Relevance and irrelevance of three effective Hamiltonians for high-temperature superconductors with CuO_2 planes

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Photoemission spectra of high-temperature cuprate-oxide superconductors are consistent with band calculations; Cu $3d$ levels are shallower than O $2p$ levels by about 1 eV. When effects of shallow and broad $3d$ and $2p$ levels are taken into account, the superexchange interaction is substantially reduced but still it is as strong as $J\simeq -0.1$ eV within the three-band periodic Anderson model called the d-p model that takes into account Cu $3d_{x^2-y^2}$, O $2p_x$, and O $2p_y$ orbits. The d-p model whose parameters are consistent with photoemission spectra is a relevant model for the cuprate oxides; the coupling constant for $d_{x^2-y^2}$-wave superconductivity, which is approximately proportional to the density of states of quasiparticles and the superexchange interaction, is large enough to explain observed critical temperatures as high as $T_c=50-100$ K. The t-J model with $t\simeq -0.21$ eV and $J\simeq -0.1$ eV is also a relevant model for the cuprate oxides. When the reduction of the superexchange interaction is taken into account, on the other hand, T_c's of the Hubbard model whose parameters are consistent with the two relevant models are substantially lower than their T_c's. [S0163-1829(99)02513-8]

I. INTRODUCTION

In order to explain high-temperature superconductivity (HTS) in the cuprate oxides with CuO_2 planes, it is indispensable to understand their normal states. When no holes are doped, they are Mott-Hubbard insulators, each of which has an energy gap across the Fermi level between the lower Hubbard band (LHB) and upper Hubbard band (UHB).[1–3] When enough holes are doped, they become metallic. However, spectra of photoemission spectroscopy (PES) or x-ray photoemission spectroscopy (XPS) of metallic oxides are almost the same as those of insulating oxides[4–6] except for small variations in the vicinity of the Fermi-level edge.[7,8] This implies that the formation of the LHB and UHB occurs similarly in insulating and metallic oxides. The energy gap between the LHB and UHB gives an estimate of the on-site repulsion between electrons. Then, the on-site repulsion between Cu $3d$ electrons in metallic oxides is almost the same as that in insulating oxides, and is larger than the unrenormalized bandwidth, which is deduced by band calculations. The small variations imply the formation of Gutzwiller's heavy quasiparticle band[9] around the Fermi level. It was demonstrated in a recent theory[10] that when holes are doped a narrow band is formed at the top of a broadband, and it was argued there that the narrow band is nothing but Gutzwiller's heavy quasiparticle band and the broadband is nothing but the LHB.[11] According to Gutzwiller's theory[9] or the recent theory,[10] effective masses of quasiparticles are approximately proportional to $1/\delta$, with δ being concentrations of doped holes. In the region of small δ's, however, effective masses estimated from experimental specific heat coefficients become lighter as δ's become smaller.[12,13] This discrepancy between theory and experiment was argued in the context of the so-called spin-gap behaviors;[14,15] Gutzwiller's heavy quasiparticles are renormalized by antiferromagnetic exchange interactions or spin fluctuations, so that their effective masses become much lighter than those predicted by Gutzwiller's theory.

It is certain that HTS in the cuprate oxides, cuprate HTS, occurs in the vicinity of the Mott-Hubbard transition. Any relevant theory of cuprate HTS should take into account that it occurs in strongly correlated electron liquids.

On the other hand, the accumulation of experimental data implies that the formation of $d_{x^2-y^2}$-wave Cooper pairs between quasiparticles in Landau's Fermi liquids is responsible for cuprate HTS. Within this theoretical framework, the coupling constant for superconductivity is approximately proportional to the density of states (DOS) of quasiparticles and a superconducting pairing interaction; they are mainly argued in this paper instead of superconducting critical temperatures T_c themselves; it is never a good idea to try to predict accurately T_c's, which sensitively depend on the coupling constant.

According to the Fermi-liquid relation,[16] the specific heat coefficient is given by

$$\gamma=\frac{2}{3}\pi^2k_B^2\rho^*(0), \tag{1.1}$$

with k_B being the Boltzmann constant and $\rho^*(0)$ the DOS per spin of quasiparticles at the Fermi level. Experimental γ's are as large as

$$\gamma\simeq 14 \text{ mJ/K}^2 \text{ eV } (\text{CuO}_2 \text{ mol}) \tag{1.2}$$

for the cuprate oxides with $T_c\simeq 50-100$ K.[12,13] Then, it follows from Eqs. (1.1) and (1.2) that

$$\rho^*(0)\simeq 3.0 \text{ states/eV spin } \text{CuO}_2. \tag{1.3}$$

It is easy to explain this large $\rho^*(0)$ in terms of the formation of Gutzwiller's heavy quasiparticles.[17]

One of the most crucial issues is the question of what attractive interaction is the main pairing interaction in cuprate HTS. In general, mutual interactions are caused by the virtual exchange of bosons or bosonic excitations. For example, the electromagnetic force is caused by that of pho-

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tons, Yukawa's nuclear force by that of pions, pairing interactions in conventional Bardeen-Cooper-Schrieffer (BCS) superconductors by that of phonons, and so on. Magnetic exchange interactions were originally derived by perturbation, implicitly or explicitly, in terms of V/U, V being transfer integrals or hybridization matrices and U the on-site repulsion.[18] They can also be derived within the framework of the virtual exchange of bosonic excitations. In this framework, for example, the superexchange interaction is caused by that of high-energy spin excitations, pair excitations of electrons in spin channels, between the LHB and UHB;[19,20] it is obvious that as long as the formation of the LHB and UHB occurs the superexchange interaction is present in not only insulating phases but also metallic phases. A magnetic exchange interaction can also be a pairing interaction.[21,22] It was argued[23] that in cuprate HTS the antiferromagnetic superexchange interaction is mainly responsible for the formation of $d_{x^2-y^2}$-wave Cooper pairs; the virtual exchange of low-energy spin excitations, which are called paramagnons, plays a less important role than the superexchange interaction. It is likely that the virtual exchange of phonons plays only a minor role in strongly correlated electron liquids such as the cuprate oxides.[24]

The exchange interaction in the cuprate oxides is antiferromagnetic and is as strong as[25,26]

$$J \simeq -(0.10-0.12)\ \text{eV}. \tag{1.4}$$

When both Eqs. (1.3) and (1.4) are phenomenologically taken into account, it is straightforward to obtain theoretically $T_c = 50-100$ K for the formation of $d_{x^2-y^2}$-wave Cooper pairs.[27–30] Within a theoretical framework of the strong on-site repulsion, the antiferromagnetic exchange interaction between nearest neighbors, and the large Fermi surface predicted by band calculations, it is absolutely definite that T_c's for the formation of $d_{x^2-y^2}$-wave Cooper pairs are much higher than those of other waves.[27,28] The main purpose of this paper is to argue what is one of the simplest and relevant effective Hamiltonians that involve both Eqs. (1.3) and (1.4).

The exchange interaction J in the t-J model is a phenomenological term. It is microscopically derived in the perturbative scheme in terms of V/U; the on-site repulsion is infinitely large in the t-J model. Then, it is certain that when holes are doped Gutzwiller's heavy quasiparticles are formed in the t-J model. When a phenomenological J as large as Eq. (1.4) is used, the t-J model must be a relevant model for cuprate HTS.[31] Actually, numerical studies imply that the ground state of the t-J model in two dimensions[32] is the condensed state of $d_{x^2-y^2}$-wave Cooper pairs in a certain region of hole concentrations.[33–35]

Because cuprate HTS occurs essentially on CuO_2 planes, it is reasonable to expect that the three-band periodic Anderson model called the d-p model that takes into account Cu $3d$, O $2p_x$, and O $2p_y$ orbits is a relevant microscopic model for cuprate HTS. The t-J model is approximately derived or mapped from the d-p model.[36] In deriving the t-J model, Zhang and Rice[36] assumed that Cu $3d$ levels are much deeper than O $2p$ levels, following an interpretation of XPS spectra[5,6,37] that

$$\epsilon_{3d} - \mu \simeq -(10-12)\ \text{eV} \tag{1.5}$$

for Cu $3d$ levels and

$$\epsilon_{2p} - \mu \simeq -3\ \text{eV} \tag{1.6}$$

for O $2p$ levels,[38] with μ being the chemical potential. On the other hand, it follows according to band calculations[39–41] that

$$\epsilon_{3d} - \mu \simeq -2.3\ \text{eV} \tag{1.7}$$

and

$$\epsilon_{2p} - \mu \simeq -3.3\ \text{eV}. \tag{1.8}$$

It is surprising if such a large discrepancy between theory and experiment is real; band calculations have given so far at least good starting points to understand many crystalline materials. If this large discrepancy is real, the theory of band calculations should be critically examined as to why it gives such a large discrepancy for the cuprate oxides. On the other hand, it is interesting to examine whether or not XPS spectra can be interpreted consistently with band calculations. This examination is another purpose of this paper.

It is reasonable to expect that the universality class of the Hubbard model is the same as that of the t-J model and the ground state of the Hubbard model is also superconducting in a certain region of hole concentrations. On the other hand, numerical studies of the Hubbard model[42–45] showed that no significant superconducting fluctuations are developed for any hole concentration, at least in the temperature region considered. These studies imply that the coupling constant of the Hubbard model is so small that its T_c's are too low to be treated by numerical studies.[32] It is interesting to examine why the coupling constant of the Hubbard model is smaller than that of the corresponding t-J model. The formation of Gutzwiller's heavy quasiparticles must occur in a similar manner in both of the t-J model, whose on-site repulsion is infinitely large, and the Hubbard model, whose on-site repulsion is as large as or larger than the unrenormalized bandwidth. Then, a possible argument is that exchange interactions involved in the Hubbard model must be weaker than those of the corresponding t-J model.

