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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 $\mathbf{Q}=(\pm 3\pi/4a, \pm\pi/a)$ and $(\pm\pi/a, \pm 3\pi/4a)$, the electron-phonon interaction can also cause the softening of Cu-O bond-stretching modes around $2\mathbf{Q}$, or around $(\pm\pi/2a, 0)$ and $(0, \pm\pi/2a)$. The softening around $2\mathbf{Q}$ is accompanied by the development of charge fluctuations corresponding to the so called $4a$ -period stripe or $(4a \times 4a)$ -period checkerboard state. However, an observation that the $4a$ -period modulating part or the $2\mathbf{Q}$ part of the density of states is almost symmetric with respect to the chemical potential contradicts a scenario in which the stabilization of a single- $2\mathbf{Q}$ or double- $2\mathbf{Q}$ charge-density wave following the complete softening of the $2\mathbf{Q}$ bond stretching modes is responsible for the ordered stripe or checkerboard state. It is proposed that the stripe or checkerboard state is simply a single- \mathbf{Q} or double- \mathbf{Q} spin-density wave, whose second-harmonic effects can explain the observed almost symmetric $2\mathbf{Q}$ part of the density of states. The strong electron-phonon interaction can play no or only a minor role in the occurrence of $d\gamma$ -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.¹ 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),²⁻⁶ 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,^{7,8} kinks in the dispersion relation of quasiparticles,^{9,10} 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 are small,¹¹ which implies that the strong electron-phonon interaction can play 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 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,^{12,13} a band splits into two subbands when the on-site repulsion U is so large that $U \geq W$,

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,¹⁴⁻¹⁶ 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,¹⁷ showing that the Gutzwiller band appears at the top of LHB when the electron density per unit cell is less than 1. 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 reduced to determining and solving self-consistently the Anderson model,¹⁸⁻²⁰ which is one of the simplest effective Hamiltonians 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 - d model is also one of the simplest effective Hamiltonians for the Kondo problem. According to Yosida's perturbation theory²¹ and Wilson's renormalization-group theory,²² the ground state of the s - d 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.²³ 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 theory²⁴ and the dynamical coherent potential approximation.²⁵ 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.²⁶ In Kondo-lattice theory,^{18–20} an *unperturbed* state is the normal Fermi liquid, which is constructed in the nonperturbative 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 midgap 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/K² mol are used,^{27,28} the Fermi-liquid relation gives^{29,30}

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

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.³¹ Since the Gutzwiller quasiparticles, which are responsible for metallic properties, play 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.³² Since the superexchange interaction constant is as strong as³³ $J = -(0.10\text{--}0.15)$ eV between nearest-neighbor Cu ions on a CuO₂ 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.^{34,35} 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 $|J|/W^* = 0.3\text{--}0.5$ for superconductivity, which is realized in the strong-coupling regime for electron correlations defined by $U/W \gtrsim 1$.

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 paper³⁶ 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 $4a$ -period stripes and $(4a \times 4a)$ -period checkerboards are observed in under-doped cuprate oxide superconductors,^{37–42} 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 $4a$ of stripes and checkerboards. The softening of the stretching modes is accompanied by the development of $4a$ -period or $(4a \times 4a)$ -period fluctuations in charge channels, which are simply stripe or checkerboard 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 checkerboards.

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 checkerboards. 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 checkerboards is critically examined in Sec. IV. An argument on the mechanism of high- T_c superconductivity is given in Sec. V. Conclusions are 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.³¹ When the broadening or finite bandwidths of UHB and LHB are ignored, the exchange interaction constant between nearest-neighbor Cu ions on a CuO₂ 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 $3d$ orbitals, ϵ_d and ϵ_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 $2p$ orbitals 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, $\epsilon_d - \epsilon_p \approx 1$ eV, by band calculations.^{43–45} 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 strong. It is assumed in this paper that $V \approx 1.6$ eV and $\epsilon_d - \epsilon_p \approx 1$ eV, as is predicted by band calculations.^{43–45} Since the on-site U should be so large that the Hubbard gap might open, it is assumed that $U \approx 5$ eV. Then, Eq. (2.1) gives $J \approx -0.27$ eV. This is about twice as large as the experimental $J = -(0.10-0.15)$ eV.³³ This discrepancy is resolved when nonzero bandwidths of UHB and LHB are considered.³¹

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

$$\mathbf{u}_i = \sum_{\lambda\mathbf{q}} \frac{\hbar v_{d,\lambda\mathbf{q}}}{\sqrt{2NM_d\omega_{\lambda\mathbf{q}}}} e^{i\mathbf{q}\cdot\mathbf{R}_i} \boldsymbol{\epsilon}_{\lambda\mathbf{q}} (b_{\lambda-\mathbf{q}}^\dagger + b_{\lambda\mathbf{q}}) \quad (2.2)$$

and

$$\mathbf{u}_{[ij]} = \sum_{\lambda\mathbf{q}} \frac{\hbar v_{p,\lambda\mathbf{q}}}{\sqrt{2NM_p\omega_{\lambda\mathbf{q}}}} e^{i\mathbf{q}\cdot\mathbf{R}_{[ij]}} \boldsymbol{\epsilon}_{\lambda\mathbf{q}} (b_{\lambda-\mathbf{q}}^\dagger + b_{\lambda\mathbf{q}}), \quad (2.3)$$

