Spin-Fluctuation-Driven Nematic Charge-Density-Wave in Cuprate Superconductors: Charge-Orbital-Spin Multimode Fluctuations Caused by Vertex Corrections

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We propose the mechanism of the nematic charge-density-wave (CDW) formation in cuprate superconductors, by investigating the vertex correction (VC) in the three-orbital $d$-$p$ Hubbard model. Due to the strong charge-spin interference given by the VC, the CDW instability at $q = (\Delta_{FS}, 0)$, $(0, \Delta_{FS})$ is strongly promoted near the magnetic critical point. Here, $\Delta_{FS}$ is the wavenumber connected by the neighboring hot spots. The obtained spin-fluctuation-driven CDW is described as the "intra-unit-cell orbital order" accompanied by the charge transfer between the neighboring atomic orbitals. The obtained nematic-type charge pattern is similar to the STM results. The CDW in cuprates has a close relation to the nematic orbital order in Fe-based superconductors.

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The rich phase diagram of cuprate high-$T_c$ superconductors has been actively discussed by many physicists. The non-Fermi-liquid-like electronic states near the optimally-doped region, including the under-doped (UD) region [5], in the nearly antiferromagnetic Fermi liquid picture [1–4], whereas strong-coupling theories were developed to describe the under-doped (UD) region [5]. In the pseudogap state of slightly UD cuprates, superconducting fluctuations play important roles [2, 4, 6–8]. However, many mysteries in the pseudogap region had been unsolved, such as the Fermi arc formation found by ARPES studies [9–12], nematic charge-density-wave (CDW) formation observed by STM studies [13–16], and small Fermi pockets detected by quantum oscillations [17].

The recent discovery of the CDW order in Y- [18–20], Bi- [21, 22], Hg- [23] and La- [24] based cuprates by X-ray scattering measurements provided a great breakthrough for solving the abovementioned mysteries of the pseudogap phenomena. All $p_x$, $p_y$, $d_{x^2-y^2}$ orbital electrons seem to contribute to the CDW formation [16, 21, 25]. This finding in the pseudogap region reveals that both spin and charge fluctuations intimately develop in cuprates. The intertwining of charge and spin order parameters had been discussed based on various models, such as $t$-$J$ type models and spin-fermion models [26–29]. The aim of this paper is to find the microscopic mechanism of the CDW and perform a quantitative analysis based on the realistic multiorbital Hubbard model for cuprates.

The wavevector of the CDW changes with doping, coinciding with the nesting vector between the neighboring hot-spots (see Fig. 1 (b)) in Y-, Bi- and Hg-based cuprates [19–23]. However, this nesting is not very relevant, so the antiferromagnetic state without any charge modulation is obtained if the mean-field-level approximations (like the RPA) are applied to the Hubbard models with realistic parameters. For this reason, the vertex correction (VC), which may be dropped or underestimated in the mean-field-level approximations, must be taken into account in the present study [30–34].

Other than cuprates, the nematic states are realized by systems near the magnetic quantum-critical-point (QCP). In Fe-pnictides, spin-nematic mechanism [35] and orbital-nematic one [30, 34, 36, 37] have been discussed intensively. In both scenarios, spin-fluctuation-driven nematicity is discussed. In the latter mechanism, the orbital-order is induced by the VC near the magnetic QCP, and this scenario is applicable even when the spin fluctuations are incommensurate, like Sr$_x$Ru$_2$O$_{4.2}$ [31, 32] and Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ with $x \geq 0.056$ ($T_N \leq 30K$). In cuprates, the VC will develop for both $d$ and $p$ orbitals since both orbitals largely contribute to the density-of-states (DOS) at the Fermi level. Thus, the multiorbital CDW order in cuprates could be explained by applying the orbital-spin mode-coupling theories [30–34, 37].

In this paper, we investigate the $d$-$p$ Hubbard model with repulsive Coulomb interactions. The charge-spin interference due to Aslamazov-Larkin (AL) type VC becomes significant near the magnetic QCP. For this reason, the CDW instability at wavevectors $q = (\Delta_{FS}, 0)$ and $(0, \Delta_{FS})$, connected by the neighboring hot-spots, is promoted by the VC. The realized nematic CDW state with inter-orbital charge transfer is consistent with the STM measurements [13–16]. Also, the Fermi arc structure and small Fermi pockets will be formed by the Brillouin zone folding [38, 39]. The strong charge-orbital-spin mode-coupling due to VC gives the multimode fluctuations, which will be ubiquitous in strongly correlated systems.

