Electronic instabilities of kagomé metals: saddle points and Landau theory

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(Dated: June 11, 2021)

We study electronic instabilities of a kagomé metal with a Fermi energy close to saddle points at the hexagonal Brillouin zone face centers. Using parquet renormalization group, we determine the leading and subleading instabilities, finding superconducting, charge, orbital moment, and spin density waves. We then derive and use Landau theory to discuss how different primary density wave orders give rise to charge density wave modulations, as seen in the AV_3Sb_5 family, with A=K,Rb,Cs. The results provide strong constraints on the mechanism of charge ordering and how it can be further refined from existing and future experiments.

I. INTRODUCTION

Two dimensional correlated metals based on transition metal ions are a classic subject for many body physics [1, 2], displaying diverse electronic phenomena such as unconventional superconductivity [3–5], charge and spin order [6, 7], nematicity [8, 9], strange metallic behavior [10–12], and more. These topics have been most heavily investigated in theory and experiment in structures based on square lattices in the cuprates [4, 13] and Fe superconductors [3, 14, 15]. Correlated metals with hexagonal/triangular symmetry are much less common, with the best-known example being the triangular lattice cobaltates [16, 17], which however are complicated by Na vacancy ordering and water intercalation [18].

Recently, a new class of kagomé metals, with chemical formula AV_3Sb_5, where A=K, Rb, or Cs, have emerged as an exciting realization of quasi-2D correlated metals with hexagonal symmetry [19]. These materials have been shown to display several electronic orders setting in through thermodynamic phase transitions: multi-component (“3Q”) hexagonal charge density wave (CDW) order below a T_c ≈ 90K [20–27], and superconductivity with critical temperature of 2.5K or smaller [20, 21, 28–35], and some indications of nematicity and one-dimensional charge order in the normal and superconducting states [21, 31, 36]. Other experiments show a strong anomalous Hall effect [37, 38], suggesting possible topological physics. Furthermore, density functional calculations identified CsV_3Sb_5 as a Z_2 topological metal [39]. Angle resolved photoemission studies show these materials to be multi-band systems with several Fermi surface components [39], including approximately nested components and a Fermi energy that is close to multiple saddle points of the dispersion, in agreement with density functional theory [39, 40]. Furthermore, strong momentum dependent charge gaps near the saddle point momenta were observed below the CDW transition temperature [41, 42].

Many of these ingredients bring to mind a storied idea of electronic instabilities enhanced by van Hove singularities near saddle points. This mechanism figured heavily in early theoretical treatments of the cuprates [43–45, and references therein]. In a two-dimensional system, the divergence of the density of states generates enhanced scattering amongst electrons near the saddle points of the bands, which may drive not only superconducting but also other charge and spin instabilities.

The same idea emerged recently in the context of doped graphene [46–48], and has been applied to the theory of magic angle graphene bilayers [49–53]. The observations in AV_3Sb_5 suggest another application. Notably, the observed period of charge order in AV_3Sb_5 within the two-dimensional kagomé plane is precisely that expected from scattering amongst the saddle points located at the hexagonal Brillouin zone face centers (denoted as \( M \)).

While the saddle point model on a 2D hexagonal lattice has been studied extensively in the literature [46–49], its application to a coherent understanding of the electronic instabilities revealed in multiple experiments remains to be understood. First, the renormalization group studies from repulsive interactions [46, 49] suggest leading spin density wave, superconductivity, and orbital moment instabilities, rather than the charge density wave order which is observed. Therefore it is natural to expect that the lattice plays some role, and thus it is important to understand the combined effect of electron-phonon and electron correlation. Second, the strong anomalous Hall effect observed below the charge density wave critical temperature suggests time-reversal symmetry breaking order may develop below T_c. It would be desirable to understand the interplay between time-reversal symmetric and broken CDW order. Third, in addition to the 2×2 charge density wave within the 2D layer, STM and x-ray studies also observed modulation in the z-direction, i.e. \( k_z \neq 0 \),...
in RbV₃Sb₅ and CsV₃Sb₅. The three-dimensional alignment of 2D charge density waves has not yet been studied theoretically.

In this paper, we explore the electronic instabilities due to interactions amongst electrons near the saddle points with hexagonal symmetry. We apply the parquet renormalization group scheme [54–57] to determine all the primary and secondary instabilities, generalizing prior work [46, 49]. We further use mean field theory to study different possible emergent density wave states, which include not only a conventional charge density wave, but also spin and orbital moment density waves. We investigate how they relate to the observed charge density wave measured in AV₃Sb₅. Through this analysis, we provide constraints on the interpretation of experimental observations, and suggestions for future theoretical and experimental studies.

The rest of this paper is structured as follows: In Sec. II, we construct a low energy continuum model by taking patches around the saddle point momenta \( \mathbf{M} \) and identify its connection to the real space tight-binding model. In Sec. III, we generalize the parquet renormalization group formulation, and discuss all stable fixed points within the patch model. In Sec. IV, we analyze the mean field theory for each fixed point solutions. This includes a Landau theory analysis of the conventional charge density wave (Sec. IV B) as well as an analysis of other leading instabilities, i.e. the orbital moment density wave (Sec. IV C) and spin density wave (Sec. IV D), and their interplay with the conventional charge density wave. In Sec. V, we discuss the implications of the results obtained in Sec. IV to experimental observations. The real space pattern on the kagomé lattice are shown in Sec. V A. To understand the three dimensional 3Q CDW order with \( k_z \neq 0 \), we study the effects of weak interlayer coupling and discuss the allowed \( k_z \) for both conventional CDW and orbital moment density wave orders. The experimentally observed anisotropic CDW order can also be explained within this picture. In Sec. V C, we discuss the critical behavior for different types of charge order instabilities. The staggered and uniform orbital moment is estimated in Sec. V D. The possibility of a magnetic field induced mixture of conventional CDW and orbital moment is also briefly discussed there. Lastly, a summary of our work and discussions on the theoretical and experimental implications are presented in Sec. VI.

II. MODEL

In this section, we introduce a simple model to study the electronic behavior in AV₃Sb₅. As explained in the introduction, STM and x-ray scattering measurements show a \( 2 \times 2 \) CDW order with wavevector \( Q_\alpha = Q_{\text{Bragg}}/2 \) [20–22, 24]. These wavevectors are equivalent to the momenta that connect the three \( \mathbf{M}_\alpha \) points in the hexagonal Brillouin zone as shown in Fig. 1(b). In addition, DFT calculations show that the band structure has saddle points at the \( \mathbf{M}_\alpha \) points near the Fermi level as shown in Fig. 2 for CsV₃Sb₅. In two-dimensional systems, a saddle point is a van Hove singularity with a logarithmically diverging density of states. Based on these two observations, we assume that the collective electronic behavior in AV₃Sb₅ is determined by the saddle points located at the \( \mathbf{M}_\alpha \) points and the interactions between them.

![FIG. 1. (a)Vanadium kagomé lattice structure in AV₃Sb₅. The actual lattice structure has a Sb atom in the center of the hexagonal faces, but they are not shown here since our work is only focused on the electronic behavior of vanadium. The space group of the full lattice is \( P6/mmm \). (b) Hexagonal Brillouin zone of AV₃Sb₅. There are three distinct M points along the Brillouin zone boundaries. The \( \mathbf{M}_\alpha \) points in the Brillouin zone are connected by three nesting vectors \( \{Q_\alpha\} \). The nesting vectors satisfy \( Q_\alpha \equiv -Q_\alpha \) up to a reciprocal lattice vector.](image)

![FIG. 2. Band structure of CsV₃Sb₅ calculated using DFT without spin-orbit coupling [58]. The Fermi energy is set to 6.81 eV. \( \Gamma_1^+, \Gamma_3^+ \) are the irreducible representations of the two saddle point bands nearest the Fermi energy at \( \mathbf{M}_1 \). The little co-group at \( \mathbf{M}_1 \) is \( D_{2h} \), and the orientation of the symmetry axes \( C_2, C_3, C'_2 \) are shown in Fig. 1. We use the notation found in Ref. [59].](image)
where $\alpha, \beta$ are patch indices, $q$ is the momentum measured from $M_\alpha$, $\varepsilon_\alpha(q)$ is the saddle point dispersion sitting at $M_\alpha$, and $\mu$ is the chemical potential measured away from the saddle point. Up to quadratic order in $q$, the saddle point dispersions take the general form,

\[
\begin{align*}
\varepsilon_1(q) &= aq_x^2 - bq_y^2, \\
\varepsilon_2(q) &= \frac{a - 3b}{4} q_x^2 + \frac{\sqrt{3}(a + b)}{2} q_x q_y + \frac{3a - b}{4} q_y^2, \\
\varepsilon_3(q) &= \frac{a - 3b}{4} q_x^2 - \frac{\sqrt{3}(a + b)}{2} q_x q_y + \frac{3a - b}{4} q_y^2,
\end{align*}
\]

where $q = (q_x, q_y)$. The parameters $a, b$ that determine the shape of the saddle point must have the same sign, $ab > 0$. Note, that the dispersion of the three patches are related by a three-fold rotation. The condition for perfect nesting is given by $a/b = 3$, but in our work we will not necessarily impose this condition unless otherwise stated.

