Origin and roles of a strong electron-phonon interaction in cuprate oxide superconductors

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A strong electron-phonon interaction arises from the modulation of the superexchange interaction by lattice vibrations. It is responsible for the softening of the half-breathing modes around \((\pm \pi/a, 0)\) and \((0, \pm \pi/a)\) in the two-dimensional Brillouin zone, with \(a\) being the lattice constant of CuO\(_2\) planes, as is studied in Phys. Rev. B 70, 184514 (2004). Provided that antiferromagnetic spin fluctuations are developed around \(Q = (\pm 3\pi/4a, \pm \pi/a)\) and \((\pm \pi/a, \pm 3\pi/4a)\), the electron-phonon interaction can also cause the softening of Cu-O bond stretching modes around \(2Q\), or around \((\pm \pi/2a, 0)\) and \((0, \pm \pi/2a)\). The softening around \(2Q\) is accompanied by the development of charge fluctuations corresponding to the so-called 4\(a\)-period stripe or \(4a \times 4a\)-period checker-board state. However, an observation that the 4\(a\)-period modulating part or the \(2Q\) part of the density of states is almost symmetric with respect to the chemical potential contradicts a scenario that the stabilization of a single-\(2Q\) or double-\(2Q\) charge density wave following the complete softening of the \(2Q\) bond stretching modes is responsible for the ordered stripe or checker-board state. It is proposed that the stripe or checker-board state is simply a single-\(Q\) or double-\(Q\) spin density wave, whose second-harmonic effects can explain the observed almost symmetric 2\(Q\) part of the density of states. The strong electron-phonon interaction can play no or only a minor role in the occurrence of \(d\text{-wave}\) superconductivity in cuprate oxides.

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I. INTRODUCTION

It is one of the most interesting and important issues in condensed-matter physics to elucidate the mechanism of high critical temperature (high-\(T_c\)) superconductivity occurring in cuprate oxides.7 The oxides are highly anisotropic quasi-two-dimensional oxides, whose main compositions are CuO\(_2\) planes. High-\(T_c\) superconductivity occurs on the CuO\(_2\) planes. There are pieces of evidence that the electron-phonon interaction is strong on the CuO\(_2\) planes: the softening of the half-breathing modes around \((\pm \pi/a, 0)\) and \((0, \pm \pi/a)\) in the two-dimensional Brillouin zone (2DBZ) with \(a\) being the lattice constant of the CuO\(_2\) planes, the softening of Cu-O bond stretching modes around \((\pm \pi/2a, 0)\) and \((0, \pm \pi/2a)\) in 2DBZ and so on. It may be argued therefore that the electron-phonon interaction must play a major role in the occurrence of high-\(T_c\) superconductivity. On the other hand, observed isotope shifts of \(T_c\) and so on. It may be argued therefore that the strong electron-phonon interaction must play no or only a minor role in high-\(T_c\) superconductivity itself. The origin and roles of the strong electron-phonon interaction should be clarified in order that the issue of high-\(T_c\) superconductivity might be solved.

Parent cuprate oxides with no doping are Mott insulators. When holes or electrons are doped into the the Mott insulators, high-\(T_c\) superconductivity appears. Cuprate oxide superconductors lie in the vicinity of the Mott metal-insulator transition or crossover. It may be argued therefore that strong electron correlations must play a crucial role not only in the occurrence of high-\(T_c\) superconductivity but also in the origin and roles of the strong electron-phonon interaction.

The Hubbard model is one of the simplest effective Hamiltonians for strongly correlated electron liquids. In Hubbard’s approximation, a band splits into two subbands when the on-site repulsion \(U\) is so large that \(U > W\), with \(W\) being the bandwidth of unrenormalized electrons. The subbands are called the upper Hubbard band (UHB) and the lower Hubbard band (LHB), and a gap between UHB and LHB is called the Hubbard gap. In Gutzwiller’s approximation, a narrow quasiparticle band appears around the chemical potential. The band and quasiparticles are called the Gutzwiller band and quasiparticles, respectively. It is plausible to speculate that the density of states has in fact a three-peak structure, with the Gutzwiller band between UHB and LHB. Both of the approximations are single-site approximations (SSA). Another SSA theory confirms the speculation showing that the Gutzwiller band appears at the top of LHB when the electron density per unit cell is less than one. The nature of the ground state of the Hubbard model depends on the nature of the Gutzwiller quasiparticles.

The SSA that considers all the single-site terms is reduce to determining and solving self-consistently the Anderson model, which is one of the simplest effective Hamiltonian for the Kondo problem. Hence, the three-peak structure corresponds to the Kondo peak between two subpeaks in the Anderson model, or in the Kondo problem. The \(s\)-model is also one of the simplest effective Hamiltonian for the Kondo problem. According to Yosida’s perturbation theory and Wilson’s renormalization-group theory, the ground state of the \(s\)-model is a singlet or a normal Fermi liquid provided...
that the Fermi surface of conduction electrons is present. Since the $s$-$d$ model is derived from the Anderson model, the ground state of the Anderson model is also a normal Fermi liquid. It is certain therefore that under the SSA the ground state of the Hubbard model is a normal Fermi liquid or a metal. Even if the Hubbard gap opens, the Fermi surface of the Gutzwiller quasiparticles is present.

The SSA can also be formulated as the dynamical mean-field theory and the dynamical coherent potential approximation. In the SSA, local fluctuations are rigorously considered but Weiss mean fields, which are responsible for the appearance of the corresponding order parameter, are ignored. Hence, the SSA is rigorous for infinite dimensions within the Hilbert subspace with no order parameter. In Kondo-lattice theory, an unperturbed state is the normal Fermi liquid, which is constructed in the non-perturbative SSA theory, and not only effects of intersite fluctuations but also ordering due to Weiss mean fields such as magnetism, superconductivity and so on are perturbatively considered. Kondo-lattice theory can also be formulated as $1/d$ expansion theory, with $d$ being the spatial dimensionality.