with \mathbf{R}_i and $\mathbf{R}_{[ij]} = (\mathbf{R}_i + \mathbf{R}_j)/2$ being positions of the i th Cu and $[ij]$ th O ions, M_d and M_p masses of Cu and O ions, $b_{\lambda\mathbf{q}}^\dagger$ and $b_{\lambda\mathbf{q}}$ creation and annihilation operators of a phonon with a polarization λ and a wave vector \mathbf{q} , $\omega_{\lambda\mathbf{q}}$ a phonon energy, $\boldsymbol{\epsilon}_{\lambda\mathbf{q}} = (\epsilon_{\lambda\mathbf{q},x}, \epsilon_{\lambda\mathbf{q},y}, \epsilon_{\lambda\mathbf{q},z})$ a polarization vector, and N the number of unit cells. Here, only longitudinal phonons are considered so that it is assumed that $\epsilon_{\lambda\mathbf{q}} = (q_x, q_y, q_z)/|\mathbf{q}|$ for \mathbf{q} within the first Brillouin zone. The \mathbf{q} dependence of $v_{d,\lambda\mathbf{q}}$ and $v_{p,\lambda\mathbf{q}}$ is crucial. For example, $v_{d,\lambda\mathbf{q}} = 0$ and $v_{p,\lambda\mathbf{q}} = O(1)$ 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

$$\mathbf{S}(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha\beta} \frac{1}{2} \boldsymbol{\sigma}^{\alpha\beta} d_{[\mathbf{k}+(1/2)\mathbf{q}]_\alpha}^\dagger d_{[\mathbf{k}-(1/2)\mathbf{q}]_\beta}, \quad (2.4)$$

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

$$\mathcal{P}_\Gamma(\mathbf{q}) = \frac{1}{2} \sum_{\mathbf{q}'} \eta_\Gamma(\mathbf{q}') \left[\mathbf{S}\left(\mathbf{q}' + \frac{1}{2}\mathbf{q}\right) \cdot \mathbf{S}\left(-\mathbf{q}' + \frac{1}{2}\mathbf{q}\right) \right], \quad (2.5)$$

with

$$\eta_s(\mathbf{q}) = \cos(q_x a) + \cos(q_y a) \quad (2.6)$$

and

$$\eta_d(\mathbf{q}) = \cos(q_x a) - \cos(q_y a). \quad (2.7)$$

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

$$\begin{aligned} \mathcal{H}_p &= iC_p \sum_{\mathbf{q}} \frac{\hbar v_{p,\lambda\mathbf{q}}}{\sqrt{2NM_p\omega_{\lambda\mathbf{q}}}} (b_{\lambda-\mathbf{q}}^\dagger + b_{\lambda\mathbf{q}}) \\ &\times \bar{\eta}_s(\mathbf{q}) \sum_{\Gamma=s,d} \eta_\Gamma\left(\frac{1}{2}\mathbf{q}\right) \mathcal{P}_\Gamma(\mathbf{q}) \end{aligned} \quad (2.8)$$

and

$$\mathcal{H}_d = iC_d \sum_{\mathbf{q}} \frac{\hbar v_{d,\lambda\mathbf{q}}}{\sqrt{2NM_d\omega_{\lambda\mathbf{q}}}} (b_{\lambda-\mathbf{q}}^\dagger + b_{\lambda\mathbf{q}}) \sum_{\Gamma=s,d} \bar{\eta}_\Gamma(\mathbf{q}) \mathcal{P}_\Gamma(\mathbf{q}), \quad (2.9)$$

with C_p and C_d being real constants, which are given in the previous paper,³⁶ and

$$\bar{\eta}_s(\mathbf{q}) = 2 \left[e_{\lambda_x} \sin\left(\frac{q_x a}{2}\right) + e_{\lambda_y} \sin\left(\frac{q_y a}{2}\right) \right] \quad (2.10)$$

and

$$\bar{\eta}_d(\mathbf{q}) = 2 \left[e_{\lambda_x} \sin\left(\frac{q_x a}{2}\right) - e_{\lambda_y} \sin\left(\frac{q_y a}{2}\right) \right]. \quad (2.11)$$

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

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

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

$$\mathbf{S}_i = \sum_{\alpha\beta} \frac{1}{2} \boldsymbol{\sigma}^{\alpha\beta} d_{i\alpha}^\dagger d_{i\beta}. \quad (2.13)$$

The carrier density per unit cell is defined by

$$n = \frac{1}{N} \sum_i \langle d_{i\sigma}^\dagger d_{i\sigma} \rangle. \quad (2.14)$$

It should be noted that the infinitely large on-site repulsion U_∞ 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 δ , is $\delta \approx 0.15$. Then, $\delta \lesssim 0.15$ and $\delta \gtrsim 0.15$ are called underdoped and overdoped 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

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

According to band calculations,^{43–45} 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 multisite 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 multisite self-energies,

$$\Sigma_\sigma(i\varepsilon_n, \mathbf{k}) = \tilde{\Sigma}_\sigma(i\varepsilon_n) + \Delta \Sigma_\sigma(i\varepsilon_n, \mathbf{k}). \quad (2.16)$$