In general, there are four different cases of the form of the dispersion that we can consider: (i) $a, b > 0$, $a/b > 1$, (ii) $a, b > 0$, $a/b < 1$, (iii) $a, b < 0$, $a/b > 1$, and (iv) $a, b < 0$, $a/b < 1$. These cases can be all be mapped to case (i) by using two transformations. First, rotating the coordinates by $\pi/2$ takes cases (iii), (iv) to cases (ii), (i) respectively. Second, a particle-hole transformation combined with the same $\pi/2$ rotation maps case (ii) to case (i) (changing the sign of $\mu$). Hence, we only need to consider case (i). Note that the latter particle-hole-like transformation becomes a symmetry when $a = b$ and $\mu = 0$.

Next, we introduce interactions to the continuum model by listing all possible electron-electron interactions between the fermions in the three patches. There are four such interactions,

\[
H_1 = \frac{1}{2N} \sum'_{\{q_1, \ldots, \{q_4\} < \Lambda} \left[ \sum_{\alpha \neq \beta} \left( g_1 c_{\alpha q_1, \sigma} c_{\beta q_2, \sigma}^\dagger c_{\alpha q_3, \sigma'} c_{\beta q_4, \sigma'}^\dagger \\
+ g_2 c_{\alpha q_1, \sigma} c_{\beta q_2, \sigma}^\dagger c_{\alpha q_3, \sigma'} c_{\beta q_4, \sigma'}^\dagger \\
+ g_3 c_{\alpha q_1, \sigma} c_{\beta q_2, \sigma}^\dagger c_{\alpha q_3, \sigma'} c_{\beta q_4, \sigma'}^\dagger \\
+ \sum_{\alpha} g_4 c_{\alpha q_1, \sigma} c_{\alpha q_2, \sigma}^\dagger c_{\alpha q_3, \sigma'} c_{\alpha q_4, \sigma'}^\dagger \right) \right],
\]

where $\sum'_{\{q_1, \ldots, \{q_4\} < \Lambda} \equiv \sum_{\{q_1, \ldots, \{q_4\} < \Lambda} \delta_{q_1 + q_2, q_3 + q_4}$, $N$ is the number of unit cells in the system, and $g_i$ are the interactions that are to be intrinsically and have units of energy. As seen in Fig. 3, the $g_1, g_2, g_3, g_4$ interactions represent inter-patch exchange, inter-patch density-density, Umklapp, and intra-patch density-density scattering processes, respectively.

The patch model introduced here has been used in previous works to study the interaction and competition between different instabilities in the Hubbard model and doped graphene [46, 60]. An important thing to note is that the continuum model defined above does not include details on the underlying structure of the lattice and the global band structure. We supplement the results of our model with the symmetry information provided by the DFT results for CsV$_3$Sb$_5$ shown in Fig. 2 [58]. This gives a one-to-one correspondence between Brillouin zone patches, $M_\alpha$, and the vanadium sites, $V_\alpha$ (see App. A). A minimal tight binding model on the kagomé lattice can be readily obtained from this correspondence to faithfully describe the saddle point fermions (see Sec. V A2 for more discussions).

FIG. 3. All possible interactions in the patch model. The cones represent the saddle point dispersion at each $M_\alpha$ and the arrows denote the scattering processes described by the interactions.

III. RENORMALIZATION GROUP ANALYSIS

FIG. 4. RG phase diagram for $g_2^{(0)} > 0$. The leading instabilities of each phase under RG are, Phase I: sSC, rSDW, iSDW, Phase II: iCDW and rCDW, and Phase III: dSC, rSDW, iCDW. The phase diagram was calculated assuming $d_1 = 1/2, g_2^{(0)} = 0.1, g_4^{(0)} = 0.3$.

While all four interactions $g_1, g_2, g_3$ and $g_4$ are marginal at tree level, they acquire leading double logarithmic corrections from particle-particle fluctuations at zero momentum ($\Pi_{pp}(0)$) and particle-hole fluctuations at momentum transfer $M_\alpha$ ($\Pi_{ph}(M_\alpha)$) at the one loop level and so can become marginally relevant. To study
the evolution of $g_i$ at energy $E$ as the fermion fluctuations from cutoff energy $\Lambda_{\text{RG}} \sim i\Lambda^2$ to $E$ are integrated out, we perform a parquet renormalization group (pRG) analysis. Following Ref. [46], the pRG equations for $g_i$ are

\[
\begin{align*}
\frac{dg_1}{dy} &= 2d_1 g_1 (g_2 - g_1), \\
\frac{dg_2}{dy} &= d_1 (g_2^2 + g_3^2), \\
\frac{dg_3}{dy} &= -g_3^2 - 2g_3 g_4 + 2d_1 g_3 (2g_2 - g_1), \\
\frac{dg_4}{dy} &= -2g_3^2 - g_4^2, \\
\end{align*}
\]  

(4)

where $y = \Pi_{\text{pp}}(0, E) \sim \ln^2(\Lambda_{\text{RG}}/E)$ is the RG time and $d_1(y) = d\Pi_{\text{pp}}(M_a)/dy$ is the “nesting parameter”, which satisfies $0 < d_1(y) \leq 1/2$. For perfect nesting, $d_1(y) = 1/2$ and is independent of RG time. For concreteness, we will consider the perfect nesting case hereafter, i.e. $d_1 \equiv 1/2$. It has been checked that other $0 < d_1(y) < 1/2$ does not qualitatively change the fixed point solutions and leading density wave instabilities.

The RG equations, having entirely quadratic $\beta$-functions (the right hand sides of the pRG equations), do not have any non-trivial controlled fixed points in the usual sense. Rather, they describe flows in the vicinity of the free fixed point: since the RG equations are perturbative, they are strictly valid only within some sphere of small radius of the origin in $g$-space. Within certain domains of this space, the flows will be unstable, i.e. they will exit the sphere of control, which indicates an instability toward a new regime, and most likely an ordered state. Within the unstable regions of phase space, RG flows that begin very close to the origin tend to converge toward particular unstable trajectories which act as attractors, and are typically straight “rays”[61, 62]. Below we follow previous works that reformulate these rays to appear as fixed points, by projecting the trajectories to a plane of constant value of one of the parameters. The stable “fixed rays” are expected to describe the asymptotic limit of arbitrarily weak but non-zero bare interaction, such that convergence to these rays is nearly perfect before the sphere of control is exited. One should keep in mind that when the bare interactions are small but not arbitrarily so, the deviations from these rays become important, and the physics will be less universal and controlled more by the actual values of the interactions, but the RG equations can still be employed.

Before considering the stable fixed rays, we note a few features of these equations. The $\beta$-functions for $g_1$ and $g_3$ contain an overall factor of $g_1$ and $g_3$, respectively. This follows from symmetry: all terms except $g_1$ conserve spin at each saddle point separately, and all terms except $g_3$ conserve the number of electrons at each saddle point separately. The conserving interactions cannot generate a non-conserving one. As a result, the sign of $g_1$ and $g_3$ remain fixed through out the RG evolution. One also notes that the $dg_2/dy > 0$ and $dg_4/dy < 0$ under the RG. Thus an initially positive $g_2$ must remain positive, and an initially negative $g_4$ remains negative.

To understand the physical meaning of the $g_i$, it is useful to define interactions that parametrize particular channels of ordering, e.g. they appear in the mean-field treatment below in Sec. IV. They were previously defined in Ref. [46, 49]. Here, we consider the interactions in the $d$-wave superconductivity ($G_{3\text{SC}} = g_3 - g_4$), $s$-wave superconductivity ($G_{3\text{SC}} = -g_3 - g_4$), real charge density ($G_{\text{CDW}} = -2g_1 + g_2 - g_3$), orbital moment density ($G_{\text{CDW}} = -2g_1 + g_2 + g_3$) \(^1\), real spin density ($G_{\text{SDW}} = g_2 + g_3$), spin flux order ($G_{\text{SDW}} = g_2 - g_3$) channels. The interactions $G_a$ are defined such that the $a$ instability develops only when $G_a > 0$.