The $d$-$p$ model, where Cu $3d$ and O $2p$ orbits are explicitly considered, is one of the simplest effective Hamiltonians for cuprate oxide superconductors. Since the on-site repulsion $U$ plays a crucial role in the $d$-$p$ model as it does in the Hubbard model, it is straightforward to extend the analysis for the Hubbard model to the $d$-$p$ model. Observed quasiparticle states, which are often called mid-gap states, are simply the Gutzwiller quasiparticle states, which can also be renormalized by intersite fluctuations. When observed specific heat coefficients as large as $\gamma \approx 14$ mJ/K$^2$mol are used, the Fermi-liquid relation gives

$$W^* = 0.3-0.4 \text{ eV}, \quad (1.1)$$

for the effective bandwidth of the Gutzwiller quasiparticles in optimal-doped cuprate oxide superconductors, where $T_c$ is the highest as a function of doping concentrations. According to field theory, the superexchange interaction arises from the virtual exchange of a pair excitation of electrons across the Hubbard gap. Since the Gutzwiller quasiparticles, which are responsible for metallic properties, plays no significant role in the virtual exchange process, the superexchange interaction is relevant even in a metallic phase, provided that the Hubbard gap opens. Cooper-pairs can also be bound by a magnetic exchange interaction. Since the superexchange interaction constant is as strong as $J = -(0.10-0.15)$ eV between nearest-neighbor Cu ions on a CuO$_2$ plane, observed high-$T_c$ can be easily reproduced. In actual, it has already been proposed that the condensation of $d_\gamma$-wave Cooper pairs between the Gutzwiller quasiparticles due to the superexchange interaction is responsible for high-$T_c$ superconductivity. Since the superexchange interaction is strong only between nearest-neighbor Cu ions, it is definite that theoretical $T_c$ of the $d_\gamma$ wave is much higher than those of other waves. In fact, high-$T_c$ superconductivity occurs in an intermediate-coupling regime $|J|/W^* = 0.3-0.5$ for superconductivity, which is realized in the strong-coupling regime for electron correlations defined by $U/W > 1$.

Since charge fluctuations are suppressed by strong electron correlations, the conventional electron-phonon interaction arising from charge-channel interactions must be weak in cuprate oxide superconductors. On the other hand, an electron-phonon interaction arising from spin-channel interactions can be strong. For example, an electron-phonon interaction arising from the modulation of a magnetic exchange interaction by phonons plays a significant role in the spin-Peierls effect. It has been shown in a previous paper that an electron-phonon interaction arising from the modulation of the superexchange interaction by phonons is strong in cuprate oxide superconductors. The electron-phonon interaction can explain the softening of the half-breathing modes around $(\pm \pi/a, 0)$ and $(0, \pm \pi/a)$ in 2DBZ. It has been predicted that the softening must be small around $(\pm \pi/a, \pm \pi/a)$ in 2DBZ. An attractive mutual interaction due to such an electron-phonon interaction is strong between quasiparticles on next-nearest-neighbor Cu ions, but is very weak between those on nearest-neighbor Cu ions. Therefore, the mutual interaction can play no significant role in the binding of $d_\gamma$-wave Cooper pairs. Observed small isotope shifts of $T_c$ can never contradict the presence of the strong electron-phonon interaction.

The so called 4$a$-period stripes and 4$a \times 4$a-period checker boards are observed in under-doped cuprate oxide superconductors, whose doping concentrations are smaller than those of optimal-doped ones. The wave numbers of Cu-O bond stretching modes, $(\pm \pi/2a, 0)$ and $(0, \pm \pi/2a)$ in 2DBZ, correspond to the period 4$a$ of stripes and checker boards. The softening of the stretching modes is accompanied by the development of 4$a$-period or $4a \times 4a$-period fluctuations in charge channels, which are simply stripe or checker-board fluctuations. It may be argued therefore that a charge density wave (CDW) following the complete softening of the bond stretching modes is responsible for ordered stripes and checker boards.

One of the purposes of this paper is to show that the strong electron-phonon interaction can also explain the softening of Cu-O bond stretching modes in cuprate oxide superconductors. The other purpose is to examine critically the relevance of the CDW scenario, whether or not the CDW is actually responsible for ordered stripes and checker boards. This paper is organized as follows: Preliminary discussions are presented in Sec. II. The derivation of the electron-phonon interaction is reviewed in Sec. II A and Kondo-lattice theory is reviewed in Sec. II B. The softening of the bond stretching modes around $(\pm \pi/2a, 0)$ and $(0, \pm \pi/2a)$ in 2DBZ is studied in Sec. III. The relevance of the CDW scenario for stripes and checker boards is critically examined in Sec. IV. An argument on the mechanism of high-$T_c$ superconductivity is given in Sec. V. Conclusion is presented in Sec. VI.
II. PRELIMINARIES

A. Electron-phonon interaction

In cuprate oxide superconductors, the superexchange interaction arises from the virtual exchange of a pair excitation of 3d electrons between UHB and LHB that are strongly hybridized subbands between Cu 3d and O 2p orbits. When the broadening or finite bandwidths of UHB and LHB are ignored, the exchange interaction constant between nearest-neighbor Cu ions on a CuO$_2$ plane is given by

$$J = -\frac{4V^4}{(\epsilon_d - \epsilon_p + U)^2} \left( \frac{1}{\epsilon_d - \epsilon_p + U} + \frac{1}{U} \right), \quad (2.1)$$

with $V$ being the hybridization matrix between nearest-neighbor O 2p and Cu 3d orbits, $\epsilon_d$ and $\epsilon_p$ the depths of Cu 3d and O 2p levels, and $U$ the on-site repulsion between Cu 3d electrons.

Doped holes reside mainly at O ions. The preferential doping suggests that O 2p levels are shallower than Cu 3d levels or that parent cuprate oxides with no hole doping must be charge-transfer insulators rather than Mott insulators; charge-transfer insulators and Mott insulators are characterized by $\epsilon_p > \epsilon_d$ and $\epsilon_p < \epsilon_d$, respectively. Since the hybridization between Cu 3d and O 2p orbits must be strong, it may also be argued that Cu 3d levels are much deeper than O 2p levels, that is, $\epsilon_p \gg \epsilon_d$ rather than $\epsilon_p > \epsilon_d$, to explain the observed preferential doping. However, the suggested level scheme of $\epsilon_p > \epsilon_d$ or $\epsilon_p \gg \epsilon_d$ disagrees with the prediction of Mott insulators, $\epsilon_d - \epsilon_p \simeq 1$ eV, by band calculations. The preferential doping does not necessarily mean that the parent cuprate oxides are charge-transfer insulators, but it simply means that the local charge susceptibility of 3d electrons is much smaller than that of 2p electrons, which implies that the effective on-site repulsion $U$ between 3d electrons is very small. It is assumed in this paper that $V \simeq 1.6$ eV and $\epsilon_d - \epsilon_p \simeq 1$ eV, as predicted by band calculations. Since the on-site $U$ should be so large that the Hubbard gap might open, it is assumed that $U \simeq 5$ eV. Then, Eq. (2.1) gives $J \simeq -0.27$ eV. This is about twice as large as the experimental $J = -(0.10-0.15)$ eV. This discrepancy is resolved when nonzero bandwidths of UHB and LHB are considered.

