Incommensurate DDW order

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We consider various incommensurate (IC) order parameters for electrons on a square lattice which reduce to $d_{x^2−y^2}$-density wave (DDW) order when the ordering wavevector $\mathbf{Q} \rightarrow (\pi, \pi)$. We describe the associated charge and current distributions and their experimental signatures. Such orders can arise at the mean-field level in extended Hubbard models. We compare the phase diagrams of these models with experiments in the underdoped cuprates, where (1) DDW order is a possible explanation of the pseudogap, and (2) there are experimental indications of incommensurability. We find various types of IC DDW and discuss their possible relevance to the physics of the cuprates. Our main finding is that IC DDW order is generally accompanied by superconducting order, but the magnitude of the IC wavevector can be small. A comparison with the analogous AF-ICSDW transition is given.

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I. INTRODUCTION

When a commensurate one-dimensional charge density wave (CDW) is doped, the resulting charges may be viewed as defects in the CDW. If the interactions between them are sufficiently strong compared to their effective kinetic energy, then they will form an ordered lattice (which can be stabilized by a crossover to 3D or effective kinetic energy, then they will form an ordered density wave (CDW). If the interactions be viewed as defects in the CDW. If the interactions

In this paper we consider various ways in which $d_{x^2−y^2}$-density wave (DDW) order can go incommensurately. Before turning to this discussion, we review the reasons for expecting DDW order to occur in the pseudogap regime of the cuprates. It has been suggested that competition between DDW order and $d$-wave superconductivity (DSC) can explain many of the anomalous properties of the pseudogap. The DDW order parameter is given by

$$\langle c_{i,k\sigma}^\dagger c_{i+k,Q\sigma} \rangle = i\Phi f(k)$$

with $f(k) = \cos(k_x) - \cos(k_y)$ and a commensurate (C) ordering wavevector $\mathbf{Q} = (\pi, \pi)$. The particle-hole condensate in \[1\] breaks translation by one lattice spacing, parity, and time-reversal but is invariant under the combination of any two of the above symmetries. In real space it is represented by currents which alternate from one plaquette to the next.

One motivation for considering DDW order is to explain the abrupt depletion of the superfluid density below the critical $x_c \approx 0.19$ in Bi2212 and similar dopings in other materials. Because the order has a $d$-wave momentum dependence, its onset would explain ARPES measurements above $T_c$ in the pseudogap. Furthermore, since DDW is a spin-singlet condensate, it would also explain the suppression of the spin susceptibility in NMR measurements and opening of a spin gap in inelastic neutron scattering. Also, the depletion of the c-axis conductivity, whose contribution mostly comes from the antinodal regions, would also be naturally ex-
plained by the development of DDW order, which gaps these regions. Direct attempts to measure DDW order through neutron scattering have neither ruled it out nor unambiguously verified its presence, but there are intriguing suggestions that it may be present. Thus, it is natural to ask whether DDW order is compatible with incommensurability. (For a discussion of the experimental signatures of DDW order, the reader is referred to the literature. The case of DDW in $La_{2-x}Ba_xCuO_4$ is discussed in. For numerical evidence of the existence of DDW in other systems, one is referred to.)

The plan of our paper is as follows. In section II we develop some preliminary intuition about the energetics of IC density wave order by analyzing the DDW susceptibility of a Fermi liquid (both the nested and non-nested cases). In section III we review some of the theory of commensurate (C) DDW order and show various ways to make it incommensurate. We also suggest the kind of microscopic physics that could lead to C and IC DDW, and in addition discuss possible experimental signatures of IC DDW. Finally, in section IV we compute the mean-field phase diagrams of an extended Hubbard model. Our main results are that (a) IC DDW develops for a wide range of parameters, but (b) the IC wavevectors can be very small. Their relevance to the cuprates may, at most, be for a rather narrow set of dopings. We also offer a physical explanation of our results, which sheds some light on the nature of C-IC DDW transition in extended Hubbard models. We note that similar incommensurate order has been found in refs.

II. SUSCEPTIBILITY NEAR HALF-FILLING

The easiest way to see that IC DDW phases could arise in effective models (which, in this paper, will, in turn, emerge from microscopic extended Hubbard models with correlated hopping terms, see section III C for details) is to consider the bare susceptibility as a function of the incommensurability wavevector $q$, where $Q = (\pi, \pi)$:

$$\chi_0(q) = \frac{1}{2\pi^2} \int_k (f(k))^2 \frac{n_F(\epsilon_k+\mu) - n_F(\epsilon_k-\mu)}{\epsilon_k - \epsilon_{k+q}}.$$  \hspace{1cm} (2)

where $f(k)$ is defined after eq. Here, for simplicity, DDW is considered without the presence of any other order. In eq. $n_F$ is the Fermi occupation number, and the energy dispersion contains nearest, $t$, and next-nearest neighbor, $t'$, hopping parameters, $\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$. The DDW equivalent of the Stoner criterion is satisfied when the right-hand-side of this equation approaches the inverse of the pertinent coupling $1/\beta$. This observation allows us to interpret the positions of the peaks of $\chi_0(q)$ as the wavevectors at which DDW order is likely to occur as we lower the temperature. A similar analysis was done by Schulz for the case of AF and IC SDW order in the Hubbard model close to half-filling, where perfect nesting at half-filling was assumed. In fact, his results can be recovered by letting $f(k) \rightarrow 1$ in if we set $t' = 0$.

