

# Discommensuration-enhanced superconductivity in the charge density wave phases of transition-metal dichalcogenides

Chuan Chen,<sup>1,2</sup> Lei Su,<sup>3</sup> A. H. Castro Neto,<sup>1,2</sup> and Vitor M. Pereira<sup>1,2</sup>

<sup>1</sup>*Centre for Advanced 2D Materials and Graphene Research Centre,  
National University of Singapore, Singapore 117546*

<sup>2</sup>*Department of Physics, National University of Singapore, Singapore 117542*

<sup>3</sup>*Department of Physics, University of Chicago, Chicago, Illinois 60637, USA*

(Dated: June 22, 2018)

We introduce a McMillan-Ginzburg-Landau theory to describe the cooperative coexistence of charge-density and superconducting order in two-dimensional crystals. With a free-energy that explicitly accounts for the competition between commensurate and incommensurate ground states, we are able to map the transition between these phases and monitor the development of discommensurations in the near-commensurate regime. Attributing the enhancement of superconducting order to density-wave fluctuations, we propose a coupling scheme that yields a phase diagram in qualitative agreement with experiments in conducting transition metal dichalcogenides. The model predicts the development of non-uniform superconductivity similar to that arising from a pair-density wave, except that the spatial texture is driven by the underlying density modulation.

PACS numbers: 71.10.Hf, 71.45.Lr, 74.20.De

Recent experiments suggest the emergent superconductivity in doped transition-metal dichalcogenides (TMDs) is closely related to fluctuations of their charge density wave (CDW) order [1–4]. The archetype example of 1T-TiSe<sub>2</sub> (TiSe<sub>2</sub> in short) supports superconductivity (SC) amidst long-range CDW correlations, as soon as the nature of the CDW changes from commensurate (C) to incommensurate (IC) under electron doping [1, 5–7] or pressure [6, 8], either in bulk or 2D samples [1, 9]. The SC stability is limited to a dome over a small range of the external parameter  $x$  (doping or pressure) in the  $T$ - $x$  phase diagram. Since (i) undoped TiSe<sub>2</sub> is non-superconducting [5], (ii) CDW correlations persist in the SC phase [10], and (iii) the SC dome is centered at the putative quantum critical point of the commensurate CDW (C-CDW) phase, it has been suggested that SC might arise (or be enhanced) as a result of CDW fluctuations [11–13].

The basic excitation of a C-CDW is called *discommensuration* [14] (DC): a localized defect (domain wall) where the phase of the density order parameter jumps by  $2\pi\nu$ , with  $\nu$  the commensurability fraction [14–16]. DCs have been observed in TiSe<sub>2</sub> by scanning tunneling microscopy (STM) [2, 3] performed above the optimal SC transition temperature ( $T_{\text{sc}}^{\text{max}} \simeq 4$  K), and are implied by inelastic scattering [7]. This suggests that the CDW converts from C to IC through a near-commensurate (NC) regime characterized by a finite density of DCs, similarly to the cases of 2H-TaSe<sub>2</sub> [14] or 1T-TaS<sub>2</sub> [17].

Although the range  $T < T_{\text{sc}}$  remains unexplored by STM, it has been proposed that DCs might develop and organize as a regular network below  $T_{\text{sc}}$ : Little-Parks magnetoresistance oscillations [18] observed in the SC phase of TiSe<sub>2</sub> films [1] hint at supercurrents flowing within an underlying periodicity; a natural speculation

ties the potential SC conduits to DCs produced by the CDW background. This picture finds indirect support in STM that reveals the enhancement of electronic density of states within DCs [2]. In addition, the onset of a DC network introduces new low-energy phonons [19, 20]. If they couple to electrons and cause a Cooper instability, the induced SC should also be closely associated to DCs. Both ingredients — high density of states and low energy modes — suggest that the underlying theory must be able to tie SC to both fluctuations and the domain structure of the electronic CDW.

Ginzburg-Landau theories have proved to be a powerful framework to describe order parameter fluctuations in both SC and CDW physics. Insensitive to microscopic details, they permit capturing the universality of the underlying physics and are frequently the only practical approach to computations with coupled order parameters, especially with non-uniformity. To investigate the potential role of CDW fluctuations in either inducing or enhancing the SC instability in conducting TMDs, we propose here an extension of McMillan’s theory for the CDW order in layered TMDs [14, 21]. It incorporates a SC order parameter coupled to the electronic density via DCs. In the vicinity of the C-IC transition (the NC regime), the predicted phase diagram reproduces the experimental one in doped TiSe<sub>2</sub> and this description naturally extends to other notable cases such as TiTe<sub>2</sub>, TaS<sub>2</sub> or TaSe<sub>2</sub>. The nature of the SC phase is interesting since the model implies its non-uniformity in the NC regime close to  $T_{\text{sc}}$ . Moreover, with decreasing temperature, SC develops as a three-step percolation transition: from 0d to 1d to 2d superconductivity. The ramifications of this non-uniform, yet ordered, SC texture to the magnetic response are discussed.

**CDW order** — The foundational work of McMillan

[14, 21] established how to tackle the C-IC transition in terms of a free energy functional with a complex order parameter. Although the approach is general, the relevant nonlinear and *umklapp* terms to retain depend on the particular ordering vectors and commensurability condition [21]. We must thus be specific and shall consider the case of TiSe<sub>2</sub>: Even though a number of TMDs are notable for their robust CDW and SC phases, the intrinsically small carrier density of TiSe<sub>2</sub> makes it easily tuneable across the C, IC and SC phases by either pressure [6] or doping [7], including field-effect doping in the atomically thin limit [1]. Both bulk [22] and monolayer [23] TiSe<sub>2</sub> undergo a second order phase transition to the C-CDW phase characterized by the formation of a 2×2 superlattice in the 2d layers. The experimentally measured density modulation  $\delta\rho(\mathbf{r})$  has a 6-fold symmetry arising from the linear combination of three plane waves with wavevectors  $\mathbf{Q}_j^C \equiv \mathbf{G}_j/2$ , where  $\mathbf{G}_j$  ( $j = 1, 2, 3$ ) are primitive reciprocal vectors related to each other by  $C_3$  rotations [22]. As the in-plane ordering is the same in both the layered bulk crystal and monolayer [23], neglecting the inter-plane interaction is appropriate to describe both cases and we will do so.

We begin by defining the complex CDW order parameters,  $\psi_j(\mathbf{r}) \equiv \varphi_j(\mathbf{r})e^{i\theta_j(\mathbf{r})}$ , according to

$$\delta\rho(\mathbf{r}) \equiv \sum_j e^{i\mathbf{r} \cdot \mathbf{Q}_j^C} \psi_j(\mathbf{r}) + \text{c.c.}, \quad (1)$$

which establishes  $\psi_j(\mathbf{r})$  as an envelope function encoding deviations of  $\delta\rho(\mathbf{r})$  from the C state. To describe the IC phase, we introduce 3 new wavevectors,  $\mathbf{Q}_j^I$ , that parametrize a uniform IC-CDW with the same  $C_3$  symmetry and further define  $\mathbf{q}_j^I \equiv \mathbf{Q}_j^I - \mathbf{Q}_j^C$ . In line with the experiments, we take  $\mathbf{Q}_j^I = (1 + \delta)\mathbf{Q}_j^C$  where  $\delta$  quantifies the incommensurability, and define  $q^I \equiv |\mathbf{q}_j^I| = \delta |\mathbf{Q}_j^C|$ .

The free energy density consists of a conventional Ginzburg-Landau portion,

$$f_0(\mathbf{r}) \equiv A \sum_j |\psi_j|^2 + B \sum_j |(i\nabla_j + \mathbf{q}_j^I) \psi_j|^2 + G \sum_j |\psi_j|^4, \quad (2a)$$

where the  $B$  term favors a solution  $\psi_j(\mathbf{r}) \propto e^{i\mathbf{q}_j^I \cdot \mathbf{r}}$  that distorts  $\delta\rho(\mathbf{r})$  towards an IC state [24]. As usual, the quadratic coefficient is assumed to vanish linearly at a critical temperature:  $t \equiv A \propto T - T_{\text{icdw}}$ , and  $t$  will be our effective temperature parameter.

The presence of multiple non-colinear wavevectors contributing to  $\delta\rho(\mathbf{r})$  entails that additional terms must be included for a consistent account of the free energy to 4th order [21, 25]. Considering the symmetries of the system, one can identify the distinct terms as described

in the Supplementary Information and obtain

$$f_1(\mathbf{r}) \equiv -\frac{E}{2} \sum_j (\psi_j^2 + \psi_j^{*2}) - \frac{3D}{2} (\psi_1\psi_2\psi_3 + \text{c.c.}) - \frac{M}{2} \sum_j (\psi_j\psi_{j+1}^*\psi_{j+2}^* + \text{c.c.}) + \frac{K}{2} \sum_{i \neq j} |\psi_i\psi_j|^2. \quad (2b)$$

This complements  $f_0(\mathbf{r})$  to make up the total free energy density governing the CDW order:  $\mathcal{F}_{\text{cdw}} \equiv \int [f_0(\mathbf{r}) + f_1(\mathbf{r})] d\mathbf{r}$ . The notation  $\psi_{j+1}$  is to be understood as running cyclically through  $j = 1, 2, 3$  (e.g.  $\psi_5 \equiv \psi_2$ ) and, except if otherwise noted, the subscript  $j$  runs over  $\{1, 2, 3\}$  in all the subsequent expressions. Physically, the last 3 terms in Eq. (2b) reflect the electrostatic cost incurred by the superposition of distinct density waves [26]. The term proportional to  $E$  is called *lock-in* energy because its competition with the  $B$  term plays a prominent role in stabilizing the C state: it lowers the total energy of a C-CDW (we set  $E > 0$ ), but averages out for an IC-CDW.