Displacements of the $i$th Cu ion and the $ij$th O ion, which lies between the nearest-neighbor ith and jth Cu ions, are given by

$$u_i = \sum_{\lambda\alpha} \frac{\hbar\nu_{p,\lambda\alpha}}{\sqrt{2NM_d\omega_{\lambda\alpha}}} e^{iq^\dagger R_i} \epsilon_{\lambda\alpha} \left( b^\dagger_{\lambda-q} + b_{\lambda q} \right), \quad (2.2)$$

and

$$u_{ij} = \sum_{\lambda\alpha} \frac{\hbar\nu_{p,\lambda\alpha}}{\sqrt{2NM_d\omega_{\lambda\alpha}}} e^{iq^{ij} R_i} \epsilon_{\lambda\alpha} \left( b^\dagger_{\lambda-q} + b_{\lambda q} \right), \quad (2.3)$$

with $R_i$ and $R_{ij} = (R_i + R_j)/2$ being positions of the $i$th Cu and $ij$th O ions, $M_d$ and $M_p$ masses of Cu and O ions, $b^\dagger_{\lambda q}$ and $b_{\lambda q}$ creation and annihilation operators of a phonon with a polarization $\lambda$ and a wave vector $q$, $\omega_{\lambda q}$ a phonon energy, $\epsilon_{\lambda\alpha} = (\epsilon_{\lambda\alpha,x}, \epsilon_{\lambda\alpha,y}, \epsilon_{\lambda\alpha,z})$ a polarization vector, and $N$ the number of unit cells. Here, only longitudinal phonons are considered so that it is assumed that $\epsilon_{\lambda\alpha} = (q_x, q_y, q_z)/|q|$ for $q$ within the first Brillouin zone. The $q$ dependence of $v_{d,\lambda q}$ and $v_{p,\lambda q}$ is crucial. For example, $v_{d,\lambda q} = 0$ and $v_{p,\lambda q} = O(1)$ for modes that bring no change in adjacent Cu-Cu distances.

Two types of electron-phonon interactions arise from the modulations of the superexchange interaction $J$ by the vibrations of O and Cu ions. When they are considered, it is convenient to define a dual-spin operator. First, a single-spin operator is defined by

$$S(q) = \frac{1}{\sqrt{N}} \sum_{k\omega\sigma} 2^{1/2} \sigma^{\alpha\beta} d_{(k+1/2)\alpha}^{(d,\lambda)} d_{(k-1/2)\beta}^{(d,\lambda)}, \quad (2.4)$$

with $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ being the Pauli matrices and $d_{k\omega\sigma}^{(d,\lambda)}$ and $d_{k\omega\sigma}^{(d,\lambda)}$ being creation and annihilation operators, respectively, of 3d electrons with wave number $k$. Then, the dual-spin operator is defined by

$$P_{\Gamma}(q) = \frac{1}{2} \sum_{q'} \eta_{\Gamma}(q') [S(q + 1/2) \cdot S(-q + 1/2)]^\dagger, \quad (2.5)$$

with

$$\eta_x(q) = \cos(q_x a) + \cos(q_y a), \quad (2.6)$$

and

$$\eta_y(q) = \cos(q_x a) - \cos(q_y a). \quad (2.7)$$

It is assumed in this paper that the $x$ and $y$ axes are within CuO$_2$ planes and the $z$ axis is perpendicular to CuO$_2$ planes. The electron-phonon interactions are simply given by

$$H_p = iC_p \sum_q \frac{\hbar\nu_{p,\lambda\alpha}}{2N M_p \omega_{\lambda\alpha}} \left( b^\dagger_{\lambda-q} + b_{\lambda q} \right) \times \tilde{\eta}_{\Gamma}(q) \sum_{\Gamma = s, d} \eta_{\Gamma}(q) P_{\Gamma}(q), \quad (2.8)$$

and

$$H_d = iC_d \sum_q \frac{\hbar\nu_{d,\lambda\alpha}}{2N M_d \omega_{\lambda\alpha}} \left( b^\dagger_{\lambda-q} + b_{\lambda q} \right) \times \sum_{\Gamma = s, d} \tilde{\eta}_{\Gamma}(q) P_{\Gamma}(q), \quad (2.9)$$

with $C_p$ and $C_d$ being real constants, which are given in the previous paper and

$$\tilde{\eta}_x(q) = 2 \left[ \epsilon_{\lambda x} \sin \left( \frac{q_x a}{2} \right) + \epsilon_{\lambda y} \sin \left( \frac{q_y a}{2} \right) \right], \quad (2.10)$$

and

$$\tilde{\eta}_y(q) = 2 \left[ \epsilon_{\lambda x} \sin \left( \frac{q_x a}{2} \right) - \epsilon_{\lambda y} \sin \left( \frac{q_y a}{2} \right) \right]. \quad (2.11)$$
B. Kondo-lattice theory

One of the simplest effective Hamiltonians for the electron part of cuprate oxide superconductors is the \(d-p\) model on a square lattice. Since the anisotropy is large, it is convenient to consider phenomenologically quasi-two-dimensional features. The \(d-p\) model is approximately mapped to the \(t-J\) model or the \(t-J\)-infinite-\(U\) model: 46

\[
\mathcal{H}_{t-J} = \sum_{ij\sigma} t_{ij} d_{i\sigma}^\dagger d_{j\sigma} - \frac{1}{2} J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)
+ U_{\infty} \sum_i d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow}, \tag{2.12}
\]

with the summation over \(\langle ij \rangle\) indicating that the summation should be made over nearest neighbors and

\[
\mathbf{S}_i = \sum_{\alpha\beta} \frac{1}{2} \sigma^{\alpha\beta} d_{i\alpha}^\dagger d_{i\beta}. \tag{2.13}
\]

The carrier density per unit cell is defined by

\[
n = \frac{1}{N} \sum_i \langle d_{i\sigma}^\dagger d_{i\sigma} \rangle. \tag{2.14}
\]

