Coexistence of Charge-Density-Wave and Pair-Density-Wave Orders in Underdoped Cuprates

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Yuxuan Wang,[1] Daniel F. Agterberg,[2] and Andrey Chubukov[3]

[1] *Department of Physics, University of Wisconsin, Madison, WI 53706, USA*
[2] *Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53211, USA*
[3] *William I. Fine Theoretical Physics Institute, and School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA*

We analyze incommensurate charge-density-wave (CDW) and pair-density-wave (PDW) orders with transferred momenta $(\pm Q,0)/(0,\pm Q)$ in underdoped cuprates within the spin-fermion model. Both orders appear due to exchange of spin fluctuations before magnetic order develops. We argue that the ordered state with the lowest energy has non-zero CDW and PDW components with the same momentum. Such a state breaks C_4 lattice rotational symmetry, time-reversal symmetry, and mirror symmetries. We argue that the feedback from CDW/PDW order on fermionic dispersion is consistent with ARPES data. We discuss the interplay between the CDW/PDW order and $d_{x^2-y^2}$ superconductivity and make specific predictions for experiments.

Introduction. The search for competitors to $\mathrm{d}_{x^2-y^2}$ superconductivity (d-SC) in underdoped cuprates has gained strength over the last few years due to mounting experimental evidence that some form of electronic charge order spontaneously emerges below a certain doping and competes with d-SC (Refs. [1–16]) The two most frequently discussed candidates for electronic order are incommensurate charge density-wave (CDW) order (Refs. [17–28, 31–34]) and incommensurate pair-density-wave order (PDW), which is a SC order with a finite Cooper pair momentum $\mathbf{Q}$ (Refs. [35–40]). Other potential candidates are loop current order [41] and CDW order with momentum near (π,π) (Ref. [42]).

CDW order in underdoped cuprates has been proposed some time ago [17] and has been analyzed in detail by several groups in the last few years within the spin-fluctuation formalism [19, 20, 22–24, 26–28] and within $t-J$ model [18, 21]. The initial discussion was focused on near-equivalence between d-SC and d-wave charge bond order (BO) with momenta (Q,Q) along zone diagonal [19, 20, 27], but charge order of this type has not been observed in the experiments. It was later found [22, 23, 26, 28] that the same magnetic model also displays a CDW order with momenta $(Q,0)$ or $(0,Q)$, which is consistent with the range of CDW wave vectors extracted from experiments [1–6, 9, 10, 29]. Such CDW order is also consistent with experiments that detect the breaking of discrete rotational and time-reversal symmetries in a (T,x) range where competing order develops [11–16]. In particular, when spin-fermion coupling is strong enough, the CDW order develops in the form of a stripe and breaks C_4 lattice rotational symmetry. A stripe CDW order with $(Q,0)/(0,Q)$ in turn gives rise to modulations in both charge density and charge current and breaks time-reversal and mirror symmetries [23, 24, 28, 33].

The agreement with the data is encouraging, but two fundamental issues with CDW order remain. First, within the mean-field approximation, T_{cdw} is smaller than the superconducting T_c (and also the onset temperature for (Q,Q) order. It has been conjectured that T_{cdw} may be enhanced by adding e.g., phonons [17], or nearest-neighbor Coulomb interaction [30] or assuming the CDW emerges from already pre-existing pseudogap [26, 31]. T_{cdw} is also enhanced by fluctuations beyond mean-field [23, 24], but whether such enhancements are strong enough to make T_{cdw} larger than T_c remains to be seen. Second, stripe CDW order cannot explain qualitative features of the ARPES data away from zone boundaries [38].

It has been argued [38] that ARPES experiments for all momentum cuts can be explained by assuming that the competing order is PDW rather than CDW. PDW order was initially analyzed for doped Mott insulators [35, 39, 40], but it also emerges in the spin-fermion model [28] with the same momentum $(Q,0)/(0,Q)$ as CDW order and its onset temperature T_{pdw} is close to T_{cdw} (the two become equivalent if one neglects the curvature of fermionic dispersion at hot spots [27, 28]). Given that PDW order explains ARPES experiments, it seems logical to consider it as a candidate for competing order. Just like CDW, the PDW order develops in the form of a stripe and breaks C_4 lattice rotational symmetry [28, 36], if, again, the coupling is strong enough. However, it does not naturally break time-reversal and mirror symmetries [37] (although it does so for a particular Fermi surface geometry [36]), and the mean-field T_{pdw} is also smaller than T_c for d-SC.