The support of $(f(k))^2$ in the integrand in $2$ is at $(0, \pi)$ and symmetry-related antinodal points of the FS since this is where the DDW order parameter is large. However, since these points are also the location of van Hove singularities, the regions around them also dominate the AF susceptibility. Thus, at least in the $t' = 0$ case, one expects that whenever an IC SDW instability occurs, an IC instability for DDW should also occur. Indeed, for both orders, the peak of $\chi_0(q)$ occurs at $q \neq 0$ for low enough temperatures and sufficiently away from half-filling, e.g. if $|\mu| \beta \geq O(1)$, as shown in Fig. 1. Note that the same analysis repeated with any other density wave or spin-density wave order would yield an IC instability as long as the dominant channels of the modulation coincide with Fermi surface points which give large contributions to the susceptibility. For instance, a $p_x$-density wave with wavevector $Q = (0, \pi) + q$ has a peak in $\chi_0$ for $q \neq 0$ away from half filling at $T \simeq 0$, in the case $t' = 0$.

A natural question to ask is: to what extent does the IC DDW instability mimic the IC SDW one? To answer this, one needs to consider specific models as we do in III C. However, two differences can be anticipated even beforehand. First, the DDW order parameter has nodes, while the AF order parameter does not. Second, in a more realistic model, one must consider competition with DSC, which also could change features of the tran-
sition to IC state. A better understanding of IC DDW order parameter is necessary to better understand the the situation away from half-filling.

III. C VS. IC ORDER

A. C Order parameter

Given that the susceptibility (2) points towards an IC instability, the next issue is what IC DDW order would look like. Before addressing this question, let us first summarize some features of the C-case. In the C case, a general singlet particle-hole condensate can be written as (neglecting the $k = k'$ contribution):

$$\langle c_{\alpha,k}^\dagger c_{\alpha,k} \rangle = i\Phi f(k) \delta^\alpha \delta_{k',k+Q}. \quad (3)$$

Here, $\Phi$ is the magnitude of the order parameter. The wavevector $2Q$ is a reciprocal lattice vector. The spin index $\alpha$ included above will be omitted in the future for simplicity unless clarity requires otherwise. In (3), the form factor $f(k)$, which can transform non-trivially under the point group of the 2-D lattice, is related to the angular momentum of the particle-hole condensate. For DDW order, $f(k) = \cos k_x - \cos k_y$ which corresponds to $l = 2$ and $d_{x^2-y^2}$ symmetry. A $p_z$-density-wave with $Q = (0, \pi)$ has $f(k) = \sin k_x$, which corresponds to $l = 1$.

In real space, (3) becomes

$$\langle c_{\alpha,k}^\dagger c_{\alpha,k} \rangle = \mathcal{V}(r, r') \Phi \cos(Q \cdot r) \quad (4)$$

where the vertices $\mathcal{V}$ of the orders discussed above are given by

$$-i\mathcal{V}^{DDW}(r, r') = \delta_{\alpha',\alpha} \delta_{r',r} + \delta_{\alpha',\alpha} \delta_{r',r} - \delta_{\alpha',\alpha} \delta_{r',r} - \delta_{\alpha',\alpha} \delta_{r',r}.$$

$$-i\mathcal{V}^{PDW}(r, r') = \delta_{\alpha',\alpha} \delta_{r',r} - \delta_{\alpha',\alpha} \delta_{r',r}. \quad (5)$$

Note that the factors of $i$ in $\mathcal{V}^{DDW}$ and $\mathcal{V}^{PDW}$ signify that the corresponding phases break time-reversal, e.g. current flows along the bonds. Positive/negative signs in $\mathcal{V}$ represent current going in/out of the vertex. Translation invariance, by default, is broken by any density wave order since there is a preferred vector $Q$, but in the C case, invariance under a subset of the lattice group is retained. DDW order, for example, is invariant under translation by linear combinations of even reciprocal lattice vectors along each bond direction. The current along the bonds is given by:

$$j_{r+\tilde{x},r+\tilde{y}} = i\hbar(\langle c_{\alpha,k}^\dagger c_{\alpha,k+\tilde{x}} \rangle - \langle c_{\alpha,k+\tilde{x}} c_{\alpha,k} \rangle) \quad (6)$$

Here $\tilde{s}$ is along either the $\tilde{x}$- or $\tilde{y}$-direction. Because of the equivalence of $Q = -Q$ in the C case, the current is simply $j_{r+r+\tilde{s},r+\tilde{s}} \sim \cos(Q \cdot \tilde{s}) \sim \langle c_{\alpha,k}^\dagger c_{\alpha,k+\tilde{s}} \rangle$. In the DDW case this results in an alternating plaquette current/checkerboard magnetic field patterns.