It should be noted that the infinitely large on-site repulsion \(U_{\infty}\) is introduced to exclude double occupancy so that \(n\) can never be larger than unity, or \(0 \leq n \leq 1\). The electron and hole pictures should be taken for the so-called hole-doped \((n < 1)\) and electron-doped \((n > 1)\) cuprate oxide superconductors, respectively, so that \(n\) is the electron density for hole-doped ones and is the hole density for electron-doped ones. The doping concentration is defined by \(\delta = 1 - n\), and the optimal concentration, where superconducting \(T_c\) is the highest as a function of \(\delta\), is \(\delta \simeq 0.15\). Then, \(\delta \lesssim 0.15\) and \(\delta \gtrsim 0.15\) are called under-doped and over-doped concentrations, respectively. When transfer integrals between nearest and next-nearest neighbors, which are denoted by \(t\) and \(t'\), are only considered, the dispersion relation of electrons or holes is given by

\[
E(k) = 2t [\cos(k_x a) + \cos(k_y a)]
+ 4t' [\cos(k_x a) \cos(k_y a)]. \tag{2.15}
\]

According to band calculations, it follows that \(t = -0.3-0.5\) eV and \(t' \approx -0.3t\) for electrons in hole-doped cuprate oxide superconductors and \(t = -(0.3-0.5)\) eV and \(t' \approx +0.3t\) for holes in electron-doped ones.

Every physical quantity is divided into single-site and multi-site terms. Calculating the single-site term is reduced to determining and solving self-consistently the Anderson model, as is discussed in the Introduction. When it is assumed that there is no order parameter, for example, the self-energy of electrons is divided into single-site and multi-site self-energies:

\[
\Sigma_\sigma(i\varepsilon_n, k) = \delta \Sigma_\sigma(i\varepsilon_n) + \Delta \Sigma_\sigma(i\varepsilon_n, k). \tag{2.16}
\]

The single-site self-energy \(\delta \Sigma_\sigma(i\varepsilon_n)\) is given by that of the Anderson model. It is expanded as

\[
\delta \Sigma_\sigma(i\varepsilon_n, k) = \delta \Sigma_\sigma(i\varepsilon_n) = \delta \Sigma_0 + (1 - \delta \phi) \varepsilon
+ (1 - \delta \phi) \frac{1}{2} \sigma g \mu B H + O(\varepsilon^2), \tag{2.17}
\]

at \(T = 0\) K in the presence of an infinitesimally small Zeeman energy \(g \mu B H\), with \(g\) the g factor and \(\mu B\) the Bohr magneton. The expansion coefficients \(\delta \Sigma_0, \delta \phi\), and \(\delta \phi\) are all real; \(\delta \phi \approx 2 \phi \gg 1\) for \(n \approx 1\). When Eq. (2.17) is used and the multi-site self-energy is ignored, the dispersion relation of the Gutzwiller quasiparticles is given by

\[
\xi_\sigma(k) = \frac{1}{\phi} \left[ \delta \Sigma_0 + E(k) - \mu \right] - \frac{1}{2} \sigma \bar{W}_s g \mu B H, \tag{2.18}
\]

with

\[
\bar{W}_s = \delta \phi \phi, \tag{2.19}
\]

being the so-called Wilson ratio for the Kondo problem.

The irreducible polarization function in spin channels is also divided into single-site and multi-site polarization functions:

\[
\pi_s(i\omega_l, q) = \bar{\pi}_s(i\omega_l) + \Delta \pi_s(i\omega_l, q). \tag{2.20}
\]

The single-site polarization function \(\bar{\pi}_s(i\omega_l)\) is given by that of the Anderson model. The spin susceptibilities of the Anderson and \(t-J\) models are given, respectively, by

\[
\chi_s(i\omega_l) = \frac{2\bar{\pi}_s(i\omega_l)}{1 - U_{\infty} \bar{\pi}_s(i\omega_l)}, \tag{2.21}
\]

and

\[
\chi_s(i\omega_l, q) = \frac{2\pi_s(i\omega_l, q)}{1 - \frac{1}{2} \frac{\bar{J}(q)}{U_{\infty}} \pi_s(i\omega_l, q)}, \tag{2.22}
\]

with

\[
\bar{J}(q) = 2J [\cos(q_x a) + \cos(q_y a)]. \tag{2.23}
\]

In Eqs. (2.21) and (2.22), the conventional factor \(\frac{1}{2} g^2 \mu B^2\) is not included. A physical picture for Kondo lattices is that local spin fluctuations at different sites interact with each other by an intersite exchange interaction. In Kondo-lattice theory, therefore, an intersite exchange interaction \(J_s(i\omega_l, q)\) is defined by

\[
\chi_s(i\omega_l, q) = \frac{\bar{\chi}_s(i\omega_l)}{1 - \frac{1}{2} J_s(i\omega_l, q) \bar{\chi}_s(i\omega_l)}, \tag{2.24}
\]

It follows that

\[
J_s(i\omega_l, q) = \bar{J}(q) + 2U_{\infty} \Delta \pi_s(i\omega_l, q). \tag{2.25}
\]

The derivation of Eq. (2.24) from Eqs. (2.21) and (2.22) is rigorous because ignored terms, which are
O[1/U_\infty \tilde{\chi}_s(i\omega_l)] vanish for infinitely large U_\infty. The term of $2U_\infty^2 \Delta \pi_s(i\omega_l, \mathbf{q})$ is composed of two terms:

$$2U_\infty^2 \Delta \pi_s(i\omega_l, \mathbf{q}) = J_Q(i\omega_l, \mathbf{q}) - 4\Lambda(i\omega_l, \mathbf{q}).$$

The first term $J_Q(i\omega_l, \mathbf{q})$ is an exchange interaction arising from the virtual exchange of a pair excitation of spin fluctuations constructed in the non-perturbative SSA theory and multi-dimensional lattice here. Although no interlayer coupling is included in the fuselage model, the nature of quasi-two-dimensional AF spin fluctuations is relevant in the softening of Cu-O bond stretching modes, as is examined below.