In this communication we build on the results of the generic Ginzburg-Landau analysis [28] and propose how to resolve the partial disagreement with experiments for pure CDW or PDW orders. We first re-iterate that pure CDW/PDW orders emerge in the forms of stripes only if the spin-fermion interaction g is strong enough. In practice, g has to be at least comparable to the upper energy cutoff of the spin-fermion model Λ (see details below). For smaller couplings the system develops a checkerboard order for which C_4 symmetry is preserved [43]. The spin-

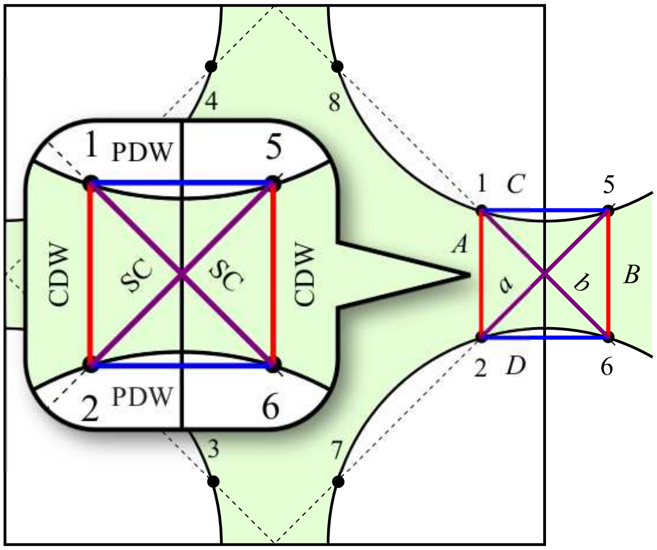

FIG. 1. The Brillouin zone, the Fermi surface, and the hot spots. We label bonds connecting hot spots as A, B, C, D, a and b. Inset: the structure of the mixed CDW/PDW state in one of the hot regions.

fermion model is a low-energy model and it is rigorously defined only when the coupling g is smaller than Λ. In this respect, stripe CDW or PDW orders emerge, only at the edge of the applicability of the model. Here we consider spin-fermion model at smaller couplings, well within its applicability range, and allow both CDW and PDW orders to develop. We show that the system develops a mixed CDW/PDW order, in which a CDW component develops between hot fermions separated along, say, Y direction and a PDW component develops between fermions separated along X direction (see Fig. 1). Because the momentum carried by an order parameter is the transferred momentum for CDW and the total momentum for PDW, the CDW order along Y and the PDW order along X actually carry the same momentum $(0, Q)$. We argue that such a state further lowers its Free energy by developing (via an emerging triple coupling) secondary homogeneous superconducting orders [28]. This effect favors the mixed CDW/PDW state over the pure checkerboard CDW or PDW states, which would otherwise all be degenerate. The mixed CDW/PDW state breaks C_4 symmetry because both orders carry either momentum $(Q, 0)$ or $(0, Q)$, but not both, and it also breaks time-reversal and mirror symmetries as the pure stripe CDW order with $(Q, 0)$ or $(0, Q)$ does.

The presence of PDW component is relevant for the interpretation of the ARPES data. Without it, the fermionic spectrum in the CDW phase would contain the lower energy branch, which never crosses Fermi level, and the upper energy branch, which would approach the Fermi level *from above* as the momentum cuts enter the arc region. As discussed in [38], this is inconsistent with the data [9] which show that the dispersion approaches the Fermi level *from below*. We show that the presence of PDW component changes the structure of fermionic dispersion in such a way that now the lower branch crosses the Fermi level in the arc region (see Fig. 2), in full agreement with ARPES experiments.

