Checkerboard order in vortex cores from pair-density-wave superconductivity

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We consider competing pair-density-wave (PDW) and d-wave superconducting states in a magnetic field. We show that PDW order appears in the cores of d-wave vortices, driving checkerboard charge-density-wave (CDW) order in the vortex cores, which is consistent with experimental observations. Furthermore, we find an additional CDW order that appears on a ring outside the vortex cores. This CDW order varies with a period that is twice that of the checkerboard CDW and it only appears where both PDW and d-wave order coexist. The observation of this additional CDW order would provide strong evidence for PDW order in the pseudogap phase of the cuprates. We further argue that the CDW seen by nuclear magnetic resonance at high fields is due to a PDW state that emerges when a magnetic field is applied.

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I. INTRODUCTION

Pair-density-wave (PDW) superconducting order has emerged as a realistic candidate for order in the charge-ordered region of the pseudogap phase of the cuprates near one-eighth filling. It naturally accounts for both superconducting (SC) correlations and for static quasi-long-range charge-density-wave (CDW) order observed near this hole doping and at temperatures below approximately 150 K [1–7], and it can explain observed signatures of broken time-reversal symmetry [8–13]. Moreover, PDW can lead to the quantum oscillations seen in the cuprates [14] and can also explain anomalous quasiparticle properties observed by angle-resolved photoemission (ARPES) measurements [7]. In addition, numerical simulations of theories of a doped Mott insulator reveal PDW order to be a competitive ground state to d-wave superconductivity [15]. It is therefore important to find experiments that can identify PDW order in the cuprates. Motivated by the observation of checkerboard CDW order inside d-wave vortex cores by scanning tunneling microscopy (STM) [16,17] and by nuclear magnetic resonance (NMR) [18,19], we examine the competition between d-wave and PDW superconductivity in applied magnetic fields. Previous theoretical studies of competing orders in a magnetic field have emphasized competing spin-density-wave (SDW) order [20,21], CDW order [20–22], and staggered flux phases [23,24] with d-wave superconductivity. Competing PDW and d-wave order has not been extensively studied (note that superconducting phase disordered PDW competing with d-wave order has been examined [25]). Here, we find that inside the vortex cores of d-wave superconductivity, PDW order drives the observed checkerboard CDW order and, in conjunction with d-wave superconductivity, it also drives an additional CDW order that appears in a ringlike region outside the vortex cores. This additional CDW order has twice the period of the observed checkerboard CDW order and serves as a smoking gun for PDW order.

In the following, we develop a phenomenological theory for competing PDW and d-wave superconductivity, sketched in Fig. 1. We assume that in zero field, only d-wave superconductivity appears at the expense of the PDW order. The PDW order can only appear when the d-wave order is weakened by the external field. This is followed by an analysis of the core structure of a single d-wave vortex, where we show that PDW order appears inside these cores, without any phase winding, generating the CDW order discussed above. Finally, we examine the behavior of this competing system as the field is further increased and identify a transition at which PDW order develops phase coherence and forms a vortex phase. At the mean-field level, PDW order simultaneously breaks gauge invariance and translational symmetry. Fluctuations can lead to two separate transitions: one for which gauge symmetry is broken and one for which translational symmetry is broken [26]. We argue that at high fields, the superconducting order is removed by phase fluctuations, leaving behind the CDW order seen through NMR experiments.

II. GINZBURG-LANDAU THEORY OF COMPETING d-WAVE AND PDW SUPERCONDUCTIVITY

To investigate the physics resulting from the $H-T$ phase diagram shown in Fig. 1, we consider a model with competing d-wave and PDW superconductivity. The PDW order parameter is represented by a four-component complex vector $\Delta_{\rm PDW}$, defined as $\Delta^\dagger_{\rm PDW}=(\Delta^*_{Q_x},\Delta^*_{-Q_x},\Delta^*_{Q_y},\Delta^*_{-Q_y})$, and the d wave is represented by one complex (scalar) field Δ_d. For an external applied field $\boldsymbol{H}$, which we will take to be along the z axis, $\boldsymbol{H}=H\boldsymbol{e}_z$, the Ginzburg-Landau free-energy density is