When we consider an IC-CDW characterized by  $\psi_j \propto e^{i\mathbf{q}_j \cdot \mathbf{r}}$ , the terms in Eq. (2b) induce higher harmonics, implying that the equilibrium IC state consists of a linear combination of all compatible harmonics, and making the analytical minimization of  $\mathcal{F}_{\text{cdw}}$  a formidable task. We tackle the problem numerically with a systematic expansion of the order parameter, as pioneered by Nakanishi *et al.* [27–29]. The method, described in the Supplementary Information, amounts to expanding each  $\psi_j(\mathbf{r})$  in terms of  $e^{i\mathbf{q}_j \cdot \mathbf{r}}$  and all the two-dimensional harmonics spawned by the nonlinear terms in Eq. (2b). Pragmatically, this converts  $\mathcal{F}_{\text{cdw}}$  from a functional of  $\psi_j(\mathbf{r})$  into a function of a countable set of amplitudes  $\Delta_{j;lmn}$  and wavevectors  $\mathbf{q}_{j;lmn}$  of the different harmonics [30]. The equilibrium solution follows from a multidimensional minimization of  $\mathcal{F}_{\text{cdw}}$  with respect to these parameters, as well as  $\mathbf{q}_j$  itself. We take  $\mathbf{q}_j \parallel \mathbf{q}_j^I$ , and introduce  $\eta \equiv |\mathbf{q}_j|/q^I$  that determines if the solution is a C-CDW ( $\eta = 0$ ), a uniformly IC-CDW ( $\eta = 1$ ), or in between (NC-CDW).

**CDW phase diagram** — As we are only interested in scrutinizing the C-IC transition and presently disregard effects that might arise from induced anisotropy, strain, etc., we map the phase diagram in the  $E$ - $t$  plane fixing the remaining parameters to the values  $A = t$ ,  $K = G = 2B(q^I)^2 = -2D = 2M = 2$ . This choice allows us to concentrate on the vicinity of the C-IC boundary shown in Fig. 1, and drive the transition via  $E$  which, formally, controls the energy gain of having a C-CDW. Physically, a *smaller*  $E$  is associated to *larger* electron densities because: (i) phenomenologically, electron doping reduces the stability of the C state in favor of an IC-CDW [1, 2, 7]; (ii) microscopically, a theory of the CDW instability in TiSe<sub>2</sub> must yield a reduction of the C-CDW order parameter with doping [13, 31, 32] and the microscopic lock-in gain, being associated with the condensation energy, is itself determined by the magnitude of the order parameter [16, 33]. For this reason, the

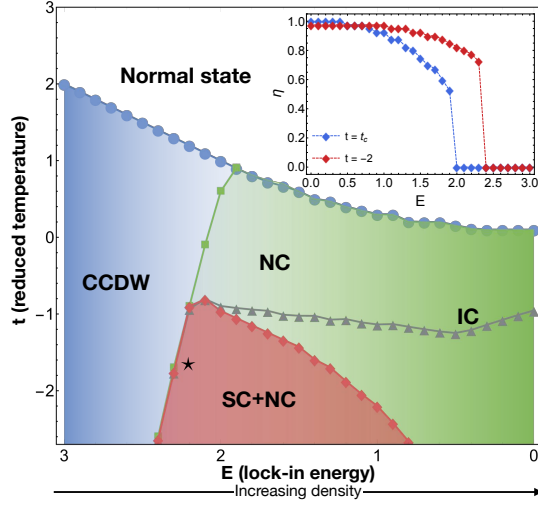


FIG. 1. Phase diagram obtained by minimizing  $\mathcal{F}_{\text{cdw}}$  (supplementary Eq. S7). When  $\mathcal{F}_{\text{cdw}} < 0$ , the system is in a CDW state and the C phase corresponds to  $\eta = 0$ . The green line represents the C-IC boundary,  $E_c(t)$ . The red line indicates the boundary of the SC phase including the linear  $E$  dependence in the CDW-SC coupling  $a_s$  of Eq. (3); it becomes the gray line if  $a_s$  is  $E$ -independent. The inset shows the equilibrium  $\eta$  at  $t_c$  (the transition is first order) and at low temperature.

horizontal  $E$  axis in the figure is reversed so that electron densities increase from left to right, as is usually presented in the experimental phase diagrams [1, 7].

The phase diagram in Fig. 1 exhibits the anticipated stability of the C state at large  $E$  (low density) and its suppression below a critical and temperature-dependent lock-in parameter:  $E_c(t)$ . Note that the critical temperature,  $t_c(E)$ , is reduced as the system progresses from the C to the IC state, in agreement with the experimental trend [1, 7]. Likewise in agreement is the abrupt loss of the C phase indicated by the relatively steep slope of the line  $E_c(t)$ . In light of our definition of  $t$  above, the asymptotic tendency  $t_c(E \rightarrow 0) \approx 0$  means that  $T_c \rightarrow T_{\text{icdw}}$ , suggesting that an IC state is ultimately preferred in the absence of lock-in energy. To be more specific, the inset shows the equilibrium value of the parameter  $\eta$  at the critical temperature of the normal-CDW phase transition and at low temperatures: It grows towards  $\eta \approx 1$  with decreasing  $E$ , implying that the dominant wavevectors contributing to  $\delta\rho(\mathbf{r})$  at each equilibrium state increasingly approach the reference IC vector  $\mathbf{Q}_I^I$ .

Knowledge of  $\eta$  is insufficient to characterize the rich spatial texture of the charge modulation which, following supplementary Eq. S6, depends on the detailed harmonic content that minimizes  $\mathcal{F}_{\text{cdw}}$ . Fig. 2(a) shows a real-space plot of  $\delta\rho(\mathbf{r})$  at the representative point close to the C-CDW boundary marked by  $\star$  in Fig. 1. The color density scale shows that there is no single periodicity. In more detail, Figs. 2(b,c) show line cuts of the phase and

amplitude of the order parameters  $\psi_j(\mathbf{r}) \equiv \varphi_j(\mathbf{r})e^{i\theta_j(\mathbf{r})}$  along the vertical dashed line in panel (a). The phase  $\theta_j(\mathbf{r})$  displays a stepwise variation with periodic phase slips of  $\pi$ . Seeing that the definition (1) implies that regions where  $\theta_j(\mathbf{r}) \approx 0 \bmod \pi$  are commensurate with the Bravais lattice, the spatial profile of the phase reveals that the equilibrium state is characterized by domains of approximately C-CDW separated by DCs at which the phase jumps by  $\pi$ . This is the NC regime; it replicates the characteristics of CDW domain walls investigated by STM slightly above  $T_{\text{sc}}$  [2, 3].

More generally, adapting the interaction terms in Eq. (2b) to a commensurability condition  $\mathbf{Q}^C = \nu\mathbf{G}$  with  $\nu$  a rational number ( $\nu = 1/2$  for  $\text{TiSe}_2$ ), one obtains a corresponding domain structure with the phase jumping by  $2\pi\nu$  across the boundary of two neighboring C domains [15, 19, 25, 28, 29]. In 1D and phase-only reductions of this problem [ $\varphi_j(\mathbf{r}) = \text{const.}$ ], the saddle-point condition for  $\mathcal{F}_{\text{cdw}}$  reduces to the static sine-Gordon equation [15, 19] and it becomes clear that a DC/domain wall corresponds to its soliton solutions. Even though the general problem of interest to us is two-dimensional, (1) still consists of a linear combination of one-dimensional CDW modulations along the direction of  $\mathbf{G}_j$ . It is thus not surprising that each  $\theta_j(\mathbf{r})$  seen in Fig. 2(b) retains the soliton-like nature characteristic of the 1D solution.

The DCs form a 2D network whose periodicity is highlighted by the yellow-dashed contours in Fig. 2(a). They expose a Kagome superlattice overlaying the C-CDW, which is the natural effect of superimposing three equivalent 1D-like DC staircases along directions  $120^\circ$  apart. For a general commensurability fraction  $\nu$ , the period of the DC network is  $L = 2\pi\nu/(\eta q^I) = \sqrt{3}a/(\eta\delta)$ , where  $a$  is the lattice constant of the crystal in the normal phase.

