Multistage Electronic Nematic Transitions in Cuprate Superconductors:
Functional-Renormalization-Group Analysis

Masahisa Tsuchiizu, Kouki Kawaguchi, Youichi Yamakawa, and Hiroshi Kontani
Department of Physics, Nagoya University, Nagoya 464-8602, Japan
(Dated: May 16, 2017)

Recently, complex phase transitions accompanied by the rotational symmetry breaking have been discovered experimentally in cuprate superconductors. To find the realized order parameters, we study various charge susceptibilities in an unbiased way, by applying the functional-renormalization-group method to the realistic $d$-$p$ Hubbard model. Without assuming the wavevector of the order parameter, we reveal that the most dominant instability is the uniform ($q = 0$) charge modulation on the $p_x$ and $p_y$ orbitals, which possesses the $d$-symmetry. This uniform nematic order triggers another nematic $p$-orbital density wave along the axial (Cu-Cu) direction at $Q_a \approx (\pi/2, 0)$. It is predicted that uniform nematic order is driven by the spin fluctuations in the pseudogap region, and another nematic density-wave order at $q = Q_a$ is triggered by the uniform order. The predicted multistage nematic transitions are caused by the Aslamazov-Larkin-type fluctuation-exchange processes.

PACS numbers: 74.72.Kf, 74.20.-z, 74.40.Kb, 75.25.Dk

In the normal state of high-$T_c$ cuprate superconductors, interesting unconventional order parameters emerge due to the strong interference among the spin, charge, and orbital degrees of freedom. These phenomena should be directly related to the fundamental electronic states in the pseudogap region. The emergence of the charge-density-wave (CDW) states inside the pseudogap region has been confirmed by the x-ray and STM measurements [1–6], as schematically shown in Fig. 1 (a). The observed CDW pattern is shown in Fig. 1 (b), in which the density modulations mainly occur on the oxygen $p_x$ and $p_y$ orbitals with antiphase ($d$-symmetry) form factor. The discovery of the CDW has promoted significant progress in the theoretical studies, such as the spin-fluctuation-driven density-wave scenarios [7–14] and the superconducting-fluctuation scenarios [15–18].

The origin and nature of the pseudogap phase below $T^*$ remain unsolved. For example, it is unclear whether the pseudogap is a distinct phase or a continuous crossover. The short-range spin-fluctuations at $T \sim T^*$ induce the large quasiparticle damping [19–21], which causes the pseudogap in the density-of-states. On the other hand, the phase transition around $T^*$ have been reported by the resonant ultrasound spectroscopy [22], ARPES analysis [23], and magnetic torque measurement [24]. Especially, Ref. [24] discovered the $C_4$ symmetry breaking (nematic) transition, and its natural candidate is the uniform CDW with $d$-symmetry schematically shown in Fig. 1 (c). Then, a fundamental question is what mechanism can account for such unconventional multistage CDW transitions. No CDW instabilities are given by the mean-field-level approximations, like the random-phase-approximation (RPA), unless large inter-site interactions are introduced [13, 25]. Therefore, higher-order many body effects, called the vertex corrections (VCs), should be essential for the CDW formation [7–13, 26].

In many spin-fluctuation-driven CDW scenarios, the CDW wavevector is given by the minor nesting vector $Q_a$ or $Q_d$ in Fig. 1 (d); $Q_a$ is the “axial-wavevector” parallel to the nearest Cu-Cu direction, and $Q_d$ is the “diagonal-wavevector”. The experimental axial CDW is obtained if the Aslamazov-Larkin VCs (AL-VCs) are taken into account [13]. In addition, the uniform ($q = 0$) CDW instability has been studied intensively based on the Hubbard models [9, 27–29]. In these studies, however, it was difficult to exclude the possibility that the CDW susceptibility has the maximum at finite $q$.

In many spin-fluctuation-driven CDW scenarios, the...
Theoretically, it is difficult to analyze the spin and charge susceptibilities with general wavevector \( q \) on equal footing, by including the VCs in an unbiased way. For this purpose, in principle, the functional renormalization-group (fRG) method would be the best theoretical method. The pioneering fRG studies \([9, 28, 30]\) were performed only in the weak-coupling region, where the obtained CDW instability is small and its \( q \)-dependence is not clear. In order to overcome this problem, we have to improve the numerical accuracy of the fRG method, and apply it to the two-dimensional Hubbard model in the strong-coupling region.