From the previous discussion, we can see a few features clearly. Real and imaginary parts of the CDW and SDW order parameters (OPs) are degenerate if $g_3 = 0$. This is because the umklapp interaction is the only one transferring charge between saddle points, so that in its absence there is a separate $U(1)$ charge rotation for each valley. Similarly, the corresponding real and imaginary parts of the CDW and SDW orders are degenerate when $g_1 = 0$. This is because only $g_1$ violates separate spin conservation at each saddle, so that when $g_1 = 0$, independent $SU(2)$ rotations may be made for each flavor, which mixes CDW and SDW orders. Thus, we see that the sign of $g_3$ decides between real and imaginary CDW/SDW, while the sign of $g_1$ decides between CDW and SDW order.

To proceed further, we determine the fixed rays and the pRG flow trajectory near them. We rewrite interactions as $g_i = \gamma_i g$, and choose $g$ as one of the interactions, which diverges as $g \sim 1/(y_{c} - y)$ along the fixed trajectory (as we verify afterwards). A proper identification of $g$ ensures that $\gamma_i$ tends to a constant value $\gamma_i^\ast$ along the fixed trajectory, and $\gamma_i^\ast = 0$ implies that the interaction $g_i$ either flows to zero or diverges slower than $1/(y_{c} - y)$. We call it a fixed point hereafter. The solutions to $\gamma_i^\ast$ can be obtained by solving a set of algebraic equations $\tilde{\beta}_i(\{\gamma\}) = 0$ for $i = 1, 2, 3, 4$, where

\[
\tilde{\beta}_i(\{\gamma\}) = \gamma_i - \frac{1}{g}(\dot{g}_i - \gamma_i g).
\]  

(5)

Among those solutions, only the stable fixed point solutions are of physical interest, as they do not flow away under small perturbations. To examine the stability of a fixed point solution, we define a matrix $T$ that is determined by the flow of $\tilde{\beta}_i$ at the fixed point, i.e.

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\(^1\) Here, iCDW stands for “imaginary charge density wave”. However, note that the latter does not necessarily mean that the charge instability must break time reversal symmetry for a generic wave vector. But at wave vector $M = -M$ up to a reciprocal lattice vector, imaginary charge density must break time-reversal symmetry, and correspond to orbital moment density wave. For similar reasoning, we use iSDW for spin flux order.
Definition

\[ \mathbf{T}_{ij} = \partial \tilde{\beta}_i / \partial \gamma_j |_{\{ \gamma \}}. \]

The RG fixed point is stable only when all the eigenvalues of \( \mathbf{T} \) are non-positive.

In addition to identifying the leading instabilities, the subleading ones are also considered here for three reasons. First, as discussed above, when the interaction strengths are not truly infinitesimal, flow to the unstable regime may occur before the fixed ray is reached. This may occur when bare couplings are small but not too close to a fixed ray, and deviate from it in a particular direction favoring a subleading instability. Second, the flow may be also cut off by imperfect nesting and/or a non-zero chemical potential (i.e. doping from the saddle point). These effects limit the convergence to the fixed ray, and deviate from it in a particular direction favoring a subleading instability. Third, a secondary instability may develop at a lower temperature, even if the primary one occurs first. To account for those possibilities, which depend upon the microscopic details, we will list the leading two instabilities at the RG fixed points.

To summarize, we list all the stable fixed point solutions for both repulsive and attractive bare interactions. In addition, we discuss an interesting semi-stable fixed point solution with only one weak unstable direction flowing out of the fixed point.

When \( g_2(0) > 0 \), there are three (semi)stable fixed points, which we take the liberty of denoting “phases” I, II, III – this is an abuse of terminology since these solutions really describe unstable rays in the full phase space, which may not correspond to a unique phase. As \( g_2(y) \) must diverge as \( \sim \frac{1}{y_c - y} \), we choose \( g(y) = g_2(y) = \frac{1}{d_1 (1 + \gamma^2) (y_c - y)}. \)

I. When \( g_3(0) < 0, g_2 \) flows to negative value at the stable RG fixed point, and we find \( \gamma_1 = 0, \gamma_2 = 1, \gamma_3 \approx -6.1, \gamma_4 \approx -5.5 \). The subleading divergence of \( g_1 \) goes as \( g_1(y) \sim (y_c - y)^{-\frac{2}{1 + \gamma_3}} \sim \frac{1}{(y_c - y)^{10.2}} \). Note that as the flow of \( g_1 \) is subleading here, the sign of \( g_1(0) \) is not qualitatively important to determine the fixed trajectory. The leading instabilities are \( G_{\text{gSC}} = 17.6g, G_{r\text{CDW}} = G_{i\text{SDW}} = 7.1g. \)

II. When \( g_1(0) < 0, g_3(0) > 0 \), and for large enough \( |g_3(0)| \), the system may flow to a semi-stable fixed point, where there is only one weak unstable direction in the 4-dimensional parameter space defined by \( \{ g_1, g_2, g_3, g_4 \} \). The fixed point solution reads \( \gamma_1 \approx -46.7, \gamma_2 = 1, \gamma_3 \approx 9.7, \gamma_4 \approx -4.4 \). The leading instabilities are \( G_{r\text{CDW}} = 104.0g, G_{i\text{CDW}} = 84.6g. \)

III. When \( g_1(0), g_3(0) > 0 \), the stable RG fixed point has been discussed a lot in the literature [46]. The fixed point solution gives \( \gamma_1 = 0, \gamma_2 = 1, \gamma_3 \approx 5.6, \gamma_4 \approx -10.0 \), where the subleading divergence of \( g_1 \) can be obtained as \( g_1(y) \sim (y_c - y)^{-\frac{2}{1 + \gamma_3}} \approx \frac{1}{(y_c - y)^{14.9}} \). The leading divergent instabilities are \( G_{\text{gSC}} = 15.6g, G_{r\text{SDW}} = G_{i\text{CDW}} = 6.6g. \)

### TABLE I

| OP    | Definition | Interaction strength (G) |
|-------|------------|--------------------------|
| rCDW  | \( N_\alpha = G_{r\text{CDW}} \sum_q \langle c_{q\sigma} c_{-q\bar{\sigma}} \rangle \) | \(-2g_1 + g_2 - g_3\) |
| iCDW  | \( \phi_\alpha = G_{i\text{CDW}} \sum_q \langle c_{q\sigma} c_{-q\sigma} \rangle \) | \(-2g_1 + g_2 + g_3\) |
| rSDW  | \( S_\alpha = G_{r\text{SDW}} \sum_q \langle c_{q\sigma} c_{q\bar{\sigma}} \rangle \) | \(g_2 + g_3\) |
| iSDW  | \( \psi_\alpha = G_{i\text{SDW}} \sum_q \langle c_{q\sigma} c_{-q\bar{\sigma}} \rangle \) | \(g_2 - g_3\) |
| aSC   | \( \Delta_x = G_{a\text{SC}} \sum_q \langle c_{q\sigma} c_{-q\bar{\sigma}} \rangle \) | \(-2g_3 - g_4\) |
| dSC   | \( \Delta_{x^2-y^2} = G_{d\text{SC}} \sum_q \langle c_{q\sigma} c_{-q\bar{\sigma}} \rangle \) | \(g_3 - g_4\) |

In Fig. 4, the phase diagram in the space of \( g_1(0), g_3(0) \) for \( g_2(0) > 0 \) is shown.

When \( g_2(0) < 0, g_2 \) may instead flow to zero. We find in this way a fourth fixed ray, which we denote Phase IV. It is described by letting \( g = g_1(y) = -\frac{1}{2d_1 (y_c - y)} \), and \( \gamma_1 = 1, \gamma_2 = 0, \gamma_3 = 0, \gamma_4 = 0 \). This solution requires \( g_1(0) < 0, g_3(0) > 0, \) and is only stable when \( g_3(0) > 0 \). Moreover, \( g_3(y) \) is also divergent and is only logarithmically smaller than \( g_1 \). We find \( g_3(y) = \frac{1}{y_c - y} \left( \ln \frac{1}{y_c - y} \right)^{-1} \). The leading instabilities are \( G_{r\text{CDW}} = G_{i\text{CDW}} = -2g = \frac{1}{d_1 (y_c - y)} \). The fixed point solution indicates that the rCDW and iCDW orders are degenerate at the leading order, but they are split by a logarithmically subdominant effect due to \( g_3 \) > 0 weakly in favor of the iCDW, i.e. \( G_{i\text{CDW}} > G_{r\text{CDW}} \).