Note that the amplitude of  $\psi_i(\mathbf{r})$  is also significantly modulated. In particular, Fig. 2(c) shows it can drop more than 30% at each DC. The high variational freedom introduced by the expansion (supplementary Eq. S6) permits the CDW to distort from the simple plane wave solution in order to minimize both the lock-in and gradient terms in Eq. (2). It can therefore be, simultaneously, as close to a C and an IC configuration as possible, which the solution in Figs. 2(a-c) accomplishes by: (i) having domains of nearly flat phase and high amplitude (C-CDW) joined by (ii) domain boundaries where, on the one hand, the phase jumps so that on spatial average  $\langle\theta_j(\mathbf{r})\rangle \approx \mathbf{q}_j^I \cdot \mathbf{r}$  and, on the other, the amplitude drops to minimize the cost in deviating from commensurability at those regions.

**Coupling to superconductivity** — It is natural to expect these DCs to couple strongly with the SC order parameter: On the one hand, the development of a DC superlattice as in Fig. 2(a) introduces new low energy phonons associated with the superlattice [19, 20]. From the perspective of SC pairing due to retarded electron-phonon interactions, the emergence of this DC lattice

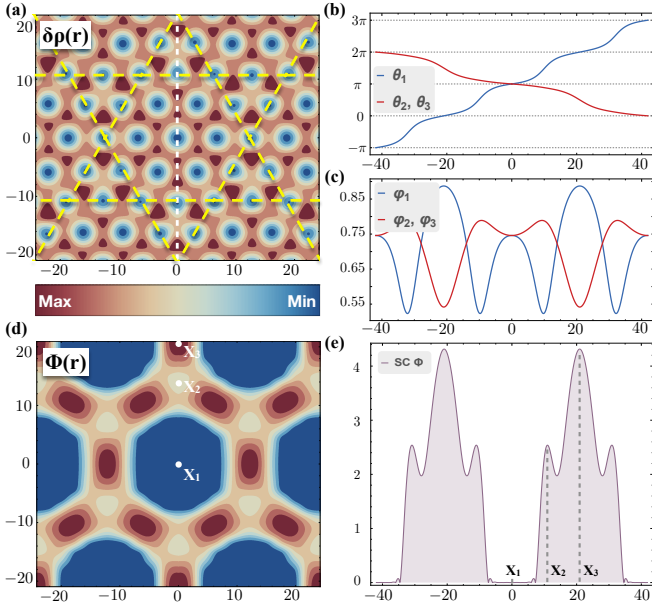


FIG. 2. (a) Real space plot of the density profile  $\delta\rho(\mathbf{r})$  at  $E = 2.2$ ,  $t = -1.7$  ( $\star$  in Fig. 1). Lengths are in units of  $\sqrt{3}a/2\pi$ , with  $a$  the lattice constant. The yellow-dashed lines mark the places where the phase of each CDW order parameter,  $\psi_j(\mathbf{r})$ , jumps by  $\pi$ . (b) and (c) respectively show the phase and amplitude of  $\psi_j(\mathbf{r})$  along the white vertical cut marked in (a). (d) The SC order parameter,  $\Phi(\mathbf{r})$ , in the same region shown in (a). (e)  $\Phi(\mathbf{r})$  along the vertical cut marked in (a).

might enhance any intrinsic pairing tendency already present in the absence of a CDW [34]. On the other hand, DCs are nothing but CDW fluctuations. While both phase and amplitude fluctuations are gapped in the C regime [16], the transition to the NC state releases them to potentially favor SC through fluctuation-induced pairing. This is the analogue of pairing induced by fluctuations of magnetic order proposed for high-temperature superconductors [35].

As a minimal approach to describe this interplay between the two orders we propose extending the conventional [36] Ginzburg-Landau free energy associated with the SC order parameter,  $\Phi(\mathbf{r})$ , and writing

$$\mathcal{F}_{\text{sc}} \equiv \int \left[ a_s(T, \nabla\psi_j) |\Phi|^2 + b_s |\nabla\Phi|^2 + c_s |\Phi|^4 \right] d\mathbf{r}. \quad (3)$$

Making  $a_s$  a function of  $\nabla\psi_j$  permits the enhancement of SC by deviations from a C-CDW. To lowest order in the interaction and inhomogeneity,  $a_s$  should have the form  $a_s = a_0 - a_1 \sum_j |\nabla\psi_j|^2$ , where  $a_0 \propto T - T_{\text{sc}}$  is the conventional quadratic coefficient and  $a_1 > 0$  so that SC is stabilized within regions of fluctuating C order (we take  $a_1$  to be  $T$ -independent). This captures phenomenologically both the effect of fluctuation-induced ( $a_0 = \text{const.}$ ) and fluctuation-enhanced ( $a_0 \propto T - T_{\text{sc}}$ ) pairing, as well as the spatial enhancement of the electronic DOS at DCs [2].

The total free energy is now  $\mathcal{F} = \mathcal{F}_{\text{cdw}} + \mathcal{F}_{\text{sc}}$  and the coupling in (3) requires one to self-consistently find the saddle point for both  $\psi_j(\mathbf{r})$  and  $\Phi(\mathbf{r})$ . As in  $\text{TiSe}_2$   $T_{\text{cdw}} \simeq 40 \text{ K}$  and  $T_{\text{sc}} \simeq 4 \text{ K} \ll T_{\text{cdw}}$  [1, 5, 8], the CDW order parameter is well developed when the SC instability appears. Combined with the fact that we are in a time-independent Ginzburg-Landau framework, this justifies solving the two problems independently and tackle Eq. (3) given the solution to the CDW alone. In practice, this entails minimizing  $\mathcal{F}_{\text{sc}}$  in the presence of the static CDW background that minimizes Eq. (2).

A representative outcome of such procedure [30] is shown in Fig. 2(d) for the CDW solution in panel (a) [37]. The most significant feature is the non-uniformity of  $\Phi(\mathbf{r})$  that follows the spatial texture of the DC network. The section plotted in Fig. 2(e) shows there is no SC within the C domains [ $\Phi(\mathbf{x}_1) = 0$ ] but only at and near the DCs, and that SC is reinforced when two DCs overlap at the vertices of the Kagome:  $\Phi(\mathbf{x}_3) \approx 2\Phi(\mathbf{x}_2)$ .

Most interestingly, it is clear from how  $\nabla\psi_j$  enters the quadratic coefficient  $a_s$  in Eq. (3) that, depending on the parameters, the development of SC in the NC regime might take place in three stages with decreasing temperature, see Fig. 3(a): (i) it begins at  $T_{\text{sc}}^{0\text{d}}$  with the nucleation of isolated SC dots at the Kagome vertices; (ii) at  $T_{\text{sc}}^{1\text{d}} \lesssim T_{\text{sc}}^{0\text{d}}$  these SC dots have grown and overlap to percolate the system in a connected network, as in Fig. 2(d); (iii) ultimately, at  $T_{\text{sc}}^{2\text{d}} \lesssim T_{\text{sc}}^{1\text{d}}$  the whole system becomes superconducting. (The SC boundaries in the phase diagram correspond to  $T_{\text{sc}}^{0\text{d}}$ .) The coupling proposed in Eq. (3) therefore predicts that, depending on the temperature, the SC order can have either a 0d, 1d or 2d character. This can be experimentally probed with temperature-dependent local spectroscopy across the SC transition. Also, in the absence of other intrinsic pairing mechanisms [38], this picture predicts that if the localization length of  $\Psi(\mathbf{r})$  is not much larger than the width of a DC, it is possible that  $T_{\text{sc}}^{2\text{d}} = 0$  in the NC region of the phase diagram. SC would then span the system, at most, through the 1d network [cf. Fig. 3(a)].

The area of SC stability in the phase diagram depends on whether the parameter  $a_1$  in Eq. (3) varies with  $E$ . If it does not, SC persists from the NC to the IC limit at temperatures below the gray line in Fig. 1. It remains in the IC limit because  $|\nabla\psi_j|$  is finite in the IC limit, thereby supporting uniform SC. This is a sensible physical outcome from a perspective of fluctuation-induced pairing because phase fluctuations of an IC-CDW are gapless. In the specific case of doped  $\text{TiSe}_2$ , however, SC seems to exist only over a dome-shaped portion of the phase diagram, over a finite density range [1, 5]. This phenomenology can be captured by replacing  $a_1 \rightarrow a_1 E$  in the parameter  $a_s$ , making it depend both implicitly (through  $\psi_j$ ) and explicitly on the lock-in parameter  $E$ . In view of the previously argued negative correlation between  $E$  and the electronic density, this amounts to mak-



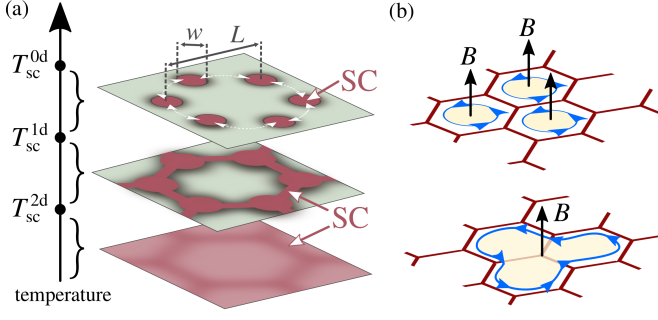


FIG. 3. (a) Schematic of the distinct non-uniform SC regimes spatially correlated with the DC network: nucleation and expansion of the SC order parameter ( $T_{sc}^{1d} < T < T_{sc}^{0d}$ ), percolation ( $T_{sc}^{2d} < T < T_{sc}^{1d}$ ), and finite everywhere. See supplementary Fig. S3 for actually calculated textures. (b) Illustration of how the connectivity in the percolation regime constrains the vortex structure, with impact in the magnetic response.

ing the coupling to CDW fluctuations weaker at higher densities, which is also physically plausible in view of screening. Indeed, the phase boundary computed in this way corresponds to the dome-shaped red line in Fig. 1: by restricting the SC phase to the NC region it renders the phase diagram qualitatively correct.