In this paper, we study the orbital-dependent spin and charge susceptibilities for various symmetries on equal footing, by analyzing the higher-order VCs in an unbiased way using the improved fRG method. We find that the uniform CDW accompanied by the antiferro spin fluctuations. This uniform nematic CDW enhances another nematic CDW instability at the wavevector \( q = Q_a \) shown in Fig. 1 (b). The present study indicates that the uniform \( p \)-orbital \( cCDW \) is induced at \( T_{CDW} < T^* \). These multistage CDW transitions in under-doped cuprates originate from the pseudogap region, and the axial \( q = Q_a \) CDW appears in the pseudogap region, and the axial \( q = Q_a \) CDW.

In the present study, we use the functional RG + constrained RPA (RG+cRPA) method. The advantage of this method had been explained in Refs. \([30, 32–34]\). Using the RPA, the higher-energy processes are calculated accurately by dropping the VCs, which are less important for higher-energy processes. The lower-energy scattering processes for \( |E_{k,\nu}| < \Lambda_0 \) are calculated by solving the RG equations, based on the \( N_p \)-patch RG scheme \([27, 35]\). Hereafter, we put \( N_p = 128 \) and \( \Lambda_0 = 0.5 \) eV. In the RG+cRPA method, the numerical accuracy of the susceptibilities is greatly improved even in the weak-coupling region since the cRPA is used for the higher-energy processes, for which the \( N_p \)-patch RG scheme is less accurate. We verified that the numerical results are essentially independent of the choice of \( \Lambda_0 \) when \( E_F \gtrsim \Lambda_0 \gg T \).

By solving the RG equations, many-body vertices are gradually renormalized as reducing the energy scale \( \Lambda_i = \Lambda_{i-1} e^{-l} \) with increasing \( l \) (\( \geq 0 \)). In principle, the renormalization of the vertex saturates when \( \Lambda_i \) reaches \( \sim T \) \([35, 36]\). Here, we introduce the lower-energy cutoff \( \Lambda_{low} \) \(( \sim T \)) in the RG equation for the four-point vertex \( \Gamma_l^{(c)} \), and stop the renormalization at \( \Lambda_i = \Lambda_{low} \); see the Supplemental Material (SM): A \([37]\) and Ref. \([9]\).

We find that the numerical accuracy and stability are improved by employing the Wick-ordered scheme of the fRG formalism, in which the cutoff function \( \Theta^{\Lambda}(e) = \Theta(\Lambda - |e|) \) is used for the Green function \([35]\). In this scheme, in principle, the VCs due to higher-energy processes are included more accurately, compared to using another cutoff function \( \Theta^{\Lambda}(e) = \Theta(|e| - \Lambda) \) based on the Kadanoff-Wilson scheme used in Ref. \([30]\).

In Figs. 2 (a) and (b), we show the \( p \)-O-CDW susceptibility \( \chi_p^{\text{orb}}(q) \) given by the RG+cRPA method for \( U = 4.32 \) eV at \( T = 0.1 \) eV. The obtained large peaks at \( q = 0 \), \( Q_a \), and \( Q_d \) originate from the VCs, since
the RPA result is less singular as seen in Fig. 2 (b). As shown in Figs. 2 (a)-(c), the most dominant peak locates at $q = 0$. This is consistent with the experimental uniform nematic transition at $T^* (> T_{CDW})$ [24]. We also obtain the peak structures at $q = Q_d$ and $Q_a$, consistently with our previous fRG study [30]. Figure 2 (c) shows that $\chi_d^{p\text{-orb}}(0)$ monotonically increase with decreasing $T$, consistently with the recent electronic nematic susceptibility measurement [38]. At low temperatures, $\chi_d^{p\text{-orb}}(Q_a)$ increases steeply and becomes larger than $\chi_d^{p\text{-orb}}(Q_d)$. Note that the temperature $T = 0.1$ eV is comparable to $T^* \sim 300$ K if the mass-enhancement factor $m^*/m_{\text{band}} \sim 3$ is taken into account.