The renormalized energy of phonons, which is denoted by $\Sigma^{(ph)}_{\lambda} (i\omega_l, \mathbf{q})$, can be perturbatively calculated in terms of $H_p$ and $H_d$, the renormalized Green function for phonons is given by

$$D^{(0)}_\lambda (i\omega_l, \mathbf{q}) = \frac{2\omega_{\lambda\mathbf{q}}}{(i\omega_l)^2 - \omega_{\lambda\mathbf{q}}^2}.$$

When the self-energy for phonons is denoted by $\Sigma^{(ph)}_{\lambda} (i\omega_l, \mathbf{q})$, which can be perturbatively calculated in terms of $H_p$ and $H_d$, the renormalized Green function for phonons is given by

$$\begin{align*}
D_\lambda (i\omega_l, \mathbf{q}) &= D^{(0)}_\lambda (i\omega_l, \mathbf{q}) + D^{(0)}_\lambda (i\omega_l, \mathbf{q}) \Sigma^{(ph)}_{\lambda} (i\omega_l, \mathbf{q}) D_\lambda (i\omega_l, \mathbf{q}) \\
&= \frac{2\omega_{\lambda\mathbf{q}}}{(i\omega_l)^2 - \omega_{\lambda\mathbf{q}}^2 - 2\omega_{\lambda\mathbf{q}} \Sigma^{(ph)}_{\lambda} (i\omega_l, \mathbf{q})}.
\end{align*}$$

The renormalized energy of phonons, which is denoted by $\omega^*_{\lambda\mathbf{q}}$, is given by

$$(\omega^*_{\lambda\mathbf{q}})^2 - \omega^2_{\lambda\mathbf{q}} - 2\omega_{\lambda\mathbf{q}} \Sigma^{(ph)}_{\lambda} (\omega^*_{\lambda\mathbf{q}} + i0, \mathbf{q}) = 0.$$

The renormalization of phonon energies is given by

$$\Delta \omega_{\lambda\mathbf{q}} = \omega^*_{\lambda\mathbf{q}} - \omega_{\lambda\mathbf{q}} = \Sigma^{(ph)}_{\lambda} (\omega_{\lambda\mathbf{q}} + i0, \mathbf{q}) - \left[ \Sigma^{(ph)}_{\lambda} (\omega_{\lambda\mathbf{q}} + i0, \mathbf{q}) \right]^2/2\omega_{\lambda\mathbf{q}} + \cdots.$$

As well as AF spin fluctuations are developed around Q due to $I_s(i\omega_l, \mathbf{q})$, $d_\sigma$-wave superconducting (SC) and charge bond order (CBO) fluctuations are also developed due to $I_s(i\omega_l, \mathbf{q})$ or $I^*_s(i\omega_l, \mathbf{q})$. Although charge fluctuations are never much developed, charge-channel fluctuations can also contribute to the softening of phonons, as well as AF, SC, and CBO fluctuations, provided that vertex corrections for the dual spin operator in spin, SC,
and CBO channels are properly treated. According to
the previous paper, the softening of the half-breathing
modes is mainly caused by the charge-channel fluctua-
tions. Since the charge-channel fluctuations are signifi-
cant in the metallic phase, the softening is large in the
metallic phase but is small in the insulating phase.

Since phonons can couple with two lines or two chan-
nels of spin fluctuations to the lowest or first order in
the dual-spin operator, as is shown in Eqs. (2.8) and
(2.9). AF spin fluctuations around \((\pm \pi/2a, 0)\) and
\((0, \pm \pi/2a)\) in 2DBZ can play a significant role in
the softening of Cu-O bond stretching modes around
\((\pm \pi/2a, 0)\) and \((0, \pm \pi/2a)\) in 2DBZ. According to Mer-
min and Wagner if the Néel temperature \(T_N\) were
nonzero in two dimensions integrated effects of two-
dimensional critical AF spin fluctuations would be di-
vergent at \(T_N\), which leads to a conclusion that \(T_N\)
must be zero in two dimensions. Their argument im-
plies that quasi-two-dimensional critical AF spin fluctua-
tions can play a crucial role in the softening, at least,
in an AF critical region of cuprate oxide superconductors
provided that the anisotropy of critical AF spin fluctua-
tions is large. In order to examine how crucial a role the
anisotropy plays in the softening, it is more convenient
to use a phenomenological expression for the spin suscepti-
bility, which includes explicitly the anisotropy factor for
AF spin fluctuations, than to calculate microscopically
the spin susceptibility for quasi-two-dimensional systems.
The superexchange interaction \(J(q)\), which is given by
Eq. (2.23), has broad peaks at \((\pm \pi/a, \pm \pi/a)\) in 2DBZ
and the exchange interaction \(J_Q(0,q)\), which is given by
Eq. (2.29), has sharp peaks at nesting wave numbers of
the Fermi surface. Therefore, it is assumed in this paper
that \(I_s(0,q)\) is maximal at \(Q = (\pm 3\pi/4a, \pm \pi/a, Q_z)\) and
\((\pm \pi/2a, \pm 3\pi/4a, Q_z)\) or that \(\chi_s(0,q)\) is maximal at \(Q,\)
and that the spin susceptibility is approximately but well described by
\[
\chi_s(i\omega_l, Q + q) = \frac{\chi_s(0,Q)k^2}{\kappa^2 + (q||a)^2 + \delta^2(q,c)^2 + \frac{|q|}{\Gamma_{AF}}}, \tag{3.7}
\]
around each of \(Q\)'s, with \(q|| = (q_x, q_y)\) being the com-
ponent parallel to CuO\(_2\) planes, \(q_c\) the component per-
pendicular to CuO\(_2\) planes, \(c\) the lattice constant along
the \(z\) axis, and \(\Gamma_{AF}\) the energy scale of AF spin fluctua-
tions. The anisotropy factor \(\delta\) is introduced to consider
quasi-two-dimensional AF spin fluctuations. The corre-
lation length within the \(x\)-\(y\) plane is \(\sigma/\kappa\) and that along
the \(z\) axis is \(\delta c/\kappa\). A cut-off \(q_c = \pi/3a\) is introduced in
such a way that \(\chi_s(i\omega_l, Q + q) = 0\) for \(|q_c| > q_c\) or
\(|q_y| > q_c\). The anisotropy of the lattice constants plays
no role when \(\delta\) and \(q_c\) are defined in these ways.