The single-site self-energy $\tilde{\Sigma}_\sigma(i\varepsilon_n)$ is given by that of the Anderson model. It is expanded as

$$\tilde{\Sigma}_\sigma(\varepsilon + i0) = \tilde{\Sigma}_0 + (1 - \tilde{\phi}_\gamma) \varepsilon + (1 - \tilde{\phi}_s) \frac{1}{2} \sigma g \mu_B H + O(\varepsilon^2) \quad (2.17)$$

at $T=0$ K in the presence of an infinitesimally small Zeeman energy $g \mu_B H$, with g the g factor and μ_B the Bohr magneton. The expansion coefficients $\tilde{\Sigma}_0$, $\tilde{\phi}_\gamma$, and $\tilde{\phi}_s$ are all real; $\tilde{\phi}_s \approx 2\tilde{\phi}_\gamma \gg 1$ for $n \approx 1$. When Eq. (2.17) is used and the multisite self-energy is ignored, the dispersion relation of the Gutzwiller quasiparticles is given by

$$\xi_\sigma(\mathbf{k}) = \frac{1}{\tilde{\phi}_\gamma} [\tilde{\Sigma}_0 + E(\mathbf{k}) - \mu] - \frac{1}{2} \sigma \tilde{W}_s g \mu_B H, \quad (2.18)$$

with

$$\tilde{W}_s = \tilde{\phi}_s / \tilde{\phi}_\gamma \quad (2.19)$$

being the so called Wilson ratio for the Kondo problem.

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

$$\pi_s(i\omega_l, \mathbf{q}) = \tilde{\pi}_s(i\omega_l) + \Delta \pi_s(i\omega_l, \mathbf{q}). \quad (2.20)$$

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

$$\tilde{\chi}_s(i\omega_l) = \frac{2\tilde{\pi}_s(i\omega_l)}{1 - U_\infty \tilde{\pi}_s(i\omega_l)} \quad (2.21)$$

and

$$\chi_s(i\omega_l, \mathbf{q}) = \frac{2\pi_s(i\omega_l, \mathbf{q})}{1 - \left[\frac{1}{4} J(\mathbf{q}) + U_\infty \right] \pi_s(i\omega_l, \mathbf{q})}, \quad (2.22)$$

with

$$J(\mathbf{q}) = 2J[\cos(q_x a) + \cos(q_y a)]. \quad (2.23)$$

In Eqs. (2.21) and (2.22), the conventional factor $\frac{1}{4} g^2 \mu_B^2$ 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 $I_s(i\omega_l, \mathbf{q})$ is defined by

$$\chi_s(i\omega_l, \mathbf{q}) = \frac{\tilde{\chi}_s(i\omega_l)}{1 - \frac{1}{4} I_s(i\omega_l, \mathbf{q}) \tilde{\chi}_s(i\omega_l)}. \quad (2.24)$$

It follows that

$$I_s(i\omega_l, \mathbf{q}) = J(\mathbf{q}) + 2U_\infty^2 \Delta \pi_s(i\omega_l, \mathbf{q}). \quad (2.25)$$

The derivation of Eq. (2.25) 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_∞ . The term of $2U_\infty^2 \Delta \pi_s(i\omega_l, \mathbf{q})$ is composed of two terms,⁴⁷

$$2U_\infty^2 \Delta \pi_s(i\omega_l, \mathbf{q}) = J_Q(i\omega_l, \mathbf{q}) - 4\Lambda(i\omega_l, \mathbf{q}). \quad (2.26)$$

The first term $J_Q(i\omega_l, \mathbf{q})$ is an exchange interaction arising from the virtual exchange of a pair excitation of the Gutzwiller quasiparticles. According to the Ward relation,⁴⁸ the static component of the single-site irreducible vertex function in spin channels is given by

$$\tilde{\lambda}_s = \tilde{\phi}_s [1 - U_\infty \tilde{\pi}_s(0)]. \quad (2.27)$$

Then, it follows that

$$U_\infty \tilde{\lambda}_s = 2\tilde{\phi}_s / \tilde{\chi}_s(0). \quad (2.28)$$

When the vertex correction $\tilde{\lambda}_s$ given by Eq. (2.28) is used, it follows that

$$J_Q(i\omega_l, \mathbf{q}) = \frac{4\tilde{W}_s^2}{\tilde{\chi}_s^2(0)} \left[P(i\omega_l, \mathbf{q}) - \frac{1}{N} \sum_{\mathbf{q}} P(i\omega_l, \mathbf{q}) \right], \quad (2.29)$$

with

$$P(i\omega_l, \mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}\sigma} \frac{f[\xi_\sigma(\mathbf{k})] - f[\xi_\sigma(\mathbf{k} + \mathbf{q})]}{\xi_\sigma(\mathbf{k} + \mathbf{q}) - \xi_\sigma(\mathbf{k}) + i\omega_l}, \quad (2.30)$$

with

$$f(\varepsilon) = \frac{1}{e^{\varepsilon/k_B T} + 1}. \quad (2.31)$$

In Eq. (2.29), the single-site term is subtracted because it is considered in the SSA. The strength of the exchange interaction is proportional to the width of the Gutzwiller band. Since the chemical potential lies around the center of the Gutzwiller band or the nesting of the Fermi surface is sharp, the exchange interaction is antiferromagnetic (AF) in cuprate oxide superconductors. The second term $-4\Lambda(i\omega_l, \mathbf{q})$ corresponds to the mode-mode coupling term in the self-consistent renormalization theory of spin fluctuations,⁴⁹ which is relevant in the weak-coupling regime for electron correlations defined by $U/W \lesssim 1$.