**Ramifications** — The feasibility of non-uniform percolative SC in the NC regime is determined by the characteristic width of DCs ( $w$ ), their separation ( $L$ , the size of the C domains), and the SC coherence length  $\xi$  ( $\sim 12$  nm in  $\text{TiSe}_2$  [39]). It is likely that  $w \lesssim \xi$ , not sufficient to permit fully developed SC grains in the temperature range  $T_{sc}^{1d} < T < T_{sc}^{0d}$  where the model predicts nucleation at the vertices of the DC network. But it might be enough to stabilize Cooper pairs within each vertex reducing the problem to that of interacting Bose particles on a lattice with a metallic background (similarly to cold atoms on an optical lattice [40], except that the periodic potential comes here from the DC network and is temperature dependent). Tunneling of non-condensed pairs among this realization of a Josephson junction array would tally with the observation [9] of an anomalous-metallic phase in  $\text{TiSe}_2$  near  $T = 0$  K [41–44], and the analysis of its vortex phases would be similar to that in references 45 and 46.

The situation in the range  $T_{sc}^{2d} < T < T_{sc}^{1d}$  has interesting implications in the presence of a magnetic field,  $B$ . First, vortices are naturally pinned by the DC lattice, even in the absence of disorder, and their motion correlated. Second, given the likelihood that  $w \lesssim \xi$ , vortices would not squeeze within DCs; the supercurrent would instead circulate along the linked network of 1D SC channels [36], as illustrated in Fig. 3(b). If  $L \gg \xi$ , we may regard this as a microscopic version of SC wire grids which have been extensively studied experimentally [47–50] and theoretically [51–55]. A distinctive feature

of these grids are oscillatory dips as a function of  $B$  in thermodynamic [47] and transport [49] properties, with period determined by rational fractions,  $f = \phi/\phi_0$ , of the flux through the grid’s elementary plaquette ( $\phi \sim BL^2$ ,  $\phi_0 \equiv h/2e$ ) [53, 54, 56]. Given that such a networked texture of the SC order parameter is a natural implication of the model studied here, it is tempting to speculate this to be the origin of Little-Parks-type resistance oscillations found in the SC/anomalous-metal phase of  $\text{TiSe}_2$  near optimum doping [1].

To put this to the test, assume the grid is hexagonal as in Fig. 2(d) ( $f = 1/4$  [54]) and take the first magnetoresistance dip at  $B \simeq 0.13$  T in the experiment of Li *et al.* [1]. Hence,  $L = [\phi_0/(2\sqrt{3}B)]^{1/2} \simeq 70$  nm. We noted above that  $L = \sqrt{3}a/(L\eta)$  where  $a = 0.35$  nm for  $\text{TiSe}_2$  [22, 57]. Since  $\eta \sim 1$  (Fig. 1), it follows that  $\delta \sim 0.01$ . In other words, interpreted from the perspective of our model, the experimental resistance oscillations indirectly suggest a CDW incommensurability factor  $\delta \sim 1\%$  and a typical distance between DCs  $L \sim 70$  nm. Compellingly, x-ray diffraction does reveal  $\delta \sim 5\text{--}15\%$  in the superconducting dome [7], which is in the same range as in other metallic TMDs [58], and STM finds DCs separated by 10’s of nm at optimum doping above  $T_{sc}$  [2]. Having in mind that Cu intercalation likely pins and disorders the DCs into an irregular network, these estimates seem in noteworthy agreement with experiments.

Experimental evidence that SC emerges with the suppression of the C-CDW in the NC regime is increasingly better documented across a large range of  $2H$  and  $1T$  TMDs [4]. These span both good metals and semimetals, as well as a number of distinct commensurability conditions. Our model straightforwardly extends to these cases, each corresponding to a particular region of the general phase diagram in Fig. 1. It thus provides a definite and universal phenomenological foundation to further explore the interplay between these two coexisting orders and their fluctuations.

VMP was supported by the Singapore Ministry of Education through grant MOE2015-T2-2-059 and AHCN by the National Research Foundation of Singapore under its Medium-Sized Centre Programme. Numerical computations were carried out at the HPC facilities of the NUS Centre for Advanced 2D Materials.

- 
- [1] L. J. Li, E. C. T. O’Farrell, K. P. Loh, G. Eda, B. Özyilmaz, and A. H. Castro Neto, *Nature* **529**, 185 EP (2015).
  - [2] S. Yan, D. Iai, E. Morosan, E. Fradkin, P. Abbamonte, and V. Madhavan, *Phys. Rev. Lett.* **118**, 106405 (2017).
  - [3] A. M. Novello, M. Spera, A. Scarfato, A. Ubaldini, E. Giannini, D. R. Bowler, and C. Renner, *Phys. Rev. Lett.* **118**, 017002 (2017).
  - [4] See reference 12 and references therein.