We also consider the interplay between CDW/PDW order and d-SC and present the phase diagram in Fig. 3. The reduction of the superconducting T_c in the coexistence region with CDW/PDW is the obvious consequence of competition for the Fermi surface. A small (of order g/Λ) drop of T_c upon entering the coexistence region is the result of a weak first-order CDW/PDW transition. There exists, however, a more subtle feature of the phase diagram. Namely, a secondary SC order is generated by CDW/PDW order, which preserves the same sign of the gap along each quadrant of the Fermi surface. Below T_c for d-SC, this secondary superconducting order couples with $d_{x^2-y^2}$ order, and the net result is the removal or shifting of the gap nodes. Simultaneously, the CDW order acquires an extra component with s-form factor, i.e., the magnitude of its s-wave portion increases. We propose to verify these through experiments.

The model We follow previous works [19, 20, 23, 28] and consider emerging charge order within the spin-fermion model [44]. This model describes interactions between itinerant electrons and their near-critical antiferromagnetic collective spin excitations in two spatial dimensions. Eight "hot" spots, defined as points on the Fermi surface separated by antiferromagnetic ordering momentum (π, π) (points 1-8 in Fig. 1), are the most relevant for destruction of a normal Fermi liquid state. The known instabilities of the spin-fermion model include d-SC (e.g. $\langle c_1 c_6\rangle$, see Fig. 1) [19, 45, 46], bond charge order (BO) with momenta $(\pm Q, \pm Q)$ (e.g. $\langle c_1^\dagger c_6\rangle$) [19, 20, 27], CDW order with momenta $(0, \pm Q)$ and $(\pm Q, 0)$ (e.g. $\langle c_1^\dagger c_2\rangle$) [23, 26, 32] and PDW order with momenta $(0, \pm Q)$ and $(\pm Q, 0)$ (e.g. $\langle c_1 c_2\rangle$) [27, 28]. The model has an approximate SU(2) particle-hole symmetry [19, 20, 27, 28, 34], which becomes exact once one linearizes the fermionic dispersion in the vicinity of the hot spots. This gives rise to near-degeneracy between d-SC and BO and between CDW and PDW.

The Ginzburg-Landau analysis We introduce four order parameters: Ψ for SC, Φ for BO, ψ for PDW, and ρ for CDW respectively. SC and BO order parameters connects hot spots along diagonal bonds, which we label as a and b in Fig. 1, while PDW and CDW connect hot spots along vertical and horizontal bonds, which we label as A, B, C, and D. We define the CDW order parameter residing on bond A as $\rho_A \sim \langle c_1^\dagger c_2\rangle$ and use analogous notations for other order parameters. The effective action is the sum of three terms:

$$\mathcal{S}_{\rm eff} = \mathcal{S}_{\rm cdw/pdw}[\rho, \psi] + \mathcal{S}_{\rm sc/bo}[\Psi, \Phi] + \mathcal{S}_{\rm int} \qquad (1)$$