Magnetic exchange interactions such as the superexchange interaction were originally derived for insulating phases where levels of magnetic electrons are deep and sharp enough.[18] According to band calculations, however, Cu $3d$ levels are shallow and broad in the cuprate oxides. In general, an exchange interaction is reduced, when exchanged bosons have nonzero lifetime broadening. Then, magnetic exchange interactions must be reduced in the cuprate oxides. One of the other purposes of this paper is to study such a reduction effect on magnetic exchange interactions in the d-p and the Hubbard models.

The structure of this paper is as follows. It is argued in Sec. II that XPS spectra are consistent with band calculations. It is argued in Sec. III that the d-p model whose parameters are consistent with XPS spectra is a relevant model for cuprate HTS. It is shown in Sec. IV that the exchange interaction involved in the Hubbard model corresponding to the relevant d-p or the relevant t-J model is weaker than Eq. (1.4). A discussion is given in Sec. V. A summary is given in Sec. VI. In the Appendix, several rigorous properties for the auxiliary-particle t-J model are argued.

II. SHALLOW Cu 3*d* LEVELS

Direct processes of XPS in the cuprate oxides are $(3d)^9+h\nu\rightarrow(3d)^8+e^-$ and $(3d)^9+h\nu\rightarrow(3d)^9\underline{L}+e^-$, where $(3d)^9$ stands for the ground state of Cu^{2+} ions, $h\nu$ for a photon, e^- for an emitted electron, and L for a $2p$ hole on O ions. On the other hand, the initial processes of resonant XPS are $(3d)^9+h\nu\rightarrow\underline{p}(3d)^{10}$ and $(3d)^9+h\nu\rightarrow\underline{p}(3d)^9 4s$, where $\underline{p}$ stands for a $2p$ or $3p$ core hole on a Cu ion. Then, the Auger processes of $\underline{p}(3d)^{10}\rightarrow(3d)^8+e^-$ and $\underline{p}(3d)^9 4s\rightarrow(3d)^7 4s+e^-$ occur. If electron correlations between O $2p$ electrons and Cu core holes are substantial, the following Auger processes also occur: $\underline{p}(3d)^{10}\rightarrow(3d)^9\underline{L}+e^-$, $\underline{p}(3d)^{10}\rightarrow(3d)^{10}\underline{L}^2+e^-$, $\underline{p}(3d)^9\overline{4s}\rightarrow(3d)^8 4s\underline{L}+e^-$, and $\underline{p}(3d)^9 4s\rightarrow(\overline{3d})^9 4s\underline{L}^2+e^-$. Because the hybridization between Cu $3d$ and O $2p$ orbits is strong, the mixing among $(3d)^8$, $(3d)^9\underline{L}$, and $(3d)^{10}\underline{L}^2$ and the mixing among $(3d)^7 4s$, $(3d)^8 4s\underline{L}$, and $(3d)^9 4s\underline{L}^2$ in final states can never be ignored in the direct and the Auger processes. If these processes are effective, an interpretation of XPS spectra consistent with band calculations is possible.

Consider a cluster of CuO_4 on a plane, which includes only a Cu $3d_{x^2-y^2}$ orbit, a Cu $4s$ orbit, and a linear combination of four O $2p$ orbits that has the x^2-y^2 symmetry:

$$\mathcal{H}_c=\sum_\sigma(\epsilon_{4s}-\mu)\hat{n}_{s\sigma}+\sum_\sigma(\epsilon_{3d}-\mu)\hat{n}_{d\sigma}+U_{dd}\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}+\sum_\sigma(\overline{\epsilon}_{2p}-\mu)\hat{n}_{p\sigma}+U_{pp}\hat{n}_{p\uparrow}\hat{n}_{p\downarrow},\tag{2.1}$$

with $\hat{n}_{\nu\sigma}$'s ($\nu=d$, s, or p) number operators. It is assumed that the on-site repulsion U_{dd} is so strong that[46]

$$\epsilon_{3d}+U_{dd}-\mu>0,\tag{2.2}$$

and that $\epsilon_{3d}-\mu<0$, $\overline{\epsilon}_{2p}+U_{pp}-\mu<0$, and $\epsilon_{4s}-\mu>0$. No hybridization between different orbits is taken into account; only excitation energies of XPS can be argued, but no line shapes can be argued.

Although the ground state of this cluster model is $(3d)(2p)^2$, it is denoted as $(3d)^9$ in this paper. The energy of the ground state is $E[(3d)^9]=(\epsilon_{3d}-\mu)+2(\overline{\epsilon}_{2p}-\mu)+U_{pp}$. Define an effective depth of $2p$ levels by

$$\epsilon_{2p}=\overline{\epsilon}_{2p}+U_{pp}.\tag{2.3}$$

Excitation energies from $(3d)^9$ are given by[47]

$$E[(3d)^9\underline{L}]-E[(3d)^9]=-(\epsilon_{2p}-\mu),\tag{2.4}$$

$$E[(3d)^8]-E[(3d)^9]=-(\epsilon_{3d}-\mu),\tag{2.5}$$

$$E[(3d)^9 4s\underline{L}^2]-E[(3d)^9]=U_{pp}+(\epsilon_{4s}-\mu)-2(\epsilon_{2p}-\mu),\tag{2.6}$$

$$E[(3d)^8 4s\underline{L}]-E[(3d)^9]=(\epsilon_{4s}-\mu)-(\epsilon_{3d}-\mu)-(\epsilon_{2p}-\mu),\tag{2.7}$$

and

$$E[(3d)^{10}\underline{L}^2]-E[(3d)^9]=U_{dd}+U_{pp}+(\epsilon_{3d}-\mu)-2(\epsilon_{2p}-\mu).\tag{2.8}$$

According to Eq. (2.4), Eq. (2.3) is nothing but the depth of $2p$ levels measured by XPS. When other Cu $3d$ orbits are explicitly taken into account, the configuration of $(3d)^7 4s$ can be treated. Its excitation energy is substantially larger than Eqs. (2.6) and (2.7):[48]

$$E[(3d)^7 4s]-E[(3d)^9]\simeq U_{dd}+(\epsilon_{4s}-\mu)-2(\epsilon_{3d}-\mu).\tag{2.9}$$

Our interpretation of XPS spectra is essentially the same as previous ones.[49,50] According to band calculations,[39,41] Cu $3d$ levels are shallower than O $2p$ levels by about 1 eV, as is shown by Eqs. (1.7) and (1.8):

$$\epsilon_{3d}-\epsilon_{2p}\simeq 1.0\ \text{eV}.\tag{2.10}$$

The main peak around 3.5 eV below the Fermi-level edge corresponds to Eqs. (2.4) and (2.5), so that

$$\epsilon_{3d}-\mu\simeq -3.0\ \text{eV}\tag{2.11}$$

and

$$\epsilon_{2p}-\mu\simeq -4.0\ \text{eV}.\tag{2.12}$$

The satellites around (10–12) eV below the Fermi-level edge correspond to Eqs. (2.6), (2.7), (2.8), and (2.9),[47,48] so that $\epsilon_{4s}-\mu\simeq(2-4)$ eV, $U_{pp}\lesssim 2$ eV, and

$$U_{dd}\simeq(4-7)\ \text{eV}.\tag{2.13}$$

Equation (2.2) is satisfied for these parameters.[46]

Note that $\epsilon_{3d}-\mu$ and $\epsilon_{2p}-\mu$ given by Eqs. (2.11) and (2.12) are lower by about 0.7 eV than those given by Eqs. (1.7) and (1.8), respectively. It is argued in Sec. III A that when the chemical potential shift due to electron correlations is taken into account this discrepancy is resolved.

III. *d-p* MODEL

A. Doped holes on Cu and O ions

When Cu $3d$ levels are actually shallow, doped holes must exist on not only O ions but also Cu ions. One of the purposes of this subsection is to examine how many holes exist on Cu ions.

Consider the *d-p* model in two dimensions:[32]

$$\mathcal{H}_{d\text{-}p}=\sum_{\mathbf{i}\sigma}(\epsilon_{3d}-\mu)d^\dagger_{\mathbf{i}\sigma}d_{\mathbf{i}\sigma}+\sum_{\nu=x,y}\sum_{\mathbf{i}\sigma}(\epsilon_{2p}-\mu)c^\dagger_{\nu\mathbf{i}\sigma}c_{\nu\mathbf{i}\sigma}+\sum_{\nu=x,y}\sum_{\mathbf{ij}\sigma}V^{(\nu)}_{\mathbf{i};\mathbf{j}}[d^\dagger_{\mathbf{i}\sigma}c_{\nu\mathbf{j}\sigma}+c^\dagger_{\nu\mathbf{j}\sigma}d_{\mathbf{i}\sigma}]+U\sum_{\mathbf{i}}d^\dagger_{\mathbf{i}\uparrow}d_{\mathbf{i}\uparrow}d^\dagger_{\mathbf{i}\downarrow}d_{\mathbf{i}\downarrow},\tag{3.1}$$

where $d^\dagger_{\mathbf{i}\sigma}$, $c^\dagger_{x\mathbf{i}\sigma}$, and $c^\dagger_{y\mathbf{i}\sigma}$ are creation operators of a Cu $3d$ electron with spin σ at $\mathbf{R_i}=a(i_x,i_y)$, an O $2p_x$ electron with spin σ at $\mathbf{X_i}=a(i_x+\frac{1}{2},i_y)$, and an O $2p_y$ electron with spin σ at $\mathbf{Y_i}=a(i_x,i_y+\frac{1}{2})$, respectively, with i_x and i_y being integers and a the lattice constant. As one of the simplest mod-

els, $V_{\mathbf{i};\mathbf{j}}^{(\nu)}$'s are assumed to be nonzero only between the nearest neighbors in such a way that[51]

$$V_{\mathbf{i};\mathbf{j}}^{(x)}=\begin{cases}(-1)^{i_x-j_x}V & \text{for } \mathbf{R_i}-\mathbf{X_j}=(\pm a/2,0),\\ 0 & \text{for other pairs}\end{cases} \tag{3.2}$$

and

$$V_{\mathbf{i};\mathbf{j}}^{(y)}=\begin{cases}(-1)^{i_y-j_y}V & \text{for } \mathbf{R_i}-\mathbf{Y_j}=(0,\pm a/2),\\ 0 & \text{for other pairs.}\end{cases} \tag{3.3}$$

In the model (3.1), U_{dd} in Sec. II is simply denoted by U; ϵ_{2p} is defined by Eq. (2.3).