When AF spin fluctuations are only considered, the
self-energy for phonons is given by
\[
\Sigma^{(ph)}_F(i\omega_l, q) = -\frac{\hbar^2}{2M_p\omega_{\lambda q}^2} \sum_{\Gamma\Gamma'} Y_{\Gamma'}(q)Y_{\Gamma}(q) \times X_{\Gamma\Gamma'}(i\omega_l, q), \tag{3.8}
\]
with
\[
Y_{\Gamma'}(q) = \tilde{\eta}_{\Gamma'}(q) \left[ C_{p\Gamma'} v_{\Gamma'\lambda q} \eta_{\Gamma'} \left( \frac{i}{2} q \right) + C_{d\Gamma'd\lambda q} \sqrt{\frac{M_p}{M_d}} \right], \tag{3.9}
\]
and
\[
X_{\Gamma\Gamma'}(i\omega_l', q) = \frac{k_B T}{N} \sum_{\eta_{\Gamma'}} \eta_{\Gamma'}(p) \eta_{\Gamma'}(p) \chi_s \left( i\omega_l' - p + \frac{1}{2} q \right) \times \chi_s \left( -i\omega_l' - p - \frac{1}{2} q \right). \tag{3.10}
\]
In Eq. (3.10), two \(\chi_s\)'s appear because of the dual-
spin operator. It should be noted that \(2Q\)'s are equiv-
alent to \((\pm \pi/2a, 0)\) and \((0, \pm \pi/2a)\): \(2Q - G = \pm \pi/a, 0)\) and \((0, \pm \pi/2a)\), with \(G = (\pm 2\pi/a, 0)\) and
\((0, \pm 2\pi/a)\) being reciprocal lattice vectors in 2DBZ. Then, Cu-O bond stretching modes around \((\pm \pi/2a, 0)\)
and \((0, \pm \pi/2a)\) in 2DBZ can be soft provided that
AF fluctuations around \(Q = (\pm 3\pi/4a, \pm \pi/a)\) and
\((\pm \pi/a, \pm 3\pi/4a)\) in 2DBZ are developed.

Since Cu-O bond stretching modes around \(2Q\) are con-
sidered, the vibrations of Cu ions are ignored, that is, it
is assumed that
\[
|C_{d\Gamma'd\lambda q}| \sqrt{\frac{M_p}{M_d}} = 0, \tag{3.11}
\]
and
\[
|C_{p\Gamma'\lambda q}| = c_p eV/\AA, \tag{3.12}
\]
where \(c_p\) is a dimensionless constant and it is likely
\(c_p = O(1). \tag{3.13}\)
Since the contribution from small \(p\) is large in the sum-
mation over \(p\) in Eq. (3.10), only the contribution from
the \(\Gamma = s\) channel is considered. Then, it follows that
\[
\Sigma^{(ph)}_s(\omega_{\lambda q} + i0, q) = -A_q \Xi(\omega_{\lambda q} + i0, q), \tag{3.14}
\]
with
\[
A_q = \frac{\hbar^2}{2M_p\omega_{\lambda q}^2} \frac{3}{4\pi} \Gamma_{AF} \left[ \chi_s(0,Q)k^2 \right]^2 \left| C_{p\Gamma'\lambda q} \right|^2, \tag{3.15}
\]
and
\[
\Xi(\omega_{\lambda q} + i0, q) = \tilde{\eta}_s^2(q) \eta_s^2 \left( \frac{i}{2} q \right) \frac{X_{ss}(\omega_{\lambda q} + i0, q)}{\Gamma_{AF} \left[ \chi_s(Q)k^2 \right]^2}. \tag{3.16}
\]
It should be noted that \(\Xi(i\omega_l, q)\) is defined as a dimen-
sionless quantity. The effective transfer integral between
nearest neighbors for the Gutzwiller quasiparticles is
\[
t^* = \tilde{t}/\phi_{\gamma}. \tag{3.17}
\]
According to Eq. (1.1), a plausible number for \(t^*\) is
\[
t^* \simeq W^*/8 \approx 40-50 \text{ meV}. \tag{3.18}
\]
According to a microscopic calculation for the spin susceptibility, it follows that $\Gamma_{AF}/|t^*| = O(1)$ and $\chi_s(0, Q)\kappa^2|t^*| = O(1)$. It is assumed, for the sake of simplicity, that the energy of Cu-O bond stretching modes is constant and is as large as

$$\omega_{\lambda q} = 50 \text{ meV}.\quad (3.19)$$

Then, $A_\mathbf{q}$ defined by Eq. (3.15) is approximately given by

$$A_\mathbf{q} \simeq 10 \times c_p^2 \frac{\Gamma_{AF}}{|t^*|} |\chi_s(0, Q)\kappa^2|t^*|^2| \text{ meV}$$

$$\simeq 10c_p^2 \text{ meV}.\quad (3.20)$$

In this paper, $T = 0 \text{ K}$ is assumed in the $\omega_t$ sum of Eq. (3.15).

The softening around one of $2Q$'s or $2Q_0$, with $Q_0 = (-3\pi/4a, \pi/a)$ in 2DBZ is considered; $2Q_0$ is equivalent to $(\pi/2a, 0)$. Figure 1 shows the dependence of $\Xi(\omega_{\lambda q} + i0, 2Q_0)$ on $\kappa$, $\delta$, $\Gamma_{AF}$, and $\chi_s$. Figure 1(a) and Fig. 1(b) show $\text{Re}[\Xi(\omega_{\lambda q} + i0, 2Q_0)]$ as a function of $\kappa$ and $\text{Re}[\Xi(\omega_{\lambda q} + i0, 0)]$ as a function of $\kappa$, respectively, for several sets of $\delta$ and $\omega_{\lambda q}/\Gamma_{AF}$. According to Eq. (3.15), $\Xi(\omega_{\lambda q} + i0, \mathbf{q})$ has a maximum, that is, $\text{Re}[\Sigma^{\text{ph}}(\omega_{\lambda q} + i0, \mathbf{q})]$ has a minimum around $2Q_0$ as a function of $\mathbf{q}$. According to Eq. (3.20), Fig. 1(a), and Fig. 1(b), it is likely that the softening at $2Q_0$ is as large as $-(10-20) \text{ meV}$ for $\kappa^2 \ll 1$ and $\delta \ll 1$. It should be noted that the softening can only be large provided that $\kappa^2 \ll 1$ and $\delta \ll 1$, as is implied by Mermin and Wagner’s argument. Integrated effects on the softening are never divergent even in the limit of $\kappa \to 0$ and $\delta \to 0$.