The enhancement of $\chi_d^{p\text{-orb}}(q)$ is caused by the spin fluctuations, due to the strong charge-spin interplay given by the VCs. The moderate peak at $Q_d$ is caused by the Maki-Thompson (MT)-VCs, given by the series of the single-fluctuation-exchange processes shown in Fig. 2 (d) [11, 12]. However, the MT-VCs cannot account for the dominant peaks at $q = 0$ and $Q_a$. Recently, it was found that the uniform nematic order in the Fe-based superconductors [26, 39] and Sr$_3$Ru$_2$O$_7$ [32, 40] is driven by the AL-VC, given by the series of the double-fluctuation-exchange processes shown in Fig. 2 (e). In fact, the first term in Fig. 2 (e) is proportional to $\sum_k \chi_{\text{spin}}(k+q)\chi_{\text{spin}}(k)$, which takes large value for $q = 0$ when $\chi_{\text{spin}}^{\text{max}} \gg 1$ [26, 41]. Later, we will demonstrate that the AL-VC causes the uniform and axial CDW instabilities in the present $d$-$p$ model.

Next, we investigate the $U$-dependences of the susceptibilities. In the inset of Fig. 3 (a), we show the $U$ dependence of $\chi_{\text{spin}}^{\text{max}} \equiv \max_q \{\chi_{\text{spin}}^{\text{spin}}(q)\}$. Thanks to the numerical accuracy of the RG+cRPA method, $\chi_{\text{spin}}^{\text{max}}$ perfectly follows the RPA result for wide weak-coupling region ($U < 4$ eV). To clarify the close interplay between spin and orbital fluctuations, we plot the peak values of $\chi_d^{p\text{-orb}}(q)$ as a function of $\chi_{\text{spin}}^{\text{max}}$ in Fig. 3 (a). In contrast to $\chi_{\text{spin}}^{\text{spin}}$, $\chi_d^{p\text{-orb}}(q)$ strongly deviates from the RPA result, indicating the significance of the VCs. With increasing $U$, the peak position of $\chi_d^{p\text{-orb}}(q)$ shifts to $q = 0$ at $\chi_{\text{spin}}^{\text{max}} \sim 2.5$, and $\chi_d^{p\text{-orb}}(0)$ exceeds the spin susceptibility for $\chi_{\text{spin}}^{\text{spin}} \sim 10$ eV$^{-1}$.

To understand the origin of the enhancement of $\chi_d^{p\text{-orb}}(q)$, we analyze the scaling flow of the effective four-point vertices for the pO-CDW with $d$ symmetry, for $U = 4.32$ eV at $T = 0.1$ eV. $l (\geq 0)$ is the scaling parameter. The scaling flows for spin channel is also shown where $Q_a$ is the nesting vector $\approx (\pi, 0.78\pi)$ or $(0.78\pi, \pi)$. (c) The optimized form factor $f_{q-a}(k)$ on the FS, which has the $d$-symmetry.
interaction for the p-O-CDW introduced as $\Gamma_{\text{p-orb}}^{\text{orb}}(q) \equiv \Gamma_{\text{spin}}^{\text{spin}}(q) + \Gamma_{\text{orb}}^{\text{orb}}(q) - \Gamma_{\text{spin}}^{\text{spin}}(q) - \Gamma_{\text{orb}}^{\text{orb}}(q)$ with $\Gamma_{\text{spin}}^{\text{spin}}(q) \equiv \sum_{k,k'}(\Gamma^s_{\delta}(k + q, k'; k + q, k') u_{\alpha}(k) \cdot u_{\beta}(k' + q) u_{\beta}^*(k'))$. Here $\Gamma^s_{\delta}$ is the charge-channel four-point vertex, which is a moderate function of the Fermi momenta in the parameter range of the present numerical study. $u_{\alpha}(k)$ is the matrix element connecting the p-orbitals ($\alpha = x, y$) and the conduction band [30]. The scaling flow of $\Gamma_{\text{p-orb}}^{\text{orb}}(q)$ is shown in Fig. 3 (b), with the scaling parameter $l = \ln(\Lambda_0/\Lambda_1)$. The negative effective interaction drives the enhancement of the corresponding instability. We also plot the effective interaction for the spin channel, $\Gamma_{\text{spin}}^{\text{spin}}(Q_s)$. For the spin-channel, $\Gamma_{\text{spin}}^{\text{spin}}(Q_s) \sim -U$ at $l = 0$, and it is renormalized like the RPA as $\Gamma_{\text{spin}}^{\text{spin}} = \Gamma_{\text{spin}}^{\text{spin}}(1 - c)\Gamma_{\text{spin}}^{\text{spin}}(l)$ for $l \lesssim \ln(\Lambda_0/\Lambda_1) = 1.6$, where $c$ is the density of states. For the charge-channel, although $\Gamma_{\text{p-orb}}^{\text{orb}}(q)$ at $l = 0$ is quite small, it is strongly renormalized to be a large negative value. This result means that the CDW instability originates from the VC going beyond the RPA.