Figure 1 (a) shows the three-orbital $d$-$p$ model for cuprates in real space. The nearest $d$-$p$, $d$-$d$, and $p$-$p$ hopping integrals are shown as $t_{dp}$, $t_{dd}$, and $t_{pp}$, respectively. We use the hopping integrals of the first-principles model for La$_2$CuO$_4$ listed in Table 2 ($N = 0$) of Ref. [40], in which the 2nd-nearest ($t'_{dp}$, $t'_{pp}$) and the 3rd-nearest ($t''_{pp}$) hopping integrals exist. In addition, we include the 3rd-nearest $d$-$d$ hopping $t_{dd}^{3rd} = -0.1eV$ to make the Fermi surface (FS) closer to Y- and Bi-based cuprates. The obtained hole-like FS for the electron fill-
ing $n = n_d + n_p = 4.9$ (hole filling is $x = 0.1$) is shown in Fig. 1 (b). We also introduce the on-site Coulomb interactions ($U_d$, $U_p$) and the nearest $d$-$p$ Coulomb interaction ($V$) shown in Fig. 1 (a). According to the first principle studies [41], $U_d \sim 8$eV, $U_p \sim 3$eV and $V \gtrsim 1$eV. Hereafter, the unit of energy is eV unless otherwise noted.

Before analyzing the $d$-$p$ Hubbard model, we study the single $d$-orbital Hubbard model to demonstrate why the GV gives the CDW. The conduction band of the $d$-$p$ model is well fitted by the dispersion of the single $d$-orbital model, $e_k = 2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y + 2t''(\cos 2k_x + \cos 2k_y)$, by putting $t = -0.5$, $t'/t = -1/6$ and $t''/t = 1/5$ [4]. In the random-phase-approximation (RPA) without the VC, the spin (charge) susceptibility is given as $\chi_{\text{RPA}}(q) = \chi^{(0)}(q)/(1 + \Delta U \chi^{(0)}(q))$: $U$ is the on-site Coulomb interaction, $\chi^{(0)}(q) = -T \sum_k G(k+q)G(k)$ is the bare bubble, and $G(k) = (\epsilon_n + \mu - e_k)^{-1}$. Here and hereafter, $q \equiv (q_x, \omega)$ and $k \equiv (k_x, \epsilon_n)$, where $\omega = 2\pi T$ and $\epsilon_n = (2n+1)\pi T$. Figure 1 (c) shows $\chi_{\text{RPA}}(q) = \chi_{\text{RPA}}(q,0)$ for $U = 1.65$, $x = 0.1$ and $T = 0.025$. The spin Stoner factor $\alpha_S \equiv \max_{q}(U \chi^{(0)}(q))$ is 0.99. In contrast, $\chi^{c}(q)$ is suppressed by $U$ within the RPA.

Next, we discuss the charge susceptibility beyond the RPA by taking the VC into account. It is given as

$$\chi^{c}(q) = \Phi^{c}(q)/(1 + U \Phi^{c}(q)), \tag{1}$$

where $\Phi^{c}(q) = \chi^{(0)}(q) + X^{c}(q)$, and $X^{c}(q)$ is the irreducible VC for the charge sector. Here, we consider the AL-type VC, which is the second-order term with respect to the fluctuations, since it is scaled by the square of the magnetic correlation length $\xi_{\text{AF}} \sim 1/(1 - \alpha_S)$ in two-dimensional systems [30, 42]. (In contrast, the Maki-Thompson type VC, given by the first-order term with respect to the fluctuations, is regular near the QCP [31, 32].) Thus, the AL-type VC gives the nematic orbital order in Fe-based superconductors and Sr$_2$RuO$_7$ near the magnetic QCP [30, 32]. The expression of the AL-type VC is given in Ref. [30], which is simplified in the $d$-orbital Hubbard model [42] at $\omega_l = 0$ as follows:

$$X^{c}(q) = \frac{2U^4}{2} \sum_p \Lambda(q;p) (\chi^{c}(p+q/2)\chi^{c}(p-q/2))$$