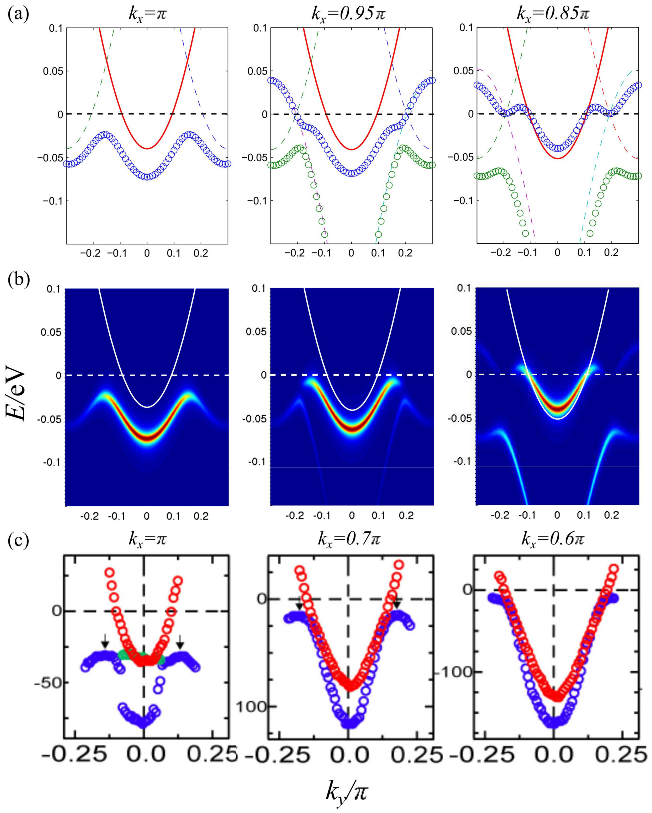

FIG. 2. Fermionic dispersion in the antinodal region in the presence of the mixed CDW/PDW order. Upper panel – the dispersion in the presence of CDW/PDW order for various k_x ($k_x = \pi$ corresponds to the cut along the Brillouin zone boundary). Middle panel– the spectral function. Thin line on both panels is the bare dispersion. Bottom panel – experimental data from Ref. [9] for comparison. The experimental data have been taken below T_c and show a gapped dispersion in a wider range of $\pi - k_x$.

The $\mathcal{S}_{\rm cdw/pdw}[\rho, \psi]$ term is of our primary interest. Keeping the SU(2) symmetry exact, we follow Ref. [28] and combine PDW and CDW orders on a given bond (say, bond A) into a 2×2 matrix order parameter

$$\Delta_A^{\mu\nu} \equiv \begin{pmatrix} \psi_A & \rho_A^* \\ -\rho_A & \psi_A^* \end{pmatrix} \equiv \sqrt{|\rho_A|^2 + |\psi_A|^2}\; U_A, \qquad (2)$$

where $\rho_A \sim c_1^\dagger c_2$, $\psi_A \sim c_1 c_2$, and U_A is a SU(2) matrix "phase". The order parameters $\Delta_{B,C,D}$ and phases $U_{B,C,D}$ are similarly defined (see Supplementary Material (SM) for details). Minimizing the Free energy, we obtain $\Gamma \equiv {\rm Tr}(U_A U_C^\dagger U_B U_D) = -2$, $\sqrt{|\rho_A|^2 + |\psi_A|^2} = \sqrt{|\rho_B|^2 + |\psi_B|^2} \equiv |\Delta_y|$, and $\sqrt{|\rho_C|^2 + |\psi_C|^2} = \sqrt{|\rho_D|^2 + |\psi_D|^2} \equiv |\Delta_x|$. Under these conditions, the CDW/PDW action becomes

$$\begin{aligned}\mathcal{S}_{\rm cdw/pdw} =& \frac{\alpha}{2}(|\Delta_x|^2 + |\Delta_y|^2) + \beta(|\Delta_x|^4 + |\Delta_y|^4) \\ &+ (\tilde{\beta} - \bar{\beta})|\Delta_x|^2|\Delta_y|^2 + O(\Delta^6) \qquad (3)\end{aligned}$$

where $\alpha \sim \Lambda/v_F^2 \times (T - T_{\rm cdw})/T_{\rm cdw}$ and $T_{\rm cdw} = T_{\rm pdw} \sim g$ (Ref. [23]). The prefactors β, $\tilde{\beta}$, and $\bar{\beta}$ are determined by different convolutions of four fermionic propagators (the square diagrams [23, 28, 32]). At $g \ll \Lambda$ we have $\beta \sim 1/(v_F^2\Lambda)$, $\tilde{\beta} \sim \log(\Lambda/g)/(v_F^2\Lambda)$, and $\bar{\beta} \sim (\Lambda/g)/(v_F^2\Lambda)$. We see that $\bar{\beta}$ is the largest term, hence the action (3) is minimized when $|\Delta| \equiv |\Delta_x| = |\Delta_y|$. Because $\tilde{\beta} - \bar{\beta} < 0$, the action is unbounded, which implies that the transition is first-order and sixth-order terms (coming from six-leg diagrams) have to be included to stabilize the order. Including these terms we obtain a first order into CDW/PDW state at $T_{\rm cdw/pdw} = T_{\rm cdw}(1 + O(g/\Lambda))$. We emphasize that this temperature is higher than the one for a pure CDW (or PDW) transition.

