Superconductivity and partial violation of spin correlation in electron stripes

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We examine the electronic state of the electron stripe which can be realized to stabilize local polarization mainly caused by the ion displacement in the *c* axis direction. In an undoped state, the electrons in the ground state are well localized to form a 2D electron-hole lattice with an antiferromagnetic (AF) order in the stripe direction. From the stability of the elementary excitation of the electron stripe, the lattice constant in the stripe direction, D_a, is restricted as 6 Å$\lesssim D_a \lesssim$8 Å. Upon doping carriers, when the AF state is partially violated due to the transfer (hopping) of the localized charges, the lower bound to D_a tends to be reduced to around 4 Å . Given the superconductivity (SC) mediated through the interaction with the elementary excitation of the electron stripe, the optimal transition temperature T_c can be written as $T_c \approx c/D_a^{5/2}$, where c is some structure-dependent constant. If the electron stripe exists in layered cuprates, where c is around 100 K$\cdot$(4 Å)$^{5/2}$, it is found that SC with T_c of order 100 K can be realized.

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I. INTRODUCTION

The interplay of the electron stripe, which has been observed on the CuO_2 plane in layered cuprates,[1–3] with high-T_c superconductivity (SC) has been extensively discussed.[4] The electron stripe, which is a 1D charge ordered state, frequently shows (fluctuating) antiferromagnetic (AF) correlation. From a theoretical point of view, the stripe formation has been examined, based mostly on the (extended) Hubbard model[5–10] or on the spin-fermion model.[11]

On the other hand, the electron stripe accompanies the ion displacement mainly in the *c* axis direction, due to the *c*-direction electric field generated by the electron stripe. Conversely speaking, the electron stripe can be realized to stabilize local polarization caused by the ion displacement,[12] provided that the chemical potential for the stripe formation should be less than about 1 eV.[13] A relevant work emphasizing the role of local polarization in the stripe formation has also been found in Ref. 14. Compared to the (extended) Hubbard model, the above stripe-polarization model has fewer parameters (essentially one parameter in the ground state) to be regarded as more simple to understand.

It seem natural to examine the possibility of high-T_c SC based on the stripe-polarization model. If we assume that SC can be realized through the interaction with the elementary excitation of the electron stripe, the optimal T_c can be written as $T_c \approx c/D_a^{5/2}$, where c and D_a represent some constant depending on the crystal structure and the electron lattice constant in the stripe direction, respectively.[15] From this relation, we are tempted to derive the lower bound to D_a so as to estimate the upper bound to T_c. Different from the lattice constant D_b perpendicular to the stripe direction, D_a is experimentally difficult to estimate, due to not only the smallness of the charge modulation but also the (partial) violation of the spin correlation.

The aim of this article is, based on the stripe-polarization model, to estimate the lower bound to D_a by examining the electronic state of the electron stripe. In an undoped state, the electron stripe shows an AF order in the stripe direction, with 6 Å$\lesssim D_a \lesssim$8 Å. Upon doping carriers, when the AF correlation should be partially violated due to the transfer (or hopping) of the localized charges along the stripe, the lower bound to D_a tends to be reduced to around 4 Å. If the electron stripe exists in layered cuprates, where $c \approx 100$ K $\cdot$(4 Å)$^{5/2}$, it is found that SC with T_c of order 100 K can be realized.

II. ELECTRON STRIPE

We begin with the model Hamiltonian H which is composed of three parts: the elastic energy due to the ion displacement in the *c* axis direction, the electron (hole) kinetic energy, and the Coulomb potential between the neutralization charges (electrons and holes) and the polarization charges $\sigma_i(x_1,x_2)$ caused by the ion displacement and between themselves, namely,[16]

$$H=\frac{1}{2}\sum_i \kappa_i \int [\sigma_i(x_1,x_2)]^2 dx_1 dx_2 - \frac{\hbar^2}{2m}\sum_{\alpha=\pm 1/2}\int \psi_\alpha^\dagger(\mathbf{x})\nabla^2\psi_\alpha(\mathbf{x})d^3\mathbf{x} + \frac{e^2}{2}\int :n^{(\mathrm{tot})}(\mathbf{x})U(\mathbf{x};\mathbf{x}')n^{(\mathrm{tot})}(\mathbf{x}'):d^3\mathbf{x}d^3\mathbf{x}', \quad (1)$$

where the summation over i extends to all ions within a single layer, $n^{(\mathrm{tot})}(\mathbf{x})=\Sigma_i\sigma_i(x_1,x_2)\delta(x_3)+\Sigma_\alpha\psi_\alpha^\dagger(\mathbf{x})\psi_\alpha(\mathbf{x})$, $U(\mathbf{x};\mathbf{x}')=1/|\mathbf{x}-\mathbf{x}'|$, and $\kappa_i=(k_i/e_i^2)(V^2/S)$ with k_i the *c*-direction force constant of the ith ion, e_i the effective charge, V the layer volume, and S the area of the CuO_2 plane.