When U is zero, the d-p model (3.1) is easily diagonalized in such a way that

$$E_{\pm}(\mathbf{k})=\frac{1}{2}(\epsilon_{3d}+\epsilon_{2p}-2\mu) \pm\frac{1}{2}\sqrt{(\epsilon_{3d}-\epsilon_{2p})^2+16V^2S(\mathbf{k})}, \tag{3.4}$$

with

$$S(\mathbf{k})=1-\frac{1}{2}[\cos(k_xa)+\cos(k_ya)], \tag{3.5}$$

for the antibonding band denoted by $+$ and the bonding band denoted by $-$, respectively, and $E_0(\mathbf{k})=\epsilon_{2p}-\mu$ for the decoupled $2p$ band. In the case of five electrons per unit cell,

$$n_e\equiv\sum_{\sigma}\langle d_{i\sigma}^{\dagger}d_{i\sigma}\rangle+\sum_{\nu\sigma}\langle c_{\nu i\sigma}^{\dagger}c_{\nu i\sigma}\rangle=5, \tag{3.6}$$

the chemical potential is at the center of the antibonding band at $T=0$ K; the dispersion relation of the antibonding band is given by[52]

$$E_{+}(\mathbf{k})=2t_{d\text{-}p}[\cos(k_xa)+\cos(k_ya)], \tag{3.7}$$

with

$$t_{d\text{-}p}=-V^2/|\epsilon_{3d}+\epsilon_{2p}-2\mu| \tag{3.8}$$

in the vicinity of the chemical potential.

Consider the case of nonzero U or $U\gg|t_{d\text{-}p}|$. Every physical property is divided into a single-site term and a multisite term. For example, the polarization function in spin channels, $\pi_s(i\omega_l,\mathbf{q})$, is written in such a way that

$$\pi_s(i\omega_l,\mathbf{q})=\tilde{\pi}_s(i\omega_l)+\Delta\pi_s(i\omega_l,\mathbf{q}), \tag{3.9}$$

where $\tilde{\pi}_s(i\omega_l)$ is the single-site term and $\Delta\pi_s(i\omega_l,\mathbf{q})$ the multisite term. The single-site term is identical to its corresponding term of the Anderson model mapped from the d-p model (3.1) in the single-site approximation (SSA) or to leading order in $1/d$, with d being the spatial dimensionality.[53–55] Then,

$$\tilde{\chi}_s(i\omega_l)=2\tilde{\pi}_s(i\omega_l)/[1-U\tilde{\pi}_s(i\omega_l)] \tag{3.10}$$

is nothing but the susceptibility of the mapped Anderson model. The local Kondo temperature T_K or k_BT_K is defined as the temperature or energy scale of local quantum spin fluctuations in such a way that

$$k_BT_K=[1/\tilde{\chi}_s(0)]_{T\to 0\,\mathrm{K}}. \tag{3.11}$$

Note that $k_BT_K/U\ll 1$ in strongly correlated systems.[56] To leading order in k_BT_K/U, the susceptibility due to d electrons in the d-p model is given by

$$\chi_s(i\omega_l,\mathbf{q})=\frac{\tilde{\chi}_s(i\omega_l)}{1-\frac{1}{4}I_s(i\omega_l,\mathbf{q})\tilde{\chi}_s(i\omega_l)}, \tag{3.12}$$

with

$$I_s(i\omega_l,\mathbf{q})=2U^2\Delta\pi_s(i\omega_l,\mathbf{q}). \tag{3.13}$$

Equation (3.12) is consistent with a physical picture of the Kondo lattice that local spin fluctuations at different sites interact with each other by an intersite exchange interaction, $I_s(i\omega_l,\mathbf{q})$, which is antiferromagnetic for the cuprate oxides. If the d-p model is actually a relevant model, the cuprate-oxide high-temperature superconductors are Kondo lattices.[57] Only low-temperature cases of $T\ll T_K$ are considered in this paper.[56]

When the self-energy of $3d$ electrons is given by $\Sigma_{\sigma}(i\varepsilon_n,\mathbf{k})$, single-particle excitations are obtained by solving

$$\begin{vmatrix}\varepsilon+i0+\mu-\epsilon_{3d}-\Sigma_{\sigma}(\varepsilon+i0,\mathbf{k}) & 2V\sqrt{S(\mathbf{k})}\\ 2V\sqrt{S(\mathbf{k})} & \varepsilon+i0+\mu-\epsilon_{2p}\end{vmatrix}=0. \tag{3.14}$$

The self-energy for $|\varepsilon_n|\gg k_BT_K$ is evaluated in the so-called Hubbard I approximation,[1] which is a SSA, so that

$$\frac{1}{i\varepsilon_n+\mu-\epsilon_{3d}-\Sigma_{\sigma}(i\varepsilon_n,\mathbf{k})}=\frac{1-n_{d-\sigma}}{i\varepsilon_n+\mu-\epsilon_{3d}} +\frac{n_{d-\sigma}}{i\varepsilon_n+\mu-\epsilon_{3d}-U}, \tag{3.15}$$

with $\varepsilon_n=(2n+1)\pi k_BT$ and $n_{d\sigma}=\langle d_{i\sigma}^{\dagger}d_{i\sigma}\rangle$ the average number of $3d$ electrons with spin σ per unit cell. Single-particle spectra are split into the LHB around $\epsilon_{3d}-\mu$ and the UHB around $\epsilon_{3d}+U-\mu$. We confine ourselves to considering the case of $n_e\simeq 5$ or $n_{d\sigma}\simeq\frac{1}{2}$. When the LHB is argued,

$$i\varepsilon_n+\mu-\epsilon_{3d}-\Sigma_{\sigma}(i\varepsilon_n,\mathbf{k})=2(i\varepsilon_n+\mu-\epsilon_{3d}) \tag{3.16}$$

can be approximately used. The dispersion relations of the antibonding and the bonding bands of the LHB are obtained in such a way that

$$E_{l\pm}^{*}(\mathbf{k})=\frac{1}{2}(\epsilon_{3d}+\epsilon_{2p}-2\mu)\pm\frac{1}{2}\sqrt{(\epsilon_{3d}-\epsilon_{2p})^2+8V^2S(\mathbf{k})}. \tag{3.17}$$

When the UHB is argued,

$$i\varepsilon_n+\mu-\epsilon_{3d}-\Sigma_{\sigma}(i\varepsilon_n,\mathbf{k})=2(i\varepsilon_n+\mu-\epsilon_{3d}-U) \tag{3.18}$$

can be approximately used. Equation (3.14) gives two solutions

$$E^*_{u\pm}(\mathbf{k})=\frac{1}{2}(\epsilon_{3d}+U+\epsilon_{2p}-2\mu)$$
$$\pm\frac{1}{2}\sqrt{(\epsilon_{3d}+U-\epsilon_{2p})^2+8V^2S(\mathbf{k})}. \quad (3.19)$$

The antibonding solution $E^*_{u+}(\mathbf{k})$ describes the dispersion relation of the UHB. The bonding solution $E^*_{u-}(\mathbf{k})$ should be discarded, because Eq. (3.18) can never apply to states around or below the chemical potential.

When a small number of holes are doped, the chemical potential should be at the top of the antibonding band of the LHB, $E^*_{l+}(\mathbf{k})$, so that

$$(\epsilon_{3d}-\mu)(\epsilon_{2p}-\mu)\simeq 4V^2. \quad (3.20)$$

The chemical potential moves upward from the band center to the band top due to electron correlations or the formation of the LHB and UHB. According to band calculations,[41] the hybridization matrix is as large as

$$|V|\simeq 1.6 \text{ eV}. \quad (3.21)$$

It follows from Eqs. (2.10), (3.20), and (3.21) that $\epsilon_{3d}-\mu \simeq -2.7$ eV and $\epsilon_{3d}-\mu\simeq -3.7$ eV. When the broadening of the LHB due to electron correlations and the hybridization is taken into account, these values will become a little large; they are consistent with Eqs. (2.11) and (2.12). In this paper, Eqs. (2.11) and (2.12), which include the chemical potential shift, are assumed for $\epsilon_{3d}-\mu$ and $\epsilon_{2p}-\mu$, respectively; Eqs. (2.13) and (3.21) are assumed for U and $|V|$, respectively.

Doped holes occupy the top of the LHB. When Eq. (3.15) or (3.16) is used, the spectral weight of $3d$ electrons in the LHB is about a half of that of $2p$ electrons. Then, it is straightforward to argue that about two-third of doped holes exist on O ions while about a third of doped holes exist on Cu ions;[58] it follows that

$$n_d=n_{d\uparrow}+n_{d\downarrow}\simeq 1-\frac{1}{3}\delta, \quad (3.22)$$

with $\delta=5-n_e$ being the concentration of doped holes. Small variations were observed in extended x-ray absorption fine structure (EXAFS) or near-edge EXAFS (NEXAFS),[59] when holes are doped. These small variations are consistent with Eq. (3.22); for example, the valence of Cu $3d$ electrons is decreased by about 1/20 per Cu ions for $\delta\simeq 0.15$ according to Eq. (3.22).