When Eq. (2.28) is used, the mutual interaction mediated by intersite spin fluctuations, which works between the Gutzwiller quasiparticles, is given by

$$(U_\infty \tilde{\chi}_s)^2 [\chi_s(i\omega_l, \mathbf{q}) - \tilde{\chi}_s(i\omega_l)] = \tilde{\phi}_s^2 I_s^*(i\omega_l, \mathbf{q}), \quad (2.32)$$

with

$$I_s^*(i\omega_l, \mathbf{q}) = \frac{I_s(i\omega_l, \mathbf{q})}{1 - \frac{1}{4} I_s(i\omega_l, \mathbf{q}) \tilde{\chi}_s(i\omega_l)}. \quad (2.33)$$

In Eq. (2.32), the single-site term is subtracted because it is considered in the SSA. The exchange interaction $I_s(i\omega_l, \mathbf{q})$ is enhanced into $I_s^*(i\omega_l, \mathbf{q})$ by spin fluctuations. The mutual interaction mediated by spin fluctuations is essentially the same as that due to the exchange interaction $I_s(i\omega_l, \mathbf{q})$ or $I_s^*(i\omega_l, \mathbf{q})$.

In Kondo-lattice theory, an *unperturbed* state is constructed in the nonperturbative SSA theory, and multisite or intersite effects are perturbatively considered in terms of $I_s(i\omega_l, \mathbf{q})$ or $I_s^*(i\omega_l, \mathbf{q})$.

III. SOFTENING OF PHONONS DUE TO ANTIFERROMAGNETIC SPIN FLUCTUATIONS

An effective Hamiltonian to be eventually examined in this paper is

$$\mathcal{H} = \mathcal{H}_{t-J} + \mathcal{H}_{\text{ph}} + \mathcal{H}_p + \mathcal{H}_d, \quad (3.1)$$

with

$$\mathcal{H}_{\text{ph}} = \sum_{\lambda\mathbf{q}} \omega_{\lambda\mathbf{q}} \left(b_{\lambda\mathbf{q}}^\dagger b_{\lambda\mathbf{q}} + \frac{1}{2} \right), \quad (3.2)$$

and \mathcal{H}_p and \mathcal{H}_d defined by Eqs. (2.8) and (2.9), respectively. The t - J model \mathcal{H}_{t-J} is defined on a square lattice in Sec. II B, but it should be defined on a quasi-two-dimensional lattice here. Although no interlayer coupling is included in \mathcal{H}_{t-J} , the nature of quasi-two-dimensional AF spin fluctuations is

phenomenologically considered, which plays one of the most crucial roles in the softening of Cu-O bond stretching modes, as is examined below.

In the absence of \mathcal{H}_p and \mathcal{H}_d , the Green function for phonons is given by

$$D_\lambda^{(0)}(i\omega_l, \mathbf{q}) = \frac{2\omega_{\lambda\mathbf{q}}}{(i\omega_l)^2 - \omega_{\lambda\mathbf{q}}^2}. \quad (3.3)$$

When the self-energy for phonons is denoted by $\Sigma_\lambda^{(\text{ph})}(i\omega_l, \mathbf{q})$, which can be perturbatively calculated in terms of \mathcal{H}_p and \mathcal{H}_d , the renormalized Green function for phonons is given by

$$\begin{aligned} D_\lambda(i\omega_l, \mathbf{q}) &= D_\lambda^{(0)}(i\omega_l, \mathbf{q}) + D_\lambda^{(0)}(i\omega_l, \mathbf{q}) \Sigma_\lambda^{(\text{ph})}(i\omega_l, \mathbf{q}) D_\lambda(i\omega_l, \mathbf{q}) \\ &= \frac{2\omega_{\lambda\mathbf{q}}}{(i\omega_l)^2 - \omega_{\lambda\mathbf{q}}^2 - 2\omega_{\lambda\mathbf{q}} \Sigma_\lambda^{(\text{ph})}(i\omega_l, \mathbf{q})}. \end{aligned} \quad (3.4)$$

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

$$(\omega_{\lambda\mathbf{q}}^*)^2 - \omega_{\lambda\mathbf{q}}^2 - 2\omega_{\lambda\mathbf{q}} \Sigma_\lambda^{(\text{ph})}(\omega_{\lambda\mathbf{q}}^* + i0, \mathbf{q}) = 0. \quad (3.5)$$

The renormalization of phonon energies is given by

$$\begin{aligned} \Delta\omega_{\lambda\mathbf{q}} &= \omega_{\lambda\mathbf{q}}^* - \omega_{\lambda\mathbf{q}} \\ &= \Sigma_\lambda^{(\text{ph})}(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q}) \\ &\quad - [\Sigma_\lambda^{(\text{ph})}(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})]^2 / 2\omega_{\lambda\mathbf{q}} + \dots, \end{aligned} \quad (3.6)$$

unless $|\Sigma_\lambda^{(\text{ph})}(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})|$ is larger than $|\omega_{\lambda\mathbf{q}}|$.