In passing, we note that purely electronic interactions generally give repulsion for all couplings, i.e. \( g_i(0) > 0 \) with \( i = 1, 2, 3, 4 \). However, other factors, such as orbital composition of the wave function near saddle points, and electron-phonon coupling, may contribute to attraction for certain \( g_i(0) \). In App. B, we consider the effect of electron-phonon coupling, and show that the renormalization to \( g_i(0) \) can be attractive for both \( \delta g_1(0) \) and \( \delta g_3(0) \) or only \( \delta g_1(0) \), depending upon the strength of the coupling and phonon modes involved.
IV. MEAN-FIELD THEORY

As shown in Sec. III, we found instabilities to superconducting, charge density wave (rCDW), orbital moment (iCDW) and spin density wave (SDW) states. In all three AV3Sb5 materials, experiments have observed charge density wave order (rCDW order) setting as the first instability of the symmetric state at a $T_c \sim 90K$, and superconductivity only at much lower temperatures. Hence, in this section, we neglect superconductivity, and discuss the ways that the remaining instabilities may lead to the specific rCDW order observed experimentally in the AV3Sb5 materials. Notably, we find that rCDW order can be induced even if rCDW is not the primary order parameter. Hence we study the formation of rCDWs both when the rCDW is and is not the primary instability, and discuss the differences in the resulting properties. We carry out the study using mean field theory.

The renormalization group analysis tells us that in phase I the rCDW is a leading instability. In Sec. IV.B, we will study this case by calculating a mean-field theory in the rCDW channel. In Sec. IV.C, we consider a iCDW-rCDW coupled mean field theory, which is relevant to phases II and IV. Here we discuss how rCDW can be induced when the iCDW is the primary order parameter. Finally, in Sec. IV.D, we consider the situation with a leading rSDW instability, relevant to phase III, and show how it may induce rCDW order.

A. Complex CDW free energy

We first obtain the Landau free energy including both rCDW and iCDW order parameters, defined as $N_\alpha$, $\phi_\alpha$ with $\alpha = 1, 2, 3$ labeling the interpatch momentum transfer $Q_\alpha$ (see Fig. 1 (b)), respectively. The patch-model interaction given in Eq. (3) can be rewritten in the form of a rCDW interaction and an iCDW interaction:

$$H_{rCDW} = -\frac{NG_{rCDW}}{2} \sum_\alpha \beta_{rC,\alpha} \tilde{\rho}_{rC,\alpha},$$

$$H_{iCDW} = -\frac{NG_{iCDW}}{2} \sum_\alpha \beta_{iC,\alpha} \tilde{\rho}_{iC,\alpha},$$

(6)

where $G_{r/iCDW}$ is the r/iCDW interaction strength defined in Sec. III and $\tilde{\rho}_{rC,\alpha} = \frac{1}{2N} \sum_{\alpha < \Lambda} \bar{c}^\dagger_{\beta q} c_{\gamma q}$, $\tilde{\rho}_{iC,\alpha} = \frac{\epsilon_{\alpha,\Lambda}}{2N} \sum_{\alpha < \Lambda} \bar{c}^\dagger_{\beta q} c_{\gamma q}$ is the rCDW and iCDW operators with momentum $Q_\alpha = M_\beta - M_\gamma$. Using the Hubbard-Stratonovich transformation we decouple the interactions in the two channels and then integrate out the Fermionic degrees of freedom. This gives us the free energy as a function of the rCDW, iCDW order parameters, $N_1, N_2, N_3, \phi_1, \phi_2, \phi_3$:

$$F_{CDW} = \frac{N}{2G_{rCDW}} \sum_{\alpha=1}^3 N_\alpha^2 + \frac{N}{2G_{iCDW}} \sum_{\alpha=1}^3 \phi_\alpha^2 - (\text{Tr} \log G^{-1}),$$

(7)

where $G^{-1}$ is defined as

$$G^{-1}(i\omega_n, q; \{N_\alpha, \phi_\alpha\}) = \left[ \begin{array}{ccc} -i\omega_n + \varepsilon_1(q) & -(N_3 - i\phi_3)/2 & -(N_2 + i\phi_2)/2 \\ -(N_3 + i\phi_3)/2 & -i\omega_n + \varepsilon_2(q) & -(N_1 - i\phi_1)/2 \\ -(N_2 - i\phi_2)/2 & -(N_1 + i\phi_1)/2 & -i\omega_n + \varepsilon_3(q) \end{array} \right].$$

Expanding the order parameter fields in Eq. (8) perturbatively, the free energy in terms of the complex charge density order parameter $\Delta_\alpha = N_\alpha + i\phi_\alpha = |\Delta_\alpha| e^{i\theta_\alpha}$ is

$$f_{CDW} = \frac{r_N + r_\phi}{2} \sum_\alpha |\Delta_\alpha|^2 + \frac{r_N - r_\phi}{2} \sum_\alpha |\Delta_\alpha|^2 \cos 2\theta_\alpha + K_2 |\Delta_1||\Delta_2||\Delta_3| \cos(\theta_1 + \theta_2 + \theta_3) + K_4 \left( \sum_\alpha |\Delta_\alpha|^2 \right)^2 + (K_3 - 2K_4) \sum_{\alpha < \beta} |\Delta_\alpha|^2 |\Delta_\beta|^2 + O(\Delta^5).$$

(9)

Here, $r_N = \frac{1}{2G_{rCDW}} + K_1$, $r_\phi = \frac{1}{2G_{iCDW}} + K_1$, and $K_1, \ldots, K_4$ are functions of temperature and chemical potential, that we will discuss in detail in Sec. IV.B. For simplicity, we first consider the case $K_3 - 2K_4 < 0$, which favors 3Q CDW. The configuration of $\theta_\alpha$ that minimizes the free energy depends on the sign of $r_N - r_\phi$:

- When $r_N < r_\phi$, i.e. $G_{rCDW} > G_{iCDW} > 0$, minimizing the 2nd term requires $\theta_\alpha = n_\alpha \pi$, with $n_\alpha \in \mathbb{Z}$. By choosing the proper $n_\alpha$, the minimization of cubic term can be readily achieved. For any $\theta_\alpha = n_\alpha \pi$, the iCDW order parameter must vanish, so the ground state only contains rCDW order.

- When $r_N = r_\phi$, i.e. $G_{rCDW} = G_{iCDW}$, the second term vanishes, and the minimization of the cubic term gives a continuously degenerate ground state manifold. To lift the degeneracy, other perturbations should be considered.

- When $r_N > r_\phi$, i.e. $0 < G_{rCDW} < G_{iCDW}$, the second quadratic and cubic terms cannot be minimized simultaneously. As a result, $\theta_\alpha \neq n_\alpha \pi/2$, with $n_\alpha \in \mathbb{Z}$. This indicates that both $N_\alpha$ and $\phi_\alpha$ are non-zero. To analyze the Free energy with iCDW as the leading instability, the iCDW-rCDW coupling must be considered.

Below, we discuss the above three scenarios and then the rSDW-rCDW coupling scenario.

B. rCDW Mean-field theory

At the RG fixed point corresponding to phase I ($g_3(0) < 0$), the rCDW is the leading density wave instability. As argued above, it is enough to consider only the rCDW...
order parameters. The mean field free energy becomes

$$ F_{rCDW} = \frac{N}{2G_{rCDW}} \sum_{\alpha=1}^{3} N_{\alpha}^{2} - (\text{Tr} \log G^{-1}), \quad (10) $$

where $G^{-1}$ is defined as

$$ G^{-1}(i\omega_n, \mathbf{q}; \{ N_{\alpha} \}) = \begin{bmatrix} -i\omega_n + \varepsilon_1(\mathbf{q}) & -N_3/2 & -N_2/2 \\ -N_3/2 & -i\omega_n + \varepsilon_2(\mathbf{q}) & -N_1/2 \\ -N_2/2 & -N_1/2 & -i\omega_n + \varepsilon_3(\mathbf{q}) \end{bmatrix}, \quad (11) $$

As a function of $N_{\alpha}$, the rCDW free energy has the symmetry of the tetrahedral point group, $T_d$. This can be deduced by applying the symmetry operations of the full space group of the lattice, $P6/mmm$, to the definitions of the rCDW order parameter. Using our knowledge of this symmetry, we can determine what solutions of the free energy are possible. In the cases that are physically relevant, the solutions of the mean-field theory belong in either the 3Q$^+$, 3Q$^-$, or 1Q rCDW configurations which are classes of rCDW states with directions:

- 3Q$^+$: \{ (111), (1\overline{1}1), (\overline{1}1\overline{1}), (\overline{1}\overline{1}1) \},
- 3Q$^-$: \{ (\overline{1}1\overline{1}), (11\overline{1}), (1\overline{1}1), (\overline{1}11) \},
- 1Q: \{ (100), (100), (010), (010), (001), (001) \}.

Indeed, by numerically solving the full free energy we will see that the solutions belong in either the 3Q$^\pm$ or 1Q rCDW classes. A detailed discussion is provided in App. C. The rCDW patterns of the 3Q$^\pm$ and 1Q states are shown in Fig. 7.