B. Gutzwiller's heavy quasiparticles

The self-energy of $3d$ electrons, $\Sigma_\sigma(i\varepsilon_n,\mathbf{k})$, is divided into a single-site term $\tilde{\Sigma}(i\varepsilon_n)$ and a multisite term $\Delta\Sigma_\sigma(i\varepsilon_n,\mathbf{k})$, so that

$$\Sigma_\sigma(i\varepsilon_n,\mathbf{k})=\tilde{\Sigma}(i\varepsilon_n)+\Delta\Sigma_\sigma(i\varepsilon_n,\mathbf{k}). \quad (3.23)$$

Note that the single-site term is also equal to its corresponding term of the mapped Anderson model. They are expanded in such a way that

$$\tilde{\Sigma}_\sigma(i\varepsilon_n)=\tilde{\Sigma}_0+[1-\tilde{\phi}_m]i\varepsilon_n+\cdots \quad (3.24)$$

and

$$\Delta\Sigma_\sigma(i\varepsilon_n,\mathbf{k})=\Delta\Sigma_0(\mathbf{k})+[1-\Delta\phi_m(\mathbf{k})]i\varepsilon_n+\cdots \quad (3.25)$$

for $|\varepsilon_n|\ll k_BT_K$. Then, the dispersion relation of quasiparticles is given by[60]

$$\xi(\mathbf{k})=\frac{1}{2}\left[\frac{\epsilon_{3d}+\Sigma_0(\mathbf{k})-\mu}{\phi_m(\mathbf{k})}+(\epsilon_{2p}-\mu)\right]$$
$$+\frac{1}{2}\sqrt{\left[\frac{\epsilon_{3d}+\Sigma_0(\mathbf{k})-\mu}{\phi_m(\mathbf{k})}-(\epsilon_{2p}-\mu)\right]^2+\frac{16V^2}{\phi_m(\mathbf{k})}S(\mathbf{k})}, \quad (3.26)$$

with

$$\phi_m(\mathbf{k})=\tilde{\phi}_m+\Delta\phi_m(\mathbf{k}) \quad (3.27)$$

and

$$\Sigma_0(\mathbf{k})=\tilde{\Sigma}_0+\Delta\Sigma_0(\mathbf{k}). \quad (3.28)$$

Note that the Fermi-surface sum rule requires

$$|\epsilon_{3d}+\Sigma_0(\mathbf{k})-\mu|\ll 2V^2/|\epsilon_{2p}-\mu| \quad (3.29)$$

in the case of $0<\delta\ll 1$.

According to Gutzwiller's theory[9] or the recent theory,[10] both of which are in SSA's, it is reasonable to assume that

$$\tilde{\phi}_m\simeq 1/(1-n_d)\simeq 3/\delta. \quad (3.30)$$

Intersite terms vanish in any SSA: $\Delta\phi_m(\mathbf{k})=0$ and $\Delta\Sigma_0(\mathbf{k})=0$. Because $|\epsilon_{2p}-\mu|\gg|\epsilon_{3d}+\Sigma_0(\mathbf{k})-\mu|/\tilde{\phi}_m$ and $|\epsilon_{2p}-\mu|^2\gg 16V^2/\tilde{\phi}_m$ in the case of $0<\delta\ll 1$, Eq. (3.26) is approximately given by

$$\xi(\mathbf{k})\simeq\frac{1}{\tilde{\phi}_m}\left\{\epsilon_{3d}+\Sigma_0(\mathbf{k})-\mu\right.$$
$$\left.-\frac{2V^2}{|\epsilon_{2p}-\mu|}[\cos(k_xa)+\cos(k_ya)]\right\} \quad (3.31)$$

for $\mathbf{k}$'s in the vicinity of the Fermi surface.

In the SSA or to leading order in $1/d$, the local Kondo temperature k_BT_K is approximately given by a quarter of the heavy-electron bandwidth,[53–55] so that

$$k_BT_K\simeq\frac{2V^2}{\tilde{\phi}_m|\epsilon_{2p}-\mu|}\simeq 0.43\ \ \delta \text{ eV} \quad (3.32)$$

and

$$\rho^*(0)\simeq\frac{1}{4k_BT_K}\simeq\frac{0.58}{\delta} \text{ states/eV spin } CuO_2. \quad (3.33)$$

Experimental T_c's as a function of δ reach their maximum around $\delta\simeq 0.15$.[13] It follows that $k_BT_K\simeq 0.064$ eV and

$$\rho^*(0)\simeq 3.9 \text{ states/eV spin } CuO_2 \quad (3.34)$$

for $\delta=0.15$. This $\rho^*(0)$ is a little larger than Eq. (1.3).

In this paper, the renormalization of quasiparticles is argued in a SSA. Intersite exchange interactions and spin fluctuations also renormalize quasiparticles. There are two types

of renormalization. One is the mass enhancement due to $\Delta\phi_m(\mathbf{k})$; $\rho^*(0)$ is enhanced furthermore. The other is the mass reduction due to $\Delta\Sigma_0(\mathbf{k})$; it was shown in the previous papers[14,15] that the $\mathbf{k}$ dependence of $\Delta\Sigma_0(\mathbf{k})$ makes quasiparticles light. A part of the discrepancy between Eqs. (1.3) and (3.34) can be explained in terms of the latter type of renormalization, at least.

The SSA is expected to be good enough in the region where local quantum spin fluctuations are more substantial than intersite spin fluctuations. In the region of $\delta \gtrsim 0.2$, Eq. (3.33) is actually consistent with $\rho^*(0)$'s of the cuprate oxides, which are estimated from experimental temperature-linear specific heat coefficients.[13]

C. Reduction of the superexchange interaction

In the previous papers,[19,20] the superexchange interaction was derived within the theoretical framework of the virtual exchange of spin excitations. In this subsection, the previous study is extended to take into account the broadening of the LHB and UHB due to electron correlations and the hybridization, which causes the broadening of exchanged spin excitations.

When the single-site vertex corrections are taken into account, a magnetic pairing interaction is given by[61]

$$Y_s(i\omega_l,\mathbf{q})=\frac{1}{4}U^2\tilde{\lambda}_s^2(i\varepsilon_n+i\omega_l,i\varepsilon_n)\chi_s(i\omega_l,\mathbf{q}), \tag{3.35}$$

with $\tilde{\lambda}_s(i\varepsilon_n+i\omega_l,i\varepsilon_n)$ being the irreducible single-site vertex function for spin channels. According to the Ward-Takahashi identity,[62] it follows that

$$\tilde{\lambda}_s(0,0)=\tilde{\phi}_s[1-U\tilde{\pi}_s(0)]=2\tilde{\phi}_s\tilde{\pi}_s(0)/\tilde{\chi}_s(0), \tag{3.36}$$

with

$$\tilde{\phi}_s=\{1-[d\tilde{\Sigma}_{\uparrow}(0)/dH^*]\}_{H^*\to 0}. \tag{3.37}$$

Here, H^* is an infinitesimally small Zeeman energy of $3d$ electrons. Note that $\tilde{\phi}_s/\tilde{\phi}_m$ is nothing but the Wilson ratio for the mapped Anderson model so that

$$\tilde{\phi}_s/\tilde{\phi}_m \simeq 2 \tag{3.38}$$

for $U/k_BT_K \gg 1$.[63] The intrasite part of Eq. (3.35) can play no essential role in the formation of Cooper pairs; the total intrasite term is definitely strongly repulsive. When intrasite terms are subtracted, Eq. (3.35) turns out to be

$$Y'(i\omega_l,\mathbf{q})\equiv Y_s(i\omega_l,\mathbf{q})-\frac{1}{N}\sum_{\mathbf{q}} Y_s(i\omega_l,\mathbf{q})$$

$$=[U\tilde{\pi}_s(0)]^2\tilde{\phi}_s^2\frac{1}{4}I^*(i\omega_l,\mathbf{q}) \tag{3.39}$$

with

$$\frac{1}{4}I^*(i\omega_l,\mathbf{q})=\frac{\frac{1}{4}I_s(i\omega_l,\mathbf{q})}{1-\frac{1}{4}I_s(i\omega_l,\mathbf{q})\tilde{\chi}_s(i\omega_l)}. \tag{3.40}$$

Here, the energy dependences of $\tilde{\lambda}_s(i\varepsilon_n+i\omega_l,i\varepsilon_n)$ are ignored, because we are concerned with low-energy processes of $|\varepsilon_n| \ll k_BT_K$ and $|\varepsilon_n+\omega_l| \ll k_BT_K$. In Eq. (3.39), N is the number of unit cells. In Eq. (3.40), the subtraction of intrasite terms is assumed.