B. IC Order Parameter

To obtain an IC version of DDW order, one first notes that DDW is chiral and hence breaks the Ising symmetry which reverses all the clockwise plaquette currents into counter-clockwise and vice versa. Therefore one can construct anti-phase domain walls as in Fig 2a. A simple caricature of a bond-oriented domain wall is given in Fig 2b. Its real space representation is

$$\langle c_{\alpha,k}^\dagger c_{\alpha,k} \rangle = \mathcal{V}^{IC}(r, r') \Phi \cos(Q \cdot r) \times (2\Theta(r_x) - 1) + \mathcal{V}^{IC} \quad (7)$$

where $\Theta(x)$ is the step function, so

$$2\Theta(x) - 1 = \sum_n A_{2n+1} \sin\left(\frac{2n+1}{L} \pi x \right) \quad (8)$$

with $A_{2n+1} = 4/\pi(2n+1)$. At the midpoint of the domain wall, the currents in the $x$-direction vanish while the currents in the $y$-direction are halved. The diagonal domain wall depicted in figure 2b has a similar representation. Note that because of the halving of the $y$-direction currents at the midpoint of the bond-domain wall in (7), we need to include the term:

$$\mathcal{V}^{IC} = \mathcal{V}^{R}(r, r') \delta_{r,0} + \mathcal{V}^{L}(r, r') \delta_{r,1} \quad (9)$$

where the new vertices $\mathcal{V}^{L,R}$ are given by:

$$-i\mathcal{V}^{L} = \delta_{\alpha',\alpha} \delta_{r',r} - \frac{1}{2} \delta_{\alpha',\alpha} \delta_{r',r+\tilde{x}} - \frac{1}{2} \delta_{\alpha',\alpha} \delta_{r',r-\tilde{x}} - \frac{1}{2} \delta_{\alpha',\alpha} \delta_{r',r+\tilde{y}} - \frac{1}{2} \delta_{\alpha',\alpha} \delta_{r',r-\tilde{y}}. \quad (10)$$

Such vertices seem necessary for IC transitions of current density waves. One could imagine situations in which the transition to a disordered state is driven by thermal proliferation of such vertices, similar to earlier analysis of the 6-vertex model. Although the analysis of such a transition is an interesting topic on its own, we will not pursue it in this paper. We are more interested in the energetics of the IC phase, so a long-wavelength mean-field treatment is sufficient.

To analyze the C-IC transition, one then considers an array of alternating domain walls with average separation $L$. Then, in the single harmonic approximation one retains only the $n = 0$ term in (8) and identifies $q = \pi / L$ with the incommensurability wavevector. The new short-range vertex contributions are also neglected in the lowest harmonic approximation. The neglect of higher harmonics should not change the transition temperature or the value of the critical doping for the onset of IC order since $\Phi$ is small and the corrections are of higher order in $\Phi$. An incommensurate instability in a clean system occurs when $L$ becomes finite. (In a disordered system, it occurs when when $L \leq L_d$, where $L_d$ is a characteristic length scale for the disorder.)

Within the single harmonic approximation, an array of anti-phase domain walls with separation
\[ |q| = |Q - (\pi, \pi)| = \pi/L, \] looks simpler in momentum space:

\[ \langle c^\dagger_k c_k \rangle = i \frac{\Phi}{2} f(k)(\delta_{k'k+Q} + \delta_{k'k-Q}). \]  

(11)

Note that in the limit \(|q| \to 0\), the above reduces to \[8\]. One could have guessed the result \[8\] by writing \(2\delta_{k'k+Q} = \delta_{k'k+Q} + \delta_{k'k-Q}\) in the commensurate case, and then let \(Q\) go incommensurate. This suggests other ways to get IC order. In particular the oddness of DDW order with respect to rotations by \(\pi/2\) and transpositions about, say, the \((\pi, \pi)\) direction lead to the following example of a DDW checkerboard pattern:

\[ \langle c^\dagger_k c_k \rangle = i \frac{\Phi}{4} f(k)(\delta_{k'k+Q} + \delta_{k'k-Q}) - \{Q \to O(Q)\} \]  

(12)

where the operation \(O(Q)\) can be either a transposition, or a rotation by \(\pi/2\). The checkerboard pattern in \[12\] corresponds to simply superimposing two domain walls rotated by \(\pi/2\) with respect to each other.

In a similar spirit, one could also investigate the possibility of non-topological domain walls, e.g. IC domains as the above, superimposed with an uniform order, so the overall order parameter does not change chirality. However, as we will see in Sec. \[IV\] much of the physics of the C-IC transition will already be transparent from the simpler choices \[11\] and \[12\] of order parameter.