We also calculate the d-electron charge susceptibility with form factor $f_q(k)$, which is given as

$$
\chi_{\text{d-orb}}^{\text{d-orb}}(q) = \frac{1}{2} \int_0^1 d\tau \langle B(q, \tau) B(-q, 0) \rangle,
$$

where $B(q) = \sum_{k,\sigma} f_q(k) d_{k+q/2,\sigma}^d d_{k-\sigma}^d$. The numerically optimized $f_q(k)$ at $q = 0$ is shown in Fig. 3 (c), which has the $B_{1g}$-symmetry that is called the d-wave bond order. Since $k$-dependence of $f_q(k)$ in Fig. 3 (c) is similar to that of $|u_x(k)|^2 - |u_y(k)|^2$, the obtained $\chi_{\text{max}}^{\text{spin}}$ dependence of $\chi_{\text{d-orb}}^{\text{d-orb}}(0)$ with the optimized form factor is similar to that of $\chi_{\text{d-orb}}^{\text{d-orb}}(0)$ shown in Fig. 3 (a).

The divergence of $\chi_{\text{d-orb}}^{\text{d-orb}}(0)$ gives rise to the uniform p-orbital polarization with $n_x \neq n_y$ shown in Fig. 1 (c). In order to discuss the CDW instabilities inside the nematic phase, we perform the RG+cRPA analysis in the presence of the uniform p-O-CDW order $H' = \Delta E_p [n_x(0) - n_y(0)]$. In Fig. 4 (a), we plot the peak values of $\chi_{\text{d-orb}}^{\text{d-orb}}(q)$ in the uniform p-O-CDW state with $\Delta E_p = 0.3$ eV. Due to $\Delta E_p > 0$, $\chi_{\text{d-orb}}^{\text{d-orb}}(q)$ at $q = Q^x_0$ (along x-axis) increases whereas that at $q = Q^y_0$ (along y-axis) decreases.

To confirm the mechanism of the nematic transition, we perform the diagrammatic calculation for the MT- and AL-VCs. These VCIs can be obtained by solving the CDW equation introduced in Ref. [42] in the study of Fe-based superconductors. We analyze the linearized CDW equation introduced in the SM: B [37] and in Ref. [43]. By solving the CDW equation, both MT- and AL-VCs shown in Figs. 2 (d) and (e) with the optimized form factors are systematically generated. Figure 4 (b) shows the eigenvalue of the linearized equation, $\lambda_q$, for $\Delta E_p = 0.3$ eV [37]. (The inset shows the results for $\Delta E_p = 0$.) Here, $\alpha_S$ is the spin Stoner factor, and the horizontal axis is proportional to $\chi_{\text{max}}^{\text{spin}}$. The CDW susceptibility is proportional to $(1 - \lambda_q)^{-1}$, and $\lambda_q$ decreases with the quasiparticle damping $\gamma$; we set $\gamma = 0.3$ eV in Fig. 4 (b) [37]. The obtained results are qualitatively consistent with the RG+cRPA results in Fig. 4 (a). In the SM: B[37], we reveal that the CDW instabilities at $q = 0$ and $q = Q^y_0$ are given by the higher-order AL-type VCs.