According to Eq. (3.40), $I_s(i\omega_l,\mathbf{q})$ is enhanced by antiferromagnetic spin fluctuations, whose development is due to $I_s(i\omega_l,\mathbf{q})$ itself.[64] Equation (3.40) is also written in such a way that

$$\frac{1}{4}I^*(i\omega_l,\mathbf{q})=\frac{1}{4}I_s(i\omega_l,\mathbf{q})+\left[\frac{1}{4}I_s(i\omega_l,\mathbf{q})\right]^2\chi_s(i\omega_l,\mathbf{q}). \tag{3.41}$$

The second term is nothing but the enhanced part. According to Eq. (3.39), $U\tilde{\pi}_s(0)\tilde{\phi}_s$ is an effective vertex function for the enhanced exchange interaction, $\frac{1}{4}I_s^*(i\omega_l,\mathbf{q})$. It follows from Eqs. (3.10) and (3.11) that

$$U\tilde{\pi}_s(0)=\frac{U/k_BT_K}{2+(U/k_BT_K)}, \tag{3.42}$$

which is about unity for $U/k_BT_K \gg 1$. Then,

$$U\tilde{\pi}_s(0)\tilde{\phi}_s \gg 1 \tag{3.43}$$

for $U/k_BT_K \gg 1$; the effective vertex function plays an essential role.[65]

In metallic phases, the virtual exchange of pair excitations of Gutzwiller's heavy quasiparticles in spin channels,[66] which is denoted by $J_Q(i\omega_l,\mathbf{q})$ here, can also play a role as well as the superexchange interaction, which is denoted by $J_s(\mathbf{q})$ here.[67] When small irrelevant terms are ignored, it follows that

$$I_s(i\omega_l,\mathbf{q})=J_s(\mathbf{q})+J_Q(i\omega_l,\mathbf{q}). \tag{3.44}$$

It was discussed in the previous paper[23] that $J_s(\mathbf{q})$ dominates $J_Q(i\omega_l,\mathbf{q})$ in the cuprate oxides. When only the nearest-neighbor terms of $J_s(\mathbf{q})$, which are the most effective, are taken into account, it follows that

$$J_s(\mathbf{q})=2J_{d\text{-}p}[\cos(q_xa)+\cos(q_ya)] \tag{3.45}$$

in the momentum-space representation, with $J_{d\text{-}p}$ being the strength between nearest neighbors. The reduction effect on $J_{d\text{-}p}$ is examined in the following.

Denote the site-diagonal part of the single-particle Green function for $3d$ electrons by $\tilde{G}_\sigma(i\varepsilon_n)$, which is also equal to the single-particle Green function of the mapped Anderson model. In this paper, a phenomenological

$$\tilde{G}_\sigma(i\varepsilon_n)=\frac{1-n_{d-\sigma}}{i\varepsilon_n+\mu-\epsilon_{3d}+\sigma H^*+i\Gamma_l\,\mathrm{sgn}(\varepsilon_n)}$$

$$+\frac{n_{d-\sigma}}{i\varepsilon_n+\mu-\epsilon_{3d}-U+\sigma H^*+i\Gamma_u\,\mathrm{sgn}(\varepsilon_n)} \tag{3.46}$$

is used in order to take into account high-energy pair excitations between the LHB and UHB. Equation (3.46) is obtained in a SSA called the Hubbard III approximation,[2] when

the DOS of unrenormalized $3d$ electrons is approximated by a Lorentzian shape. Although the level width Γ_l of the LHB is equal to the level width Γ_u of the UHB in this approximation, it is assumed that Γ_l and Γ_u are different from each other. The site-diagonal part of the single-particle Green function for $2p$ electrons is assumed to be given by

$$G_{\nu\nu'\sigma}(i\varepsilon_n)=\delta_{\nu\nu'}\frac{1}{i\varepsilon_n+\mu-\epsilon_{2p}+i\Gamma_p\,\mathrm{sgn}(\varepsilon_n)}, \tag{3.47}$$

instead of Eq. (3.18) of Ref. 20. Here, $\nu(\nu')$ is $2p_x$ or $2p_y$. According to the Ward-Takahashi identity,[62] it follows that for $|\varepsilon_n|\gg k_BT_K$

$$\begin{aligned}\tilde{\lambda}_s(i\varepsilon_n,i\varepsilon_n)&=[1-U\tilde{\pi}_s(0)]\left[\frac{d}{dH^*}\frac{1}{\tilde{G}_\uparrow(i\varepsilon_n)}\right]_{H^*\to 0}\\ &\simeq-\frac{\tilde{\pi}_s(0)}{\tilde{G}_\uparrow^2(i\varepsilon_n)}\left[\frac{1}{i\varepsilon_n+\mu-\epsilon_{3d}+i\Gamma_l\,\mathrm{sgn}(\varepsilon_n)}\right.\\ &\quad\left.-\frac{1}{i\varepsilon_n+\mu-\epsilon_{3d}-U+i\Gamma_u\,\mathrm{sgn}(\varepsilon_n)}\right].\end{aligned} \tag{3.48}$$

Here, higher-order terms in $k_BT_K/|\epsilon_{3d}+U-\mu|$ and $k_BT_K/|\mu-\epsilon_{3d}|$ are ignored, and

$$\left[\frac{dn_{d\sigma}}{dH^*}\right]_{H^*\to 0}=\frac{1}{2}\sigma\tilde{\chi}_s(0) \tag{3.49}$$

is made use of.

Following the treatment of Ref. 20, it is straightforward to calculate $J_{d\text{-}p}$ so that

$$J_{d\text{-}p}=[U\tilde{\pi}_s(0)]^2J'_{d\text{-}p}\ , \tag{3.50}$$

with $U\tilde{\pi}_s(0)$ given by Eq. (3.42), and

$$\begin{aligned}J'_{d\text{-}p}=\frac{2V^4}{\pi}\mathrm{Im}\Bigg[&-\frac{2}{(z_l-z_p)^3}\ln\frac{-z_l}{-z_p}+\frac{1}{(z_l-z_p)^2}\left(\frac{1}{z_l}+\frac{1}{z_p}\right)\\ &-\frac{2}{(z_u-z_p)^3}\ln\frac{-z_u}{-z_p}+\frac{1}{(z_u-z_p)^2}\left(\frac{1}{z_u}+\frac{1}{z_p}\right)\\ &+\frac{2\ln(-z_l)}{(z_u-z_l)(z_l-z_p)^2}-\frac{2\ln(-z_u)}{(z_u-z_l)(z_u-z_p)^2}\\ &-\frac{2(z_l+z_u-2z_p)\ln(-z_p)}{(z_l-z_p)^2(z_u-z_p)^2}-\frac{2}{z_p(z_l-z_p)(z_u-z_p)}\Bigg].\end{aligned} \tag{3.51}$$

Here, z_l, z_p, and z_u are given by

$$z_l=\epsilon_{3d}-\mu-i\Gamma_l,\quad z_p=\epsilon_{2p}-\mu-i\Gamma_p, \tag{3.52}$$

and

$$z_u=\epsilon_{3d}+U-\mu-i\Gamma_u\,. \tag{3.53}$$

There are two types of reduction effects. One is due to nonzero Γ_l, Γ_u, and Γ_p. This can be regarded as the effect of the broadening of exchanged spin excitations. The other is due to $U\tilde{\pi}_s(0)<1$ or finite U/k_BT_K.

In the limit of $U/k_BT_K\to+\infty$, $\Gamma_l/|V|\to+0$, and $\Gamma_u/|V|\to+0$, Eqs. (3.50) and (3.51) are reduced to the well-known result

$$J^{(0)}_{d\text{-}p}=-\frac{4V^4}{(\epsilon_{3d}+U-\epsilon_{2p})^2}\left[\frac{1}{U}+\frac{1}{\epsilon_{3d}+U-\epsilon_{2p}}\right]. \tag{3.54}$$

For example, consider the parameter region of

$$4.5\ \text{eV}\leqslant U\leqslant 5.0\ \text{eV}. \tag{3.55}$$

These U's are consistent with Eq. (2.13). When Eqs. (2.11), (2.12), and (3.21) are used, it follows that

$$J^{(0)}_{d\text{-}p}=-(0.27-0.35)\ \text{eV}. \tag{3.56}$$

These $|J^{(0)}_{d\text{-}p}|$'s are about 3 times as large as Eq. (1.4).

When $\epsilon_{3d}\simeq\epsilon_{2p}$ is taken into account in Eq. (3.17), the bandwidth of the LHB is estimated in such a way that

$$W_l\simeq 4V\simeq 6.4\ \text{eV}. \tag{3.57}$$

When the strong hybridization between $3d$ and $2p$ levels is considered, it is reasonable to assume that

$$\Gamma_l=\Gamma_p=cW_l\,. \tag{3.58}$$

In this scheme, c is a constant a little smaller than $1/\pi=0.318\ldots$. The bandwidth of the UHB is estimated from Eq. (3.19) in such a way that

$$W_u\simeq(1.4-1.5)\ \text{eV} \tag{3.59}$$

for U's given by Eq. (3.55). In this paper,

$$\Gamma_u=cW_u \tag{3.60}$$

is approximately used. The reduction due to nonzero $\Gamma_l=\Gamma_p$ and Γ_u is substantial, so that $J'_{d\text{-}p}=-(0.10-0.15)$ eV for U's given by Eq. (3.55) and $c=0.22$. When $k_BT_K=0.1$ eV is used, it follows that $[U\tilde{\pi}_s(0)]^2\simeq 0.92$; the reduction due to $[U\tilde{\pi}_s(0)]^2$ is small. Then, we obtain

$$J_{d\text{-}p}=-(0.09-0.14)\ \text{eV}. \tag{3.61}$$

Although the $J_{d\text{-}p}$'s depend on c, Eq. (3.61) is at least consistent with Eq. (1.4).

When a similar value of $J_{d\text{-}p}$ to Eq. (3.61) is assumed and both $J_Q(i\omega_l,\mathbf{q})$ and the enhancement effect are taken into account, it is straightforward to obtain $T_c=50-100$ K.[23] The d-p model whose parameters are given by Eqs. (2.11), (2.12), (3.21), and (3.55) is a relevant model for cuprate HTS.