The constraint $\Gamma \equiv {\rm Tr}(U_A U_C^\dagger U_B U_D) = -2$ leaves the ground state hugely degenerate – the order parameter manifold is $\mathrm{SO}(4) \times \mathrm{SO}(4)$ (Ref. 28). This manifold includes pure CDW and pure PDW checkerboard states and mixed CDW/PDW states. To select the actual ground state configuration we note that, if CDW and PDW orders have components which carry the same momentum $\mathbf{Q}$, the Free energy is further lowered by creating a secondary order whose magnitude is a product of CDW and PDW order parameters. This secondary order is a homogeneous SC with equal sign of the gap along each quadrant of the FS [28] One can straightforwardly check that the reduction of the Free energy is maximal when in a nominally checkerboard state CDW occurs along vertical bonds and PDW occurs along horizontal bonds or vise versa, i.e., each order develops in the form of a stripe. This corresponds to either $\psi_{A,B} = \rho_{C,D} = 0$ (as in the inset of Fig. 1) or $\psi_{C,D} = \rho_{A,B} = 0$, the choice breaks C_4 lattice rotation symmetry. Furthermore, the stripe CDW order parameters ρ_A and ρ_B and PDW order parameters ψ_C and ψ_D get separately coupled by fermions away from hot spots, and the coupling between ρ_A and ρ_B locks the relative phase of ρ_A and ρ_B such that $\rho_B = \pm i\rho_A$ (Ref. [23]). The choice of the sign breaks time-reversal and mirror symmetries. The coupling between ψ_C and ψ_D does not lock their phases.

Feedback from CDW/PDW order on fermions We now show that the feedback from stripe CDW/stripe PDW order on the fermionic dispersion at $k \sim (\pi, 0)$, taken as a function of k_y for various $k_x = \pi - \delta k_x$, yields results in quite reasonable agreement with ARPES data [9, 10]. Previous studies have shown [23] that a pure CDW order can explain the ARPES spectrum for a cut along the BZ boundary, but not for cuts that are closer toward BZ center (see Ref. [38, 47]). To obtain the dispersion along various cuts in the presence of both CDW and PDW, we have extended our analysis of the CDW/PDW order to a finite momentum range away from the hot spots. We find that at the BZ boundary, the CDW order has a larger amplitude due to better FS nesting but the PDW component increases as the cuts move towards the hot spots. We present the details in SM and show the

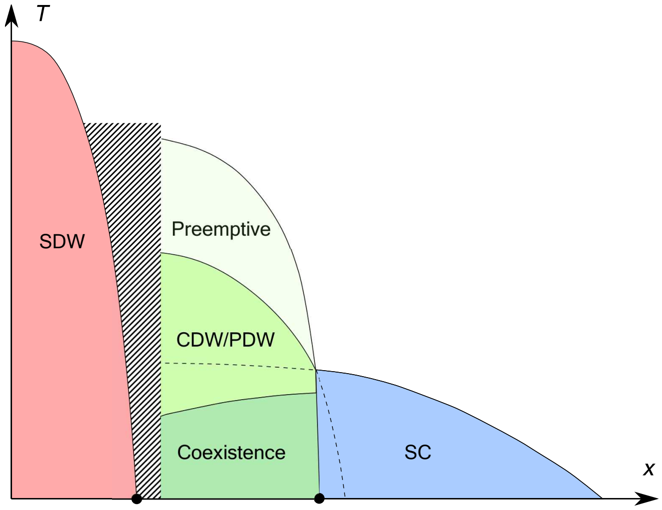

FIG. 3. The phase diagram. The transition into CDW/PDW state is weakly first-order and the superconducting T_c drops by a finite amount upon entering into coexistence region. In the region labeled as "pre-emptive" discrete C_4 and time-reversal/mirror symmetries are broken but continuous $U(1)$ translational symmetry (associated with the locking of the common phases of ρ_A and ρ_B) remains unbroken [23]. In the shaded region, Mott physics develops and the onset temperature of charge ordering shrinks.

results in Fig. 2. There are three key features in our scenario that are qualitatively consistent with experiment: (1) at the BZ boundary ($k_x = \pi$), the locus of minimum excitation energy shifts from k_F to a larger value $k_G \approx Q/2$, where Q is the CDW momentum, (2) as k_x decreases, the excitation approaches the Fermi level from below, and (3) at k_x when the Fermi arc emerges, the fermionic dispersion becomes flat for $|k_y| > k_F$. These features are also reproduced by pure PDW order [38] and from a spatially homogeneous self-energy arising from a d-wave CDW order peaked at (π, π) [21]. However, both these scenarios do not immediately explain the observation of broken time-reversal symmetry or CDW order with small incommensurate momentum. To obtain quantitative agreement with the experiments, we would need to know how CDW and PDW order parameters depend on frequency. This would require one to model the bare dispersion far away from k_F and solve complex integral equations for frequency-dependent order parameters.