Finally, we explain why $\Lambda_{\text{low}}$ should be set small. The RG equation for the $q = 0$ vertex, $\Gamma^s_{\delta}(k; k') \equiv \Gamma_{\delta}(k; k'; k')$, is given as $d\Gamma^s_{\delta}(k; k')/dl \propto \Lambda_0 \delta(\langle E_k \rangle) - \Lambda_0 \Gamma^s_{\delta}(k; k') \Gamma^s_{\delta}(k'; k')$ (other two terms), where $\delta$ is the derivative of the Fermi distribution function. Since the factor $\Lambda_0$ is small for $\Lambda_1 \gtrsim 4T$, the obtained $\Gamma_{\delta}$ is strongly reduced if $\Lambda_{\text{low}} \gg T$. In contrast, $\Gamma^{s+e}$ for $q \neq 0$ is not so sensitive to $\Lambda_{\text{low}}$. For this reason, the renormalization effect of $\Gamma_{\delta}$ is understood for $q \approx 0$ if $\Lambda_{\text{low}} \gg T$. Then, the obtained $\chi_{\text{d-orb}}^{\text{d-orb}}(0)$ is suppressed to be smaller than the peak values at $q \neq 0$ if a large cutoff $\Lambda_{\text{low}} \gg T$ is used, similarly to the previous results for $\Lambda_{\text{low}} = \pi T$ [30]. In the present study, large $\chi_{\text{d-orb}}^{\text{d-orb}}(0)$ is correctly obtained thanks to the use of the small cutoff $\Lambda_{\text{low}} = T$.

In summary, we studied the spin-fluctuation-driven CDW instabilities in the d-p Hubbard model in an unbiased way, by using the RG+cRPA method. When $\chi_{\text{max}}^{\text{spin}}$ is as large as 10 eV$^{-1}$, the CDW susceptibility $\chi_{\text{d-orb}}^{\text{d-orb}}(q)$ develops divergently at $q = 0$, which leads to the uniform p-O-CDW order with $n_x \neq n_y$. Under this nematic CDW state, the axial p-O-CDW instability is strongly magnified even if the deformation of the FS is small. These multistage CDW transitions originate from the higher-order AL-type VCs. We predict that the short-range spin-fluctuations drive the uniform nematic CDW around $T^*$ and the axial $q = Q_0$ CDW at $T_{\text{CDW}}$ successively. Although the uniform CDW order cannot simply explain the pseudogap formation, the large quasiparticle damping [19–21] due to the short-range spin-fluctuations may
induce the pseudogap for $T \lesssim T^\ast$.

We are grateful to Y. Matsuda, T. Hanaguri, T. Shibauchi, Y. Kasahara, Y. Gallais, W. Metzner, T. Enss, L. Classen, and S. Onari for fruitful discussions. This work was supported by Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science, and Technology, Japan.
A: RG equation for the four-point vertex

In the main text, we analyzed the $d$-$p$ Hubbard model by using the RG+cRPA method [1]. This method is the combination of the fRG theory and the cRPA. The RG+cRPA method enables us to perform reliable numerical study in the unbiased way. In this method, we introduce the original cutoff energy $\Lambda_0$ in order to divide each band into the higher and the lower energy regions: The higher-energy scattering processes are calculated by using the cRPA: The lower-energy scattering processes are analyzed by solving the RG equations, in which the initial vertices in the differential equation are given by the cRPA.

In the present model, the bare Coulomb interaction term on $d$-electrons is given as

$$H_U = \frac{1}{4} \sum_i \sum_{\sigma \sigma'} U^{0: \sigma \sigma'}_i d^\dagger_{i\sigma} d_{i\sigma'} d^\dagger_{ip} d_{ip}, \quad \text{(S1)}$$

$$U^{0: \sigma \sigma'}_{i} = \frac{1}{2} U^{0:s}_{i} \delta_{\sigma \sigma'} \cdot \tilde{\sigma}_{\rho \rho'} + \frac{1}{2} U^{0:i}_{i} \delta_{\sigma \sigma'} \delta_{\rho \rho'}, \quad \text{(S2)}$$

where $U^{0:s} = U$ and $U^{0:i} = -U$.