- [5] E. Morosan, H. W. Zandbergen, B. S. Dennis, J. W. G. Bos, Y. Onose, T. Klimczuk, A. P. Ramirez, N. P. Ong, and R. J. Cava, *Nat. Phys.* **2**, 544 (2006).
- [6] Y. I. Joe, X. M. Chen, P. Ghaemi, K. D. Finkelstein, G. a. de la Peña, Y. Gan, J. C. T. Lee, S. Yuan, J. Geck, G. J. MacDougall, T. C. Chiang, S. L. Cooper, E. Fradkin, and P. Abbamonte, *Nature Physics* **10**, 421 (2014), 1309.4051.
- [7] A. Kogar, G. A. de la Pena, S. Lee, Y. Fang, S. X.-L. Sun, D. B. Lioi, G. Karapetrov, K. D. Finkelstein, J. P. C. Ruff, P. Abbamonte, and S. Rosenkranz, *Phys. Rev. Lett.* **118**, 027002 (2017).
- [8] A. F. Kusmartseva, B. Sipos, H. Berger, L. Forró, and E. Tutiš, *Phys. Rev. Lett.* **103**, 236401 (2009).
- [9] L. Li, C. Chen, K. Watanabe, T. Taniguchi, Y. Zheng, Z. Xu, V. M. Pereira, K. P. Loh, and A. H. C. Neto, arXiv:1803.10936 (2018), 1803.10936.
- [10] M. Spera, A. Scarfato, E. Giannini, and C. Renner, arXiv (2017), 1710.04096.
- [11] H. Barath, M. Kim, J. F. Karpus, S. L. Cooper, P. Abbamonte, E. Fradkin, E. Morosan, and R. J. Cava, *Phys. Rev. Lett.* **100**, 106402 (2008).
- [12] B. Wang, Y. Liu, K. Ishigaki, K. Matsubayashi, J. Cheng, W. Lu, Y. Sun, and Y. Uwatoko, *Phys. Rev. B* **95**, 220501 (2017).
- [13] C. Chen, B. Singh, H. Lin, and V. M. Pereira, arXiv:1712.04967 (2017), 1712.04967.
- [14] W. L. McMillan, *Phys. Rev. B* **14**, 1496 (1976).
- [15] P. Bak and V. J. Emery, *Phys. Rev. Lett.* **36**, 978 (1976).
- [16] G. Grüner, *Density Waves in Solids* (Addison-Wesley, 1994).
- [17] R. E. Thomson, B. Burk, A. Zettl, and J. Clarke, *Phys. Rev. B* **49**, 16899 (1994).
- [18] W. A. Little and R. D. Parks, *Phys. Rev. Lett.* **9**, 9 (1962).
- [19] W. L. McMillan, *Phys. Rev. B* **16**, 4655 (1977).
- [20] K. Nakanishi and H. Shiba, *J. Phys. Soc. Japan* **45**, 1147 (1978).
- [21] W. L. McMillan, *Phys. Rev. B* **12**, 1187 (1975).
- [22] F. J. Di Salvo, D. E. Moncton, and J. V. Waszczak, *Phys. Rev. B* **14**, 4321 (1976).
- [23] P. Chen, Y.-H. Chan, X.-Y. Fang, Y. Zhang, M.-Y. Chou, S.-K. Mo, Z. Hussain, A.-V. Fedorov, and T.-C. Chiang, *Nature communications* **6**, 8943 (2015).
- [24] The actual magnitude of  $\mathbf{q}_f^L$  does not play a role in the subsequent energy minimization because it can be absorbed into the definition of  $B$ .
- [25] A. E. Jacobs and M. B. Walker, *Phys. Rev. B* **21**, 4132 (1980).
- [26] Being a result of interactions among different waves, the form of  $f_1(\mathbf{r})$  is specific to the case of  $\text{TiSe}_2$ . But, as mentioned, the formalism is general and straightforwardly applied to other near-commensurate conditions [27, 29].
- [27] K. Nakanishi, H. Takater, Y. Yamada, and H. Shiba, *J. Phys. Soc. Jpn.* **43**, 1509 (1977).
- [28] K. Nakanishi and H. Shiba, *J. Phys. Soc. Jpn.* **43**, 1839 (1977).
- [29] K. Nakanishi and H. Shiba, *J. Phys. Soc. Jpn.* **44**, 1465 (1978).
- [30] Additional details are provided in the Supplementary Information file.
- [31] C. Monney, E. F. Schwier, M. G. Garnier, N. Mariotti, C. Didiot, H. Cercellier, J. Marcus, H. Berger, A. N. Titov, H. Beck, and P. Aebi, *New J. Phys.* **12**, 125019 (2010).
- [32] J. van Wezel, P. Nahai-Williamson, and S. S. Saxena, *Phys. Rev. B* **83**, 024502 (2011).
- [33] P. A. Lee, T. M. Rice, and P. W. Anderson, *Solid State Commun.* **14**, 703 (1974).
- [34] The small Fermi surfaces characteristic of 1T TMDs suggest that conventional BCS pairing is inefficient.
- [35] D. Scalapino, *J. Low Temp. Phys.* **117**, 179 (1999).
- [36] M. Tinkham, *Introduction to Superconductivity: Second Edition* (McGraw Hill, Inc., New York, 1996).
- [37] The gray SC boundary in Fig. 1 was obtained with  $a_0 = 10t + 60$  (chosen to approximate  $T_{sc} : T_{cdw}$  to the experimental ratio at the dome's tip),  $a_1 = 500 \times 2.1$ , and  $b_s = c_s = 1$ . The red boundary was obtained by setting  $a_1 = 500E$  instead.
- [38] In the specific case of  $\text{TiSe}_2$ , the small Fermi surface suggests a feeble conventional BCS-type mechanism so that fluctuations might indeed dominate the SC stability.
- [39] E. Morosan, L. Li, N. P. Ong, and R. J. Cava, *Phys. Rev. B* **75**, 104505 (2007).
- [40] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).
- [41] D. Das and S. Doniach, *Phys. Rev. B* **60**, 1261 (1999).
- [42] D. Dalidovich and P. Phillips, *Phys. Rev. B* **64**, 052507 (2001).
- [43] B. Spivak, P. Oreto, and S. A. Kivelson, *Phys. Rev. B* **77**, 214523 (2008).
- [44] A. Kapitulnik, S. A. Kivelson, and B. Spivak, arXiv:1712.07215 (2017).
- [45] J. W. Reijnders and R. A. Duine, *Phys. Rev. Lett.* **93**, 060401 (2004).
- [46] J. W. Reijnders and R. A. Duine, *Phys. Rev. A* **71**, 063607 (2005).
- [47] B. Pannetier, J. Chaussy, R. Rammal, and J. C. Villegier, *Phys. Rev. Lett.* **53**, 1845 (1984).
- [48] H. D. Hallen, R. Seshadri, A. M. Chang, R. E. Miller, L. N. Pfeiffer, K. W. West, C. A. Murray, and H. F. Hess, *Phys. Rev. Lett.* **71**, 3007 (1993).
- [49] X. S. Ling, H. J. Lezec, M. J. Higgins, J. S. Tsai, J. Fujita, H. Numata, Y. Nakamura, Y. Ochiai, C. Tang, P. M. Chaikin, and S. Bhattacharya, *Phys. Rev. Lett.* **76**, 2989 (1996).
- [50] M. D. Stewart, A. Yin, J. M. Xu, and J. M. Valles, *Science* **318**, 1273 (2007).
- [51] S. Teitel and C. Jayaprakash, *Phys. Rev. Lett.* **51**, 1999 (1983).
- [52] S. Alexander, *Phys. Rev. B* **27**, 1541 (1983).
- [53] Q. Niu and F. Nori, *Phys. Rev. B* **39**, 2134 (1989).
- [54] Y.-L. Lin and F. Nori, *Phys. Rev. B* **65**, 214504 (2002).
- [55] J. Berger and J. Rubinstein, *Connectivity and superconductivity*, Vol. 62 (Springer Science & Business Media, 2001).
- [56] K. Park and D. A. Huse, *Phys. Rev. B* **64**, 134522 (2001).
- [57] B. Singh, C. H. Hsu, W. F. Tsai, V. M. Pereira, and H. Lin, *Phys. Rev. B* **95**, 245136 (2017).
- [58] D. E. Moncton, J. D. Axe, and F. J. Disalvo, *Phys. Rev. Lett.* **34**, 734 (1975).

---

## SUPPLEMENTARY MATERIAL

---

### **Discommensuration-enhanced superconductivity in the charge density wave phases of transition-metal dichalcogenides**

Chuan Chen,<sup>1,2</sup> Lei Su,<sup>3</sup> A. H. Castro Neto,<sup>1,2</sup> and Vitor M. Pereira<sup>1,2</sup>

<sup>1</sup>*Centre for Advanced 2D Materials and Graphene Research Centre,  
National University of Singapore, Singapore 117546*

<sup>2</sup>*Department of Physics, National University of Singapore, Singapore 117542*

<sup>3</sup>*Department of Physics, University of Chicago, Chicago, Illinois 60637, USA*

(Dated: June 18, 2018)

## SI. TRANSFORMATION OF THE ORDER PARAMETER UNDER SYMMETRY OPERATIONS OF THE SYSTEM

In order to establish a Ginzburg-Landau free energy, we begin with considering the symmetries of the system. Monolayer  $\text{TiSe}_2$  has four types of symmetry: translational,  $C_3$  rotation, mirror (along  $\Gamma M$ 's) and inversion. Using the fact that the commensurate wavevectors are  $\mathbf{Q}_j^C \equiv \mathbf{G}_j/2$ , where  $\mathbf{G}_j$  ( $j = 1, 2, 3$ ) are primitive reciprocal vectors related by 120 degree rotations, the order parameters transform as follows.

1. Under translation by a Bravais lattice vector,

$$\begin{aligned}
 \delta\rho'(\mathbf{r}) &= \delta\rho(\mathbf{r} - \mathbf{R}_{b,l}) \\
 &= \sum_j e^{i\frac{\mathbf{G}_j}{2} \cdot (\mathbf{r} - \mathbf{R}_{b,l})} \psi_j(\mathbf{r} - \mathbf{R}_{b,l}) + c.c \\
 &= \sum_j e^{i\frac{\mathbf{G}_j}{2} \cdot \mathbf{r}} e^{-i\frac{\mathbf{G}_j}{2} \cdot \mathbf{R}_{b,l}} \psi_j(\mathbf{r} - \mathbf{R}_{b,l}) + c.c \\
 \psi'_j(\mathbf{r}) &= e^{-i\frac{\mathbf{G}_j}{2} \cdot \mathbf{R}_{b,l}} \psi_j(\mathbf{r} - \mathbf{R}_{b,l})
 \end{aligned} \tag{S1}$$

2. Under a  $C_3$  rotation,

$$\begin{aligned}
 \delta\rho'(\mathbf{r}) &= \delta\rho(C_3^{-1}\mathbf{r}) \\
 &= \sum_j e^{i\frac{\mathbf{G}_j}{2} \cdot (C_3^{-1}\mathbf{r})} \psi_j(C_3^{-1}\mathbf{r}) + c.c \\
 &= \sum_j e^{i\frac{\mathbf{G}_{j-1}}{2} \cdot \mathbf{r}} \psi_j(C_3^{-1}\mathbf{r}) + c.c \\
 &= \sum_j e^{i\frac{\mathbf{G}_j}{2} \cdot \mathbf{r}} \psi_{j+1}(C_3^{-1}\mathbf{r}) + c.c \\
 \psi'_j(\mathbf{r}) &= \psi_{j+1}(C_3^{-1}\mathbf{r})
 \end{aligned} \tag{S2}$$

3. Under a mirror operation,

$$\begin{aligned}
 \psi'_1(x, y) &= \psi_1(-x, y) \\
 \psi'_2(x, y) &= \psi_3(-x, y) \\
 \psi'_3(x, y) &= \psi_2(-x, y)
 \end{aligned} \tag{S3}$$

4. Under an inversion,  $\mathcal{I}$ ,

$$\psi'_j(\mathbf{r}) = \psi_j^*(-\mathbf{r}) \tag{S4}$$



## SII. FREE ENERGY DERIVED FROM THE SYMMETRIES OF THE SYSTEM

After taking into account the symmetry of the system, assuming higher order coupling terms do not play a significant role, and only focusing on the simplest types of coupling which can capture the *lock-in* effect of the commensurate charge density wave (described by the  $E$ -term) and the interaction between the three density waves, one arrive at the free energy in Eq. (2):

$$f(x) = A \sum_j |\psi_j|^2 + B \sum_j \left| \left( i \frac{\partial}{\partial x_{\parallel,j}} + \mathbf{q}_j^I \right) \psi_j \right|^2 + C \sum_j \left| \frac{\partial}{\partial x_{\perp,j}} \psi_j \right|^2 - \frac{3D}{2} (\psi_1 \psi_2 \psi_3 + \psi_1^* \psi_2^* \psi_3^*) \\ - \frac{E}{2} \sum_j (\psi_j^2 + \psi_j^{*2}) + G \sum_j |\psi_j|^4 + \frac{K}{2} \sum_{i \neq j} |\psi_i \psi_j|^2 - \frac{M}{2} \sum_j (\psi_j \psi_{j+1}^* \psi_{j+2}^* + c.c) \quad (\text{S5})$$

In view of the  $C_6$  rotational symmetry of the CDW and given that we are not interested in the development of other CDW phases due to induced anisotropy, strain, or disorder, we make the gradient term isotropic by choosing  $B = C$ .