IV. *t-J* AND HUBBARD MODELS

Consider the *t-J* model on the simple square lattice:[32,51]

$$\mathcal{H}_{t\text{-}J}=\sum_{i\sigma}(\epsilon_d-\mu)a^\dagger_{i\sigma}a_{i\sigma}+t\sum_{\langle ij\rangle\sigma}a^\dagger_{i\sigma}a_{j\sigma}-\frac{1}{2}J\sum_{\langle ij\rangle\nu}\sum_{\alpha\beta}\left(a^\dagger_{i\alpha}\frac{1}{2}\sigma^{\alpha\beta}_\nu a_{i\beta}\right)\sum_{\gamma\delta}\left(a^\dagger_{j\gamma}\frac{1}{2}\sigma^{\gamma\delta}_\nu a_{j\delta}\right)+U_D\sum_i a^\dagger_{i\uparrow}a_{i\uparrow}a^\dagger_{i\downarrow}a_{i\downarrow}, \tag{4.1}$$

with t the transfer integral, the summation $\langle ij\rangle$ over the nearest neighbors, $\sigma^{\alpha\beta}_\nu$ the $(\alpha\beta)$th component of the Pauli matrix ($\nu=x,\ y,$ or z), and

$$U_D/|t|\to+\infty. \tag{4.2}$$

No doubly occupied sites can exist because of Eq. (4.2).

A question is what t and J should be used in order that the *t-J* model might be a relevant model for cuprate HTS. The susceptibility of the *t-J* model is written in the same form as Eq. (3.12); local spin fluctuations and intersite interactions between them should be the same as or at least similar to those of the *d-p* model. When Eq. (1.4) or (3.61) is used for J, the virtual exchange of high-energy spin excitations is phenomenologically taken into account.[68]

Because the *t-J* model is also mapped to the Anderson model in the SSA,[69] local quantum spin fluctuations are uniquely characterized by the local Kondo temperature T_K. Then, t should be determined in such a way that T_K of the *t-J* model might be the same as T_K of the *d-p* model or that the dispersion relations of heavy quasiparticles might be the same as or at least similar to each other between the two models. The self-energy is expanded in such a way that

$$\Sigma_{J\sigma}(i\varepsilon_n,\mathbf{k})=\Sigma_{J0}(\mathbf{k})+[1-\phi_{Jm}(\mathbf{k})]i\varepsilon_n+\cdots \tag{4.3}$$

for $|\varepsilon_n|\ll k_BT_K$. The dispersion relation of quasiparticles is given by

$$\xi_J(\mathbf{k})=\frac{1}{\phi_{Jm}(\mathbf{k})}\{\Sigma_{J0}(\mathbf{k})+2t[\cos(k_xa)+\cos(k_ya)]-\mu\}. \tag{4.4}$$

In the Gutzwiller approximation, it follows that

$$\phi_{Jm}(\mathbf{k})\simeq 1/\delta. \tag{4.5}$$

Because Eq. (4.4) should be approximately equal to Eq. (3.31), it follows that

$$t=-\frac{\phi_{Jm}}{\phi_m}\frac{V^2}{|\epsilon_p-\mu|}\simeq-\frac{V^2}{3|\epsilon_p-\mu|}\simeq-0.21\ \text{eV}. \tag{4.6}$$

Here, the $\mathbf{k}$ dependence of $\phi_m(\mathbf{k})$ and $\phi_{Jm}(\mathbf{k})$ is ignored; they are simply denoted as ϕ_m and ϕ_{Jm}. Because the chemical potential is at the top of the LHB, it follows that $\epsilon_d-\mu\simeq-4|t|\simeq-0.85$ eV.

The *t-J* model whose parameters are given by Eqs. (1.4) and (4.6) is a relevant model for cuprate HTS; its low-energy properties, including critical temperatures T_c, are almost the same as those of the relevant *d-p* model within the theoretical framework of Landau's Fermi liquids. However, electrons in the LHB of the *t-J* model obtained in this way do not correspond to electrons in the antibonding LHB of the *d-p* model. A little larger t than Eq. (4.6) should be used to describe the antibonding LHB. The *t-J* model cannot describe consistently both low-energy and high-energy properties of the cuprate oxides.

Next, examine whether or not the Hubbard model on the simple square lattice,[32,51]

$$\mathcal{H}_H=\sum_{i\sigma}(\epsilon_d-\mu)a^\dagger_{i\sigma}a_{i\sigma}+t\sum_{\langle ij\rangle\sigma}a^\dagger_{i\sigma}a_{j\sigma}+U\sum_i a^\dagger_{i\uparrow}a_{i\uparrow}a^\dagger_{i\downarrow}a_{i\downarrow}, \tag{4.7}$$

can be a relevant model for cuprate HTS. As long as only low-energy properties are considered, it is possible that U in the Hubbard model is different from U in the *d-p* model. In this section,

$$10|t|\leqslant U\leqslant 5.0\ \text{eV} \tag{4.8}$$

is assumed in order that the formation of the LHB and UHB might occur. The mass renormalization factor in such a case is not so different from that in the case of $U/|t|\to+\infty$. Then, Eq. (4.6) should be used for t in the Hubbard model (4.7).

When Eq. (3.46) is used, the superexchange interaction between the nearest neighbors is calculated in the same approximation as that in Sec. III C so that

$$J_H=[U\tilde{\pi}_s(0)]^2RJ_H^{(0)}, \tag{4.9}$$

with $U\tilde{\pi}_s(0)$ given by Eq. (3.42),

$$R=1-\frac{1}{\pi}\left[\tan^{-1}\left(\frac{\Gamma_l}{\mu-\epsilon_d}\right)+\tan^{-1}\left(\frac{\Gamma_u}{\epsilon_d+U-\mu}\right)\right] \tag{4.10}$$

and

$$J_H^{(0)}=-4t^2/U. \tag{4.11}$$

In the limit of $U/k_BT_K\to+\infty$, $\Gamma_l/|t|\to+0$, and $\Gamma_u/|t|\to+0$, Eq. (4.9) is reduced to Eq. (4.11), which is the well-known result. It follows that

$$J_H^{(0)}=-(0.035-0.084)\ \text{eV} \tag{4.12}$$

for $t=-0.21$ eV and $U=(2.1-5.0)$ eV.

It is reasonable to assume that $\Gamma_l=\Gamma_u=8|t|c$ with $c\lesssim 1/\pi$. When $c=0.22$ and $k_BT_K=0.1$ eV are used, it follows that $[U\tilde{\pi}_s(0)]^2=0.83-0.92$ and $R=0.78-0.84$. Then, we obtain[68]

$$J_H=-(0.027-0.054)\ \text{eV}. \tag{4.13}$$

These $|J_H|$'s are substantially smaller than Eq. (1.4); T_c's of the Hubbard model whose parameters are consistent with those of the relevant *t-J* model are much lower than T_c's of the relevant *t-J* or the relevant *d-p* model.

V. DISCUSSION

It is one of the most crucial issues which is the case, the scheme of deep Cu $3d$ levels or the scheme of shallow Cu $3d$ levels. In the scheme of shallow Cu $3d$ levels, a problem to be resolved is to explain Cu $2p$ or $3p$ resonant XPS spec-

tra; it was argued that a strong resonant behavior of the peaks around 10–12 eV below the Fermi-level edge must be evidence for deep Cu $3d$ levels.[70] On the other hand, there are also discrepancies in the scheme of deep Cu $3d$ levels. Spectra of NEXAFS imply that the ground state is mainly composed of $(3d)^9$ and the component of $(3d)^{10}\underline{\mathrm{L}}$ is small.[59] Then,

$$E[(3d)^{10}\underline{\mathrm{L}}]-E[(3d)^9]\gg|V| \tag{5.1}$$

should be satisfied, with

$$E[(3d)^{10}\underline{\mathrm{L}}]-E[(3d)^9]=U+(\epsilon_{3d}-\mu)-(\epsilon_{2p}-\mu)$$
$$\simeq U-(7-9)\ \text{eV}. \tag{5.2}$$

In Eq. (5.2), Eqs. (1.5) and (1.6) are used. When no holes are doped, the cuprate oxides are insulators. Not only Eq. (2.2) but also

$$\epsilon_{3d}+U-\mu>W_u/2 \tag{5.3}$$

should be satisfied in order that the UHB might be empty. Both Eqs. (5.1) and (5.3) require that U should be about 10 eV or larger than 10 eV. However, such large U's are unlikely for Cu $3d$ electrons. It is difficult to explain both Eqs. (1.3) and (1.4) within the scheme of deep Cu $3d$ levels. Furthermore, band calculations totally contradict the scheme of deep Cu $3d$ levels. Because it seems to be difficult to resolve these discrepancies within the scheme of deep Cu $3d$ levels, it is interesting to try to explain Cu $2p$ or $3p$ resonant XPS spectra within the scheme of shallow Cu $3d$ levels. For example, it is interesting to examine which is actually the main Auger process among those argued in Sec. II.

There are two differences in the derivation of the t-J model from the d-p model between Zhang and Rice's[36] and this paper. One is that the level schemes of Cu $3d$ and O $2p$ levels are different between the two derivations. The other is more crucial than this difference. The derivation by Zhang and Rice follows an assumption that the so-called Zhang-Rice singlet is formed in each CuO_4 cluster. On the other hand, the derivation in this paper follows the idea that strongly correlated electron liquids described by the d-p model or the t-J model are Kondo lattices; local quantum spin fluctuations are uniquely characterized by the local Kondo temperature of the mapped Anderson model. The crossover demonstrated in the real-space renormalization study of the Kondo effect[63] implies that, in general, a singlet state formed in a small cluster is quantitatively or physically different from that in a large cluster, that is, the singlet ground state of the s-d or the Anderson model. The transfer integral between the local singlets in small clusters is different from that given by Eq. (4.6).