The antisymmetric full four-point vertex $\Gamma(k + \mathbf{q}, \mathbf{k}; \mathbf{k}' + \mathbf{q}, \mathbf{k}')$, which is the dressed vertex of the bare vertex $\tilde{U}$ in Eq. (S2) in the microscopic Fermi liquid theory, is depicted in Fig. S1 (a). Reflecting the SU(2) symmetry of the present model, $\Gamma$ is uniquely decomposed into the spin-channel and charge-channel four-point vertices by using the following relation:

$$\Gamma^{\sigma \sigma' \rho \rho'}(k + \mathbf{q}, k; k' + \mathbf{q}, k') = \frac{1}{2} \Gamma^{\sigma \sigma'}(k + \mathbf{q}, k; k' + \mathbf{q}, k') \tilde{\sigma}_{\rho \rho'} + \frac{1}{2} \Gamma^{\rho \rho'}(k + \mathbf{q}, k; k' + \mathbf{q}, k') \delta_{\sigma \sigma'} \delta_{\rho \rho'} \quad \text{(S3)}$$

where $\sigma, \sigma', \rho, \rho'$ are spin indices, and $\tilde{\sigma}$ is the Pauli matrix vector. We stress that $\Gamma^{\rho \rho'}$ are fully antisymmetrized, so the requirement by the Pauli principle is satisfied. We note that $\Gamma^{\sigma \sigma'} = \frac{1}{2} \Gamma^{\sigma \sigma'} + \frac{1}{2} \Gamma^{\sigma \sigma'}$, $\Gamma^{\rho \rho'} = \frac{1}{2} \Gamma^{\rho \rho'} - \frac{1}{2} \Gamma^{\rho \rho'}$, and $\Gamma^{\sigma \sigma' \rho \rho'} = \Gamma^{\rho \rho'}$.

In the RG formalism, the four-point vertex function is determined by solving the differential equations, called the RG equations. In the band representation basis, the explicit form of the RG equations is given by [2]:

$$\frac{d}{d\Lambda} \Gamma_{\text{RG}}(k_1, k_2; k_3, k_4) = -\frac{T}{N} \sum_{k,k'} \left[ \frac{d}{d\Lambda} G(k) G(k') \right] \quad \text{(S4)}$$

where $G(k)$ is the Green function multiplied by the Heaviside step function $\Theta(\Lambda - |E_{k,\nu}|)$, and $k$ is the compact notation of the momentum, band, and spin index: $k = (\mathbf{k}, \epsilon_n, \nu, \sigma)$. The diagrammatic representation of the RG equations is shown in Fig. S1 (b). First two contributions in the right-hand-side represent the particle-hole channels and the last contribution is the particle-particle channel.

In a conventional fRG method, $\Lambda_0$ is set large than the bandwidth $W_{\text{band}}$, and the initial value is given by the bare Coulomb interaction in Eq. (S2). In the RG+cRPA method, we set $\Lambda_0 < W_{\text{band}}$, and the initial value is given by the constraint RPA to include the higher-energy processes without over-counting of diagrams [1].

In the main text, we introduced the lower-energy cutoff $\Lambda_{\text{low}} \sim T$ in the RG equation for the four-point vertex: Eq. (S4). For this purpose, we multiply the cutoff function $\left( (\Lambda_{\text{low}}/\Lambda)^{\zeta} + 1 \right)^{-1}$ to the right-hand-side of Eq. (S4). Here, $\zeta$ is a parameter determining the width of this smooth cutoff, and we set $\zeta = 10$ in the main text. We do not introduce the lower-energy cutoff in the RG equation for the susceptibilities.

![FIG. S1: (Color online) (a) Definition of the full four-point vertex $\Gamma^{\sigma \sigma' \rho \rho'}(k + \mathbf{q}, k; k' + \mathbf{q}, k')$ in the microscopic Fermi liquid theory. (b) The one-loop RG equation for the four-point vertex. The crossed lines represent the electron Green function with cutoff $\Lambda$. The slashed lines represent the electron propagations having the energy shell $\Lambda$.](image-url)
B: Analysis of the linearized CDW equation

In the main text, we analyzed the $d$-$p$ Hubbard model for cuprate superconductors in an unbiased manner using the RG+cRPA method. We find that the nematic CDW with $d$-form factor is the leading instability. The axial nematic CDW instability at $q = Q_a$ is the second strongest, and its strength increases under the static uniform CDW order. This result leads to the prediction that uniform nematic CDW occurs at the pseudogap temperature $T^*$, and the axial CDW at wavevector $q = Q_a$ is induced under $T^*$.