$$\mathcal{F}=\frac{\boldsymbol{B}^2}{2}-\boldsymbol{B}\cdot\boldsymbol{H}+\mathcal{F}_{d\text{-wave}}+\mathcal{F}_{\rm PDW}+\mathcal{F}_{\rm Int}, \tag{1}$$

where $\boldsymbol{B}=\nabla\times\boldsymbol{A}$ is the magnetic field and $\boldsymbol{A}$ is its vector potential. $\mathcal{F}_{\rm PDW}$ describes the pair-density wave $\Delta_{\rm PDW}$, and $\mathcal{F}_{\rm Int}$ is its coupling to the d-wave order that obeys

$$\mathcal{F}_{d\text{-wave}}=\frac{1}{2}|\boldsymbol{D}\Delta_d|^2+\alpha_d|\Delta_d|^2+\frac{\beta_d}{2}|\Delta_d|^4, \tag{2}$$

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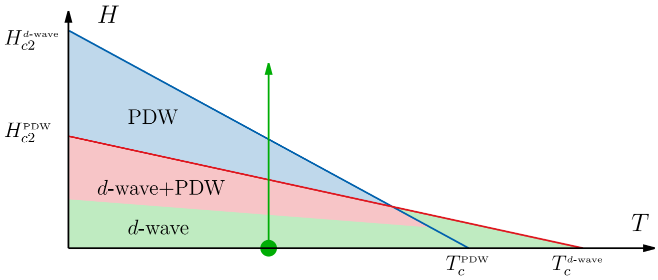

FIG. 1. (Color online) Sketch of the field/temperature phase diagram of the model with competing order. For low applied fields, the d wave (Δ_d) is present, and it completely suppresses the PDW ($\Delta_{\rm PDW}$). This is the green (lower) region of the phase diagram. When increasing the external field, the d-wave order is substantially suppressed, eventually triggering a phase transition where the PDW overcomes the competition with the d wave and develops a nonzero averaged density. For sufficiently low temperatures, the second critical field of the PDW order exceeds that of the d-wave order. As a result, further increase of the external field completely suppresses the d-wave order, leaving only $\Delta_{\rm PDW}$, which survives up to $H = {\rm H}_{c2}^{\rm PDW}$, as shown in the blue (upper) region of the diagram. The PDW order qualitatively accounts for the emergence of CDW at high fields, provided the superconducting order of the PDW is suppressed by phase fluctuations.

with $\boldsymbol{D} = \nabla + ie\boldsymbol{A}$. Symmetry arguments dictate that the free energy of the PDW has the following structure [5]:

$$\begin{aligned}\mathcal{F}_{\rm PDW} =& \frac{1}{2}\sum_{\hat{q},j} k_{\hat{q},j}|D_j\Delta_{\hat{q}}|^2 + \sum_{\hat{q}}\left(\alpha + \frac{\beta}{2}|\Delta_{\hat{q}}|^2\right)|\Delta_{\hat{q}}|^2\\ &+ \gamma_1(|\Delta_{\mathcal{Q}_x}|^2|\Delta_{-\mathcal{Q}_x}|^2 + |\Delta_{\mathcal{Q}_y}|^2|\Delta_{-\mathcal{Q}_y}|^2)\\ &+ \gamma_2(|\Delta_{\mathcal{Q}_x}|^2 + |\Delta_{-\mathcal{Q}_x}|^2)(|\Delta_{\mathcal{Q}_y}|^2 + |\Delta_{-\mathcal{Q}_y}|^2)\\ &+ \frac{\gamma_3}{2}(\Delta^*_{\mathcal{Q}_x}\Delta^*_{-\mathcal{Q}_x}\Delta_{\mathcal{Q}_y}\Delta_{-\mathcal{Q}_y} + \text{c.c.}).\end{aligned} \tag{3}$$