Effects of high-energy processes on low-energy properties are often taken into account in a phenomenological manner. Because the superexchange interaction is due to the virtual exchange of high-energy spin excitations between the LHB and UHB, it is reasonable to add

$$-\frac{1}{2}\Delta J\sum_{\langle ij\rangle\nu}\sum_{\alpha\beta}\left(a_{i\alpha}^{\dagger}\frac{1}{2}\sigma_{\nu}^{\alpha\beta}a_{i\beta}\right)\sum_{\gamma\delta}\left(a_{j\gamma}^{\dagger}\frac{1}{2}\sigma_{\nu}^{\gamma\delta}a_{j\delta}\right), \tag{5.4}$$

to the Hubbard model in order to take into account phenomenologically the presence of O $2p$ bands in actual cuprate oxides. It is interesting to study numerically such an extended Hubbard model with $U>8|t|$ and $\Delta J=-(0.04-0.07)$ eV. If the addition of such relatively small ΔJ brings about a substantial enhancement of superconducting fluctuations at $T\ll T_K$, the ground state of the Hubbard model must be superconducting a little away from half filling; it can be confirmed that the Hubbard model belongs to the same universality class as the d-p and the t-J models.

The situation for the d-p model is similar to that for the Hubbard model. When $U=5.5$ eV is used, for example, it follows that $J_{d\text{-}p}\simeq-0.06$ eV; it is significantly smaller than Eq. (1.4). The actual strength of the superexchange interaction may be a little different from that argued in Sec. III C. Critical temperatures T_c sensitively depend on the coupling constant. If the T_c's of the d-p model are a little lower or a little higher than the experimental T_c's, it is reasonable to add a phenomenological antiferromagnetic or ferromagnetic exchange interaction to the d-p model.

When $t\simeq-0.40$ eV is used instead of $t\simeq-0.21$ eV given by Eq. (4.6), for example, it follows that $J_H^{(0)}=-(0.13-0.16)$ eV for $U=(4.0-5.0)$ eV. The reduction effects are substantial, so that $J_H=-(0.10-0.11)$ eV for $c=0.22$. These $|J_H|$'s are almost the same as Eq. (1.4). Because the DOS of quasiparticles for $|t|\simeq0.40$ eV is about a half of that for $|t|\simeq0.21$ eV, T_c's of this Hubbard model are also much lower than T_c's of the relevant d-p or the relevant t-J model. It is difficult to explain both of Eqs. (1.3) and (1.4) within the Hubbard model.

It was argued in the previous paper[23] that the superexchange interaction involved in the Hubbard model with $|t|\simeq0.4$ eV and $U\simeq6$ eV is as strong as $J=-(0.10-0.12)$ eV; the reduction effects were not taken into account there. The previous argument[23] is irrelevant from a microscopical point of view. Not only the superexchange interaction but also effective masses of quasiparticles appearing in the previous paper should be regarded as phenomenological ones.

The pairing mechanism due to the virtual exchange of paramagnons, the so-called spin fluctuation mechanism, is consistent with that argued in this paper. According to Eq. (3.35), the effective interaction appearing in the spin fluctuation mechanism is given by

$$\overline{U}=\frac{1}{2}U\tilde{\lambda}_s(0)=U\tilde{\pi}_s(0)\tilde{\phi}_s k_B T_K. \tag{5.5}$$

When $U/k_BT_K\gg1$, $\overline{U}$ is as large as or a little smaller than a half of the unrenormalized bandwidth. When the superexchange interaction is effective, spin fluctuations or $\chi_s(i\omega_l,\mathbf{q})$ in the whole region of the Brillouin zone contribute to the formation of Cooper pairs. In such a case, $\chi_s(i\omega_l,\mathbf{q})$ in Eq. (3.35) should be accurately treated for the whole $\mathbf{q}$'s.

The word ''paramagnons'' is usually used for low-energy spin excitations in paramagnetic states. It is inadequate to use it for spin excitations whose excitation energies are much larger than both of the total exchange interaction and the quasiparticle bandwidth, such as spin excitations between the LHB and UHB. It is reasonable to argue that the first term in Eq. (3.41) is an exchange interaction whose main part is the superexchange interaction. In the second term of Eq. (3.41),

$[\frac{1}{4}I_s(i\omega_l,\mathbf{q})]^2$ plays a role of a cutoff function for $\mathbf{q}$. Only spin fluctuations in a narrow region of the Brillouin zone are effective; an expansion form can be approximately used for $\chi_s(i\omega_l,\mathbf{q})$ in Eq. (3.41). It is also reasonable to argue that the enhancement of the exchange interaction, the second term in Eq. (3.41), is mainly due to paramagnons.

The weak-coupling region is defined in such a way that $0<U/|t_{d\text{-}p}|\ll 8$ for the d-p model and $0<U/|t|\ll 8$ for the Hubbard model. Strictly speaking, the treatment in this paper cannot apply to the weak-coupling region. However, its naive application to the weak-coupling region suggests that magnetic exchange interactions corresponding to J_H given by Eq. (4.9) and $J_{d\text{-}p}$ given by Eq. (3.50) are small because of the reduction effects, and that superconducting T_c's are very low in the weak-coupling region of not only the Hubbard model but also the d-p model. Numerical studies for the case of $U/|t_{d\text{-}p}|>8$ or $U/|t|>8$ are interesting in order to confirm that their ground states are superconducting in a certain region of hole concentrations.

VI. SUMMARY

Photoemission spectra of high-temperature cuprate-oxide superconductors are interpreted consistently with band calculations; Cu $3d$ levels are shallower than O $2p$ levels by about 1 eV. The chemical potential shift due to the formation of the lower Hubbard band and upper Hubbard band is responsible for small differences about 0.7 eV in the depths of $3d$ and $2p$ levels between experiment and theory. It is argued that about a third of doped holes exist on Cu ions and about two-thirds exist on O ions.

When shallow and broad $3d$ and $2p$ levels are considered in the d-p model, the superexchange interaction is substantially reduced; it is reduced from $J\simeq -0.3$ eV to $J\simeq -0.1$ eV within the d-p model whose parameters are consistent with band calculations and photoemission spectra: $\epsilon_{3d}-\mu\simeq -3.0$ eV for the depth of $3d$ levels, $\epsilon_{2p}-\mu\simeq -4.0$ eV for the depth of $2p$ levels, $|V|\simeq 1.6$ eV for the hybridization energy between $3d$ and $2p$ levels, and $U\simeq(4.5-5.0)$ eV for the on-site repulsion between $3d$ electrons. The reduced one is consistent with the experimental one. Because both of the formation of Gutzwiller's heavy quasiparticles and the superexchange interaction as strong as $J\simeq -0.1$ eV are involved, such a d-p model is one of the simplest and relevant effective Hamiltonians for the cuprate oxides; the superexchange interaction is the main pairing interaction, which is responsible for the formations of $d_{x^2-y^2}$-wave Cooper pairs between Gutzwiller's heavy quasiparticles.

Within the Gutzwiller approximation, effective masses of quasiparticles in the t-J model whose transfer integral between the nearest neighbors is as large as $t\simeq -0.21$ eV are almost the same as those in the relevant d-p model. Then, the t-J model with $t\simeq -0.21$ eV and $J\simeq -0.1$ eV is also a relevant model for the cuprate oxides. When the reduction of the superexchange interaction is taken into account, on the other hand, both of the formation of heavy quasiparticles and the pairing interaction in the cuprate oxides cannot be explained within the Hubbard model.

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APPENDIX: RIGOROUS PROPERTIES OF THE AUXILIARY-PARTICLE t-J MODEL

When four kinds of auxiliary particles are introduced in the same manner as Barnes',[71] the t-J model, Eq. (4.1), is mapped to the following auxiliary-particle model:

$$\begin{aligned}\overline{\mathcal{H}}_{t\text{-}J}=&\sum_{i\sigma}(\epsilon_d-\mu)s_{i\sigma}^{\dagger}s_{i\sigma}+\sum_i \epsilon_b b_i^{\dagger}b_i\\&+\sum_i(2\epsilon_d-2\mu+U_D)d_i^{\dagger}d_i+t\sum_{\langle ij\rangle\sigma}\overline{a}_{i\sigma}^{\dagger}\overline{a}_{j\sigma}\\&-\frac{1}{2}J\sum_{\langle ij\rangle\nu}\sum_{\alpha\beta}\left(s_{i\alpha}^{\dagger}\frac{1}{2}\sigma_{\nu}^{\alpha\beta}s_{i\beta}\right)\sum_{\gamma\delta}\left(s_{j\gamma}^{\dagger}\frac{1}{2}\sigma_{\nu}^{\gamma\delta}s_{j\delta}\right)\\&+\frac{1}{2}U_{\infty}\sum_i(Q_i-1)^2,\end{aligned}\tag{A1}$$

with $\epsilon_b=0$,

$$\overline{a}_{i\sigma}^{\dagger}=s_{i\sigma}^{\dagger}b_i+\sigma d_i^{\dagger}s_{i-\sigma},\tag{A2}$$

$$Q_i=\sum_{\sigma}s_{i\sigma}^{\dagger}s_{i\sigma}+b_i^{\dagger}b_i+d_i^{\dagger}d_i,\tag{A3}$$

and

$$U_{\infty}/|t|\to+\infty.\tag{A4}$$

There are two methods of statistics for auxiliary particles. In one method, s particles, which are created by $s_{i\sigma}^{\dagger}$, are fermions while b and d particles, which are created by $b_i^{\dagger}$ and $d_i^{\dagger}$, are bosons. In the other method, s particles are bosons while b and d particles are fermions. We take the former method following mean-field resonating valence bond (RVB) theories, where s particles are called spinons and b particles are called holons.[72] It is easy to show that Q_i at each site is a constant of motion and

$$[\overline{\mathcal{H}}_{t\text{-}J},Q_i]=0.\tag{A5}$$

The model (A1) has local gauge symmetries. The mapping from the t-J model (4.1) to the model (A1) is exact only when the local constraint

$$Q_i=1\text{ for any }i\text{ site}\tag{A6}$$

is satisfied; the last term in the model (A1) is introduced in order to satisfy the local constraint of Eq. (A6). The creation operator of electrons, $a_{i\sigma}^{\dagger}$, in the t-J model corresponds to $\overline{a}_{i\sigma}^{\dagger}$; it is easy to show that

$$\overline{a}_{i\sigma}^{\dagger}\overline{a}_{j\tau}+\overline{a}_{j\tau}\overline{a}_{i\sigma}^{\dagger}=\delta_{ij}\delta_{\sigma\tau}\tag{A7}$$

within the restricted Hilbert space of Eq. (A6).