\[
\lambda_q \Sigma_q(k) = \Delta \Sigma_q(k) + \Delta \Sigma_q(k) + \Delta \Sigma_q(k) + \Delta \Sigma_q(k) + \Delta \Sigma_q(k) + \cdots
\]

\[
\lambda_q \Sigma_q(k) = \frac{U}{2} \Sigma_q(k) + \frac{1}{2} \chi^0(q) + \chi^0(q) + \chi^0(q) + \chi^0(q) + \chi^0(q) + \cdots
\]

\[
\lambda_q \Sigma_q(k) = \Sigma_q(k) + \Sigma_q(k) + \Sigma_q(k) + \Sigma_q(k) + \Sigma_q(k) + \cdots
\]

\[
\lambda_q \Sigma_q(k) = \Sigma_q(k) + \Sigma_q(k) + \Sigma_q(k) + \Sigma_q(k) + \Sigma_q(k) + \cdots
\]

FIG. S2: (color online) (a) Schematic linearized CDW equation for general wavevector $q$. (b) Examples of the VCs generated by solving the linearized CDW equation. (c) Higher-order AL processes.

In this section, we study the CDW formation mechanism in cuprate superconductors based on the diagrammatic method, in order to find what many-body processes cause the CDW order. Theoretically, the CDW order is given as the symmetry-breaking in the self-energy $\Delta \Sigma(k)$. According to Refs. [3, 4], the self-consistent CDW equation is given as

\[
\Delta \Sigma(k) = (1 - P_{A_1}) T \sum_q V(q) G(k + q), \quad (S5)
\]

where $P_{A_1}$ is the $A_1g$-symmetry projection operator, and $G(k) = (G_0^{-1}(k) - \Delta \Sigma(k))^{-1}$ is the Green function with the symmetry-breaking term $\Delta \Sigma$. $V(q) = U^2 \left( \frac{1}{2} \chi^0(q) + \frac{1}{2} \chi^0(q) - \chi^0(q) \right) + U$, where $\chi^0(q) = \chi^0(q)/(1 + \Sigma(q))/(1 + U^2 \chi^0(q))$ and $\chi^0(q) = -T \sum_k G(k + q) G(k)$.

In order to analyze the CDW state with arbitrary wavevector $q$, we linearize Eq. (S5) with respect to $\Delta \Sigma$:

\[
\lambda_q \Sigma_q(k) = T \sum_{k'} K(q; k, k') \Delta \Sigma_q(k'), \quad (S6)
\]

where $\lambda_q$ is the eigenvalue for the CDW for the wavevector $q$. The CDW with wavevector $q$ appears when $\lambda_q = 1$, and the eigenvector $\Delta \Sigma_q(k)$ gives the CDW form factor. The kernel $K(q; k, k')$ is given in Fig. S2 (a), and its analytic expression is given as [4]:

\[
K(q; k, k') = \left( \frac{3}{2} V_0^0(k - k') + \frac{1}{2} V_0^0(k - k') \right) \times G_0(k' + q/2) G_0(k' - q/2) - T \sum_p \left( \frac{3}{2} V_0^0(p + q/2) V_0^0(p - q/2) + \frac{1}{2} V_0^0(p + q/2) V_0^0(p - q/2) \right) \times G_0(k - p) (\Lambda_q(k'; p) + \Lambda_q(k'; -p)), \quad (S7)
\]

where $V_0^0(q) = U + U^2 \chi_0^0(q)$, $V_0^0(q) = -U + U^2 \chi_0^0(q)$, and $\Lambda_q(k; p) \equiv G_0(k + \frac{3}{2} Q_0(k - k; p) G_0(k - \frac{3}{2} Q_0(k - k; p))$. The subscript 0 in Eq. (S7) represents the functions with $\Delta \Sigma = 0$.

By solving the linearized CDW equation (S6), many higher-order vertex corrections (VCs) are systematically generated. Some examples of the generated VCs are shown in Fig. S2 (b). If we drop the Hartree term and MT term in $K(q; k, k')$, we obtain the series of higher-order AL-VCs shown in Fig. S2 (c). The AL terms drive the $q = 0$ CDW instability since its functional form $\propto \sum_k \chi^s(k + q) \chi^s(k)$ is large for $q \approx 0$ [5].

\[
\lambda_q \chi^s(k) = \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \cdots
\]

\[
\lambda_q \chi^s(k) = \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \cdots
\]

\[
\lambda_q \chi^s(k) = \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \cdots
\]

FIG. S3: (color online) (a) $q$-dependences of $\lambda_q$, $\lambda_q^{AL}$ and $\lambda_q^{AL,2nd}$, (b) $q$-dependences of $\lambda_q$ and $\lambda_q^{MT}$. (c) $\lambda_q$ at $q = 0$, $Q_a$ and $Q_s$ as function of $\alpha_S$. (d) Form factor for $q = 0$ (d-wave).