Here, we neglect variations along the z axis, thus $j = x,y$ is the spatial index, while $\hat{q}$ is a wave-vector index: $\hat{q} = \mathcal{Q}_x, -\mathcal{Q}_x, \mathcal{Q}_y, -\mathcal{Q}_y$. In the following, another convenient index, $q = \mathcal{Q}_x, \mathcal{Q}_y$, will also be used. The coefficients $k_{\hat{q},j}$ of the kinetic term satisfy the relation $k_{\pm\mathcal{Q}_x,x} = k_{\pm\mathcal{Q}_y,y} \equiv 1 - k$ and $k_{\pm\mathcal{Q}_x,y} = k_{\pm\mathcal{Q}_y,x} \equiv 1 + k$, and k measures the anisotropy of the system [27]. Here $\mathcal{Q}_x$ represents the wave vector $\boldsymbol{\mathcal{Q}}_x = (\mathcal{Q},0)$, $\mathcal{Q}_y$ represents $\boldsymbol{\mathcal{Q}}_y = (0,\mathcal{Q})$, and $\Delta_{\mathcal{Q}_x}$ represents the gap associated with the pairing between the fermion states $|\boldsymbol{k} + \boldsymbol{\mathcal{Q}}_x,\uparrow\rangle$ and $|\boldsymbol{k},\downarrow\rangle$, where $\boldsymbol{k}$ is the momentum and $\uparrow$, $\downarrow$ denote the spin states. Our choice of the wave vectors and model for the PDW order is motivated by the recent proposal of Amperean pairing by Lee [7], for which it has been shown that PDW order can account for both the anomalous quasiparticle properties observed by ARPES and the CDW order (at momenta $2\boldsymbol{\mathcal{Q}}_x$ and $2\boldsymbol{\mathcal{Q}}_y$) observed in the pseudogap phase of $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ (Bi2201). Depending on the parameters γ_i, the free energy of the PDW sector (3) allows five possible distinct ground states [5]. We choose parameters such that, in the noncompeting case, the PDW ground state has the form $\Delta^\dagger_{\rm PDW} = \Delta^*_0(1,1,i,i)$. This PDW ground state is the same as that proposed in Ref. [7] and is also found to be a ground state in the spin-fermion model [28,29].

Both Δ_d and $\Delta_{\rm PDW}$ interact with the magnetic field (through the kinetic terms) and are therefore indirectly coupled. They also directly interact through $\mathcal{F}_{\rm Int}$:

$$\begin{aligned}\mathcal{F}_{\rm Int} =& \gamma_4|\Delta_d|^2\left(|\Delta_{\mathcal{Q}_x}|^2 + |\Delta_{-\mathcal{Q}_x}|^2 + |\Delta_{\mathcal{Q}_y}|^2 + |\Delta_{-\mathcal{Q}_y}|^2\right)\\ &+ \frac{\gamma_5}{2}([\Delta^*_{\mathcal{Q}_x}\Delta^*_{-\mathcal{Q}_x} + \Delta^*_{\mathcal{Q}_y}\Delta^*_{-\mathcal{Q}_y}]\Delta_d{}^2 + \text{c.c.}).\end{aligned} \tag{4}$$

The first term in (4) is a biquadratic coupling between the d wave and the pair-density wave $\sim \gamma_4|\Delta_d|^2|\Delta_{\rm PDW}|^2$. The coexistence of both order parameters is penalized for positive values γ_4 and, when strong enough, only one of the condensates supports a nonzero ground-state density. Our choice of parameters is such that when $H = 0$, Δ_d has lower condensation energy and $\Delta_{\rm PDW}$ is completely suppressed because of the interaction terms (4). Moreover, as CDW order emerges at high field, we require $\Delta_{\rm PDW}$ to have a higher second critical field (${\rm H}_{c2}^{\rm PDW}$) than Δ_d (${\rm H}_{c2}^{d\text{-wave}}$). These conditions lead to Fig. 1. We note that, in principle, the existence of the competing PDW order can allow for the PDW-driven CDW order to appear in zero field in the vicinity of inhomogeneities or due to fluctuations in some materials. Indeed, CDW order has been observed in $YBa_2Cu_3O_{6.67}$ in zero field through high-energy x-ray diffraction [30] (this CDW order is enhanced by magnetic fields).