By assuming we are near the rCDW transition where the rCDW order parameters are sufficiently small, we can expand the free energy to fourth order in $N_{\alpha}$. The resulting Landau theory is

$$ f_{rCDW} = \left( \frac{1}{2G_{rCDW}} + K_1 \right) \sum_{\alpha} N_{\alpha}^{2} + K_2 N_1 N_2 N_3 $$

$$ + K_4 \left( \sum_{\alpha} N_{\alpha}^{2} \right)^2 + (K_3 - 2K_4) \sum_{\alpha<\beta} N_{\alpha}^2 N_{\beta}^2 + O(N^5), \quad (12) $$

where $f_{rCDW}$ is the free energy density. The definitions of the coefficients $K_1, \ldots, K_4$ which are functions of chemical potential and temperature are given in App. D. The coefficients can be evaluated asymptotically in the limit $\mu, k_B T \ll t \Lambda^2$ and can also be found in App. D.

Fig. 5 shows the temperature dependence of these coefficients when $\mu/t \Lambda^2 = 0.01$. Notice that the coefficients exhibit a change in behavior at the cross-over temperature $k_B T \sim \mu$. In addition, the $K_2, K_3, K_4$ coefficients change sign near the cross-over temperature. When the quartic coefficients become negative, the Landau theory expression given by Eq. (12) becomes unstable, but in those regions stability can be restored by including sixth-order terms to the free energy.

Eq. (12) has a third order term, $K_2$, that couples all three rCDW order parameters. This is allowed by symmetry since this term is even under time-reversal symmetry and the sum of the three nesting wave vectors satisfies $\sum_{\alpha} Q_{\alpha} = 0$. This term introduces a preference for 3Q$^+$ or 3Q$^-$ rCDW states depending on the sign of $K_2$.

On the other hand, when $K_3 - 2K_4 > 0$, the fourth order term sets a preference for 1Q rCDW states. When $K_3 - 2K_4 < 0$, this fourth order term prefers the 3Q$^\pm$ states equally.

When $a/b = 3$, Fig. 5 shows that $K_2 < 0$ when $\mu/k_B T \lesssim 2.14$ in the asymptotic limit. In addition, $K_3 - 2K_4 < 0$ for $\mu \ll k_B T$. Hence, in this region, all terms in the rCDW Landau theory prefer the 3Q$^+$ rCDW state. The transition to the 3Q$^+$ rCDW state must be a first-order transition because the free energy can become negative before the second-order term vanishes due to the third-order term. One thing to note is that the rCDW order parameter is not necessarily small near the first-order rCDW transition, so the results of the Landau theory must be treated with caution. We can avoid this issue by numerically solving the full free energy.

The full free energy defined in Eqs. (10), (11) has four tunable parameters: temperature $T$, chemical potential $\mu$, the rCDW interaction strength $G_{rCDW}$, and the nesting ratio $a/b$. As explained in Sec. II, we only need to consider the case $a, b > 0$. Given this condition, we can introduce a convenient reparametrization,

$$ a = \frac{\delta + \sqrt{3 + \delta^2}}{\sqrt{3}} t, $$

$$ b = -\frac{\delta + \sqrt{3 + \delta^2}}{\sqrt{3}} t, \quad (13) $$

where $t > 0$ and $\delta \in \mathbb{R}$. We see that $t$ represents the
Recall that $r$ degree of nesting. Under this parametrization, $a/b \geq 1$ for $\delta \geq 0$ and $a/b < 1$ for $\delta < 0$. In particular, $a/b = 3$ (perfect nesting) for $\delta = 1$.

For different values of $G_{\text{rCDW}}$ and $\delta$, we generate a phase diagram in the $T - \mu$ plane. The results shown in Fig. 6 are representative samples of the the entire parameter space where the continuum model holds—$k_B T, \mu, G_{\text{rCDW}} \ll \Lambda^2$. We see that when the system is doped to the saddle point ($\mu = 0$) or below it, only the 3Q+ rCDW forms. As you dope the system above the saddle point, 1Q and/or 3Q- rCDW regions can emerge. In addition, for $\delta = 1.6$, the 1Q rCDW region is small and vanishes for sufficiently small $G_{\text{rCDW}}$ as seen in Figs. 6(c), 6(f). Similarly, at perfect nesting and more generally $\delta \sim 1$, the 3Q- rCDW region vanishes for sufficiently small $G_{\text{rCDW}}$ as seen in Fig. 6(b). Clearly, the 3Q+ rCDW region is largest in all phase diagrams which is consistent with the Landau theory discussed above.

### C. iCDW-rCDW mean field theory

Now, we consider how a fundamental iCDW order can induce subsidiary rCDW order. To do so, we consider a iCDW-rCDW coupled mean field theory. We are particularly interested in the regime, motivated by the RG results for phases II and IV, in which iCDW and rCDW are close in energy and can compete.

It is convenient to express Eq. (9) in terms of $N_\alpha$ and $\phi_\alpha$:

$$f_{\text{CDW}} = r_\phi \sum_{\alpha=1}^{3} \phi_\alpha^2 + r_N \sum_{\alpha=1}^{3} N_\alpha^2$$

$$+ K_2 (N_1 N_2 N_3 - \phi_2 \phi_3 N_1 - \phi_1 \phi_3 N_2 - \phi_2 \phi_1 N_3)$$

$$+ K_4 \left( \sum_{\alpha=1}^{3} \phi_\alpha^2 + N_\alpha^2 \right)^2$$

$$+ (K_3 - 2K_4) \sum_{\alpha < \beta} (\phi_\alpha^2 + N_\alpha^2)(\phi_\beta^2 + N_\beta^2) + O(\phi^6, N^5).$$

(14)

Recall that $r_\phi = \left( \frac{1}{2G_{\text{icDW}}} + K_1 \right)$, $r_N = \left( \frac{1}{2G_{\text{icDW}}} + K_1 \right)$.

We assume $G_{\text{icDW}} > G_{\text{rCDW}} > 0$, so that iCDW is the leading instability. Note that time-reversal symmetry forbids the term cubic in $\phi$, i.e. $\phi_1 \phi_2 \phi_3$. As a result, the order parameter manifold for $\phi_\alpha$ alone has cubic symmetry $O_h$. In addition, the 3Q± classes which were distinct for the case of rCDW are now related under time-reversal symmetry and part of the larger 3Q class which is defined as the union of the 3Q± classes. Close to and below the transition temperature for iCDW, the iCDW-rCDW coupling can be treated as a perturbation.

First, we consider the iCDW Landau theory. The order parameter manifold for $\phi_\alpha$ is determined by quartic terms proportional to $K_3$ and $K_4$. The first term $K_4 (\sum_{\alpha=1}^{3} \phi_\alpha^2)^2$ is positive definite and isotropic, so the selection of the ground state configuration is determined by the term $(K_3 - 2K_4) \sum_{\alpha < \beta} \phi_\alpha^2 \phi_\beta^2$. Specifically, (i) when $K_3 > 2K_4$, the 1Q iCDW state is favored, (ii) when $K_3 = 2K_4$, the $\phi_\alpha$ ground state configuration is degenerate at quartic order, and requires higher order terms to break the degeneracy, (iii) when $K_3 < 2K_4$, the 3Q iCDW is favored. From the asymptotic solution shown in Fig. 5 at $\mu/t\Lambda^2 = 0.01$, we see that when $k_B T_c/t\Lambda^2 \lesssim 0.01$, and the 1Q iCDW is stable. When $k_B T/t\Lambda^2 \gtrsim 0.01$, $K_3 - 2K_4 < 0$. Thus 3Q iCDW develops if $T_c$ sits in this range of temperature, and it may become unstable to 1Q iCDW as temperature lowers. On the other hand, when $\mu \ll k_B T$, we find $K_3 - 2K_4 < 0$ in the low temperature regime when $k_B T/t\Lambda^2 < 0.025$ (see App. D). Thus 3Q iCDW should be stable at $\mu \sim 0$. This transition is a continuous phase transition in contrast to the rCDW case because of the absence of a third-order term. The real space pattern for 1Q and 3Q iCDW orders are presented in Sec. V A 2.

Next, we substitute the iCDW order parameter in Eq. (14) with the iCDW saddle point solution, $|\phi_\alpha| = \phi_0$, and obtain the free energy for rCDW OPs. For 1Q iCDW, no rCDW can be induced. For 3Q iCDW, as the cubic term $K_2$ contains term linear in $N_\alpha$ through coupling to two iCDW OPs at another momenta, considering up to quadratic term in $N$, we find $\{N_1, N_2, N_3\} = N_0 \{1, \pm 1, \pm 1\}$ up to any permutations of the signs between $N_\alpha$, where $N_0 \sim K_2^{1/2}$. Here, $T - T_{\text{rCDW}} \sim \left( \frac{1}{2G_{\text{rCDW}}} + K_1 \right) > 0$. So the sign of $N_0$ is determined by the sign of $K_2$. Since $K_2 < 0$ for $\mu/T \approx 2.14$, $N_0 < 0$, the induced rCDW order must be the 3Q− one. As temperature further lowers to $T < T_{\text{rCDW}}$, the quartic term in $N_\alpha$ should be included so that the free energy is stable. We checked that the rCDW order remains the 3Q− one for $K_2 < 0$ and vice versa.