Figure S3 (a) shows the obtained $q$-dependence of $\lambda_q$ for $\alpha_S = 0.995$ at $T = 50$ meV, when the quasiparticle damping is $\gamma = 0.3$ eV. Here, $\lambda_q$ is the largest at $q = 0$, and the second largest maximum is at $q = Q_s$. $\alpha_S \equiv U \max_q \left\{ \chi_0^0(q) \right\}$ is the spin Stoner factor. We also show the eigenvalue $\lambda_q^{AL}$ (and the second-largest eigenvalue $\lambda_q^{AL,2nd}$), which is obtained by dropping the Hartree

\[
\lambda_q \chi^s(k) = \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \chi^s(k) + \cdots
\]
and MT terms in the kernel. That is, \( \lambda_{q}^{AL} \) is given by the higher-order AL processes shown in Fig. S2 (c). At \( q = 0 \) and \( Q_a \), \( \lambda_{q}^{AL} \) is almost equal to the true eigenvalue \( \lambda_q \).

In the present analysis, we dropped the \( \epsilon_n \)-dependence of \( \Delta \Sigma_q(k) \) by performing the analytic continuation \( (i\epsilon_n \to \epsilon) \) and putting \( \epsilon = 0 \). We also dropped the \( \epsilon_n \)-dependence of the quasiparticle damping \( \gamma \). Due to these simplifications, the obtained \( \lambda_q \) is overestimated. Therefore, we do not put the constraint \( \lambda_q < 1 \) here.

In Fig. S3 (b), we show the eigenvalue \( \lambda_{q}^{MT} \), which is obtained by dropping the Hartree and AL terms in the kernel. It is much smaller than \( \lambda_q \) at \( q = 0 \) and \( Q_a \), whereas \( \lambda_q \) at \( q = Q_d \) is comparable to the true eigenvalue. Therefore, the origin of the CDW instability at \( q = 0 \) and \( Q_a \) is the AL process, whereas that at \( q = Q_d \) is mainly the MT process.

Figure S3 (c) shows the eigenvalues at \( q = 0, Q_a, \) and \( Q_d \) as function of \( \alpha_S \). As the spin susceptibility increases \( (\alpha_S \gtrsim 0.98) \), \( \lambda_q \) is drastically enlarged by the VCs, and \( \lambda_{q=0} \) becomes the largest due to the AL processes. The form factor at \( q = 0 \), \( \Delta \Sigma_0(k) \), has the \( d \)-wave symmetry as shown in Fig. S3 (b).

In summary, we analyzed the linearized CDW equation based on the \( d-p \) Hubbard model, by including both the MT and AL VCs into the kernel. When the spin fluctuations are strong \( (\alpha_S \gtrsim 0.98) \), the uniform nematic CDW has the strongest instability. The axial CDW instability is strongly magnified under the uniform CDW order, as we explain in the main text. The obtained results are consistent with the results by the RG+cRPA in the main text. Thus, it is concluded that the higher-order AL processes give the CDW orders at \( q = 0 \) and \( Q_a \).

[1] M. Tsuchiizu, Y. Ohno, S. Onari, and H. Kontani, Phys. Rev. Lett. 111, 057003 (2013); M. Tsuchiizu, Y. Yamakawa, S. Onari, Y. Ohno, and H. Kontani, Phys. Rev. B 91, 155103 (2015).
[2] R. Tazai et al., Phys. Rev. B 94, 115155 (2016).
[3] S. Onari, Y. Yamakawa, and H. Kontani, Phys. Rev. Lett. 116, 227001 (2016).
[4] K. Kawaguchi, Y. Yamakawa, M. Tsuchiizu, and H. Kontani, unpublished.
[5] S. Onari and H. Kontani, Phys. Rev. Lett. 109, 137001 (2012).