III. PDW-DRIVEN CDW ORDER

We take CDW order to be denoted by $\rho(\boldsymbol{r}) = \sum_{\hat{q}} e^{i\hat{\boldsymbol{q}}\cdot\boldsymbol{r}}\rho_{\hat{q}}$ (note that $\rho_{-q} = \rho_q^*$). The coupling between ρ_{2q} (with $q = \mathcal{Q}_x, \mathcal{Q}_y$) and PDW order is given by [5–7]

$$\sum_{q=\mathcal{Q}_x,\mathcal{Q}_y} \alpha_2|\rho_{2q}|^2 + \epsilon_2(\rho_{2q}\Delta_{-q}\Delta^*_q + \rho_{-2q}\Delta_q\Delta^*_{-q}). \tag{5}$$

Assuming that the CDW order is induced by the PDW order, we find that

$$\rho_{\pm 2q} = \rho^*_{\mp 2q} = -\frac{\epsilon_2}{\alpha_2}\Delta_{\pm q}\Delta^*_{\mp q}. \tag{6}$$

The CDW order given by ρ_{2q} corresponds to that observed in the pseudogap phase in zero field and to the checkerboard order observed inside the d-wave vortex cores. An important feature of this work is that the interplay between d-wave and PDW orders gives rise to an additional contribution to the CDW order. In particular, this coupling is given by [5–7]

$$\begin{aligned}\sum_{q=\mathcal{Q}_x,\mathcal{Q}_y} \alpha_1|\rho_q|^2 + \epsilon_1(\rho_q[\Delta_{-q}\Delta^*_d + \Delta^*_q\Delta_d]\\ + \rho_{-q}[\Delta_q\Delta^*_d + \Delta^*_{-q}\Delta_d]).\end{aligned} \tag{7}$$

Differentiation with respect to ρ^*_q and ρ_q yields the relations (this also assumes the CDW order is purely induced)

$$\rho_{\pm q} = \rho^*_{\mp q} = -\frac{\epsilon_1}{\alpha_1}(\Delta_{\pm q}\Delta^*_d + \Delta_d\Delta^*_{\mp q}). \tag{8}$$

The contributions $\rho_{\mathcal{Q}}$ and $\rho_{2\mathcal{Q}}$ to the CDW are reconstructed according to

$$\rho_{n\mathcal{Q}} = \sum_{q=\mathcal{Q}_x,\mathcal{Q}_y} \rho_{nq}e^{in\boldsymbol{q}\cdot\boldsymbol{r}} + \rho_{-nq}e^{-in\boldsymbol{q}\cdot\boldsymbol{r}}, \tag{9}$$

which shows the nth-order contribution to the CDW. The CDW order $\rho_{\mathcal{Q}}$ has twice the periodicity of $\rho_{2\mathcal{Q}}$ and is not an induced order of the pure $\Delta_{\rm PDW}$: it only appears when both Δ_d and $\Delta_{\rm PDW}$ coexist. Consequently, ρ_Q is a signature of the appearance of $\Delta_{\rm PDW}$ in a d-wave superconductor. Note that the existence of ρ_Q requires superconducting phase coherence for both the PDW and d-wave orders (strictly speaking, coherence in the phase difference between these two orders will suffice). We note that an observation of ρ_Q has been reported [31], and below we make predictions about the structure of ρ_Q around a vortex in Δ_d.

IV. VORTEX PROPERTIES AND CHECKERBOARD PATTERN

In order to investigate the interplay of $\Delta_{\rm PDW}$ and Δ_d, within the framework sketched in Fig. 1, we numerically minimize the free energy (1), both for single vortices and for a finite sample in an external field. The theory is discretized within a finite element formulation [32] and minimized using a nonlinear conjugate gradient algorithm (for detailed discussion on the numerical methods, see, for example, [33]).