In addition to AF spin fluctuations that are developed around \mathbf{Q} due to $I_s(i\omega_l, \mathbf{q})$, $d\gamma$ -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 developed much, 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,³⁶ the softening of the half-breathing modes is mainly caused by the charge-channel fluctuations. Since the charge-channel fluctuations are significant 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 channels 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 $(\pm 3\pi/4a, \pm \pi/a)$ and $(\pm \pi/a, \pm 3\pi/4a)$ 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 Mermin and Wagner,⁵⁰ if the Néel temperature T_N were nonzero in two dimensions, integrated effects of two-dimensional critical AF spin fluctuations would be divergent at T_N , which leads to a conclusion that T_N must be zero in two dimensions. Their argument implies that quasi-two-dimensional critical AF spin fluctuations 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 fluctuations 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 susceptibility, 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 $J(\mathbf{q})$, which is given by Eq. (2.23), has broad peaks at $(\pm\pi/a, \pm\pi/a)$ in 2DBZ, and the exchange interaction $J_Q(0, \mathbf{q})$, 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 $I_s(0, \mathbf{q})$ is maximal at $\mathbf{Q} = (\pm 3\pi/4a, \pm\pi/a, Q_z)$ and $(\pm\pi/a, \pm 3\pi/4a, Q_z)$ or that $\chi_s(0, \mathbf{q})$ is maximal at \mathbf{Q} , and that the spin susceptibility (2.24) is approximately but well described by

$$\chi_s(i\omega, \mathbf{Q} + \mathbf{q}) = \frac{\chi_s(0, \mathbf{Q})\kappa^2}{\kappa^2 + (q_{\parallel}a)^2 + \delta^2(q_z c)^2 + \frac{|\omega_{\parallel}|}{\Gamma_{\text{AF}}}}, \quad (3.7)$$

around each of the \mathbf{Q} 's, with $\mathbf{q}_{\parallel} = (q_x, q_y)$ being the component parallel to CuO_2 planes, q_z the component perpendicular to CuO_2 planes, c the lattice constant along the z axis, and Γ_{AF} the energy scale of AF spin fluctuations. The anisotropy factor δ is introduced to consider quasi-two-dimensional AF spin fluctuations. The correlation length within the x - y plane is a/κ and that along the z axis is $\delta c/\kappa$. A cutoff $q_c = \pi/3a$ is introduced in such a way that $\chi_s(i\omega, \mathbf{Q} + \mathbf{q}) = 0$ for $|q_x| > q_c$ or $|q_y| > q_c$. The anisotropy of the lattice constants plays no role when δ and q_c are defined in these ways.

When AF spin fluctuations are only considered, the self-energy for phonons is given by³⁶

$$\Sigma_{\lambda}^{(\text{ph})}(i\omega, \mathbf{q}) = -\frac{\hbar^2}{2M_p \omega_{\lambda\mathbf{q}}} \frac{3}{4^2} \sum_{\Gamma\Gamma'} Y_{\Gamma}(\mathbf{q}) Y_{\Gamma'}(\mathbf{q}) X_{\Gamma\Gamma'}(i\omega, \mathbf{q}), \quad (3.8)$$

with

$$Y_{\Gamma}(\mathbf{q}) = \bar{\eta}_s(\mathbf{q}) \left[C_p v_{p,\lambda\mathbf{q}} \eta_{\Gamma} \left(\frac{1}{2} \mathbf{q} \right) + C_d v_{d,\lambda\mathbf{q}} \sqrt{\frac{M_p}{M_d}} \right] \quad (3.9)$$

and

$$X_{\Gamma\Gamma'}(i\omega, \mathbf{q}) = \frac{k_B T}{N} \sum_{\omega', \mathbf{p}} \eta_{\Gamma}(\mathbf{p}) \eta_{\Gamma'}(\mathbf{p}) \chi_s \left(i\omega', \mathbf{p} + \frac{1}{2} \mathbf{q} \right) \times \chi_s \left(-i\omega' - i\omega, -\mathbf{p} + \frac{1}{2} \mathbf{q} \right). \quad (3.10)$$

In Eq. (3.10), two χ_s 's appear because of the dual-spin operator. It should be noted that $2\mathbf{Q}$'s are equivalent to $(\pm\pi/2a, 0)$ and $(0, \pm\pi/2a)$: $2\mathbf{Q} - \mathbf{G} = (\pm\pi/2a, 0)$ and $(0, \pm\pi/2a)$, with $\mathbf{G} = (\pm 2\pi/a, 0)$ 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 $\mathbf{Q} = (\pm 3\pi/4a, \pm\pi/a)$ and $(\pm\pi/a, \pm 3\pi/4a)$ in 2DBZ are developed.