$$+ 3 \chi^{(0)}(q)\chi^{c}(p-q/2)\Lambda(q;p), \tag{2}$$

$$\Lambda(q;p) = T \sum_k G(k+q/2)G(k-q/2)G(k-p), \tag{3}$$

where $p = (p_x, \omega_m)$, and $\Lambda(q;p) = \Lambda(q;p) + \Lambda(q;-p)$. The AL-type VC is important in strongly correlated systems since it is proportional to $U^4$. The dominance of the AL-type VC in $\chi^{c}$ and the validity of the SC-VC theory [30] are recently verified by applying the functional RG method [32, 33]. In the SC-VC method [30], we calculate both $\chi_{\text{RPA}}^{c,s}$ and $X_{\text{RPA}}^{c,s}$ self-consistently. In the present model, however, we verified that the positive feedback effect from $\chi^{c}$ to $X^{c}$, which is important in Fe-pnictides [30], is very small. Also, we can neglect the VC for the spin channel since it is less important as verified in Refs. [30–32]. Thus, we can safely replace $\chi_{\text{RPA}}^{c,s}$ in Eq. (2) with $\chi_{\text{RPA}}^{s,c}$ in the present study.

Figure 1 (d) shows the obtained $X^{c}(q)$ for $U = 1.65$ ($\alpha_S = 0.99$), which shows the maximum at $Q_c = (\delta_x, 0)$ and $Q'_c = (0, \delta_x)$, and the relation $\delta_x \approx 0.08$. The CDW instability will be caused by the large $X^{c}(Q_c)$, which is much larger than $\max_{q} \chi^{(0)}(q) \approx 0.6$. Here, the $q$-dependence of $X^{c}(q)$ is mainly given by the three-point vertex. To show this, we approximate the AL-type VC for $\alpha_S \lesssim 1$ as

$$X^{c}(q) \sim U^4|\Lambda(q;Q_s)|^2 C^{s}(q), \tag{4}$$

where $Q_s = (\pi, \pi)$ and $C^{s}(q) \equiv T \sum_p \chi_{\text{RPA}}^{s,c}(p+q/2)\chi_{\text{RPA}}^{s,c}(p-q/2)$. Figure 1 (e) shows the $q$-dependences of $|\Lambda(q;Q_s)|^2$ and $C^{s}(q)$ along the $q_x$-axis. Thus, the large peak of $X^{c}(q)$ at $q = (\delta_x, 0)$ originates from the three-point vertex. In fact, the integrand of Eq. (3) is large in magnitude when $k + q/2, k - q/2, k - Q_s$ are on the FS and connected by the nesting vector. For this reason, $|\Lambda(q;Q_s)|^2$ takes the maximum value when
$q \approx (\Delta_{FS},0)$, because of the nesting between the hot spots shown in Fig. 1 (b).

Although the charge VC becomes very large near the magnetic QCP, $\chi(q)$ in Eq. (1) cannot exceed $1/U$. In real compounds, however, strong attractive interaction $-g(q)$ due to the buckling mode with $q \sim Q_c$ had been predicted by the first principle study [43]. In this case, $U$ in Eq. (1) is replaced with $U-2g(q)$, and then $\chi^c(Q_c)$ can be strongly enlarged if $U-2g(Q_c)$ is negative. In Fig. 1 (f), we show the strong developed $\chi^c(q)$ obtained for $U = 1.65$ and $g(q) = 1.16$. Below, we show that the CDW due to the VC is much easily realized in the three-orbital $d$-$p$ model with degenerate $p_x$ and $p_y$ orbitals, without introducing $e$-$p$ interactions.