Typical single vortex solutions (see Fig. 2) clearly show that the components of the PDW order acquire small, yet nonzero density at the center of the d-wave vortex core. As a result, the CDW order is also nonzero at the vortex core. Far from the vortex, the $\Delta_{\rm PDW}$ decays to zero, and the induced CDW is suppressed as well. Figure 3 shows the magnitude of the total CDW order as well as the contributions from different orders in $\mathcal{Q}$. Here, we used the values $\mathcal{Q} = \pi/d$ and $d = 4a_0$, where a_0 is the Cu-Cu distance in cuprates and, in qualitative accordance with experimental data [34], we take the d-wave coherence length to be $\xi_d = 13a_0$. ρ_{2Q} forms a checkerboard pattern that extends significantly outside the vortex core, and this is consistent with the observations.

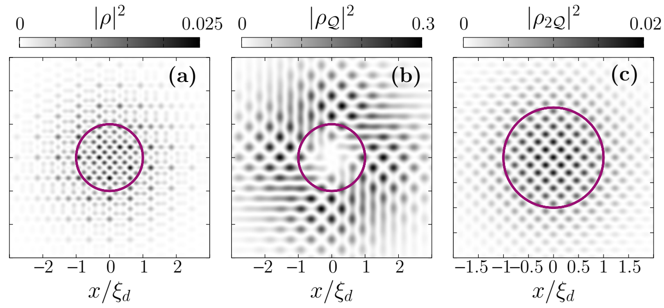

FIG. 3. (Color online) The (a) charge-density-wave order and the contributions of (b) ρ_Q and (c) ρ_{2Q}, as defined in (9). The parameters are the same as in Fig. 2 except that $\gamma_5 = 1.0$. The circle of radius ξ_d, the coherence length of the d wave, indicates the size of the vortex core. ρ_Q and ρ_{2Q} are shown for unit value of the ratios ϵ_1/α_1 and ϵ_2/α_2, while ρ, the total charge density, is shown for $\epsilon_1/\alpha_1 = 1$ and $\epsilon_2/\alpha_2 = 0.1$. As a result, ρ shows a checkerboard in the vortex core. Furthermore, since ρ_Q varies with twice the wavelength as ρ_{2Q}, away from the core, every other peak in ρ is magnified.

In addition to this checkerboard order, we also find that ρ_Q, which varies at twice the wavelength of ρ_{2Q}, is nonzero and also has a nontrivial structure. More precisely, at the singularity in the d wave, $\rho_Q = 0$, and when Δ_d becomes nonzero, ρ_Q also becomes nonzero. Since $\Delta_{\rm PDW}$ exhibits no phase winding, ρ_Q inherits the phase winding of Δ_d. A phase winding in ρ_Q implies a dislocation in the corresponding real-space order [35]. Consequently, the CDW order associated with ρ_Q has a dislocation at the vortex core. Since ρ_Q is suppressed in vortex cores, the checkerboard pattern that appears there is essentially due to ρ_{2Q}. The contribution of ρ_Q to the CDW becomes important at distances larger than ξ_d. Moreover, as it varies with a doubled wavelength, every other charge peak is magnified in a region outside the core. Note that away from the vortex, ρ_Q is suppressed at a much slower rate than ρ_{2Q}. Furthermore, if ρ_Q is observable at all, then it should vanish at $H_{c2}^{d\text{-wave}}$, while ρ_{2Q} will persist to much higher fields.