Finally, note that within the single harmonic approximation, \[11\] and \[12\] are current-conserving only to lowest order in \(q\). For the purpose of clarifying the energetics of the IC order close to the C-IC transition, or in the cases where the magnitude of the incommensurability is small, this lowest order approximation is good enough. Our numerical results, Sec. \[IV\] a posteriori show that we are in such regime.

### C. Microscopic Models

We will consider the above order parameters in the context of the following Hamiltonian:

\[ \mathcal{H} = -t_{ij} \sum_{\langle i,j \rangle} \left( c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) - t_c \sum_{\langle i,j \rangle, \langle i',j' \rangle} \langle i',j' \rangle \langle i,j \rangle \, c^\dagger_{i\sigma} c_{j\sigma}^\dagger c^\dagger_{i'\sigma} c_{j'\sigma} + V \sum_{\langle i,j \rangle} n_{i\uparrow} n_{j\uparrow} \]  

(13)

In this formula, \(t_{ij}\) is hopping with \(t_{ij} = t\) for nearest neighbors, \(t_{ij} = t'\) for next nearest neighbors and \(t_{ij} = 0\) otherwise, \(t_c\) is a correlated hopping term which simultaneously hops an electron from site \(j\) to site \(i\) and hops an electron from \(i'\) into the vacated site \(j\). The on-site and nearest-neighbor repulsions are, respectively, \(U\) and \(V\). The indices \(i, j\) signify lattice sites and \(\sigma\) the spin.

We will consider this Hamiltonian at the mean-field level. At this level, the energetics of DDW order is the same as for a ‘BCS-reduced’ Hamiltonian for DDW order of the form:

\[ \mathcal{H}_{DDW} = -g_{DDW} \int f(k) f(k') c^\dagger_{k+Q\sigma} c_{k'\sigma} c^\dagger_{k\sigma'} c_{k'\sigma'}, \]  

(14)

with \(g_{DDW} = 24t_c + 8V\). A similar reduced Hamiltonian for d-wave superconductivity has \(g_{DSC} = 12t_c - 8V\). Note that the processes responsible for both DSC and DDW are essentially kinetic.

A Hamiltonian of the form \[13\] has one important virtue: it has a \(d\)-wave superconducting ground state over a range of dopings (and an antiferromagnetic ground state at half-filling). Since this is the \textit{sine qua non} for any description of the cuprates, we believe that this is a good starting point. One may object that correlated hopping terms have to be put in by hand in a microscopic Hamiltonian. However, they naturally arise even from the one-band Hubbard model away from half-filling, where their contribution can be computed in \(t/U\) perturbation theory:

\[ t_c \simeq x \frac{e^3}{U^2} \]  

(15)

At dopings \(x = 0.1\), for \(t/U \sim 0.2\), we would have \(g_{DDW} = 2g_{DSC} \sim 0.1t = J/2\). Thus, not far away from half-filling, correlated hopping terms are certainly not negligible.
D. Mean Field Theory

Let us generalize the mean field description of C DDW to the IC case. The path we will take is similar to that in Sec. III B, where we wrote down the commensurate order parameter without making use of the Q → –Q symmetry, and as a result the generalization to incommensurate Q was straightforward. We thus obtain a functional F(μ, Δi, q), equation (20), whose minimization yields self-consistently both the order parameters Δi and the deviation from commensurability q = Q – π. The only subtlety, as we discuss at the end of this section, is that although F reduces to the mean-field free energy in the C phase, in the IC phase it is not the free energy even within the single harmonic approximation. Instead, minimization of F is equivalent to a variational search of the ground state.

Our derivations generalize the treatment of Nayak and Pivovarov26 of competition of C DDW with DSC and possibly AF. The C DDW mean field Hamiltonian we start with is:

\[ H_{\text{DDW}} = \int_{k \in \text{RBZ}} \{ i \frac{W_k}{2} c_{k\sigma}^\dagger c_{k+Q\sigma} + Q \rightarrow -Q \} + \text{h.c.} \]  \hspace{1cm} (16)

where \( W_k = \frac{W}{2} f(k) \).

Note that in (16) the \( Q \rightarrow -Q \) symmetry for incommensurate \( Q \) is not equivalent to the Hermiticity of the Hamiltonian due to the k-dependence of \( W_k \) (e.g., \( \langle c_{k\sigma}^\dagger c_{k+Q\sigma} \rangle = iW_k \neq \langle c_{k\sigma}^\dagger c_{k-Q\sigma} \rangle^* = -iW_k-Q \) for IC \( Q \)). This is unlike the case of AF order, where the interaction is simply

\[ H_{\text{AF}} = \int_{k \in \text{RBZ}} \phi (c_{k\uparrow}^\dagger c_{k+Q\uparrow} - c_{k\downarrow}^\dagger c_{k-Q\downarrow}) + \text{h.c.} \]  \hspace{1cm} (17)

and we have \( \langle c_{k\sigma}^\dagger c_{k-Q\sigma} \rangle = \phi = \langle c_{k\sigma}^\dagger c_{k-Q\sigma} \rangle^* \).