Since Cu-O bond-stretching modes around $2\mathbf{Q}$ are considered, the vibrations of Cu ions are ignored, that is, it is assumed that

$$|C_d v_{d,\lambda\mathbf{q}}| \sqrt{M_p/M_d} = 0 \quad (3.11)$$

and

$$|C_p v_{p,\lambda\mathbf{q}}| = c_p \text{ eV}/\text{\AA}, \quad (3.12)$$

where c_p is a dimensionless constant, and it is likely that³⁶

$$c_p = O(1). \quad (3.13)$$

Since the contribution from small \mathbf{p} is large in the summation over \mathbf{p} in Eq. (3.10), only the contribution from the $\Gamma = s$ channel is considered. Then, it follows that

$$\Sigma_{\lambda}^{(\text{ph})}(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q}) = -A_{\mathbf{q}} \Xi(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q}), \quad (3.14)$$

with

$$A_{\mathbf{q}} = \frac{\hbar^2}{2M_p \omega_{\lambda\mathbf{q}}} \frac{3}{4^2} \Gamma_{\text{AF}} [\chi_s(0, \mathbf{Q})\kappa^2]^2 |C_p v_{p,\lambda\mathbf{q}}|^2 \quad (3.15)$$

and

$$\Xi(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q}) = \bar{\eta}_s^2(\mathbf{q}) \eta_s^2 \left(\frac{1}{2} \mathbf{q} \right) \frac{X_{ss}(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})}{\Gamma_{\text{AF}} [\chi_s(\mathbf{Q})\kappa^2]^2}. \quad (3.16)$$

It should be noted that $\Xi(i\omega, \mathbf{q})$ is defined as a dimensionless quantity. The effective transfer integral between nearest neighbors for the Gutzwiller quasiparticles is

$$t^* = t/\tilde{\phi}_{\gamma}. \quad (3.17)$$

According to Eq. (1.1), a plausible number for t^* is

$$|t^*| \simeq W^*/8 \simeq 40\text{--}50 \text{ meV}. \quad (3.18)$$

According to a microscopic calculation for the spin susceptibility, it follows that $\Gamma_{\text{AF}}/|t^*| = O(1)$ and $\chi_s(0, \mathbf{Q})\kappa^2 |t^*| = O(1)$. It is assumed, for the sake of simplicity, that the energy of Cu-O bond-stretching modes is constant and is as large as

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

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

$$A_{\mathbf{q}} \simeq 10 \times c_p^2 \frac{\Gamma_{\text{AF}}}{|t^*|} [\chi_s(0, \mathbf{Q})\kappa^2 |t^*|]^2 \text{ meV} \simeq 10c_p^2 \text{ meV}. \quad (3.20)$$

In this paper, $T=0$ K is assumed in the ω' sum of Eq. (3.10).

The softening around one of $2\mathbf{Q}$'s or $2\mathbf{Q}_0$, with $\mathbf{Q}_0 = (-3\pi/4a, \pi/a)$ in 2DBZ, is considered; $2\mathbf{Q}_0$ is equivalent to $(\pi/2a, 0)$. Figure 1 shows the dependence of $\Xi(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})$ on κ , δ , Γ_{AF} , and \mathbf{q} ; Figs. 1(a) and 1(b) show $\text{Re}[\Xi(\omega_{\lambda\mathbf{q}} + i0, 2\mathbf{Q}_0)]$ as a function of κ^2 and $\text{Re}[\Xi(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})]$ as a function of q_x , respectively, for several sets of δ and $\omega_{\lambda\mathbf{q}}/\Gamma_{\text{AF}}$. According to Fig. 1(b), $\Xi(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})$ has a maximum, that is, $\text{Re}[\Sigma_{\lambda}^{(\text{ph})}(\omega_{\lambda\mathbf{q}} + i0, \mathbf{q})]$ has a minimum around $2\mathbf{Q}_0$ as a function of \mathbf{q} . According to Eq. (3.20),

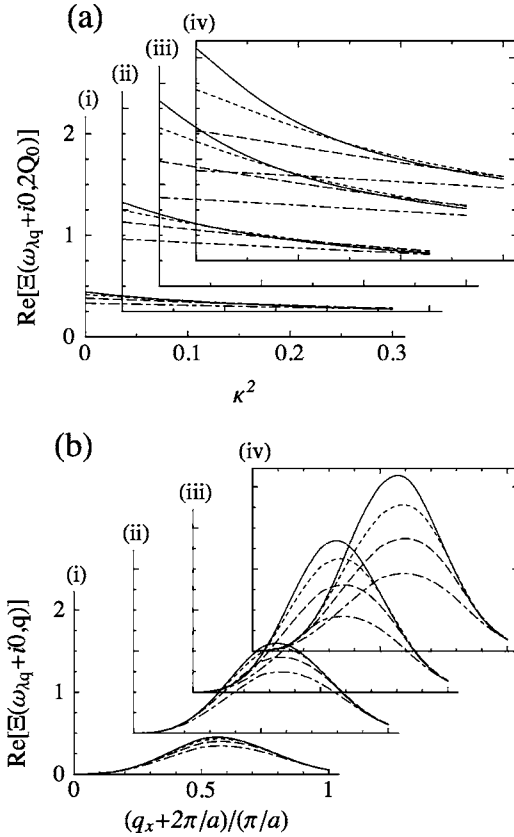


FIG. 1. (a) $\text{Re}[\Xi(\omega_{\lambda q}+i0, 2\mathbf{Q}_0)]$ as a function of κ^2 , with $\mathbf{Q}_0 = (-3\pi/4a, \pi/a)$, and (b) $\text{Re}[\Xi(\omega_{\lambda q}+i0, \mathbf{q})]$ as a function of q_x ($-2\pi/a \leq q_x \leq -\pi/a$) for $q_y = 2\pi/a$. For the anisotropy factor, (i) $\delta=1$, (ii) $\delta=10^{-1/2}$, (iii) $\delta=10^{-1}$, and (iv) $\delta=10^{-3}$. In each figure, solid, dotted, dashed, and dashed chain lines are for $\omega_{\lambda q}/\Gamma_{\text{AF}}=0.2, 0.4, 0.8,$ and 1.6 , respectively.