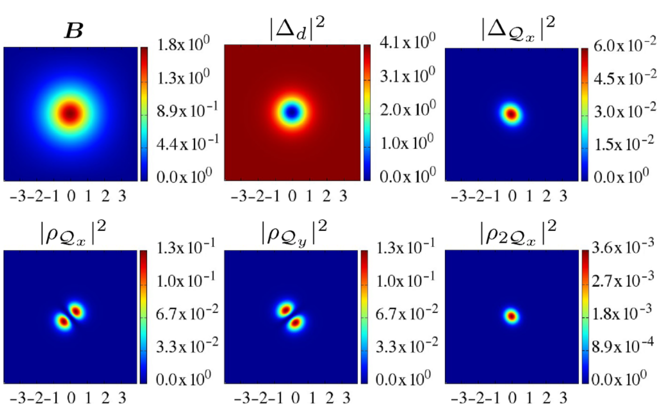

FIG. 2. (Color online) The core structure of a single d-wave vortex. The parameters are $(\alpha,\beta) = (-5,10)$ and $\gamma_2 = \gamma_1/2 = 10\gamma_5 = 3$, while the parameters for the d-wave order are $(\alpha_d,\beta_d) = (-2.5,0.61)$. The parameters of the interaction (4) that directly couple the PDW and the d-wave order are $\gamma_4 = 2$, $\gamma_5 = 0.5$ and the gauge coupling constant is $e = 0.4$. The d-wave order has nonzero ground-state density and has a vortex, while the components of the PDW are zero in the ground state. At the core of the Δ_d vortex, because there is less density, it is beneficial for the components Δ_d of the PDW to condense, as shown in the right panel of the first line (here we show only Δ_{Q_x} as the other components behave similarly). The second line displays the induced CDW: ρ_{2q} (6) and ρ_q (8) (note ρ_{2Q_y} is similar to ρ_{2Q_x}).

V. FIELD-INDUCED PDW AND CDW ORDERS

To investigate the evolution of the PDW and d-wave orders in external field $\boldsymbol{H}$, for parameters corresponding to Fig. 1, we minimize the free energy (1), while imposing $\nabla \times \boldsymbol{A} = \boldsymbol{H}$ at the (insulating) boundary of the domain. We follow the vertical line sketched in Fig. 1. That is, starting from $H = 0$, the field is sequentially increased after the solution for the current value of H is found. Typical results illustrating such a simulation are shown in Fig. 4. In low fields, only Δ_d has a nonzero ground-state density and, as a result of the competition with Δ_d in the interacting terms (4), $\Delta_{\rm PDW}$ is fully suppressed (or vanishingly small).

Above the first critical field, vortices in Δ_d, carrying a small amount $\Delta_{\rm PDW}$ in their core, start entering the system. The averaged PDW over the whole sample $\langle|\Delta_{\rm PDW}|\rangle$ is still vanishingly small. With increasing field, the density of vortices increases and they start to overlap [36]. That is, $|\Delta_{\rm PDW}|$ and