In order to check with earlier results on the C-IC transition of AF order in the weak coupling Hubbard model22 (see Sec. III B, we will also include a term like (17) in our full reduced Hamiltonian. Of course, in the strong coupling, \( U > t \), limit, one is not justified in treating AF as a Fermi surface instability, especially close to half filling. A \( t – J \) description is more appropriate in this case. However, as mentioned in Sec. III C both DDW and DSC are essentially kinetic in origin within the extended Hubbard model, so even in the strong onsite repulsion limit, there is a good justification to use mean field theory to describe their competition away from half filling.

In the C case, the standard DSC term in our reduced Hamiltonian is:

\[ H_{\text{DSC}} = \int_{k \in \text{RBZ}} \Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow} + \text{h.c.} \]  \hspace{1cm} (18)

where \( \Delta_k = \frac{\Delta}{2} f(k) \). Using a Nambu basis \( \Psi_k = (c_{k\uparrow}, c_{k+Q\uparrow}, c_{-k\downarrow}, c_{-k-Q\downarrow}) \), the full Hamiltonian \( H = H_{\text{kin}} + H_{\text{AF}} + H_{\text{DDW}} + H_{\text{DSC}} \) can be rewritten as \( H - \mu N = \int_{\text{RBZ}} \Psi_k^\dagger \cdot A \cdot \Psi_k \) where

\[ A \equiv \begin{pmatrix} c_k - \mu & iG_k + \phi & \Delta_k & 0 \\ c_k^* - \mu & c_k^* + Q - \mu & 0 & \Delta_{-k-Q} \\ 0 & c_k & -c_k + \mu & iG_{-k} - \phi \\ 0 & c_k^* & c_k & -c_k^* + \mu \end{pmatrix} \]  \hspace{1cm} (19)

with \( G_k = (W_k - W_k + Q)/2 \). The action derived from the above Hamiltonian yields, upon integrating the Fermions out, the free energy in the ordered state:

\[ \mathcal{F}_q = \mathcal{F}_{\text{quad}} + \sum_{s = \pm} \int_{k \in \text{RBZ}} \{ (s \epsilon_k - \mu - \frac{2}{\beta} \ln 2 \cosh(\frac{\beta E_s}{2})) \} \]  \hspace{1cm} (20)

with \( \pm E_s, s = \pm 1 \) the energy eigenvalues of (19), and

\[ \mathcal{F}_{\text{quad}} = \frac{\phi^2}{g_{\text{DDW}}} + \frac{W_0^2}{g_{\text{DDW}}} + \frac{\Delta_0^2}{g_{\text{DSC}}} \]  \hspace{1cm} (21)

If we assume \( Q \rightarrow -Q \) symmetry, \( E_s \) would be given by:

\[ E_s(k) = \sqrt{\Delta_k^2 + (\mu - \epsilon_+(k)) + s \sqrt{\Phi_k^2 + \epsilon^2(k)}} \]  \hspace{1cm} (22)

where \( \epsilon_\pm(k) = (\epsilon_k \pm \epsilon_{k+Q})/2 \) and \( \Phi_k^2 = W_k^2 + \phi^2 \).

However, in the IC case, \( Q \rightarrow -Q \) need not hold, in which case the above would generalize to:

\[ E_s(k) = \sqrt{\Delta_k^2 + (\mu - \epsilon_+(k)) + s \sqrt{\Phi_k^2 + \epsilon^2(k)}} + D_q(\Delta^2_{\text{DSC}}, \Phi_k^2, \epsilon_k, \mu) \]  \hspace{1cm} (23)

The effect of a nonzero incommensurability \( Q \) can be seen not only in the appearance of the terms \( f_\pm^2(k) \equiv (f^2(k) \pm f^2(k + Q))/2 \) and \( f_k \equiv (f(k) + f(k + Q))/2 \), but also in the DSC-and doping-dependent function \( D_q \).

Our final step before letting \( Q \) be incommensurate is
to pass the integration in (20) from RBZ to BZ:

$$F - F_{\text{quad}} = \int_{RBZ} f_s(\mu, \beta, \Delta_i) = \frac{1}{2} \int_{BZ} f_s(\mu, \beta, \Delta_i)$$ (24)

Once we convert the RBZ integrals to BZ integrals as in (24), we numerically minimize (see Sec. IV) the resulting ‘free energy’ with respect to both the order parameters $\Delta_i$ and the deviation from commensurability $q$.