Fig. 1(a), and Fig. 1(b), it is likely that the softening at $2\mathbf{Q}_0$ is as large as $-(10-20)$ 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;⁵⁰ integrated effects on the softening are never divergent, even in the limit of $\kappa \rightarrow 0$ and $\delta \rightarrow 0$.

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^{7,8} as large as $-(10-20)$ meV around $2\mathbf{Q}_0$ or $2\mathbf{Q}$.

Since the softening is small when κ^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 $(\pm 3\pi/4a, \pm \pi/a)$ and $(\pm \pi/a, \pm 3\pi/4a)$ 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.^{7,8}

IV. STRIPES AND CHECKERBOARDS

Since the $4a$ -period and $(4a \times 4a)$ -period correspond to $2\mathbf{Q}$, with $\mathbf{Q} = (\pm 3\pi/4a, \pm \pi/a)$ and $(\pm \pi/a, \pm 3\pi/4a)$, a plausible scenario for the stripes and checkerboards is that the complete softening is followed by the stabilization of CDW with $2\mathbf{Q}$. In general, the $2\mathbf{Q}$ component of the density of states, $\rho_{2\mathbf{Q}}(\varepsilon)$, as a function of ε is composed of symmetric and asymmetric components with respect to the chemical potential or $\varepsilon=0$. The asymmetric component is large when CDW with $2\mathbf{Q}$ is stabilized as a fundamental $2\mathbf{Q}$ effect. According to an experiment,³⁷ the symmetric component is larger than the asymmetric one, which contradicts the scenario of CDW even if the softening of the $2\mathbf{Q}$ modes is large and the $2\mathbf{Q}$ fluctuations are well developed. On the other hand, the symmetric component is large when the $2\mathbf{Q}$ modulation is due to a simple second-harmonic effect of an ordered SDW with \mathbf{Q} .⁵¹ The second-harmonic effect of the SDW can explain the observed almost symmetric $\rho_{2\mathbf{Q}}(\varepsilon)$. When stripes and checkerboards are really static orders, stripes must be due to single- \mathbf{Q} SDW and checkerboards must be due to double- \mathbf{Q} SDW. It is predicted that magnetizations of the two waves must be orthogonal to each other in double- \mathbf{Q} SDW.^{52,53} 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, SDW is never a homogeneous phase but is an inhomogeneous phase, which is composed of many domains. If the transition temperatures of SDW can be different in different domains, no significant specific anomaly can be observed. It is plausible that SDW is a disorder-induced SDW.⁴⁷

On the other hand, it is proposed⁴² that a stripe or a checkerboard 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,⁴⁷ 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, namely the spin-fluctuation mechanism and the exchange-interaction mechanism, are essentially the same. 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 (2.24) 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 $J = -(0.10-0.15)$ eV,³³ 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 $(\pm\pi/2a, 0)$ and $(0, \pm\pi/2a)$. Although the softening of the bond-stretching modes is responsible for stripe and checkerboard 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 checkerboard states. The ordered stripe or checkerboard state must be simply a single- \mathbf{Q} or double- \mathbf{Q} spin-density-wave state, whose \mathbf{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 quasiparticles 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 checkerboard fluctuations. Since the superexchange interaction is as strong as $J = -(0.10-0.15)$ 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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- ¹J. G. Bednortz and K. A. Müller, *Z. Phys. B: Condens. Matter* **64**, 189 (1986).
- ²R. J. McQueeney, Y. Petrov, T. Egami, M. Yethiraj, G. Shirane, and Y. Endoh, *Phys. Rev. Lett.* **82**, 628 (1999).
- ³L. Pintschovius and M. Braden, *Phys. Rev. B* **60**, R15039 (1999).
- ⁴R. J. McQueeney, J. L. Sarrao, P. G. Pagliuso, P. W. Stephens, and R. Osborn, *Phys. Rev. Lett.* **87**, 077001 (2001).
- ⁵L. Pintschovius, W. Reichardt, M. Braden, G. Dhalenne, and A. Revcolevschi, *Phys. Rev. B* **64**, 094510 (2001).
- ⁶M. Braden, W. Reichardt, S. Shiryayev, and S. N. Barilo, *Physica C* **378-381**, 89 (2002).
- ⁷L. 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).
- ⁸D. Reznik, L. Pintschovius, M. Ito, S. Iikubo, M. Sato, H. Goka, M. Fujita, K. Yamada, G. D. Gu, and J. M. Tranquada, *Nature (London)* **440**, 1170 (2006).
- ⁹P. 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).
- ¹⁰T. Sato, H. Matsui, T. Takahashi, H. Ding, H.-B. Yang, S.-C. Wang, T. Fujii, T. Watanabe, A. Matsuda, T. Terashima, and K. Kadowaki, *Phys. Rev. Lett.* **91**, 157003 (2003).
- ¹¹J. P. Franck, *Physical Properties of High Temperature Superconductors IV*, edited by D. M. Ginsberg (World Scientific, Singapore, 1994), p. 189.
- ¹²J. Hubbard, *Proc. R. Soc. London, Ser. A* **276**, 238 (1963).
- ¹³J. Hubbard, *Proc. R. Soc. London, Ser. A* **281**, 401 (1964).
- ¹⁴M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963).
- ¹⁵M. C. Gutzwiller, *Phys. Rev.* **134**, A923 (1964).
- ¹⁶M. C. Gutzwiller, *Phys. Rev.* **137**, A1726 (1965).
- ¹⁷F. J. Ohkawa, *J. Phys. Soc. Jpn.* **58**, 4156 (1989).