In the next stage, we study the three-orbital $d$-$p$ model, and derive the CDW without introducing $e$-$p$ interactions. We denote $(c_1(k), c_2(k), c_3(k)) \equiv (d_{x^2-r^2}(k), p_x(k), p_y(k))$. Here, we consider $U_d$, $U_p$, and $V$ shown in Fig. 1 (a). In case of $U_d = 4.06$ and $U_p = 0$ for $n = 4.9$ and $T = 0.05$ ($\alpha_S = 0.99$), the obtained $\chi_d^{RPA}(q)$ for $d$ orbital is similar to that for the single $d$-orbital model in Fig. 1 (c) in appearance, and $\max_q(\chi_d^{RPA}(q)) \approx 25$. In cuprates, the $p$-orbital DOS is large at the Fermi level although it is smaller than the $d$-orbital DOS [44]. For this reason, due to the large $\chi_d^{RPA}(q)$, both $d$ orbital and $p$ orbital AL-type VCs are strongly enhanced near the magnetic QCP. The expression of the VC in multiorbital models, $\tilde{X}^c(q)$, is given in Ref. [30]. For $U_d = 4.06$, the obtained $X_g^c(q) \equiv X_{g,1;1}^c(q)$ is as large as the VC in the single-orbital model shown in Fig. 1 (d). Also, $X_{g,x}^c(q) \equiv X_{3,3;2}^c(q)$ is shown in Fig. 2, (a), which is about one-third of $X_g^c(q)$ in magnitude, and it has the peak at $Q_c = (\delta_x, 0)$ ($Q'_c = (0, \delta_y)$) since the $p_y$ ($p_x$) orbital has large weight around $Y$ ($X$) point. In the presence of the VC's, the charge susceptibility with respect to $n_{py}(q)$ and $n_{px}(q)$, is given by the $3 \times 3$ matrix form:

$$\chi^c(q) = \hat{\Phi}^c(q)\{1 - \tilde{\Gamma}^c(q)\hat{\Phi}^c(q)^{-1}\},\quad (5)$$

where $\hat{\Phi}^c(q) = \chi^{(0)}(q) + \tilde{X}^c(q)$. $\xi_{m,m'}^{(0)}(q) = -T \sum_k G_{m,m'}(k+q)G_{m',m}(k)$, and $\tilde{X}^c(q)$ is the bare Coulomb interaction matrix for the charge sector, which is given as $\Gamma_{1,1} = -U_d, \Gamma_{2,2} = \Gamma_{3,3} = -U_p, \Gamma_{1,2} = -2V \cdot 2 \cos(q_x/2)$ and $\Gamma_{1,3} = -2V \cdot 2 \cos(q_y/2)$.

Due to large VC near the magnetic QCP, the charge susceptibilities are strongly enhanced without introducing $e$-$p$ interactions. In Figs. 2 (b)-(d), we show the largest three susceptibilities, $\chi_d^{c}(q) \equiv \chi_{1;1}^{c}(q)$, $\chi_{2;1}^{c}(q) \equiv \chi_{2;2}^{c}(3,3;2)(q)$, and $\chi_{d,x,y}^{c}(q) \equiv \chi_{d,x,y}^{c,2}(1,1;1)(q)$ at $n = 4.9$, in the case of $U_d = 4.06$ ($\alpha_S = 0.99$). Also, we put $V = 0.65$ to achieve the charge Stoner factor $\alpha_C = 0.99$. Both $\chi_d^{c}$ and $\chi_y^{c}$ show large positive values at $q = Q_c$, whereas $\chi_{d,x}^{c}$ develops negatively. Thus, $(d, p_y)$ orbitals form the "antiphase CDW state" at $q = Q_c$, and two possible charge distribution patterns for $Q_c = (\pi/2, 0)$ are shown in Figs. 2 (c) and (f). The intra-unit-cell nematic charge order in (e) looks similar to the recent STM results [13, 14, 16]. (The correlations between $p_2$ orbital and others are weak in the $Q_c = (\delta_x, 0)$ CDW. However, the antiphase CDW with respect to the nearest ($n_x, n_y$) develop if we introduce small Coulomb interaction $V_{p_2,p_2}$. Moreover, the Fermi arc structure found by ARPES [9-12] would be formed by the single-Q or double-Q CDW order [38, 39]. Note that the Fermi arc structure similar to cuprates was recently reported in Sr$_2$IrO$_4$ [45].

Here, we discuss the reason why the CDW state due to AL-type VC can be realized in the $d$-$p$ model for $V > 0$, without including the $e$-$p$ interactions. To discuss the charge susceptibilities at $q = Q_c$, we consider only $\Phi^c_d = \Phi^c_{1;1}$ and $\Phi^c_y = \Phi^c_{3;3}$ in Eq. (5) to simplify the discussion. For $U_p = 0$, the obtained results at $q \approx Q_c$ are