By using the Slater determinant for the N-particle state and by eliminating $\sigma_i(x_1,x_2)$ from the stability condition of $\partial\langle H\rangle/\partial\sigma_i(x_1,x_2)=0$, the expectation value of H can be written as

$$\langle H\rangle=\sum_i \langle\varphi_i|\hat{K}|\varphi_i\rangle+\frac{1}{2}\sum_{i,j}[\langle\varphi_i|\hat{D}_{ij}|\varphi_j\rangle-\langle\varphi_i|\hat{E}_{ij}|\varphi_j\rangle], \quad (2)$$

where $\langle \mathbf{x}|\hat{K}|\mathbf{x}'\rangle = -\hbar^2/(2m)\cdot\delta(\mathbf{x}-\mathbf{x}')\nabla^2$, $\langle \mathbf{x}|\hat{D}_{ij}|\mathbf{x}'\rangle = e_i e_j \langle \mathbf{x}|\varphi_i\rangle[U(\mathbf{x}-\mathbf{x}') - (1-\gamma\partial_{|x_3|})^{-1}U(\mathbf{x}_+ - \mathbf{x}'_-)]\langle\varphi_j|\mathbf{x}'\rangle$, and $\langle \mathbf{x}|\hat{E}_{ij}|\mathbf{x}'\rangle = e_i e_j \langle \mathbf{x}|\varphi_j\rangle U(\mathbf{x}-\mathbf{x}')\langle\varphi_i|\mathbf{x}'\rangle$, with $\gamma^{-1} = 2\pi\Sigma_{i\in V}\kappa_i^{-1}$, $\partial_{|x_3|} = \partial/\partial|x_3|$, and $\mathbf{x}_\pm = (x_1, x_2, \pm|x_3|)$.

Assuming the translation invariance of the corresponding Hartree–Fock equation under $x_1 \to x_1 + D_a, x_2 \to x_2 + D_b$, we can obtain two states: an itinerant state and a well localized one. In general, the mixed phase of the itinerant and localized states cannot be allowed under the translation invariance of the Hartree–Fock equation. However, in the stripe configuration, where the localized electrons and holes are equal in number, the mixed phase is compatible with the translation invariance.[17] This can be understood by considering that the Coulomb interaction of the itinerant charge with the localized electron cancels out that with the localized hole. Here it should be noticed that not all the charge configurations such that the localized electrons and holes are equal in number can be realized. Consider, for example, the checkerboard configuration, where the localized electrons and holes are alternately aligned in the x_1 and x_2 axis directions. From the stability condition of $\partial\langle H^{(\mathrm{tot})}\rangle/\partial D_i = 0$ $(i=a,b)$, where $H^{(\mathrm{tot})} = H - \mu\Sigma_\alpha \psi_\alpha^\dagger \psi_\alpha$, with μ the chemical potential, it has been found that this configuration cannot be allowed.[17] This can be understood as follows. Rewriting the stability condition as $2E_0 = \Sigma_{i=a,b} D_i(\partial E_0/\partial D_i)$, where $E_0 = \langle H^{(\mathrm{tot})}\rangle/N$, with N the total lattice number, and using $E_0 = \text{const.} + a/D_a^3 + b/D_b^3 + (\text{higher order terms})$, where $a,b<0$ due to the attractiveness between the lattice, we find that $E_0 > 0$. This is inappropriate due to the positiveness of the total energy despite the magnitude of μ.

Thus in the following, we deal with only the stripe configuration. Since in the mixed phase the localized and the itinerant states can be treated independently, we concentrate on the electronic state of the localized charges. In the localized state (assuming half filling, for simplicity), it is natural that the localized electrons and holes should be oscillating around their equilibrium points. Adding the ion kinetic energy term to H, can obtain the wave number $\mathbf{q}$-dependence of the acoustic "phonon" ω of the 2D electron-hole lattice oscillation. From the stability of the acoustic phonon ($\omega^2 > 0$) for $D_a^2 \ll D_b^2$ [this condition is well satisfied in layered cuprates,[13] where D_a (D_b) is chosen as a lattice constant in the direction parallel (perpendicular) to the stripe], it is required that[15]

$$(0<)\,\epsilon < \delta < 3\epsilon, \tag{3}$$

where $\epsilon = (\langle x_2^2\rangle - \langle x_1^2\rangle)/\langle x_3^2\rangle$ and $\delta = [\langle x_1^2\rangle - \langle x_3^2\rangle - 2\gamma\langle|x_3|\rangle + O(\gamma^2)]/\langle x_3^2\rangle$, with $\langle x_n^2\rangle (n=1,2,3)$ the square of the spatial spread of the localized wave function in the x_n axis direction. If this condition were violated, the localized state in itself would be unstable.