FIG. 3: Phase diagram of DDW competing with DSC. Both $g_{\text{DDW}} = 0.05eV$ and $g_{\text{DSC}} = 0.03eV$ are large (compare to Figs. 6 and 8) $t = 0.5eV$. The next nearest neighbor hopping, $t' = -0.05eV$, is small compared to typical values fitted to ARPES[2], but IC order was nevertheless robust away from half-filling. Inset: IC wavevector $q$ at $T = 0.01eV$ as a function of doping. Wavevectors are in units of $\pi/a$, where $a$ is the lattice spacing.

FIG. 4: Again $g_{\text{DDW}} = 0.04eV$, $g_{\text{DSC}} = 0.02eV$ are ‘large’ (note temperature scale) similar to Fig. 4 with $t = 0.5eV$. However this time we take a more realistic $t' = -0.12eV$. Again IC order is robust at dopings relevant for the pseudogap. Inset: IC wavevector $q$ at $T = 0.01eV$ as a function of doping. See Fig. 10 for a more detailed view of $q$ (and also Fig. 4 for the case of $t' = -0.06eV$).

IV. NUMERICAL RESULTS

To obtain the phase diagrams for the models in (20), for various fixed dopings $x$ and temperatures $T$, we minimize $F = F(\Delta_i, q)$ with respect to both the order parameters $\Delta_i$ (as was done previously in the C-case[29]) and the IC wavevector magnitude $q$. Each choice of IC order parameter (e.g. bond or diagonal) corresponds to a separate minimization procedure. To distinguish which IC order dominates at a particular point in $(x, T)$ space, we compared the free energies of the orders considered, and chose the IC phase of minimal energy. Note that, as given in (20), the free energy is a function of $\mu$, so to obtain the dependance on the doping $x$, we first perform a Legendre transformation and minimize instead $F(x) = F(\mu(x)) + \mu(x)N$ where the chemical potential is obtained from $1 - x = \partial f/\partial \mu$ with $f = F/N_0$.

Our approach is slightly different than that previously used in the C-case[29]. There, the competition between AF, DDW and DSC was analyzed, and some sensitivity on the details of the microscopics was found. Phase diagrams resembling that of the cuprates were obtained. The general trend was that any phase diagram which included $d$-wave superconductivity also had DDW order competing with it. By changing the bare coupling constants, rather different phase diagrams could be obtained and these generally did not have superconductivity.

In our treatment here, we do not consider the competition with AF order, which is not a Fermi surface instability anyway in the context of the cuprate superconduc-
In (20), we still include AF, but only in order to check with previous results \( t_q \) of IC AF order away from half filling in the weak coupling \( g_{AF} < t \) limit. On the other hand, the AF order appearing at half filling in the cuprates is a strong coupling phenomenon. A reduced Hamiltonian \( H \) is the wrong starting point at half filling in the limit \( U > t \).

Therefore, we only consider competition between DDW and DSC and look for IC order in this case. All the phase diagrams constructed this way are robust in the sense that DDW and DSC are found to coexist at mean field level for almost all reasonable values of the coupling constants.

Sample phase diagrams are shown in Figs. 3-6. In all of them, IC order is present at dopings \( 0.15 \lesssim x \lesssim 0.2 \) where DDW and DSC compete. In the first two of these figures, we vary \( t' \) at relatively high \( g_{DDW} \) and \( g_{DSC} \), while in the last two we explore the phase diagram for more realistic DDW and DSC couplings (compare the temperature scales to those in the cuprates). Note the complexity of Figs. 3, Figs. 6 compared to Figs. 5, Figs. 4. At realistic couplings, the IC wavevector profile is complicated, and furthermore DSC order appears in more than one doping region within the DDW dome. In fact, the appearance of incommensurability seems correlated with the appearance of DSC. A more systematic analysis to be discussed below reveals that generally the types of C-IC transitions that were produced in our phase diagrams fall into two categories: (a) those which correspond to motion of the bare Fermi surface away from commensurate nesting (shaded regions); (b) those which appear near certain ‘magic’ filling fractions. Case (a) is similar to the familiar C-IC mechanism discussed by Schulz, while case (b) appears to be a consequence of negative effective stiffness at special fractions, the exact nature of which at present is not clear. In both cases \( q \) is independent of the onset of DSC. Fig. 7 but because incommensurability relieves the DDW-DSC competition, the onset of DSC correlates to the presence of IC DDW.

Let us first discuss (a). It is well known that in the weak-coupling Hubbard model at \( t' = 0 \), the AF insta-
bility at half-filling is driven IC for any non-zero doping (see Sec. 2). The source of the C-IC transition can be traced to the approximate nesting of the bare Fermi surface (FS) at IC wavevectors away from half-filling. Close to half-filling, this picture would produce a linear deviation from commensurability, \( q \sim |\mu - \mu_c| \sim x - x_c \), Fig. 8. The incommensurability (deviation from \((\pi, \pi)\)) is horizontal or vertical, not diagonal, as we would expect because the bare susceptibility is more divergent due to a greater overlap between nested portions of the Fermi surface.