Interplay between CDW/PDW order and $d_{x^2-y^2}$ superconductivity We next consider other terms in the effective action in Eq. (1). The term $\mathcal{S}_{\rm sc/bo}$ has been analyzed in [20, 27, 32]. When SU(2) symmetry is exact, d-SC and BO orders are degenerate and the action has four Goldstone modes. Once SU(2) symmetry is broken by FS curvature, only d-SC order develops below T_c. We assume that this is the case and keep only d-SC component Ψ in $\mathcal{S}_{\rm sc/bo}$, i.e. reduce it to $\mathcal{S}_{\rm sc/bo} = \alpha_s|\Psi|^2 + \beta_s|\Psi|^4$ with $\alpha_s \sim \Lambda/v_F^2 \times (T - T_c)/T_c$, $T_c \sim g$, and $\beta_s \sim \Lambda/(v_F g)^2$. The coupling between CDW/PDW and d-SC orders is again obtained by evaluating the square diagrams. The calculation yields $\mathcal{S}_{\rm int} = \beta'|\Delta|^2|\Psi|^2$ with $\beta' \sim 1/(v_F^2 g)$. Note that the magnitude of the coupling is phase sensitive, hence the phase locking between ρ_A and ρ_B at $\pm\pi/2$ is important (see SM for details).

The analysis of the full action is straightforward and we show the results in Fig. 3. The mean-field temperature $T_{\rm cdw/pdw} \geq T_{\rm cdw}$ is comparable to T_c near the SDW boundary but is enhanced by fluctuations [23, 26, 31]. We assume that this enhancement lifts $T_{\rm cdw/pdw}$ above T_c at large ξ. Because CDW/PDW transition is first-order, T_c jumps upon entering into the coexistence region, but the jump is again small in g/Λ. Similar behavior has been recently observed in Fe-pnictides [51]. At small T, the CDW/PDW and d-SC orders coexist.

The phase diagram in Fig. 3 is similar to that for pure CDW order [23], but there are some extra features. First, the combination of CDW/PDW orders induces a secondary SC order [28] with a non-zero gap along zone diagonal (s-wave or d_{xy}). In the coexistence region with d-SC this order Ψ_s couples with d-SC order Ψ and, as a result, gap nodes either get shifted ($d + s$ state) or removed ($d + e^{i\theta}s$ state). A similar coupling has been examined in the context of the Fe-pnictides [52]. A finite gap along zone diagonals has been observed in ARPES at doping $x < 0.1$ (Ref. [53]) and also inferred from Raman spectroscopy [54]. Second, by the same logic, the d-SC and PDW orders induce a secondary s-wave CDW order with the same momentum as the primary one. We propose a search for SC gap opening or node shifting and enhancement of s-component of CDW order in the coexistence region.

Conclusions In this letter we proposed a state with unidirectional CDW and PDW orders which carry the same momentum. We argued that this state is a member of the ground state manifold of the low-energy spin-fermion model and its energy is further reduced by induction of a secondary SC order. We further argued that CDW/PDW state has a number of features consistent with experiments: it breaks both C_4 and time-reversal symmetry and the feedback from CDW/PDW order on fermions reproduces the ARPES data from the BZ boundary to the tip of the Fermi arc. The transition into CDW/PDW state is weakly first-order and occurs at a higher transition temperature than that for a pure unidirectional CDW or PDW orders. We considered the interplay between CDW/PDW order and d-SC, and found that a SC gap becomes non-zero along zone diagonals. We proposed to search for this gap opening in the region where charge order and d-SC coexist.

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