## SIII. HARMONIC EXPANSION

### SIII.A. Outline of the method

When we consider an IC-CDW characterized by a certain  $\mathbf{q}_j$ , the various terms in Eq. (2b) induce higher harmonics of it. Hence, the equilibrium IC state must consist of a linear combination of infinite compatible harmonics. This fact must be explicitly accounted for in order to properly describe: the C-IC transition, the fact that the equilibrium  $\mathbf{q}_j$  changes with temperature, as well as the order of the phase transitions<sup>1,2</sup>. In addition, despite the insight provided by phase-only models<sup>3,4</sup>, both the phase and amplitude of the order parameter should be considered to properly describe the stable CDW as, not a uniform plane wave solution, but a wave periodically distorted in real space to accommodate the competing  $E$  and  $B$  terms in the free energy<sup>2,5,6</sup>. These two aspects, combined with the fact that the saddle-point equations are nonlinear, make the analytical minimization of  $f_{\text{cdw}}(\mathbf{r})$  a formidable problem, except in simplified cases<sup>5,6</sup>.

A pragmatic approach consists in making a systematic harmonic expansion of the order parameter and minimizing the free energy numerically, as pioneered by Nakanishi *et al.*<sup>7-9</sup>. Accordingly, we consider the expansion

$$\psi_j(\mathbf{r}) = \Delta_{j;0} + \sum_{\substack{0 \leq l,m,n \leq N \\ l \cdot m \cdot n = 0}} \Delta_{j;lmn} \exp(i\mathbf{q}_{j;lmn} \cdot \mathbf{r}), \quad (\text{S6})$$

where  $\mathbf{q}_{j;lmn} \equiv (2l+1)\mathbf{q}_j + 2m\mathbf{q}_{j+1} + 2n\mathbf{q}_{j+2}$  are the harmonics of  $\mathbf{q}_j$  generated by  $f_1(\mathbf{r})$  and  $l, m, n$  are positive integers smaller than a cutoff  $N$ . Eq. (S6) captures both the C ( $\Delta_{j;lmn} = 0$ ) and an arbitrary IC wave ( $\mathbf{q}_{j;lmn} \neq 0$  and  $\Delta_{j;lmn} \neq 0$ ) modulated in amplitude and phase. Although  $\{\Delta_{j;0}, \Delta_{j;lmn}\} \in \mathbb{C}$  in general, we make the simplifying assumptions  $\Delta_{j;0} \equiv \Delta_0 \in \mathbb{R}$ ,  $\Delta_{j;lmn} \equiv \Delta_{lmn} \in \mathbb{R}$ ,  $\mathbf{q}_j \parallel \mathbf{q}_j^I$ , and  $|\mathbf{q}_j| \equiv \eta q^I$ , which are all compatible with the experimental density modulation  $\delta\rho(\mathbf{r})$ . Under these conditions, the free energy functional becomes a function of real parameters [a total of  $(N+1)^3 - N^3 + 2$ ],

$$\mathcal{F}_{\text{cdw}}[\eta, \Delta_0, \Delta_{lmn}] \equiv \int [f_0(\mathbf{r}) + f_1(\mathbf{r})] d\mathbf{r}, \quad (\text{S7})$$

where  $\Delta_0$ ,  $\Delta_{lmn}$ ,  $\eta$ , are determined to minimize  $\mathcal{F}_{\text{cdw}}$  (the explicit form of  $\mathcal{F}_{\text{cdw}}$  is given below).

We performed the multidimensional minimization of  $\mathcal{F}_{\text{cdw}}$  numerically with respect to  $\Delta_0$  and  $\Delta_{lmn}$  at fixed  $\eta$ , subsequently scanning the latter in a fixed range. As Eq. (2) penalize deviations of  $\mathbf{q}_j$  from  $\mathbf{q}_j^I$  (via the  $B$  term) and from 0 (via the  $E$  term), it is sufficient to scan the range  $\eta \in [0, 1]$  to obtain the global minimum. We verified that the expansion (S6) converges rapidly (cf. Fig. S2), and used the quite sufficient cutoff  $N = 3$  in all subsequent calculations.

### SIII.B. Explicit form of the harmonic-expanded free energy

Substituting the order parameter given by Eq. (S6) into Eq. (2) and after some algebra, the free energy can be shown to be equal to:

$$\begin{aligned}
\mathcal{F}_{\text{cdw}}/3 = & \sum_{\substack{l,m,n \geq 0 \\ l+m+n=0}} \sum_i \left[ A + B(\mathbf{q}_{i;lmn} - \mathbf{q}_i^I) \cdot (\mathbf{q}_{i;l'm'n'} - \mathbf{q}_i^I) + 2 \left( G + \frac{K}{2} \right) |\Delta_0|^2 \right] \\
& \times \Delta_{i;lmn} \Delta_{i;l'm'n'}^* \delta(l-l', m-m', n-n') \\
& - \frac{E}{2} \sum_i [\Delta_{i;lmn} \Delta_{i;l'm'n'} \delta(l+l'+1, m+m', n+n') + c.c.] \\
& - \frac{3D}{2} [\Delta_{1;lmn} \Delta_{2;l'm'n'} \Delta_{3;l''m''n''} \delta(l+n'+m'', m+l'+n'', n+m'+l'') + c.c.] \\
& - \frac{M}{2} \sum_i [\Delta_{i;lmn} \Delta_{i+1;l'm'n'}^* \Delta_{i+2;l''m''n''}^* \delta(l-n'-m''+1, m-l'-n'', n-m'-l'') + c.c.] \\
& + G \sum_i \Delta_{i;lmn} \Delta_{i;l'm'n'}^* \Delta_{i;l''m''n''} \Delta_{i;l'''m'''n'''}^* \delta(l-l'+l''-l''', m-m'+m''-m''', n-n'+n''-n''') \\
& + \frac{K}{2} \sum_{i \neq j} \Delta_{i;lmn} \Delta_{i;l'm'n'}^* \Delta_{j;l''m''n''} \Delta_{j;l'''m'''n'''}^* \delta(l-l'+m''-m''', m-m'+n''-n''', n-n'+l''-l''') \\
& + \sum_i \left( A + B(q_i^I)^2 - E \right) |\Delta_{i;0}|^2 + \left( G + \frac{K}{2} \right) |\Delta_{i;0}|^4.
\end{aligned} \tag{S8}$$

Here, the  $\delta$ -function is defined as

$$\delta(l, m, n) = \begin{cases} 1, & l = m = n, \\ 0, & \text{otherwise.} \end{cases} \tag{S9}$$

In principle, complex  $\Delta_{j;lmn}$ 's should be used, however, as mentioned in the main text, we studied the case when  $\Delta_{j;0} = \Delta_0$ ,  $\Delta_{j;lmn} = \Delta_{lmn}$  and are real. Under these assumptions,

the free energy expansion simplifies to:

$$\begin{aligned}
\mathcal{F}_{\text{cdw}}/3 = & \left( A + \tilde{B} - E \right) \Delta_0^2 + \left( G + \frac{K}{2} \Delta_0^4 \right) + \sum_{\substack{l,m,n \geq 0 \\ l \cdot m \cdot n = 0}} \left[ A + \tilde{B} \tilde{\mathbf{q}}_{lmn}^2 + 2 \left( G + \frac{K}{2} \right) |\Delta_0|^2 \right] \Delta_{lmn} \Delta_{lmn} \\
& - E \Delta_{lmn} \Delta_{l'm'n'} \delta(l + l' + 1, m + m', n + n') \\
& - D \Delta_{lmn} \Delta_{l'm'n'} \Delta_{l''m''n''} \delta(l + n' + m'', m + l' + n'', n + m' + l'') \\
& - M \Delta_{lmn} \Delta_{l'm'n'} \Delta_{l''m''n''} \delta(l - n' - m'' + 1, m - l' - n'', n - m' - l'') \\
& + G \Delta_{lmn} \Delta_{l'm'n'} \Delta_{l''m''n''} \Delta_{l'''m'''n'''} \delta(l - l' + l'' - l''', m - m' + m'' - m''', n - n' + n'' - n''') \\
& + K \Delta_{lmn} \Delta_{l'm'n'} \Delta_{l''m''n''} \Delta_{l'''m'''n'''} \delta(l - l' + m'' - m''', m - m' + n'' - n''', n - n' + l'' - l''')
\end{aligned} \tag{S10}$$

where  $\tilde{\mathbf{q}}_{lmn}^2 = 4\eta^2[(l^2 + m^2 + n^2) - (lm + ln + mn)] + 2(2l - m - n)\eta(\eta - 1) + (\eta - 1)^2$ , with  $\eta = |\mathbf{q}_j|/q^I$ , notice that the  $(q^I)^2$  has been absorbed into  $\tilde{B} = B(q^I)^2$ .