In solving the condition of Eq. (3) to obtain the allowed region for (D_a, D_b), it should be noticed that the phonon energy ω for a typical value of $D_a \approx 5$ Å ($\lesssim D_b$) is around 0.03 K,[15] while the unit lattice energy $\langle H\rangle/N$ (N represents the total lattice number) is on the order of 1 eV.[13] Thus the values of a and b should be substantially equivalent to those obtained in the tight-binding limit. Furthermore for simplicity, we adopt the variational method instead of solving the corresponding Hartree–Fock equation directly.

If the electrons and holes are well localized, the trial function of $\langle \mathbf{x}|\varphi_i\rangle$ can be written using a Gaussian form as $\langle \mathbf{x}|\varphi_i\rangle \to \varphi(x_1 - i_1 D_a, x_2 - i_2 D_b, x_3)$, where $\varphi(\mathbf{x}) = \Pi_{n=1}^3 \phi_{\Delta_n}(x_n)$ with $\phi_{\Delta_n}(x_n) = \exp[-(x_n/2\Delta_n)^2]/\sqrt{(2\pi)^{1/2}\Delta_n}$. Here $\Delta_n (n=1,2,3)$ is a variational parameter to be derived from the stability condition of $\partial\langle H\rangle/\partial\Delta_n = 0$. In this case, the spin state of the (i_1, i_2)-site electron (or hole), denoted by $|\sigma_{i_1 i_2}\rangle$, is restricted from the orthogonality of $|\varphi_i\rangle$. For $2\Delta_1 (\approx 2\Delta_2) \sim D_a \ll D_b$, where the overlap of the wave function cannot be neglected in the stripe direction, it is required that $\langle \sigma_{\pm 1\,0}|\sigma_{0\,0}\rangle = 0$, which from the translation invariance indicates the antiferromagnetic (AF) configuration in the stripe direction.

Now we evaluate $\langle H\rangle$ in the AF state:

$$\langle H\rangle \to \langle H\rangle_{\mathrm{AF}} = N(K_{\mathrm{AF}} + D_{\mathrm{AF}} - E_{\mathrm{AF}}), \tag{4}$$

where K_{AF}, D_{AF}, and E_{AF} correspond to the terms proportional to $\hat{K}$, $\hat{D}_{ij}$, and $\hat{E}_{ij}$, respectively. Substituting the trial function into Eq. (2), we obtain $K_{\mathrm{AF}} = [\hbar^2/(8m)]\Sigma_{n=1}^3 (1/\Delta_n^2)$, and D_{AF} using the Poisson's summation formula: $\Sigma_n f(n) = \Sigma_n \int f(k)\exp(2\pi i k n)dk$ as $D_{\mathrm{AF}} = (e^2/2)\Sigma_{n,m}\mathcal{D}_{nm}$, where $\mathcal{D}_{nm}$ is given by (see Appendix)

$$\mathcal{D}_{nm} = \frac{2\pi}{D_a D_b}\frac{e^{[\alpha_n^2(\Delta_3^2-\Delta_1^2)+\beta_m^2(\Delta_3^2-\Delta_2^2)]}}{\gamma_{nm}} \times \left[\mathrm{erfc}(\gamma_{nm}\Delta_3) - \frac{1}{1+\gamma\gamma_{nm}}\mathrm{erfc}^2\left(\frac{\gamma_{nm}\Delta_3}{\sqrt{2}}\right)\right], \tag{5}$$

with $\alpha_n = 2\pi n/D_a$, $\beta_m = (1+2m)\pi/D_b$, and $\gamma_{nm} = \sqrt{\alpha_n^2 + \beta_m^2}$. Furthermore, we can evaluate E_{AF} as

$$\begin{aligned} E_{\mathrm{AF}} &= \frac{1}{2}\sum_{n,m}(-1)^m |\langle\sigma_{00}|\sigma_{nm}\rangle_{\mathrm{AF}}|^2 \mathcal{E}_{nm} \\ &\simeq \frac{1}{2}\sum_n |\langle\sigma_{00}|\sigma_{n0}\rangle_{\mathrm{AF}}|^2 \mathcal{E}_{n0} (\text{for } D_b \gg 2\Delta_2) \\ &= \frac{\sqrt{\pi}}{2}\frac{\Delta_1}{D_a}\mathcal{E}_{00}\sum_n (e^{-\alpha_n^2\Delta_1^2} + e^{-\alpha_{n+1/2}^2\Delta_1^2}), \end{aligned} \tag{6}$$