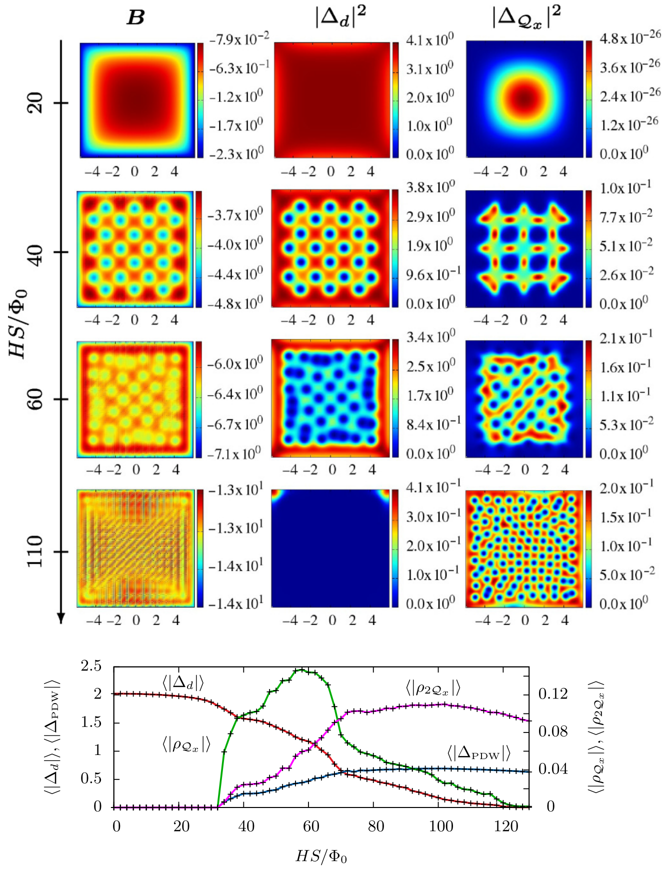

FIG. 4. (Color online) Simulation over a finite sample with increasing values of the external field (values are shown on the left) for the same parameters as in Fig. 3. The first column shows the magnetic flux, the second column shows $|\Delta_d|^2$, and the last column shows $|\Delta_{Q_x}|^2$ (other components of the PDW behave similarly to Δ_{Q_x}). The graph at the bottom shows order parameters averaged over the sample, as functions of the applied field. There, we show the densities of the d-wave and PDW order, as well as the induced CDW contributions ρ_{Q_x} and ρ_{2Q_x}. Above a certain external field (here $HS/\Phi_0 = 32$), because of the suppression of the d-wave order, the PDW develops a nonzero expectation. The appearance of the PDW in an external field is also accompanied by induced CDW order.

$|\Delta_d|$ do not have "enough room" to recover their ground-state values. At this point, the lumps of $\Delta_{\rm PDW}$, previously isolated in vortex cores, interconnect and $\Delta_{\rm PDW}$ acquires a phase coherence globally. This behavior was also found to occur in a similar system with competing orders [37]. At this phase transition, not only does $\langle|\Delta_{\rm PDW}|\rangle$ become nonzero, but the induced CDW, $\rho_{\pm q}$ and $\rho_{\pm 2q}$, also become nonzero on average (see Fig. 4). We conjecture that this phase transition is related to that seen though NMR [38].

When the PDW order is on average nonzero, energetic considerations dictate that it should acquire phase winding as well. Indeed, when two condensates have nonzero density, the energy of configurations that has winding in only one condensate diverges (at least logarithmically) with the system size. As a result, vortices in $\Delta_{\hat q}$ are created when $\langle|\Delta_{\rm PDW}|\rangle \neq 0$ [37]. Note that as it is still beneficial to have nonzero $\Delta_{\rm PDW}$ inside the vortex cores of Δ_d, the singularities that are formed due to the winding in $\Delta_{\hat q}$ do not overlap with those of Δ_d [and they do not overlap with each other due to the terms γ_i in (3), which favor core splitting]. Thus, the CDW order still appears within the vortex cores of Δ_d. Since all the vortices that are created do not overlap with each other, the magnetic induction is smeared out and is much more spatially uniform than in usual vortex phases.

For fields above the second critical field of Δ_d, only the PDW order survives. As a result, the contribution ρ_Q to the induced CDW also vanishes and the observed CDW order above $H_{c2}^{d\text{-wave}}$ is solely that induced by the PDW (that is ρ_{2Q}). In this state, at the mean-field level, the vortices in $\Delta_{\hat q}$ do not overlap, as the terms with γ_i in (3) favor vortex core splitting. In principle, the parameters γ_i can also be chosen so that the $\Delta_{\hat q}$ cores coincide for some or all PDW components. This will not change the qualitative physics associated with the competition between Δ_d and $\Delta_{\rm PDW}$. However, it will affect the resulting high-field regime. In either case, we expect superconducting phase fluctuations to play an important role in the high-field phase. In particular, it is known that for type-II superconductors, high magnetic fields significantly enhance the role of fluctuations [39,40]. Phase fluctuations will remove the superconducting long-range order of the PDW state, but the CDW order can still survive [26]. A related mechanism was also considered in a different but related model of superconductivity [41].

VI. CONCLUSIONS

We have considered a model of competing pair-density-wave and d-wave superconductivity. The superconducting state in the Meissner phase is purely d wave. With increasing external field, vortices in the d-wave superconductor are formed and they carry PDW and induced CDW order in their core. When these vortices significantly interact, the lumps of PDW order acquire global phase coherence and both PDW and d-wave superconductivity coexist. In the regions where both PDW and d-wave order exist, the induced CDW order features a ρ_Q contribution that exists at twice the periodicity of the CDW order observed in the pseudogap phase at zero fields. The observation of ρ_Q can serve to identify the existence of PDW order in the pseudogap phase.

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