A similar scenario happens in the case of DDW order. However, two notable differences from the AF case are present. First, DDW is less sensitive to \( t'/t \), since it is driven mainly by antinodal regions of high density of states (d.o.s.). Therefore, while there is no AF instability without nesting (at half-filling AF Fermi surface instability is only possible if \( g_{AF} \gtrsim O(t') \)), DDW is still possible in this regime. This suggests that whenever the antinodal regions of the bare FS evolve away from the anti-nodal regions (which happen to also be regions with a high density of states as a result of the presence of van Hove singularities), a C-IC transition is likely to occur.

\[ \frac{1}{2} + \frac{x}{4}\pi \]

\[ 0.02 \quad 0.04 \quad 0.06 \quad 0.08 \quad 0.10 \]

\[ 0.02 \quad 0.04 \quad 0.06 \quad 0.08 \quad 0.10 \]

\[ 0.10 \quad 0.08 \quad 0.06 \quad 0.04 \quad 0.02 \]

\[ q \quad 0.2 \]

\[ T \]

\[ X \]

\[ x_c - x \]

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The same phenomenon can be viewed from the opposite perspective: when DDW order becomes incommensurate, there are regions in which it is suppressed (as in the domain walls of Fig. 2). Superconductivity can occur more easily there. Hence, incommensurability alleviates the competition between DSC and DDW order at the mean-field level, thereby enhancing superconductivity. Of course, IC order appears to suppress superconductivity in the cuprates, but this could be due to effects beyond a simple mean-field theory.

When the superconducting order parameter becomes strong enough, it may become energetically favorable for phase separation to occur. We can guess when this occurs from the usual Maxwell construction whenever the mean field chemical potential $\mu(x)$ does not vary monotonically. This appears to occur at a few isolated ‘magic’ doping values. However, in a real system, proximity to a second order critical point\cite{32}, Coulomb repulsion\cite{33}, or disorder
could drive the system in a state of mesoscopic phase separation. Moreover, the lattice pins any IC density wave order, so once the system is IC in order to minimize the free energy, the deviation from commensurability $q$ would be pinned at a finite value. Finally, it is important to remember that disorder could have important effects. It would not only disorder the array of domain walls, but could lead to droplets of one phase in regions of another.

We stress that while the general trend towards IC order may be clear, many of the quantitative aspects are not clear, in particular the precise copings at which DDW order becomes incommensurate. It is not clear to us why such C-IC transitions happen near ‘magic’ filling fractions. The fact that similar behavior occurs in the case of AF order suggests that the tendency of phase separation at ’magic’ filling fractions is a general trend for a variety of density wave order. Because the AF only case was explored upon taking the $g_{DDW,DSC} \rightarrow 0$ limit in the full free energy, it is not clear yet whether the tendency of phase separation at ‘magic’ filling fractions is a general feature of density waves competing with other order parameters, or of the lattice. It might be worth reconsidering the AF case in the presence of other order parameters (such as DDW, DSC). What makes our results surprising is that unlike in the frustrated phase separation picture for stripe formation, there is no Coulomb repulsion present. Hence, there is no obvious connection between phase separation and incommensurability. (Please note that while IC DDW order can induce charge density wave order at twice the wavevector, we have not included this effect, which we expect to be small, in our calculation.) Therefore, while Coulomb repulsion may play a role in determining the CDW spacing at $x = 1/8$ in $LaCuO_2$, in our calculation, the phase separation at ‘magic’ fractions can only arise as interplay between the lattice, competing order physics and energetics. What exactly is the combination of the three deserves some future research.

V. EXPERIMENTAL SIGNATURES

According to the discussion following (25) it seems likely that within the DSC state a competing DDW order parameter is IC as it develops. Hence, we briefly describe the experimental signatures that would distinguish between C and IC DDW order. Originally, C DDW was also named ‘hidden order’ in the context of the pseudogap, because most of the experimental signatures associated with it are indirect. The magnetic field, created by the alternating currents around neighboring plaquettes, is too small to be detected by neutron scattering ($B \simeq 1 - 30$ G for $\Delta_{DDW} \sim 30$ meV). At the same time, because of the symmetry of the C DDW magnetic field, there is no signature in NMR. The charge of the C DDW state is uniform so STM would not show signatures, unless they are associated with interference of nodal quasi-particles due to scattering off impurities. It has been argued recently that such interference disperses weakly enough to account for the pseudogap d.o.s. incommensurate modulations observed by STM. For a further discussion of the signatures of C DDW, the reader is referred to the literature.[3, 10, 13, 17, 18, 19, 20, 21].

FIG. 13: Example of the low temperature ($T = 0.001$ eV) staircase IC spectrum of AF around ‘magic’ filling fractions. The parameters we have taken here are $g_{AF} = -t' = 0.04$ eV, $t = 0.5$ eV. Inset: $\mu(x)$ is non-monotonic at both jumps of $q(x)$, but is smoothly decreasing whenever $q$ is pinned.