where $\mathcal{E}_{nm} = e^2\int \varphi^*(\mathbf{x})\varphi(\mathbf{x}-\mathbf{x}_{nm})U(\mathbf{x}-\mathbf{x}')\varphi(\mathbf{x}')\varphi^*(\mathbf{x}'-\mathbf{x}_{nm})$ with $\mathbf{x}_{nm} = (nD_a, mD_b)$. Here in the second equality, the spin correlation perpendicular to the stripe can be neglected due to $D_b \gg \Delta_2$; and in the third equality, use has been made of the AF configuration: $|\langle\sigma_{00}|\sigma_{n0}\rangle_{\mathrm{AF}}|^2 = \cos^2(\pi n/2)$, and the sum over n has been converted into momentum space using the Poisson's summation formula.

Before evaluating the stability condition of $\partial\langle H\rangle_{\mathrm{AF}}/\partial\Delta_i = 0$, we estimate the values of γ and D_b (while D_a is regarded as a parameter). Rewriting $V = lS$, we find that $2\pi\gamma = l^2 S_0/\Sigma_{i\in S_0}(e_i^2/k_i)$, where S_0 represents the unit CuO_2 plane, whose magnitude is around 14 Å^2. If we take l as half

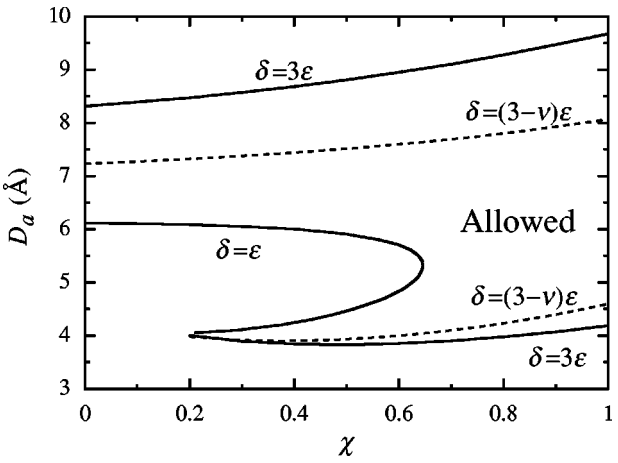

FIG. 1. Allowed region of D_a for $D_b=15$ Å. The area surrounded by the lines for $\delta=\epsilon$ and $\delta=3\epsilon$ guarantees the condition of $\omega^2>0$, while the area surrounded by the lines for $\delta=\epsilon$ and $\delta=(3-\nu)\epsilon$ guarantees $g>0$, where g, representing the superconducting coupling constant, is given by Eq. (15).

the distance between the Cu ion and its apical O ion, namely, $l\simeq(2.3/2)$ Å, γ can be estimated as $\gamma\approx 0.03$ Å for $e_{\mathrm{Cu}}\approx|e_{\mathrm{O}}|\approx 2e$ and $k_{\mathrm{Cu}}\approx k_{\mathrm{O}}\approx 50$ kdyne/cm.[18–20] The value of D_b, different from D_a, can be easily estimated using the period of the charge modulation in the direction perpendicular to the stripe direction. Considering that D_b corresponds to half the modulation period in the b-axis direction (in Bi-based cuprates, for example, the modulation period is around 30 Å),[21,22] we find that $D_b\approx 15$ Å.

From $\partial\langle H\rangle_{\mathrm{AF}}/\partial\Delta_i=0$, the condition of Eq. (3) (in this case, $\langle x_n^2\rangle_{\mathrm{AF}}=\Delta_n^2$ $(n=1,2,3)$ and $\langle|x_3|\rangle_{\mathrm{AF}}=\sqrt{2/\pi}\Delta_3$) indicates that for $D_b=15$ Å the allowed region for D_a is bound as 6 Å$\lesssim D_a\lesssim$8 Å (see Fig. 1 at $\chi=0$). The reason of the existence of the upper and lower bounds to D_a can be qualitatively understood as follows. As D_a increases as $D_a\gg 2\Delta_1$, with $D_b(\gg 2\Delta_2)$ fixed, the interlattice energy tends to be neglected. In this case, the wave function turns out to be isotropic on the ab plane, with the result of $\Delta_1\simeq\Delta_2$, namely, ϵ_{AF} $(=\epsilon$ with $\langle H\rangle\to\langle H\rangle_{\mathrm{AF}})$ tends to be vanishing, which would violate the condition of $\epsilon_{\mathrm{AF}}>0$ in Eq. (3) unless $\delta_{\mathrm{AF}}\to 0$. Considering that δ_{AF} remains positive in the limit of $D_a, D_b\gg 2\Delta_1$,[13] we find that there exists the upper bound to D_a. On the other hand, as D_a decreases, $\langle x_1^2\rangle_{\mathrm{AF}}$ tends to decrease due to the enhancement of repulsive force between the electrons in the stripe direction (while the D_a-dependence of $\langle x_2^2\rangle_{\mathrm{AF}}$ and $\langle x_3^2\rangle_{\mathrm{AF}}$ can be neglected compared to that of $\langle x_1^2\rangle_{\mathrm{AF}}$). Accordingly, ϵ_{AF} (δ_{AF}) tends to increase (decrease) to finally violate the condition of $\epsilon_{\mathrm{AF}}<\delta_{\mathrm{AF}}$. This is why there exists the lower bound to D_a.