## SIV. DETAILS OF THE NUMERICAL MINIMIZATION

### SIV.A. Solving for the equilibrium CDW order parameter

Once all the parameters of the free energy are set, to find the absolute minimum of the free energy defined above, we begin by fixing  $\eta$  and obtaining the saddle points in the multidimensional space spanned by the real parameters  $\Delta_0$  and  $\Delta_{lmn}$ . The saddle points are determined by numerically solving the Euler-Lagrangian equations for  $\Delta$ 's. The result of this step is a curve of the minimum free energy as a function of  $\eta$ ,  $\mathcal{F}_{\text{cdw}}^{\text{min}}(\eta)$ , examples of which are shown in Fig. S1 for different effective temperatures.

The calculations require setting an harmonic cutoff  $N$  that restricts the expansion to terms with  $0 \leq l, m, n \leq N$ . The number of variational parameters is then given by  $(N + 1)^3 - N^3 + 2$ , which takes into account the constraint that at least one of  $l, m, n$  must be zero ( $l \cdot m \cdot n = 0$ ), and includes  $\Delta_0$  and  $\eta$ . The convergence of the harmonic expansion is relatively fast and we verified that  $N = 3$  yields a good compromise without affecting the accuracy of the results in the range of parameters studied. A typical example of the rapid decay of the higher harmonics is shown in Fig. S2(b).

Since we are minimizing numerically a 39-dimensional function, in order to reduce the chance of finding just a local minimum, we stochastically repeat each minimization multiple

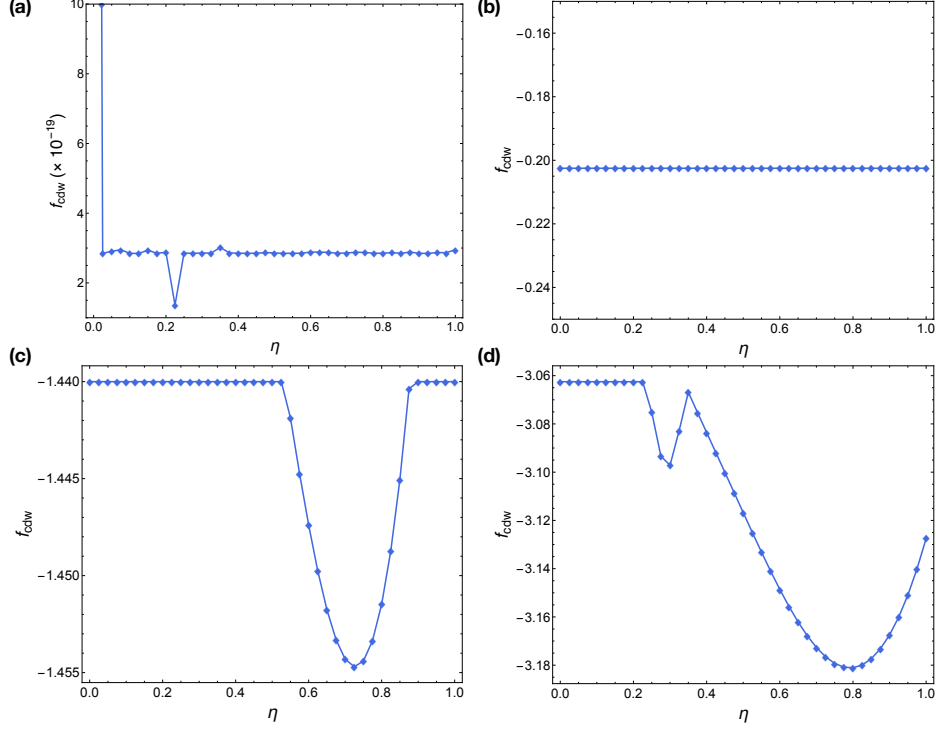


FIG. S1. Minimum of the CDW free energy (in arbitrary units) with respect to  $\eta$  at  $E = 2.2$ . (a) For  $t = 1.2$ , the minimum free energy is numerically zero for all  $\eta$  (note the extremely magnified vertical scale to emphasize the threshold of numerical accuracy), indicating a normal state. (b) At  $t = 0.3$ , the minimum of free energy is independent of  $\eta$  and negative. Only the harmonic amplitude  $\Delta_0$  is finite (not shown), which defines a C-CDW state. (c-d) For  $t = -1.2$  and  $t = -2.3$ , the minimum free energy is obtained at a finite  $\eta$ , which implies an I-CDW state.

times (typically 200 repetitions) feeding random initial values to the minimization routine and extract the absolute minimum. Moreover, we verified that the same results are obtained with independent implementations of the minimization procedure in Mathematica and Matlab which use different algorithms for absolute minimization.

The equilibrium state is identified by the harmonic content of the order parameter for the value of  $\eta$  that yields the absolute minimum of the free energy, as illustrated in Fig. S1. There are three possible outcomes: (i) If  $\mathcal{F}_{\text{cdw}}^{\min}(\eta) = 0$  as in Fig. S1(a), the equilibrium corresponds to the normal state, without either CCDW or ICDW. (ii) If  $\mathcal{F}_{\text{cdw}}^{\min}(\eta) \leq 0$  but constant with  $\eta$  as in Fig. S1(b), we have a CCDW state [which is always confirmed by inspecting that  $\Delta_0$  is the only non-zero component of  $\psi(\mathbf{r})$ ]. (iii) Otherwise,  $\mathcal{F}_{\text{cdw}}^{\min}(\eta)$  will have a global minimum at a given  $\eta$ , as in the cases shown in Fig. S1(c) and Fig. S1(d), which indicates that the



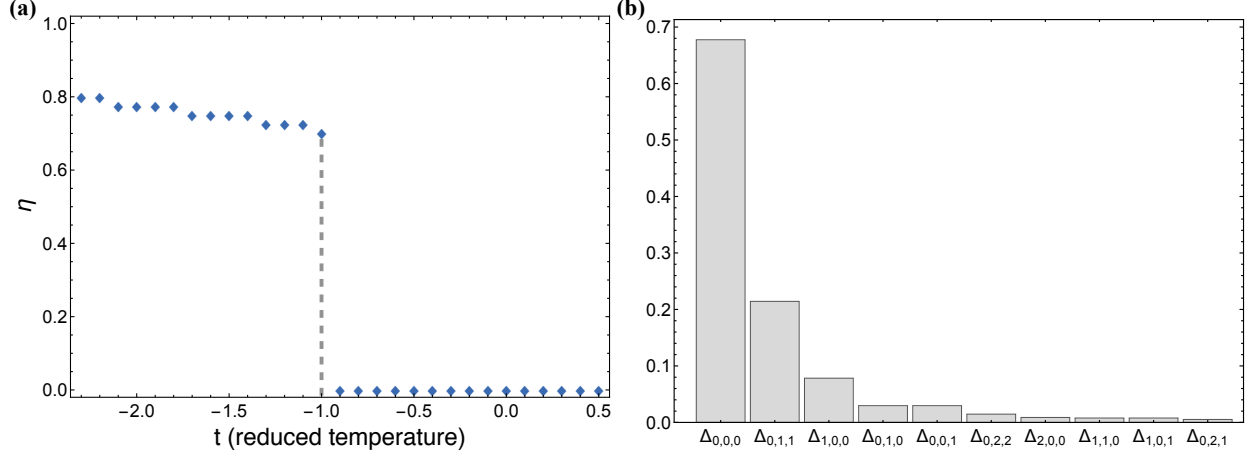


FIG. S2. Results from numerical minimization of free energy. (a) Plot of  $\eta$  versus  $t$  at a  $E = 2.2$ . The jump at  $t \approx -1$  indicates a first order nature of the C-IC phase transition. (b) The ten largest  $\Delta$ 's at  $(E, t) = (2.2, -1.7)$ . Since  $\Delta_{0,0,0}$  is the largest, the CDW phase is not commensurate at this point in the phase diagram.

equilibrium state is an ICDW. As can be seen from Fig. S2(a), due to the finite jump of  $\eta$  at the transition temperature, the C-IC transition is of first order.