FIG. 14: At higher temperatures $q(x)$ regains its linearity around $x_c$ as predicted by Schuller. Here $T = 0.035$ eV and all other parameters are as in Fig. 13. Inset: $\mu(x)$ is monotonic throughout, suggesting that at higher temperatures, the C-IC transition is driven purely by IC nesting of the FS away from half-filling.
An IC DDW is more easily detectable directly. The local electronic density of states would be modulated due to the IC order parameter, and hence could be observable by STM. Secondly, the IC modulations of the staggered currents would produce NMR line splitting of both the Cu and O atoms when the applied magnetic fields are perpendicular to the a-b planes. This is in sharp contrast with IC SDW, where there is an NMR line-splitting due to spatially modulated local magnetization, which is directed along the a-b plane.

Let us estimate the modulated magnetic field strength arising from IC DDW (the reader is referred to where similar considerations are applied to the case of orbital antiferromagnetism proposed to exist in URu$_2$Si$_2$). Suppose we have an array of domain walls, Fig. 2, along the y-axis. Deep between the domains the field is zero as in the case of C DDW. Along a domain at $x = 0$, where the field is maximal, again most of the fields cancel except those created by the vertical alternating currents of strength $I_0$ at $x = -a$ and those of strength $I_0/2$ at $x = a$. Equivalently this would be the field of a single vertical array of alternating currents of strength $I_0/2$ at $x = -a$:

$$B_{\text{max}} = \frac{\mu_0}{4\pi a_0} \sum_i (-1)^i \frac{I_0}{2} (\cos(\theta_{i+1}) - \cos(\theta_i))$$

(26)

where $\cos \theta_i = [(i - 1)a + y_0]/[\sqrt{(i - 1)a + y_0}^2 + x_0^2]$ and $(x_0, y_0) = (a/2, 0)$ for O, Cu atoms respectively. Clearly at $y_0 = 0$, Cu, atoms the field is zero by symmetry. For O atoms the sum can be performed yielding $4\pi B_{\text{max}}/\mu_0 = 0.14I_0$. In the dilute domain limit, this field is independent of the distance between the domains.

For a sinusoidal current modulation, $B_{\text{max}}$ would depend on the modulation length $l_q = 1/q$. If $I(y, x) = I(y)\sin(qx)$ then a good estimate of $B_{\text{max}}$ is given by with $I_0$ replaced by $dI_0 = 2qaI_0 = 2I_0/n$ where $n$ is the periodicity of the modulation (in units of the lattice spacing). Therefore, for large $n$ we obtain $4\pi B_{\text{max}}/\mu_0 = 0.24I_0/n$.

VI. CONCLUSION

Incommensurate order is an important possibility when competing orders are considered. At a first-order transition the system is phase separated and hence necessarily inhomogeneous. If the competition between the orders is weak, coexistence is possible, but modulations of the competing orders are likely to be induced. The effects of the lattice, disorder, long-range Coulomb repulsion and proximity to criticality is to generally stabilize incommensurability on mesoscopic length scales. This is unlike the case of, say, the liquid to vapor phase transition where the competition results in phase separation on macroscopic length scales.

In the case of DDW and DSC, the competition is certainly weak within the framework of the extended Hubbard models we have considered. Because the processes stabilizing both orders are of similar nature and are at the same time smaller than all of onsite repulsion, exchange and hopping, it does not cost much energy to convert DDW order into DSC and vice versa. A simple resolution of the competition is for DDW order to become incommensurate. We find that this occurs for some doping levels, but the incommensuration tends to be relatively small. Such IC DDW could, in principle, be observable at low temperatures by NMR since it creates an inhomogeneous magnetic field at O atoms perpendicular to the a-b plane. Most of NMR experiments test for much stronger magnetic fields parallel to the a-b plane on the Cu atoms, and at higher temperatures such IC DDW phase would be smeared by thermal fluctuations, which may explain why such IC order, if it exists, hasn’t been seen by experiment.

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35 The AF only limit was taken by simply letting $\theta_{DW,0}\to 0$ in the total free energy.  

36 There is a neat way of thinking about IC DDW at finite $\mu$ as the analog of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state of DSC in a magnetic field parallel to the plane. In the absence of next-nearest neighbor hopping, the two mean fields are related via a particle-hole transformation in the same way commensurate DDW is related to DSC at half-filling. However, while in the latter case one can rotate C DDW to DSC, in the case of finite $\mu$, the particle-hole transformation cannot interchange FFLO and IC DDW. While the mean-field Hamiltonians of IC DDW and the FFLO are related by a particle-hole transformation, the spectra are not -- in the IC DDW state there is a splitting to a generally uncountably many bands (if $Q/q$ is irrational as we discussed in Sec. since the order parameter connects $k$ and $k + Q$ while in the case of DSC there is no such splitting. We are indebted to the authors of the authors of *for pointing out their work to us.*