However, the allowed region of D_a should be altered, if the AF state in the stripe direction is (partially) violated. On doping itinerant charges, it seems natural that the AF ground state should be excited by the itinerant charges. In this case, the AF correlation is (partially) violated due to the overlap of the wave function. The indistinguishability between the localized and itinerant charges implies that the partially violated AF state can be interpreted as being caused by the transfer (or hopping) of the localized charges, so that the following argument may be applied to layered cuprates. Before dealing with the partially violated AF state, we will examine the limiting state where the AF correlation in the stripe direction is completely violated and to be regarded as a paramagnetic (PM) state. In this case, the electronic state can be written as a superposition of the ground state and the excited state in the stripe direction, while it remains in its ground state in the other directions due to the negligibility of the overlap of the wave function. Then the trial function of $\varphi(\mathbf{x})$ should be modified as $\varphi(\mathbf{x})\to\varphi'(\mathbf{x})=\Pi_{n=1}^{3}\phi'_{\Delta_n}(x_n)$, where

$$\phi'_{\Delta_1}(x_1)=\left[\cos\zeta+\sin\zeta\cdot\left(\frac{x_1-\Delta D_a}{\Delta_1}\right)\right]\phi_{\Delta_1}(x_1-\Delta D_a), \tag{7}$$

and $\phi'_{\Delta_n}(x_n)=\phi_{\Delta_n}(x_n)$ for $n=2,3$. Here we have taken account of the first excited state of the harmonic oscillator in the stripe direction, and neglected the higher-order excited states. The parameter ΔD_a is conveniently introduced so as to satisfy $\langle x_1\rangle_{\mathrm{PM}}=0$, that is, $\Delta D_a/\Delta_1=-\sin 2\zeta$. Furthermore, the parameter ζ can be derived from the orthogonality condition of $\int\phi'^{*}_{\Delta_1}(x-nD_a)\phi'_{\Delta_1}(x)dx=0$ with $n=\pm 1$ as

$$\sin\zeta=2\frac{\Delta_1}{D_a}. \tag{8}$$

As far as $(2\Delta_1/D_a)^2\ll 1$, the orthogonality conditions for $n=\pm 2,\pm 3,\ldots$ can be automatically guaranteed, due to the negligibility of the overlap of the wave function.

Under the substitution of Eq. (7), $\langle H\rangle$ can be transformed as $\langle H\rangle\to\langle H\rangle_{\mathrm{PM}}=N(K_{\mathrm{PM}}+D_{\mathrm{PM}}-E_{\mathrm{PM}})$, where $K_{\mathrm{PM}}=K_{\mathrm{AF}}+\sin^2\zeta\cdot\hbar^2/(4m\Delta_1^2)$, and D_{PM} can be written as

$$D_{\mathrm{PM}}=\frac{e^2}{2}\sum_{n,m} f_n\mathcal{D}_{nm}, \tag{9}$$

with $f_n=(1-\sin^2\zeta\cdot\alpha_n^2\Delta_1^2)^2+\sin^2 2\zeta\cdot\alpha_n^2\Delta_1^2$. Furthermore, E_{PM} can be written by averaging the spin configuration as

$$E_{\mathrm{PM}}\simeq\frac{1}{4}\left(\mathcal{E}'_{00}+\sum_n\mathcal{E}'_{n0}\right)\quad(\text{for } D_b\gg 2\Delta_2), \tag{10}$$

where we have used the PM spin configuration as $|\langle\sigma_{00}|\sigma_{n0}\rangle_{\mathrm{PM}}|^2\to(1+\delta_{n0})/2$, and $\mathcal{E}'_{n0}$ corresponds to $\mathcal{E}_{n0}$ in which $\varphi(\mathbf{x})$ and $\varphi(\mathbf{x}')$ are replaced by $\varphi'(\mathbf{x})$ and $\varphi'(\mathbf{x}')$, respectively.