Spontaneous breaking local gauge symmetries are impossible.[73] One of the purposes of this appendix is to show that even fluctuations corresponding to broken local gauge symmetries identically vanish when the local constraint of Eq. (A6) is rigorously taken into account.

Because local gauge symmetries are never broken, it is obvious that

$$\langle s_{i\sigma}^{\dagger} s_{j\sigma}\rangle = \delta_{ij}\langle s_{i\sigma}^{\dagger} s_{i\sigma}\rangle, \ \ \langle b_i^{\dagger} b_j\rangle = \delta_{ij}\langle b_i^{\dagger} b_i\rangle, \tag{A8}$$

and $\langle d_i^{\dagger} d_j\rangle = \delta_{ij}\langle d_i^{\dagger} d_i\rangle = 0$. Auxiliary particles are localized in the sense that intersite elements of these matrices identically vanish; they are itinerant through exchange processes caused by the fourth term in Eq. (A1). The situation for auxiliary particles is exactly the same as that for electrons in localized magnetic systems: the localization of electrons themselves and the itineracy of spin excitations. It is obvious that no Fermi surface of auxiliary fermions exists.[74]

Denote the chronological ordering operator by T_τ and the Heisenberg representation of an operator O by $O(\tau) \equiv \exp(\overline{\mathcal{H}}_{t\text{-}J}\tau) O \exp(-\overline{\mathcal{H}}_{t\text{-}J}\tau)$. It is easy to show that in the limit of $U_\infty/|t| \to +\infty$

$$\langle T_\tau s_{i\sigma}(\tau) s_{j\sigma}^{\dagger}\rangle = \begin{cases} -\delta_{ij}\langle s_{i\sigma}^{\dagger} s_{i\sigma}\rangle & \text{for } \tau = -0^+ \\ 0 & \text{for other } \tau, \end{cases} \tag{A9}$$

$$\langle T_\tau b_i(\tau) b_j^{\dagger}\rangle = \begin{cases} \delta_{ij}\langle b_i^{\dagger} b_i\rangle & \text{for } \tau = -0^+ \\ 0 & \text{for other } \tau, \end{cases} \tag{A10}$$

and $\langle T_\tau d_i(\tau) d_j^{\dagger}\rangle = 0$ for any τ, with 0^+ being the inverse of an infinitely large positive energy. Then, single-particle Green functions of auxiliary particles identically vanish so that

$$S_{ij\sigma}(i\varepsilon_n) \equiv -\int_0^{\beta} d\tau e^{i\varepsilon_n \tau}\langle T_\tau s_{i\sigma}(\tau) s_{j\sigma}^{\dagger}\rangle = 0, \tag{A11}$$

$$B_{ij}(i\omega_l) \equiv -\int_0^{\beta} d\tau e^{i\omega_l \tau}\langle T_\tau b_i(\tau) b_j^{\dagger}\rangle = 0, \tag{A12}$$

and

$$D_{ij}(i\omega_l) \equiv -\int_0^{\beta} d\tau e^{i\omega_l \tau}\langle T_\tau d_i(\tau) d_j^{\dagger}\rangle = 0 \tag{A13}$$

for finite ε_n and ω_l, with $\beta = 1/k_B T$. It is easy to understand that auxiliary particles are confined in the sense that no single-particle excitations are possible.[75] It is also easy to understand the absence of single-particle excitations from a physical argument that when the local constraint of Eq. (A6) is taken into account it is definitely impossible to add or remove an auxiliary particle.

According to Eq. (A12), fluctuations of holon condensation identically vanish. In a similar manner, it is straightforward to show that

$$\int_0^{\beta} d\tau e^{i\omega_l \tau}\langle T_\tau s_{i_1\sigma}(\tau) s_{i_2\sigma'}(\tau) s_{i_3\sigma'}^{\dagger} s_{i_4\sigma}^{\dagger}\rangle = 0. \tag{A14}$$

Fluctuations of spinon-pair condensation identically vanish. The absence of these fluctuations questions the validity of not only the mean-field approximation[76–78] where itinerant spinons and holons or, more precisely speaking, nonzero intersite $\langle s_{i\sigma}^{\dagger} s_{j\sigma}\rangle$ and $\langle b_i^{\dagger} b_j\rangle$ are assumed but also the introduction of intersite gauge fields that are associated with itinerant spinons and holons.[79,80]

It is obvious that the second-order phase transition of holon condensation or spinon-pair condensation never occurs in this model.[81] If the first-order transition of holon condensation or spinon-pair condensation occurred, some sites would be empty and some other sites would be occupied by two or more than two auxiliary particles. As long as the local constraint of Eq. (A6) is satisfied, the first-order transition of neither holon condensation nor spinon-pair condensation occurs in this model.

In the functional-integral method, the local constraint is usually imposed by the introduction of the so-called auxiliary λ fields.[82] Note that

$$\begin{aligned} &\frac{\Delta\tau}{2\pi}\int_{-\infty}^{+\infty} d\lambda_i(\tau) \exp\left\{-\Delta\tau\left[i\lambda_i(\tau)[Q_i(\tau)-1] + \frac{\lambda_i^2(\tau)}{U_\infty}\right]\right\} \\ &\quad = \frac{\Delta\tau}{2\pi}\int_{-\infty}^{+\infty} d\lambda_i(\tau) \exp\left\{-\Delta\tau\left[\frac{1}{2}U_\infty[Q_i(\tau)-1]^2 \right.\right. \\ &\quad \left.\left. + \frac{1}{U_\infty}\{\lambda_i(\tau) + iU_\infty[Q_i(\tau)-1]\}^2\right]\right\} \end{aligned} \tag{A15}$$

for any U_∞ and any $\Delta\tau$. In the limit of $U_\infty/|t| \to +\infty$, Eq. (A15) gives $\delta(Q_i(\tau)-1)$. When we compare both sides of Eq. (A15), it is obvious that the two treatments of the local constraint, the introduction of the last term in Eq. (A1) and that of the λ fields, are equivalent to each other. In general, broken symmetries cause only relatively small differences in the total free energy.[83] Then, it is reasonable that the saddle-point approximation for the functional integral, which corresponds to the mean-field approximation, gives an approximate free energy of the original t-J model.[84] However, this treatment can never verify broken local gauge symmetries.

In conclusion, broken local gauge symmetries in the saddle-point or mean-field approximation correspond to no physical phenomena in the original t-J model. The intersite gauge fields that are associated with itinerant spinons and holons correspond to no physical phenomena in the original t-J model either.

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[30] When electron correlations are taken into account in the SSA, the superexchange interaction as weak as $J=-(0.02-0.04)$ eV can explain experimental T_c's, as was argued in Refs. 27 and 28. This means that theoretical T_c's obtained in Refs. 27 and 28 are too high. This discrepancy was argued in Ref. 23, where electron correlations were taken into account beyond the SSA.
[31] In Ref. 22, Anderson argued from a little different theoretical point of view from that of this paper that the Hubbard or the *t-J* model is a relevant model for cuprate HTS.
[32] Any ordered state is impossible at nonzero temperatures in two dimensions because of the divergence of thermal fluctuations. Because this divergence is logarithmic, weak three dimensionality is enough to suppress the divergence and to give nonzero and substantially high T_c's. Weak three dimensionality is implicitly assumed in this whole paper. It is reasonable to expect that temperatures where significant superconducting fluctuations start to develop in two dimensions give approximate T_c's of such quasi-two-dimensional systems.
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[47] When excitation energies of two-$2p$-hole states are argued, correlations between two $2p$ holes should be treated beyond the scheme of this paper, for example, in the configuration-interaction scheme. Then, U_{pp}'s in Eqs. (2.6) and (2.8) depend on the configuration of two $2p$ holes. The effective U_{pp} is large when two $2p$ holes are on an O ion, while it is small when they are on different O ions. This is one of the possible mechanisms responsible for the two-peak structure of the satellites in XPS spectra.
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[57] This formulation is general. Then, not only the cuprate oxides but also many other strongly correlated electron liquids can be regarded as Kondo lattices in this sense.

[58] Heavy quasiparticles are mainly composed of $3d$ electrons. However, the contribution to Eq. (3.22) from the heavy-quasiparticle band can be ignored, because the Fermi-surface volume obeys the Fermi-surface sum rule and the spectral weight of the heavy-quasiparticle band is small because of the mass-renormalization factor.

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[66] Note that $J_Q(i\omega_l,\mathbf{q})$ works between itinerant electrons. Its strength is proportional to the bandwidth of quasiparticles, as was argued in Ref. 20. It is different from the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction, which is caused by the virtual exchange of pair excitations of conduction electrons in spin channels and works between localized magnetic moments in metals.

[67] Because the characteristic energy of exchanged bosons is as large as U, the energy dependence of the superexchange interaction can be ignored in the low-energy region of $|\varepsilon_n| \ll k_BT_K$ and $|\varepsilon_n+\omega_l| \ll k_BT_K$.

[68] The virtual exchange of pair excitations of Gutzwiller's heavy quasiparticles is also present in metallic phases of the t-J model and the Hubbard model.

[69] The on-site repulsion of a mapped Anderson model is the same as that of a periodic model. Then, the Anderson model mapped from the t-J model, whose on-site repulsion is infinitely large, is different from that mapped from the d-p model with finite on-site repulsion.

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