It is definite that $\kappa^2 \ll 1$ in the critical region of antiferromagnetic ordering or spin density wave (SDW), and it is certain that the anisotropy is as large as $\delta < 10^{-3}$ in cuprate oxide superconductors. Then, the second-harmonic effect of AF spin fluctuations can explain the observed softening as large as $-(10-20) \text{ meV}$ around $2Q_0$ or $2Q$.

Since the softening is small when $\kappa^2$ is large or AF spin fluctuations are not developed, it must be small in overdoped cuprate oxide superconductors, whose doping concentrations are larger than those of optimal-doped ones. When AF spin fluctuations are developed similarly or differently between $\pm3\pi/4a, \pm\pi/a$ and $\pm\pi/a, \pm3\pi/4a$ because of the anisotropy of the Fermi surface within 2DBZ, the softening must also occur similarly or differently between the $x$ and $y$ axes or between $(\pm\pi/2a, 0)$ and $(0, \pm\pi/2a)$. These two predictions are consistent with observations.

IV. STRIPES AND CHECKERBOARDS

Since the $4a$-period and $4a \times 4a$-period correspond to $2Q$, with $Q = (\pm3\pi/4a, \pm\pi/a)$ and $(\pm\pi/a, \pm3\pi/4a)$, a plausible scenario for the stripes and checker boards is that the complete softening is followed by the stabilization of CDW with $2Q$. In general, the $2Q$ component of the density of states, $\rho_{2Q}(\epsilon)$, as a function of $\epsilon$ is composed of symmetric and asymmetric components with respect to the chemical potential or $\epsilon = 0$. The symmetric component is large when CDW with $2Q$ is stabilized as a fundamental $2Q$ effect. According to an experiment, the symmetric component is larger than the asymmetric one, which contradicts the scenario of CDW even if the softening of the $2Q$ modes is large and the $2Q$ fluctuations are well developed. On the other hand, the symmetric component is large when the $2Q$ modulation is due to a simple second-harmonic effect of an ordered SDW with $Q$. The second-harmonic effect of the SDW can explain the observed almost symmetric $\rho_{2Q}(\epsilon)$. When stripes and checker-boards are really static orders, stripes must be due to single-$Q$ SDW and checker-boards must be due to double-$Q$ SDW. It is predicted that magnetizations of the two waves must be orthogonal to each other in double-$Q$ SDW. It is interesting to examine whether the prediction actually holds in cuprate oxide superconductors.
The appearance or stabilization of SDW is a transition rather than a crossover. However, no specific heat anomaly has been reported so far except for the anomaly due to superconductivity. The absence of any specific heat anomaly implies that, even if SDW is stabilized, the transition temperatures of SDW can be different in different domains, no significant specific anomaly can be observed. It is plausible that SDW is an disorder-induced SDW.

On the other hand, it is proposed that a stripe or a checker-board at rather high temperatures must be an exotic ordered state, that is, a fluctuating state in a quantum disordered phase. It should be examined whether it is actually such an exotic state. Another possibility is that it is a rather normal low-energy fluctuating state, whose energy scale is as small as that of the soft phonons. The other possibility is the disorder-induced SDW which can behave as a fluctuating state because it is inhomogeneous.

V. ATTRACTIVE INTERACTION

Although the electron-phonon interaction plays no or only a minor role in the formation of $d\gamma$-wave Cooper pairs, as is discussed in the Introduction, isotope shifts of $T_c$ can arise from the depression of superconductivity by the $2\mathbf{Q}$ fluctuations, whose development depends on the mass of O ions.

In Kondo-lattice theory, cuprate oxide superconductors can be relevantly treated as one of the typical Kondo lattices. According to Eq. (2.32), which is one of the most crucial results of Kondo-lattice theory, two mechanisms of attractive interactions, the spin-fluctuation mechanism and the exchange-interaction mechanism, are essentially the same as each other. However, the attractive interaction mediated by low-energy spin fluctuations such as those observed by low-energy neutron inelastic scatterings or those described by the phenomenological spin susceptibility is physically different from the attractive interaction due to the superexchange interaction, which arises from the exchange of a pair excitation of

electrons in spin channels across the Hubbard gap because the energy scales of spin fluctuations or spin excitations are totally different from each other in the two physical processes. The main part of the attractive interaction in cuprate oxide superconductors must be the superexchange interaction rather than the interaction mediated by low-energy AF spin fluctuations. Since the superexchange interaction is as strong as $J = -(0.10-0.15) \text{ eV}$, observed high $T_c$ can be easily reproduced, as is discussed in the Introduction.

VI. CONCLUSION

In cuprate oxides superconductors, the electron-phonon interaction arising from the modulation of the superexchange interaction by lattice vibrations is strong enough to cause the softening of not only the half-breathing modes around $(\pm \pi/a, 0)$ and $(0, \pm \pi/a)$ in the two-dimensional Brillouin zone but also Cu-O bond stretching modes around $(\pm 2\pi/2a, 0)$ and $(0, \pm 2\pi/2a)$. Although the softening of the bond stretching modes is responsible for stripe and checker-board fluctuations in charge channels, the stabilization of a charge density wave state following the complete softening of the bond stretching modes can never be any relevant scenario for ordered stripe and checker-board states. The ordered stripe or checker-board state must be simply a single-Q or double-Q spin density wave state, whose Q’s are $(\pm 3\pi/4a, \pm \pi/a)$ and $(\pm \pi/a, \pm 3\pi/4a)$. The strong electron-phonon interaction can play no or only a minor role in the binding of $d\gamma$-wave Cooper pairs in cuprate oxide superconductors, because the attractive interaction arising from the virtual exchange of a phonon is never strong between quasi-particles on nearest-neighbor Cu ions on a CuO$_2$ plane. However, isotope shifts of $T_c$ can arise from the depression of superconductivity by the stripe or checker-board fluctuations. Since the superexchange interaction is as strong as $J = -(0.10-0.15) \text{ eV}$ between nearest-neighbor Cu ions, the superexchange interaction must be mainly responsible for the binding of the $d\gamma$-wave Cooper pairs in cuprate oxide superconductors.