In the PM state, the expectation value of x_1^2 is evaluated from Eq. (7) as

$$\langle x_1^2\rangle_{\mathrm{PM}}=(1-2\sin^2\zeta+4\sin^4\zeta)\Delta_1^2, \tag{11}$$

so that Eq. (3) requires that under the stability condition of $\partial\langle H\rangle_{\mathrm{PM}}/\partial\Delta_n=0$ $(n=1,2,3)$, the allowed region of D_a should be given by 4 Å$\lesssim D_a\lesssim$10 Å (see Fig. 1 at $\chi=1$). From Fig. 1, it is found that the upper bound to D_a in the PM state is larger than that in the AF state. This can be understood by considering that for $D_a>2\sqrt{2}\Delta_1(\sim 5$ Å), namely, $\sin^2\zeta<1/2$, it is found from Eq. (11) that the relation of

$\langle x_1^2\rangle_{\rm PM}<\Delta_1^2$ is satisfied (while $\langle x_1^2\rangle_{\rm AF}=\Delta_1^2$), which implies that $\epsilon_{\rm PM}>\epsilon_{\rm AF}$ and $\delta_{\rm PM}<\delta_{\rm AF}$ for the same $\Delta_n(n=1,2,3)$. Thus the upper value of D_a such that $\delta_{\rm PM}=3\epsilon_{\rm PM}$ tends to be larger than that in the AF state. It is also found that for 4 Å$\lesssim D_a\lesssim$10 Å, the relation of $\epsilon_{\rm PM}<\delta_{\rm PM}$ is always satisfied; there is no region for D_a such that $\epsilon_{\rm PM}\geqslant\delta_{\rm PM}$. This can be understood as follows. As D_a decreases from 10 Å to 4 Å, Δ_1 tends to decrease due to the same reason as in the case of the AF state. Thus for $D_a\gtrsim 2\sqrt{2}\Delta_1(\sim 5$ Å), where $\langle x_1^2\rangle_{\rm PM}\lesssim\Delta_1^2$ is satisfied, $\epsilon_{\rm PM}$ ($\delta_{\rm PM}$) tends to increase (decrease), to approach the relation of $\epsilon_{\rm PM}=\delta_{\rm PM}$. However, as D_a decreases further so as to satisfy $D_a\lesssim 2\sqrt{2}\Delta_1$, $\epsilon_{\rm PM}$ ($\delta_{\rm PM}$) conversely tends to decrease (increase) despite the decrease of Δ_1, due to the relation of $\langle x_1^2\rangle_{\rm PM}>\Delta_1^2$, to finally violate the condition of $\delta_{\rm PM}<3\epsilon_{\rm PM}$ without reaching the relation of $\epsilon_{\rm PM}=\delta_{\rm PM}$.

We have examined two idealized electronic states: the AF and PM ones. In an actual situation, however, where the energy of the itinerant charges is not large enough, the AF correlation in the electron stripe cannot be completely violated due to the partial transfer of the localized charges. In this case, the electronic state is difficult to evaluate, because the spin correlation may fluctuate in space and time. Despite the difficulty, it may be convenient to assume that the intermediate state can be written as a mixture of the AF and PM states such that

$$\langle H\rangle_\chi=(1-\chi)\langle H\rangle_{\rm AF}+\chi\langle H\rangle_{\rm PM}\ \ (0<\chi<1). \tag{12}$$

This effective Hamiltonian is expected to well represent the qualitative behavior of the AF spin fluctuation caused by the transfer of the localized charges. In accordance with Eq. (12), the expectation value of x_1^2 can be parameterized in a similar way as $\langle x_1^2\rangle_\chi=(1-\chi)\langle x_1^2\rangle_{\rm AF}+\chi\langle x_1^2\rangle_{\rm PM}$. From the stability condition of $\partial\langle H\rangle_\chi/\partial\Delta_n=0$, the allowed region for D_a is schematically shown in Fig. 1. It is found from Fig. 1 that the lower bound to D_a for $\chi>0$ tends to be smaller than that for $\chi=0$. This is because as χ increases, ϵ tends to be smaller due to the increase of $\langle x_1^2\rangle_\chi$, so that D_a such that $\delta=\epsilon$ tends to be reduced.