- ¹⁸F. J. Ohkawa, *Phys. Rev. B* **44**, 6812 (1991).
- ¹⁹F. J. Ohkawa, *J. Phys. Soc. Jpn.* **60**, 3218 (1991).
- ²⁰F. J. Ohkawa, *J. Phys. Soc. Jpn.* **61**, 1615 (1992).
- ²¹K. Yosida, *Phys. Rev.* **147**, 223 (1966).
- ²²K. G. Wilson, *Rev. Mod. Phys.* **47**, 773 (1975).
- ²³F. J. Ohkawa, cond-mat/0606644 (unpublished). 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.
- ²⁴A. Georges and G. Kotliar, *Phys. Rev. B* **45**, 6479 (1992).
- ²⁵Y. Takehashi and P. Fulde, *Phys. Rev. B* **69**, 045101 (2004).
- ²⁶W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).
- ²⁷J. W. Loram, K. A. Mirza, J. R. Cooper, and W. Y. Liang, *Phys. Rev. Lett.* **71**, 1740 (1993).
- ²⁸N. Momono, M. Ido, T. Nakano, M. Oda, Y. Okajima, and K. Yamaya, *Physica C* **233**, 395 (1994).
- ²⁹J. M. Luttinger and J. C. Ward, *Phys. Rev.* **118**, 1417 (1960).
- ³⁰J. M. Luttinger, *Phys. Rev.* **119**, 1153 (1960).
- ³¹F. J. Ohkawa, *Phys. Rev. B* **59**, 8930 (1999).
- ³²J. E. Hirsch, *Phys. Rev. Lett.* **54**, 1317 (1985).
- ³³K. B. Lyons, P. A. Fleury, L. F. Schneemeyer, and J. V. Waszczak, *Phys. Rev. Lett.* **60**, 732 (1988).
- ³⁴F. J. Ohkawa, *Jpn. J. Appl. Phys., Part 2* **26**, L652 (1987).
- ³⁵F. J. Ohkawa, *J. Phys. Soc. Jpn.* **56**, 2267 (1987).
- ³⁶F. J. Ohkawa, *Phys. Rev. B* **70**, 184514 (2004).
- ³⁷C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik, *Phys. Rev. B* **67**, 014533 (2003).
- ³⁸M. Vershinin, S. Mirsa, S. Ono, Y. Abe, Y. Ando, and A. Yazdani, *Science* **303**, 1995 (2004).
- ³⁹T. Hanaguri, G. Lupien, Y. Kohsaka, D.-H. Lee, M. Azumas, M. Takano, H. Takagi, and J. C. Davis, *Nature (London)* **430**, 1001

- (2004).
- ⁴⁰N. Momono, A. Hashimoto, Y. Kobatake, M. Oda, and M. Ido, *J. Phys. Soc. Jpn.* **74**, 2400 (2005).
- ⁴¹K. 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).
- ⁴²S. A. Kiverson, I. P. Bindloss, E. Fradkin, V. Oganesyan, J. M. Tranquada, A. Kapitulnik, and C. Howald, *Rev. Mod. Phys.* **75**, 1201 (2003).
- ⁴³K. Takegahara, H. Harima, and A. Yanase, *Jpn. J. Appl. Phys., Part 2* **26**, L352 (1987).
- ⁴⁴N. Hamada, S. Massidda, A. J. Freeman, and J. Redinger, *Phys. Rev. B* **40**, 4442 (1989).
- ⁴⁵O. K. Andersen, O. Jepsen, A. I. Liechtenstein, and I. I. Mazin, *Phys. Rev. B* **49**, 4145 (1994).
- ⁴⁶F. C. Zhang and T. M. Rice, *Phys. Rev. B* **37**, R3759 (1988).
- ⁴⁷F. J. Ohkawa, *J. Phys. Soc. Jpn.* **74**, 3340 (2005).
- ⁴⁸J. C. Ward, *Phys. Rev.* **68**, 182 (1950).
- ⁴⁹See, for example, T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism*, Springer Series in Solid-State Sciences Vol. 56 (Springer-Verlag, Berlin, 1985).
- ⁵⁰N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**, 1133 (1966).
- ⁵¹F. J. Ohkawa, *Phys. Rev. B* **73**, 092506 (2006).
- ⁵²F. J. Ohkawa, *J. Phys. Soc. Jpn.* **67**, 535 (1998).
- ⁵³F. J. Ohkawa, *Phys. Rev. B* **66**, 014408 (2002).