \sum_k \langle a_k^+ a_k \rangle,$$

$$U_{\mathrm{sd}}^c = \frac{2|g_{\mathrm{sd}}^c|^2 \hbar\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - (\hbar\omega_q)^2}\left(\frac{2N_0 s(s+1)}{3k_{\mathrm{B}}T_{\mathrm{c}}}\right)^2 (n_0^c)^2,$$

$$(J_{\mathrm{sd},0}^c)^2 = J_{\mathrm{O}}^2 \Lambda^c(T), \qquad n_0^c \simeq n(q)$$

for the c-axis, N_0 becomes N'_0, $f(\varepsilon_{\mathrm{F}})$ is the Fermi–Dirac distribution, $g_{\mathrm{sd}}^c = g_{\mathrm{sd}}(J_{\mathrm{sd}} \to J_{\mathrm{sd},0}^c)$, $N(\varepsilon_{\mathrm{F}})$ is the density of states at the Fermi level, J_{O} is the exchange interaction between the O(3s) orbital of the copper oxide plane and the $\tilde{\mathrm{O}}$(3s) orbital of the non-copper oxide plane,

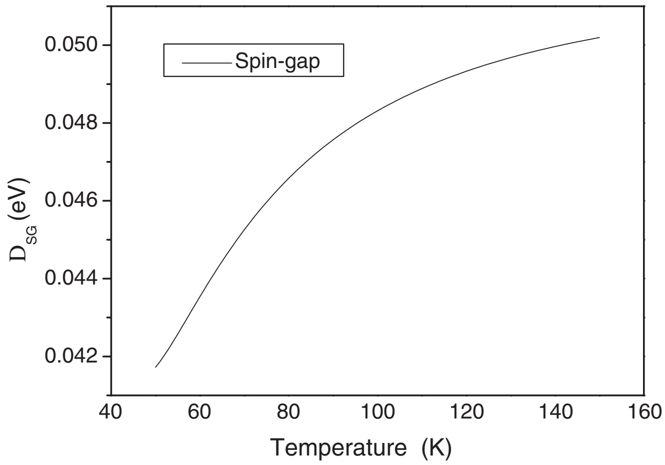

Figure 2. The variation of spin-gap with temperature. We use the parameters such as $J_O = 0.1$ eV, $J_{\tilde{O}} = 0.1$ eV, $U_c = 3.5$ eV, $U^c_{sd}|_{T_c} = -5$ eV, $U_{sd}|_{T_c} = -7$ eV, $T_c = 100$ K, $t^2/t^2_{ab} = 0.001$, $\tilde{t}^2/t^2_c = 0.000\,01$, $T_{PG} = 150$ K.

and $T = T_M$ below T_M, where $s(s+1)/3k_BT_M \equiv s/g\mu_B H_i$, H_i is the local internal field, g is the electron Lande factor, μ_B is the Bohr magneton and T_M is the saturation temperature of spin-flip.

For the spin-$\frac{1}{2}$ ladder of two legs with an ab-chain and a c-chain, the spin-gap [3, 4] is given by

$$\frac{\Delta_{SG}}{J^{ab}_O} = 1 - \frac{J^c_O}{J^{ab}_O} + \frac{1}{2}\left(\frac{J^c_O}{J^{ab}_O}\right)^2, \tag{11}$$

where J^{ab}_O is the effective exchange integral between oxygen sites in ab-planes and J^c_O is that along the c-axis and the spin-gap happens below T_{PG}. According to Dirac's work [8], an exchange interaction is given by

$$J_{\rm Dirac} = \int d\vec{r}_1\, d\vec{r}_2\, \frac{e^2}{|\vec{r}_2 - \vec{r}_1|}\, \mathrm{Re}[\phi^*_a(\vec{r}_1)\phi^*_b(\vec{r}_2)\phi_b(\vec{r}_1)\phi_a(\vec{r}_2)] \simeq \int dq\, U_c(q)\frac{t^2}{t^2_0}, \tag{12}$$

where t is the hopping integral and $t_0 = t(q=0)$ and ϕ_i is an atomic orbital for the ith atom. The exchange interactions become

$$J^{ab}_O = J_O + (U_{sd}(q) + U_c(q))\frac{t^2}{t^2_{ab}}, \tag{13}$$

$$J^c_O = J_{\tilde{O}} + (U^c_{sd}(q) + U_c(q))\frac{\tilde{t}^2}{t^2_c} \simeq J_{\tilde{O}}, \tag{14}$$

where J_O is the pure exchange integral between oxygen sites in the ab-plane and $J_{\tilde{O}}$ that along the c-axis, t is the hopping integral in the ab-plane, $\tilde{t}$ that along the c-axis, t_{ab} and t_c are critical constants, $U_{sd} \propto -\frac{1}{T^2}$ for $T \geqslant T_M$, and

$$U_{sd} < 0, \qquad U^c_{sd} < 0, \qquad \text{below } T_{PG}. \tag{15}$$

Our spin-gap has a temperature dependence different from the other theoretical predictions [9]. As shown in figure 2, the spin-gap below T_c varies rapidly and that above T_c changes slowly (almost flatly). If the hopping increases, the effective exchange interaction in the ab-plane decreases so that the spin-gap is also reduced from equations (13), (14). This explains that the overdoped HTSC materials have no spin-gaps because of higher hoppings. Because $|U_{\rm sd} + U_{\rm c}|$ is much larger than $|U_{\rm sd}^{c} + U_{\rm c}|$, we neglect $|U_{\rm sd}^{c} + U_{\rm c}|$ in equation (14). In underdoped HTSC materials, $|U_{\rm sd} + U_{\rm c}|\frac{t^2}{t_{ab}^2}$ is smaller by one order of magnitude than $J_{\rm O}$, so the temperature dependence of the spin-gap is very weak. Since the resistivity ratio between that along the c-axis and that in ab-planes is larger than 100, we choose the small value of $\tilde{t}^2/t_{\rm c}^2 = 10^{-5}$ to evaluate the spin-gap. We regard the HTSC materials as a spin-$\frac{1}{2}$ ladder of two legs with an ab-chain and a c-chain, which consist of oxygen spins. All measurements on pseudo-gaps, that is, nuclear relaxation rates, resistivity, etc are only for charge-gap type except the inelastic neutron scattering experiments for the spin-gap [10].

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