$$\chi_d^{c}(q) = \Phi_d^{c}(q)/D(q),\quad (6)$$

and

$$\chi_y^{c}(q) = \Phi_y^{c}(q)\{1 + U_d \Phi_d^{c}(q)/D(q)\},\quad (7)$$

where $D(q) = 1 + \Phi_d^{c}(q), \Phi_y^{c}(q) = -4V \Phi_y^{c}(q) \cdot \chi_d^{c}(q)$, and $\Phi_y^{c}(q) \equiv \Phi^c_y(Q_c)$. Near the magnetic QCP, $\Phi_y^{c}(Q_c) \gg 1$ is expected due to the VC. Then, the enhancement of charge susceptibilities in Fig. 2 (b)-(d) are realized when $\Phi_y^{c}(Q_c) > U_d/16V^2$. This condition will be satisfied near the magnetic QCP, because of the relation $U_d/16V^2 \ll 1$ in the first principle study [41].

In the RPA without the VC, $\tilde{\chi}^c(q)$ diverges when $V$ is larger than 2.7, which exceeds the double of $V$ given
by the first principle studies. Worse still, the divergence occurs at $q = 0$ in the present model. Thus, the VC is indispensable to realizing the stripe CDW state. Note that the RPA analysis on a $d$-$p$ model with $V_{d-p}$ was performed in Ref. [46].

In our theory, the CDW originates from purely repulsive interactions, and the $e$-$ph$ interaction is unnecessary. In real compounds, the Coulomb interaction driven CDW fluctuations couple to the lattice due to finite e-phonon interactions, and Kohn anomaly will be induced. [43, 47, 48].

Finally, we discuss the close relation between the CDW in cuprates and the nematic orbital order in Fe-pnictides. In both systems, the charge-spin interference, which is given in the AL-type VC, causes the inter-orbital charge transfer near the magnetic QCP [30, 34]. In Fe-pnictides, both $q = 0$ and $q \neq 0$ 3d-orbital orders/fluctuations have been discussed intensively [26, 30, 34, 49], and both fluctuations will contribute to the superconductivity.

In summary, we found that the spin-fluctuation-driven CDW occurs in cuprates, due to the charge-spin interference given by the AL-type VCs. Both spin fluctuations at $Q_s \approx (\pi, \pi)$ and orbital-antiphase charge fluctuations at $Q_c \approx (\Delta_{FS}, 0), Q_c' \approx (0, \Delta_{FS})$ mutually develop. We predict that the charge-orbital-spin “multimode fluctuations” emerge ubiquitously in cuprates, Fe-pnictides, and other strongly correlated electron systems, caused by the multimode-coupling by AL-type VCs.

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FIG. 3: (color online) (a) $\delta_s$, $\delta_c$, and $\Delta_{FS}$ obtained in the $d$-$p$ model as functions of $x = 5 - n$. (Inset) The values of $V$ required to give the CDW. (b) The values of $V_{CDW}^{-1}$ as a function of $x$, which will depict a qualitative behavior of $T_{CDW}$. Note that $Q_s$ shifts to 0 for $x \leq 0.02$. (Inset) $\alpha_S(x)$ (i)-(iii) are shown. (c) Schematic phase diagram of cuprates.

Now, we study the hole carrier ($x = 5 - n$) dependence of the CDW state. Figure 3 (a) shows the obtained $\delta_s$, $\delta_c$, and $\Delta_{FS}$ for $U_p = 0$, by choosing $U_d$ and $V$ so as to satisfy $\alpha_S = \alpha_C = 0.99$. The inset of (a) shows the obtained $V$, which is much smaller than the first principle value of $V$ even for $U_p = 2$. We find that $\delta_s$ increases as $x \rightarrow 0$, with satisfying the relation $\delta_s \approx \Delta_{FS}$. These results are observed in Y-, Bi- and Hg-based compounds [19–23]. On the contrary, $\delta_s$ decreases for $x \rightarrow 0$, as observed by neutron scattering studies.

In La-based compounds, the relation $\delta_c \approx 2\delta_s(\approx x)$ is satisfied [24], differently from other compounds. In principle, this relation could be explained by the present spin-fluctuation-driven CDW, if $C^\alpha(q)$ shows a peak at $2Q_s = (2\delta_s, 0), (0, 2\delta_s)$, which could be realized if $\chi^\alpha(q)$ shows prominent incommensurate peaks as discussed in Ref. [33]. It is our future problem to explain the relation $\delta_c \approx 2\delta_s$ in La-based compounds by constructing a realistic tight-binding model.

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