III. SUPERCONDUCTIVITY

In this section, we estimate T_c by assuming that SC can be realized through the interaction of the doped itinerant charge with the acoustic phonon of the 2D electron-hole lattice oscillation.[15] To guarantee the strong coupling regime, we conveniently adopt the (simplified version of) McMillan theory, where T_c can be given by

$$T_c=\hbar\omega_{\rm D}f(g), \tag{13}$$

with $f(g)=1.13\exp[-(1+g)/(g-\Delta g)]$. Here $\Delta g(\sim 0.1)$ represents the (screened) Coulomb repulsion. In a mean field theory, the coupling constant g can be written on the analogy with the 3D electron-phonon interaction as[23]

$$g=\frac{\pi\hbar^2}{2m}\frac{1}{Mc^2}\frac{1}{D_aD_b}, \tag{14}$$

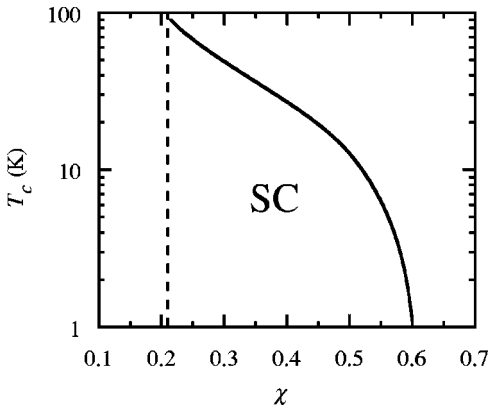

FIG. 2. χ-dependence of the critical temperature T_c for $D_a=4.05$ Å and $D_b=15$ Å, where c' is chosen as the value of layered cuprates.

where M represents the effective mass of the oscillator, and $1/c^2=(1/\Sigma_{\mathbf{q}})\Sigma_{\mathbf{q}}(q^2/\omega^2-0_+)$. Using an explicit expression for Mc^2, we can rewrite g as[15]

$$g=\frac{\pi}{3}\frac{a_{\rm B}D_a}{\langle x_3^2\rangle}\frac{\lambda h_\lambda(u)}{au(u+\lambda)}, \tag{15}$$

where $a_B[=\hbar^2/(me^2)]$ represents the Bohr radius, and $h_\lambda(u)=1+\lambda u(2-\lambda^2-\lambda u-u^2)$ with $\lambda=D_a/D_b$ and $u=\sqrt{1+b/a}$.

Under the condition of Eq. (3), it is found from Eq. (15) that g tends to diverge as u approaches 0, that is, the strong coupling regime can be realized for $\omega(\theta=0)\to 0$. The softening of ω in the stripe direction enhances the value of g, which is directly expected from the expression for $1/c^2$. As u increases, $h_\lambda(u)/[u(u+\lambda)]$ decreases monotonically and becomes negative for $u>u_0$, where $h_\lambda(u_0)=0$ with $u_0>0$. Thus the condition of $g>0$ (or $0<u<u_0$) requires that

$$\epsilon<\delta<(3-\nu)\epsilon, \tag{16}$$

where $\nu=8/(4+u_0^2)$. Note that $0<\nu<2$. For $D_b=15$ Å, we schematically show the allowed region for (χ,D_a) such that $g>0$, which is indeed inside the region such that $\omega^2>0$.

On the other hand, the magnitude of $\omega_{\rm D}$, which corresponds to the average of ω, is given by[15]

$$\hbar\omega_{\rm D}\approx c'/D_a^{5/2}, \tag{17}$$

where c' stands for some constant depending on the crystal structure [in layered cuprates, for example, $c'\approx 240$ K $\cdot(4$ Å$)^{5/2}$, so that c and c' are related to $c/c'=1.13e^{-1}$ in the strong coupling limit]. To obtain high T_c, we should take small D_a such that $g\gg 1$. If we tentatively choose D_a for $\delta=\epsilon$ as small as possible, that is, $D_a=4.05$ Å, at which $\chi=0.210$, then the χ-dependence of T_c can be estimated from Eqs. (13), (15), and (17), with the result schematically shown in Fig. 2, where c' has been chosen as the value of layered cuprates. Considering that χ tends to increase with increasing the carrier density n, we find that Fig. 2 indicates the n-dependence of T_c.