#### SIV.B. Explicit form of the SC free energies

As described in the main text, we considered two explicit forms of the Ginzburg-Landau free energy for the SC amplitude  $\Phi(\mathbf{r})$  that differ only in whether the constant that couples it to the CDW order parameter depends on the lock-in energy  $E$ . In the first form the free energy in Eq. (3) reads explicitly

$$\mathcal{F}_{\text{sc}} = \int \left[ \left( a_0 - a_1 \sum_j |\nabla \psi_j|^2 \right) |\Phi|^2 + b_s |\nabla \Phi|^2 + c_s |\Phi|^4 \right] d\mathbf{r}, \quad (\text{S11})$$

where the constants were chosen as follows:  $a_0 = 10t + 60$ , where  $t$  represents the reduced temperature,  $t = (T - T_{\text{sc}})/T_{\text{sc}}$ , and the factors 10 and 60 have been chosen so that  $T_{\text{sc}}/T_{\text{cdw}}$  at the C-NC boundary reproduces the experimental ratio found for those critical temperatures at optimal doping;  $a_1 = 500 \times 2.1$  so that the maximum  $T_{\text{sc}}$  in this calculation matches the one obtained on the basis of Eq. (S12) at the calculated tip of the SC dome;  $b_s = c_s = 1$  for simplicity since, presently, we are interested only in the qualitative characteristics of the solution and its relation to the DC network, and not in the specific details of how stiff the SC

order parameter is, which is controlled by  $b_s$ , but regarding which no experimental evidence or data exists yet.

Since all constants are independent of  $E$  in this scheme, the effect of the lock-in energy enters only indirectly via the dependence of the CDW texture on  $E$ . Using this free energy and these parameters, the SC transition occurs at the gray line shown in the phase diagram of Fig. (1).

The second scheme discussed in the main text makes the coupling depend explicitly on  $E$ . This means that the free energy reads explicitly

$$\mathcal{F}_{\text{sc}} = \int \left[ \left( a_0 - a_1 E \sum_j |\nabla \psi_j|^2 \right) |\Phi|^2 + b_s |\nabla \Phi|^2 + c_s |\Phi|^4 \right] d\mathbf{r}, \quad (\text{S12})$$

where the constants are chosen as above,  $a_0 = 10t + 60$ ,  $b_s = c_s = 1$ , except that  $a_1 = 500$  now. In this case, the effect of the lock-in energy  $E$  appears both explicitly, as a prefactor to the interaction, and implicitly, through its effect on  $\psi_j(\mathbf{r})$ .

#### SIV.C. Solving for the equilibrium superconducting order parameter

We must determine the solution  $\Phi(\mathbf{r})$  that minimizes the free energy  $\mathcal{F}_{\text{sc}}$  in either of the forms written in (S11) or (S12). For every point  $(E, t)$  in the parameter space of the phase diagram, we replace  $\psi_j(\mathbf{r})$  by the corresponding equilibrium solution arising from the minimization of  $\mathcal{F}_{\text{cdw}}$ . Since  $\psi_j(\mathbf{r})$  is non-uniform in space outside the C-CDW phase, this turns the equations (S11) and (S12) into non-uniform Ginzburg-Landau problems.

Numerically, we solve the Euler-Lagrange equations for  $\Phi(\mathbf{r})$  using the CDW texture  $(\sum_j |\nabla \psi_j(r)|^2)$  itself as the initial trial solution which is then relaxed under periodic boundary conditions consistent with the CDW and discommensuration network.

### SV. REAL-SPACE SUPERCONDUCTING ORDER

Fig. S3 shows the real space SC order in different cases. At temperature right below the  $T_{\text{sc}}^{(0)}$ , isolated SC islands emerge at the intersection of three CDW DCs and forms a Kagome lattice, as shown in panel (a1-2). At very low temperature ( $T < T_{\text{sc}}^{(2)}$ ), the area of SC network expands and is able to cover the entire space, a 2D SC regime is achieved. Due to the linear dependence on  $E$  in the CDW and SC coupling  $a_1$ , when  $E$  decreases, the SC

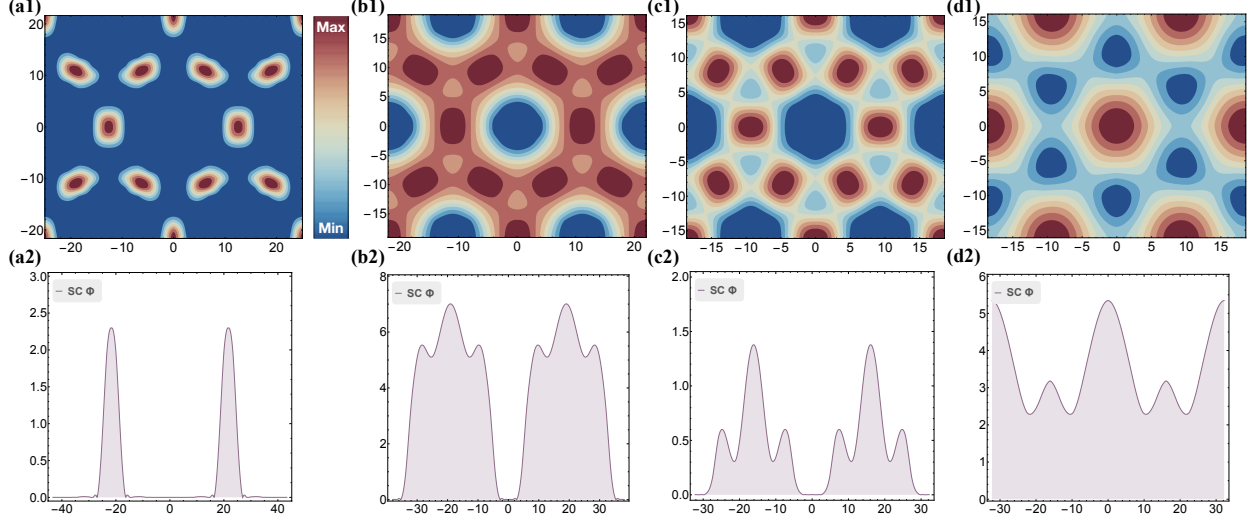


FIG. S3. Real space plots of the SC order parameter,  $\Phi(\mathbf{r})$ , computed for the CDW state at specific points  $(E, t)$  of the phase diagram shown in Fig. (1) of the main text. Each panel in the bottom row shows a vertical section along the line  $x = 0$  of the density plot directly above it. (a)  $(E, t) = (2.2, -1.1)$ : right below  $T_{\text{sc}}^{0\text{d}}$ , SC order nucleates on isolated 0d regions that coincide with the vertices of the Kagome lattice defined by the intersection of DCs. (b)  $(E, t) = (2.2, -3)$ : reducing the temperature from  $T_{\text{sc}}^{0\text{d}}$ , stabilizes the SC state further. Both the amplitude and spatial extent of the SC order parameter increase monotonically. The case shown corresponds to a temperature below the percolation threshold,  $T < T_{\text{sc}}^{1\text{d}}$ . (c)  $(E, t) = (1, -2.4)$ : the linear dependence of the CDW-SC coupling constant  $a_s$  with  $E$  weakens the SC amplitude when the lock-in energy is reduced. (d)  $(E, t) = (0, -2)$ : unlike the previous cases, here  $\Phi(\mathbf{r})$  has been obtained using an  $E$ -independent coupling  $a_s$ , as described in the text in relation to the gray SC boundary line in Fig. (1). With no lock-in energy ( $E = 0$ ), the equilibrium CDW solution approximates a homogeneously IC state (i.e., one without DCs). SC is therefore stabilized over the whole system.

order gets suppressed so one can get the dome shape of SC phase as shown in the phase diagram from main text. If the  $E$ -dependence is removed, in the IC phase (with very small  $E$ ), because of the strong fluctuation of CDW order parameter (relative to CCDW), it can still support a SC order, as shown in panel Fig. S3(d1-2).

- 
- <sup>1</sup> D. E. Moncton, J. D. Axe, and F. J. Disalvo, *Phys. Rev. Lett.* **34**, 734 (1975).
- <sup>2</sup> K. Nakanishi and H. Shiba, *J. Phys. Soc. Japan* **45**, 1147 (1978).
- <sup>3</sup> W. L. McMillan, *Phys. Rev. B* **14**, 1496 (1976).
- <sup>4</sup> P. Bak and V. J. Emery, *Phys. Rev. Lett.* **36**, 978 (1976).
- <sup>5</sup> S. A. Jackson, P. A. Lee, and T. M. Rice, *Phys. Rev. B* **17**, 3611 (1978).
- <sup>6</sup> A. E. Jacobs and M. B. Walker, *Phys. Rev. B* **21**, 4132 (1980).
- <sup>7</sup> K. Nakanishi, H. Takater, Y. Yamada, and H. Shiba, *J. Phys. Soc. Jpn.* **43**, 1509 (1977).
- <sup>8</sup> K. Nakanishi and H. Shiba, *J. Phys. Soc. Jpn.* **43**, 1839 (1977).
- <sup>9</sup> K. Nakanishi and H. Shiba, *J. Phys. Soc. Jpn.* **44**, 1465 (1978).