### D. rSDW-rCDW Mean-field theory

In phase III of the RG phase diagram, the rSDW is the leading density wave instability. Here, we consider how rCDW order can emerge as a subsidiary order through rSDW-rCDW coupling. By rewriting the full interaction, Eq. (3), using the rSDW operators the rSDW interaction term is

$$H_{\text{rSDW}} = \frac{-NG_{\text{rSDW}}}{2} \sum_\alpha \hat{\rho}_{\text{rS}, \alpha} \cdot \hat{\rho}_{\text{rS}, \alpha},$$

(15)

where $\hat{\rho}_{\text{rS}, \alpha} = \sum_{|q|<\Lambda} c_{\alpha q} \bar{c}_{\alpha q}$ is the spin density operator. Assuming the interaction in rCDW channel is also attractive, but much weaker than that of rSDW, we can decouple the interactions in the rSDW and rCDW channel using a Hubbard-Stratonovich transformation, integrate out the Fermionic degrees of freedom, and expand the resulting mean field free energy to fourth order in the rSDW and rCDW order parameters. This gives
FIG. 6. rCDW phase diagrams calculated in the $k_B T - \mu$ plane. $\tilde{G}_{r\text{CDW}}$ is defined as the dimensionless rCDW strength. $\delta$ parametrizes nesting as defined in Eq. (13). The phase diagrams correspond to the case $t, \delta > 0$ ($a, b > 0$ and $a/b > 1$). The phase diagrams for $t, \delta < 0$ ($a, b > 0$ and $a/b < 1$) are related to these phase diagrams under the exchange $3Q+ \leftrightarrow 3Q-$ and reflection in the $\mu = 0$ axis.

us the rSDW free energy (which may be added to the rCDW free energy in Eq. (12)):

$$f_{r\text{SDW}} = \left( \frac{1}{2G_{r\text{SDW}}} + \frac{K_1}{4} \right) \sum_{a} |S_a|^2 + \frac{K_2}{4} (N_1 S_2 \cdot S_3 + N_2 S_3 \cdot S_1 + N_3 S_1 \cdot S_2) + \frac{K_3}{16} \sum_{\alpha < \beta} |S_\alpha|^2 |S_\beta|^2 + \frac{K_4}{16} \sum_{\alpha} |S_\alpha|^4 + K_5 \sum_{\alpha < \beta} |S_\alpha \cdot S_\beta|^2 + K_6 (S_1 \cdot S_2 \times S_3)^2 + \cdots$$

Here $K_3, K_6$ are new symmetry-allowed coefficients. The important aspect of this Landau theory is the third-order term which couples the rSDW and rCDW order parameters. This term is allowed by symmetry since it is invariant under time-reversal and lattice translation symmetry.

Close to the transition temperature $T_c$ for the rSDW order, the rSDW-rCDW coupling term can be treated as a perturbation and we can first solve the rSDW Landau theory. Like the iCDW OPs, the $3Q+$ and $3Q-$ classes are related under time-reversal symmetry so we only need to consider the $3Q$ and $1Q$ rSDW classes. This Landau theory has previously been studied in Ref. [47]. For chemical potential sufficiently close to the saddle point, the solution to the SDW Landau theory is a uniaxial $3Q$ rSDW phase where all three rSDW order parameters
have the same magnitude and are oriented along the same axis, i.e. \( S^\alpha_\alpha = s_n a_\alpha \), where \( a_\alpha = \pm 1 \). If we substitute this solution into Eq. (16) and add the terms from Eq. (12), we get a free energy that is a function of just the rCDW OPs:

\[
\begin{align*}
  f_{rCDW} + f_{SDW} |_{S_\alpha = S^\alpha_\alpha} &= \left( \frac{1}{2G_{rCDW}} + K_1 \right) \sum_\alpha N^2_\alpha \\
  &+ K_2 |s|^2 (n_2 n_3 N_1 + \text{cyc. perms.}) + K_2 N_1 N_2 N_3 \\
  &+ K_4 \left( \sum_\alpha N^2_\alpha \right)^2 + (K_3 - 2K_4) \sum_{\alpha<\beta} N^2_\alpha N^{2}_{\alpha} N^2_{\beta}. 
\end{align*}
\] (17)

For \( K_3 - 2K_4 < 0 \), all terms prefer the 3Q+ rCDW state, so the system can develop a rCDW state.

V. EXTENSIONS AND EXPERIMENTAL IMPLICATIONS

In this section, we discuss various aspects of the different CDW phases, and how they may be differentiated experimentally.

A. Real space r/iCDW patterns

It is interesting to consider the real space patterns of charges and currents associated with the rCDW and iCDW order parameters.

Our continuum model does not carry any details of the lattice, so we rely on symmetry information provided by DFT calculations [58]. Importantly, as the saddle point band at the three \( M \) points are even under inversion, it can be shown that among the d-orbitals of vanadium atoms, only the \( \alpha \)-th vanadium atom in the unit cell contributes to the Bloch state at \( M_\alpha \) (see App. A). Furthermore, the DFT calculation shows that the saddle points consist mostly of d-orbitals of vanadium atoms. Motivated by these observations, we consider nearest-neighbor hopping on the Kagomé lattice as the minimal tight binding model that should capture the essential physics from fermions near the saddle points. For convenience, the lattice coordinate for the three sublattices is expressed as \( r_\alpha = R + \delta_\alpha \), where \( R \) is the coordinate for a unit cell, which is taken at the center of the triangular plaquette with the green sublattice facing to the left in Fig. 1(a). \( \delta_1 = (- \frac{1}{2\sqrt{3}}, 0) \), \( \delta_2 = (\frac{1}{4\sqrt{3}}, \frac{1}{2}) \) and \( \delta_3 = (\frac{1}{4\sqrt{3}}, -\frac{1}{2}) \).

The tight-binding Hamiltonian reads

\[
\hat{H}_0 = t_1 \sum_{(r_\alpha, r_\alpha + e_\beta)} \{ d_{r_\alpha}^{\dagger} d_{r_\alpha + e_\beta} + d_{r_\alpha + e_\beta}^{\dagger} d_{r_\alpha} \}, 
\] (18)

where \( (r_\alpha, r_\alpha + e_\beta) \) is the NN bond and \( e \) is defined such that \( r_\gamma = r_\alpha + e_\beta \) where \( \{ \beta, \alpha, \gamma \} \) is a permutation of \( \{1, 2, 3\} \). This gives \( e_1 = \frac{1}{2} (-1, 0) \), \( e_2 = \frac{1}{2} (-\frac{\sqrt{3}}{2}, \frac{1}{2}) \) and \( e_3 = \frac{1}{2} (\frac{\sqrt{3}}{2}, \frac{1}{2}) \).

Due to the one-to-one correspondence between patch label \( M_\alpha \) and sublattice label \( V_\alpha \) of vanadium atoms, the real space fermions on vanadium atoms can be expressed as

\[
d_{r_\alpha} = \frac{1}{\sqrt{N}} \sum_k e^{i k \cdot R_{\alpha,k}} \approx \frac{1}{\sqrt{|q|<\Lambda}} \sum e^{i M_\alpha \cdot R_{\alpha,q}}, \quad (19)
\]

where \( c_{\alpha q} \) denotes the saddle point fermion near \( M_\alpha \) as defined in the continuous model (Eq. (1)). As both rCDW and iCDW order parameters are condensates of inter-patch fermion density operators, the associated real space order must be a bond order on the Kagomé lattice. For simplicity, we will consider only nearest-neighbor (NN) bond order as an example.

1. rCDW pattern

The rCDW order parameter is time-reversal even, and contribute to bond density modulation as

\[
\langle \delta \hat{\rho}_{r_\alpha, r_\alpha + e_\beta} \rangle = \langle \delta \hat{\rho}_{r_\alpha', r_\alpha} \rangle = \text{Re} \left[ \langle d_{r_\alpha}^{\dagger} d_{r_\alpha + e_\beta} \rangle \right] = \frac{N_\alpha \gamma}{G_{rCDW}} \cos(M_\alpha \cdot R - M_\gamma \cdot R'), \quad (20)
\]

where \( r_\alpha' = r_\alpha + e_\beta = R' + \delta_\alpha \), with \( \gamma \neq \alpha \neq \beta \). In Fig. 7, the rCDW charge bond density modulation is shown for the 3Q± and 1Q rCDW states.