IV. DISCUSSION

Here we discuss, based on the stripe-polarization model, the validity of the realization of the electron stripe with $D_a \sim 5$ Å by considering the incommensurate spin fluctuation (ISF) observed in layered cuprates. In $La_{2-x}Sr_xCuO_4$ ($T_c = 37.5$ Å at $x=0.15$), ISF appears in the superconducting phase ($0.05 \lesssim x \lesssim 0.15$) with the incommensurate period λ_a around 5.4 Å,[24,25] which corresponds to about $\sqrt{2}$ times the crystal *a*-lattice constant. Assuming that λ_a corresponds to D_a, we find from Fig. 1 that for $D_a \approx 5.4$ Å (in this case, the maximum T_c can be estimated from the stripe-polarization model as 47 K, so that the actual magnitude of D_a may be slightly larger than 5.4 Å so as to accord with the observed T_c, which, however, is not crucial, because the reduction of T_c can be caused by the thermal phase fluctuation, typical of layered cuprates), the partially violated AF stripe can be realized in the superconducting phase. A similar ISF observed in underdoped $YBa_2Cu_3O_{6.6}$ (with the incommensurate period almost equal to that of LSCO[26]) can also be explained by using the stripe-polarization model. However, in optimally doped YBCO, where D_a can be estimated from T_c (≈ 90 K) as about 4.5 Å, ISF is difficult to observe, which can be understood by considering that (more than) half of the AF correlation is violated. The same may be true for optimally doped Bi- and Tl-based cuprates.

V. SUMMARY

We have obtained the allowed region for the lattice constant D_a of the electron stripe which is realized to stabilize local polarization caused by the ion displacement in the *c* axis direction. The lower bound to D_a is estimated as about 4 Å, where the AF correlation in the stripe direction should be partially violated, due to the transfer of the localized charges. Although the partially violated AF state is originally caused by the excitement by the doped itinerant charges, the indistinguishability between the localized and itinerant charges implies that the partially violated AF state can be interpreted as a state caused by the transfer (or hopping) of the localized charges. Given that the magnitude of D_a in general is incommensurate to the crystal lattice constant, it can be stated that the partially violated AF correlation corresponds to the incommensurate magnetic fluctuation, which has been observed in superconducting LSCO and YBCO. Assuming that the SC mediated through the interaction with the acoustic phonon of the electron stripe, where the optimal T_c can be written for layered cuprates as $T_c^{(\mathrm{opt})}(\mathrm{K}) \approx 100/[D_a(4\ \text{Å})]^{5/2}$, we find that SC with $T_c \approx 100$ K can be realized in the layered cuprate where the AF correlation is partially violated.

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APPENDIX: DERIVATION OF EQ. (5)

In the AF state, D_{AF} can be written as $D_{\mathrm{AF}} = (e^2/2)\Sigma_{n,m}\mathcal{D}_{nm}$, where

$$\mathcal{D}_{nm} = (-1)^m \int U_D(\mathbf{x};\mathbf{x}')|\varphi(\mathbf{x})|^2 |\varphi(\mathbf{x}'-\mathbf{x}_{n,m})|^2 \, d^3\mathbf{x} d^3\mathbf{x}', \tag{A1}$$

with $U_D(\mathbf{x};\mathbf{x}') = U(\mathbf{x};\mathbf{x}') - (1-\gamma\partial_{|x_3|})^{-1} U(\mathbf{x}_+;\mathbf{x}'_-)$, and $\mathbf{x}_{n,m} = (nD_a, mD_b, 0)$. Substituting the trial function of the Gaussian form into Eq. (A1) and using the Poisson's summation formula over *n* and *m*, we can replace $\mathcal{D}_{nm}$ as

$$\mathcal{D}_{nm} \to \frac{2\pi}{D_a D_b} \frac{e - (\alpha_n^2 \Delta_1^2 + \beta_m^2 \Delta_2^2)}{\gamma_{nm}} I_{nm}, \tag{A2}$$

where $\alpha_n = 2\pi n/D_a$, $\beta_m = (1+2m)\pi/D_b$, $\gamma_{nm} = \sqrt{\alpha_n^2 + \beta_m^2}$, and

$$\begin{aligned} I_{nm} &= \int_{-\infty}^{\infty} dx_3 \, dx_3' |\phi_{\Delta_3}(x_3)|^2 |\phi_{\Delta_3}(x_3')|^2 \\ &\quad \times \left[e^{-|x_3 - x_3'|\gamma_{nm}} - \frac{e^{-(|x_3|+|x_3'|)\gamma_{nm}}}{1+\gamma\gamma_{nm}} \right] \\ &= \int_{-\infty}^{\infty} dx_3 |\phi_{\sqrt{2}\Delta_3}(x_3)|^2 e^{-|x_3|\gamma_{nm}} \left[1 - 2\frac{\mathrm{erf}(|x_3|/2\Delta_3)}{1+\gamma\gamma_{nm}} \right]. \end{aligned} \tag{A3}$$

Using the integral formula:[27]

$$\int_0^{\infty} dx e^{-px-c^2x^2} \,\mathrm{erf}\,(cx) = \frac{\sqrt{\pi}}{4c} \exp\left(\frac{p^2}{4c^2}\right) \mathrm{erfc}^2\left(\frac{p}{2\sqrt{2}c}\right) \tag{A4}$$

for $|\arg c| < \pi/4$, we finally obtain Eq. (5).

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