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1 J. G. Bednortz and K. A. Müller, Z. Phys. B 64, 189 (1986).
2 R. J. McQueeney, Y. Petrov, T. Egami, M. Yethiraj, G. Shirane, and Y. Endoh, Phys. Rev. Lett. 82, 628 (1999).
3 L. Pintschovius and M. Braden, Phys. Rev. B 60, R15039 (1999).
4 R. J. McQueeney, J. L. Sarrao, P. G. Pagliuso, P. W. Stephens, and R. Osborn, Phys. Rev. Lett. 87, 077001 (2001).
5 L. Pintschovius, W. Reichardt, M. Braden, G. Dhalenne, and A. Revcolevschi, Phys. Rev. B 64, 094510 (2001).
6 M. Braden, W. Reichardt, S. Shiryaev and S. N. Barilo, Physica C 378-381, 89 (2002).
7 L. Pintschovius, D. Reznik, W. Reichardt, Y. Endoh, H. Hiraka, J. M. Tranquada, H. Uchiyama, T. Masui, and S. Tajima, Phys. Rev. B 69, 214506 (2004).
8 D. Reznik, L. Pintschovius, M. Ito, S. Ikubo, M. Sato, H. Goka, M. Fujita, K. Yamada, G. D. Gu, and J. M. Tranquada, Nature, 440, 1170 (2006).
9 P. D. Johnson, T. Valla, A. V. Fedorov, Z. Yusof, B. O. Wells, Q. Li, A. R. Moodenbaugh, G. D. Gu, N. Koshizuka,
C. Kendziora, Sha Jian, and D. G. Hinks, Phys. Rev. Lett. 87, 177007 (2001).
10 T. Sato, H. Matsui, T. Takahashi, H. Ding, H.-B. Yang, S.-C. Wang, T. Fujii, T. Watanabe, A. Matsuda, T. Terashima, and K. Kadawaki, Phys. Rev. Lett. 91, 157003 (2003).
11 J. P. Franck, Physical Properties of High Temperature Superconductors IV, ed. D. M. Ginsberg (World Scientific, Singapore, 1994) p189.
12 J. Hubbard, Proc. Roy. Soc. London Ser. A 276, 238 (1963).
13 J. Hubbard, Proc. Roy. Soc. London Ser. A 281, 401 (1964).
14 M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963).
15 M. C. Gutzwiller, Phys. Rev. 134, A923 (1963).
16 M. C. Gutzwiller, Phys. Rev. 137, A1726, (1965).
17 F. J. Ohkawa, J. Phys. Soc. Jpn. 58, 4156 (1989).
18 F. J. Ohkawa, Phys. Rev. B 44, 6812 (1991).
19 F. J. Ohkawa, J. Phys. Soc. Jpn. 60, 3218 (1991).
20 F. J. Ohkawa, J. Phys. Soc. Jpn. 61, 1615 (1992).
21 K. Yosida, Phys. Rev. 147, 223 (1966).
22 K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).
23 F. J. Ohkawa, cond-mat/0606644. It is possible that under the SSA the normal Fermi-liquid ground state is degenerate with a non-normal Fermi liquid state provided that the chemical potential is just at the singular point of the density of states, for example, just at the logarithmic van Hove singularity of two dimensional systems.
24 A. Georges and G. Kotliar, Phys. Rev. B 45, 6479 (1992).
25 Y. Kakehashi and P. Fulde, Phys. Rev. B 69, 45101 (2004).
26 W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
27 J. W. Loram, K. A. Mirza, J. R. Cooper, and W. Y. Liang, Phys. Rev. Lett. 71, 1740 (1993).
28 N. Momono, M. Ido, T. Nakano, M. Oda, Y. Okajima, and K. Yamaya, Physica C 233, 395 (1994).
29 J. M. Luttinger and J. C. Ward: Phys. Rev. 118, 1417 (1960);
30 J. M. Luttinger, Phys. Rev. 119, 1153 (1960).
31 F. J. Ohkawa, Phys. Rev. B 59, 8930 (1999).
32 J. E. Hirsch, Phys. Rev. Lett. 54, 1317 (1985).
33 K. B. Lyons, P. A. Fleury, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. Lett. 60, 732 (1988).
34 F. J. Ohkawa, Jpn. J. Appl. Phys. 26, L652 (1987).
35 F. J. Ohkawa, J. Phys. Soc. Jpn. 56, 2267 (1987).
36 F. J. Ohkawa, Phys. Rev. B 70, 184514 (2004).
37 C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, Phys. Rev. B 67, 014533 (2003).
38 M. Vershinin, S. Mirsa, S. Ono, Y. Abe, Y. Ando, and A. Yazdani, Science 303, 1995 (2004).
39 T. Hanaguri, G. Lupien, Y. Kohsaka, D.-H. Lee, M. Azuma, M. Takano, H. Takagi, and J. C. Davis, Nature 430, 1001 (2004).
40 N. Momono, A. Hashimoto, Y. Kobatake, M. Oda, and M. Ido, J. Phys. Soc. Jpn. 74, 2400 (2005).
41 K. McElroy, D.-H. Lee, J. E. Hoffman, K. M. Lang, J. Lee, E. W. Hudson, H. Eisaki, S. Uchida, and J. C. Davis, Phys. Rev. Lett. 94, 197005 (2005).
42 S. A. Kiverson, I. P. Bindloss, E. Fradkin, V. Oganesyan, J. M. Tranquada, A. Kapitulnik, and C. Howald, Rev. Mod. Phys. 75, 1202 (2003).
43 T. Takegahara, H. Harima, and Y. Yanase, Jpn. J. Appl. Phys. Part 1, 26, L352 (1987).
44 N. Hamada, S. Massidda, A. J. Freeman, and J. Redinger, Phys. Rev. B 40, 4442 (1989).
45 O. K. Andersen, O. Jepsen, A. I. Liechtenstein, and I. I. Mazin, Phys. Rev. B 49, 4145 (1994).
46 F. C. Zhang and T. M. Rice, Phys. Rev. B 37, R3759 (1988).
47 F. J. Okhawa, J. Phys. Soc. Jpn. 74, 3340 (2005).
48 J. C. Ward, Phys. Rev. 68, 182 (1950).
49 See, for example, T. Moriya, Spin Fluctuations in Itinerant Electron Magnetism, Springer Series in Solid-State Sciences, Vol. 56 (Springer-Verlag, Berlin, Heidelberg, New York, Tokyo, 1985).
50 N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966).
51 F. J. Okhawa, Phys. Rev. B 73, 092506 (2006).
52 F. J. Okhawa, J. Phys. Soc. Jpn. 67, 535 (1998).
53 F. J. Okhawa, Phys. Rev. B 66, 014408 (2002).