FIG. 7. Real space rCDW bond order pattern of the 3Q± and 1Q configurations. Configurations in the 3Q± classes are related by translation. Configurations in the 1Q class are related by translation and a three-fold rotation. (a) Bond ordering corresponding to the 3Q+ rCDW class. The bond ordering forms hexagonal and triangular plaquettes. (b) Bond ordering corresponding to the 3Q− rCDW class. The bond ordering forms a `star-of-David’ pattern. (c) Bond ordering pattern corresponding to the 1Q rCDW class. The pattern has alternating bond strength along one direction and uniform strength in the other two bond directions.

2. iCDW pattern

The iCDW order parameter breaks time-reversal symmetry and corresponds to bond current in real space. Note, that the current operator is well defined only when
where $t = -\{\text{the bond current pattern for} \phi \text{ from} \phi_{23}, \phi_{31}, \phi_{12} = \phi_0 \{1,0,0\} \}$. (b) Bond current from $\{\phi_{23}, \phi_{31}, \phi_{12} = \phi_0 \{1,1,1\}$ The sign of $\phi_0$ is taken as negative here.

the charge is conserved, which is indeed the case in both the high temperature disordered phase and iCDW phase. As a result, in the equilibrium phase, the current operator must satisfy

$$\sum_{r_n \rightarrow r'_n} \hat{j}_{r_n,r'_n} = 0.$$ (21)

By comparing the continuity equation and the equation of motion for charge density, we find the current operator on the NN bonds as (see App. E):

$$\hat{j}_{r_n,r'_n} = \hat{j}_{r_n,r_n+\delta r_\alpha,r_{n+\delta r_\alpha}} = \frac{ie}{\hbar} t_1 \left( d_{r_n}^\dagger \delta r_\alpha + d_{r_{n+\delta r_\alpha}}^\dagger \delta r_\alpha \right),$$ (22)

where $t_1$ is the NN hopping defined in Eq. (18). From Eq. (19), the bond current expectation value can be expressed in terms of iCDW order parameter as

$$\langle \hat{j}_{r_n,r_n+\delta r_\alpha} \rangle = \langle \hat{j}_{r_n,r_n+\delta r_\alpha} \rangle = -\frac{2e}{G_{\text{CDW}}} \frac{\langle M_{\alpha} R - M_{-\alpha} R' \rangle}{\langle c_{\alpha,q}^\dagger c_{\gamma,q} \rangle} \phi_{\alpha \gamma},$$ (23)

where again we used $r'_n = r_n + e_\beta = R' + \delta_\beta$, with $\gamma \neq \alpha \neq \beta$. From Eq. (23), the real space bond current pattern from $\phi_{23}$ are shown in Fig. 8 (a). The linear combinations of them can form loop current, as an example, we show the bond current pattern for $\{\phi_{23}, \phi_{31}, \phi_{12} = \phi_0 \{1,1,1\}$ in Fig. 8 (b).

The primary order parameter for the iCDW is a loop current. However, as was discussed in Sec. IV C, from the form of the $K_2$ coupling terms in Eq. (14), a 3Q iCDW will also induce charge order. In particular we see that a 3Q iCDW induces either a 3Q+ or 3Q− state depending upon the sign of $K_2$. Notably, the charge order is quadratic in the iCDW order parameter, $N_\alpha \sim \phi^2$, which could be detectable near the transition temperature.

B. Three-dimensional coupling

Here we extend the Landau theory to consider the implications of coupling of CDW order parameters between nearby layers, adding a layer index $z = 0,1,2 \cdots$ numbered beginning from the top layer. We assume this coupling is weak, so can be approximated by the leading terms linear in the order parameters in each layer, and decays rapidly with the distance between layers. Hence,

$$f_{\perp} = \sum_{z=0}^{\infty} \sum_{\delta=1}^{\infty} (K_{\perp,\delta} N_{\alpha,z} N_{\alpha,z+\delta} + L_{\perp,\delta} \phi_{\alpha,z} \phi_{\alpha,z+\delta}).$$ (24)

We assume that all the inter-layer interactions are weak compared to the intra-layer terms in the free energy, so that the form of the order within each layer is established by the latter, and the intra-layer terms serve to select particular relative orientations of the different symmetry-breaking states in nearby layers. Here we expect $|K_{\perp,1}| \gg |K_{\perp,2}|$ and $|L_{\perp,1}| \gg |L_{\perp,2}|$ so that terms with $\delta > 1$ can be neglected unless they are required to break degeneracies.

1. Three-dimensional ground states

Now we discuss the resulting three-dimensional ordered structures. First consider the imaginary CDW, within the 3Q phase. Within a given layer, $\phi_\alpha$ may take one of the values $\phi_\alpha = \{\phi_0(\{\pm 1, \pm 1, \pm 1\)\}$, where all 8 signs are possible, and $|\phi_0|$ is fixed by single-layer energetics. If $L_{\perp,1} < 0$, the minimum energy iCDW order parameter is identical in all layers, $\phi_{\alpha,z} = \phi_\alpha$. If instead, $L_{\perp,1} > 0$, the minimum energy configuration is “antiferromagnetic”, $\phi_{\alpha,z} = (\pm 1)^z \phi_\alpha$. The two cases above correspond to an ordering wavevector with the z-component $k_z = 0, \frac{1}{2}$, in lattice units. Note that $k_z = 1/2$ is the wavevector for the current order, but the induced real CDW order would have $q_z = 0$ in both cases.

Now consider the real CDW, in either the 3Q+ or 3Q− states. Within a single layer, $N_\alpha$ may take just four values, with $N_\alpha = N_0 n_\alpha$, with $n_0 \alpha = 1$ and $n_1 n_2 n_3 = 1$. For $K_{\perp,1} < 0$, we again obtain a “ferromagnetic” state, with $N_\alpha,z = N_\alpha$. For $K_{\perp,1} > 0$, however, the situation is distinct from the iCDW case, because an overall sign change in $N_\alpha$ is not permitted. Instead, for a given state $n_{\alpha,z}$, the inter-layer coupling equally favors $n_{\alpha,z+1}$ in any of the three states not equal to $n_{\alpha,z}$. For $N$ layers, the total degeneracy of ground states, consider just the $K_{\perp,1}$ interaction, is $4 \times 3^{N-1}$, a macroscopic degeneracy including states with arbitrary wavevectors $k_z$. 

FIG. 8. Real space iCDW (current) bond order pattern of the (a) 1Q and (b) 3Q states. All 3Q configurations are related by translations or time-reversal (changing the sign of the currents). Configurations in the 1Q class are related by translation (i.e. reversing the current direction) and a three-fold rotation. Note that the 1Q state is macroscopically time-reversal symmetric, because it is invariant under the combination of time-reversal and translation. (a) Bond current in the 1Q class, with $\{\phi_{23}, \phi_{31}, \phi_{12} = \phi_0 \{0,1,0\}$, (b) Bond current from $\{\phi_{23}, \phi_{31}, \phi_{12} = \phi_0 \{1,1,1\}$. The sign of $\phi_0$ is taken as negative here.
We must therefore consider further neighbor interactions. The problem can be mapped to a 4-state Potts model, by defining the four allowed configurations of $N_z$ in a single layer as $\sigma = 1 \cdots 4$. The interaction energy becomes

$$f_\perp = \sum_{\sigma=0}^{\infty} \sum_{\delta=1}^{\infty} K_{\perp,\delta} N_0^2 \left( 4\delta_{\sigma_1, \sigma_{\perp, \delta}} - 1 \right),$$  \hspace{1cm} (25)$$

which illustrates the $S_4$ permutation symmetry of a Potts model. This is a 4-state Potts system with competing further-neighbor interactions, which has a rich statistical mechanics for general couplings, similar to that of the ANNNI model, a paradigm for devil’s staircases, commensurate and incommensurate phases, and transitions between them. Here because each Potts spin represents an entire 2d layer, the energies involved are proportional to the area of a layer, and hence much larger than $k_B T$. Therefore, we are interested only in the ground states of the Potts chain. In this limit, the ground states are generally commensurate, but can have very large unit cells (in the $z$ direction), and the Devil’s staircase can rise. We limit our discussion to the simplest cases, and assume $|K_{\perp,\delta}| \ll |K_{\perp,\delta+1}|$ as expected on grounds of locality.

The simplest situation is $K_{\perp,2} < 0$, in which case second neighbor layers prefer to be parallel. We have then alternate layers in successive layers, $\sigma_2 = \sigma_1$ for $z$ even and $\sigma_2 = \sigma_2$ for $z$ odd, with $\sigma_1 \neq \sigma_2$. In terms of the rCDW vector $\mathbf{n}$, $n_{\alpha,\pm z} = n_{\alpha}(1)$ for $z$ even and $n_{\alpha,\pm z} = n_{\alpha}(2)$ for $z$ odd, such that $n_{\alpha}(1) \cdot n_{\alpha}(2) = -1$. This corresponds to the wavevector $k_z = 1/2$ in lattice units. Note that the three-dimensional degeneracy of this state is $4 \times 3 = 12$.

If $K_{\perp,2} > 0$, then we require both nearest neighbor and second neighbor Potts spins to differ in the ground state. After choosing the first layer, there are 3 choices for the second layer, and then 2 choices for the third layer, which must be distinct from the first two layers. This implies the smallest possible periodicity of the ground state is 3. It may, however, be larger. Indeed for the fourth layer, there are still 2 choices remaining, and the ground state is not determined. To fix this degeneracy, we may yet consider the third neighbor coupling. If $K_{\perp,3} < 0$, then we favor a return to the original state. The entire configuration becomes determined, with a periodicity of 3, and a representative sequence in Potts variables like $\sigma_2 = 1, 2, 3, 1, 2, 3, 1, 2, 3, \cdots$. These configurations correspond to a “chiral” ordering of the layers, consistent with a 3-fold screw axis. Alternatively, if $K_{\perp,3} > 0$, then we obtain a four layer periodicity, $\sigma_2 = 1, 2, 3, 4, 1, 2, 3, 4, \cdots$. These two situations have smaller ordering wavevectors in the $z$ direction, $k_z = 1/3, 1/4$, respectively. Note that the relatively simple results quoted here are the result of assuming a strict hierarchy of interactions, with couplings decaying rapidly in strength with the separation of layers. Otherwise much more complex states may arise in the Potts chain.

We conclude that a distinct difference between the iCDW and rCDW is the presence of periodicities larger than 2 in the $c$ direction. Appearance of such a periodicity (i.e. $k_z = 1/3, 1/4$) would provide clear experimental evidence in favor of the real over the imaginary CDW.

2. Rotational symmetry breaking

In the previous discussion, we determined the relative ordering between layers assuming the order parameter within each layer is rigid. Now we consider a higher order effect: the back-influence of the inter-layer interaction on the order parameter within a single layer. In particular, in the case of rCDW order, this leads to a breaking of $C_3$ rotational symmetry within a given layer. This can be understood as follows. All 4 of the 2d ordered states in the 3Q+ or 3Q− states preserve $C_3$ symmetry around the centers of one of the four hexagons within the quadrupled unit cell, but not around the other three. In the states with $k_z > 0$, the centers of neighboring layers are not aligned. Consequently there is no rotation axis which preserves all layers. In the chiral $k_z = 1/3$ states, there is instead a screw axis, which preserves macroscopic $C_3$ symmetry of the crystal in the bulk. This symmetry is however broken at the surface. In the states with $k_z = 1/2, 1/4$, there is not even macroscopic $C_3$ symmetry.

In all cases, if one observes the order within a single layer, its neighbors will influence its order and lower the symmetry. The situation is simplest for the top layer. Assume the system develops long-range order, and therefore we may treat the inter-layer interaction in a mean field sense. We therefore replace the coupling to the second layer from the top (the strongest such coupling) by a term of the form

$$f_{\perp,0} = K_{\perp,1} \langle N_{\alpha,1} \rangle N_{\alpha,0}. \hspace{1cm} (26)$$

This term appears as a “field” on the order parameter in the top layer ($z = 0$). In for example the $k_z = 1/2$ phase, we may take $\langle N_{\alpha,1} \rangle = N_0(1, 1, 1)$. Then this configurations in the first layer are “pushed” away from the $(1, 1, 1)$ direction. For example, if the top layer chooses the $(1, 1, 1)$ state, the inter-layer coupling will shift it to the form $N_{\alpha,0} = N_0(1 - \delta, -1 - \delta, -1 - \delta)$, with $0 < \delta \ll 1$. Note that $|N_1| < |N_2| = |N_3|$. The consequence is that the two dimensional Bragg peaks associated to density oscillations in the top layer develop two unequal magnitudes. This is a sign of the rotational symmetry breaking. Indeed, one can define a two-dimensional vector $\mathbf{v}_{z,z'} = -\mathbf{v}_{z',z}$

$$\mathbf{v}_{z,z'} = \sum_{\alpha} \langle n_{\alpha,\pm z} n_{\alpha,\pm z'} \rangle \mathbf{a}_{\alpha}, \hspace{1cm} (27)$$

where $\mathbf{a}_{\alpha}$ are the 2d triangular Bravais lattice vectors with $\mathbf{a}_z = -\mathbf{a}_1 - \mathbf{a}_2$. The vector $\mathbf{v}_{z,z'}$ is oriented along one of the three principle directions and selects this axis. This rotational symmetry breaking effect exists within each layer in all the $3Q\pm$ rCDW phases except the uniform $k_z = 0$ one. Rotational symmetry is also broken.
in the bulk (i.e. in an infinite system in the $z$ direction) except when it is restored macroscopically by an arrangement of layers that constitutes a screw axis. The latter occurs only for the $k_z = 1/3$ case detailed above. Rotational symmetry breaking is, however, absent both in individual layers and in bulk, in the 3Q $i$CDW states, providing another means to differentiate the $i$CDW from the rCDW experimentally.

C. Critical behavior

We briefly discuss the expected critical behavior at the ordering temperature for some important cases based on the symmetries and order parameters. This question is motivated by the presence of a cubic term in the rCDW Landau theory, which might suggest a first order transition to the CDW state, which to our knowledge is not observed experimentally. While a full understanding is somewhat involved, we argue below that both thermal fluctuations in two dimensions and three-dimensional coupling stabilize a continuous transition within most scenarios.

1. Two dimensions

If we neglect inter-layer coupling, the problem becomes two dimensional, and we must be wary of applying a mean field Landau theory analysis to critical properties, since it is well known that two dimensional systems have strong thermal fluctuations.

For the case of the 3Q+ or 3Q− rCDW, as discussed in Sec. V B 1, the ordering can be described by a four state Potts model. At mean field level, the $q$-state Potts models have first order transitions for $q \geq 3$, consistent with the Landau analysis. It is well-known, however, that in two dimensions the $q = 3, 4$ Potts models in fact have continuous transitions described by conformal field theory. In particular, the $q = 4$ Potts model is equivalent to the Ashkin-Teller model, and has known critical exponents with logarithmic corrections due to marginal operators (see e.g. Ref.[63]).

In the case of the 3Q iCDW, the order parameter has a degeneracy of 8 and transforms under full cubic $O_h$ symmetry, and we have seen that it can be expressed as an $O(3)$ vector with cubic anisotropy. In two dimensions, this problem has been analyzed by Schick[64], who concludes that the transition to the 3Q phase (called “corner cubic anisotropy” in this reference) may be either continuous (and in the Ising universality class, surprisingly) or first order.

2. Three dimensions

The two dimensional critical behavior is valid at best in a regime close but not too close to the critical point, where a crossover to three-dimensional behavior must occur. The nature of the true three-dimensional critical regime is, however, dependent on the type of inter-layer couplings, and thereby the three-dimensional order parameter. As discussed in Sec. V B 1, this is rather complicated for the rCDW problem, and we will not offer a complete analysis. The simplest case is the $k_z = 0$ one, which occurs when the inter-layer coupling favors ferromagnetically aligned rCDWs. Then the symmetry remains unchanged from the four state Potts model. However, in three dimensions, this model has a first order transition. Thus in this case a first order transition is predicted. If instead one of the $k_z > 0$ orderings occur, the situation is less clear, but it is manifestly not a Potts model transition. It is natural to think that the Landau analysis is more correct in three dimensions. Based on this reasoning, for the cases $k_z = 1/2$ and $k_z = 1/4$, a cubic term in the order parameter is no longer allowed by momentum conservation. Thus a continuous transition may be expected. The case $k_z = 1/3$ seems to allow a cubic term but we will not pursue it further here.

With three-dimensional coupling, the iCDW order develops either at $k_z = 0$ or $k_z = 1/2$. In both cases, the three-dimensional order parameter remains an $O(3)$ vector with cubic anisotropy, and the ground state degeneracy is unchanged from 8 (this can be seen because even in the $k_z = 1/2$ can a translation by one layer is equivalent to time-reversal). Hence the transition should be in the $O(3)$ cubic universality class, which is known to be continuous, and is discussed e.g. in Ref.[65].

D. Magnetic moment induced by iCDW order

The iCDW order can induce both staggered magnetic moment due to the loop current and uniform magnetic moment. Here, we estimate the magnitude from each contribution.

First, we note that the bond current obtained in Eq. (23) is linear in $\phi$, consequently, only the Fourier component at $M$ contributes to the bond current, and there is no uniform magnetic moment induced by the bond current. To estimate the staggered magnetic moment, we consider the 3Q iCDW order as an example. As shown in Fig. 8 (b), the bond current forms loop current around both the honeycomb and triangular plaquettes. Treating each plaquette as a current loop, its magnetic moment and the magnetic field it induces can be obtained following the standard magnetostatics [66]. Due to the $2 \times 2$ sublattice structure, there are two types of honeycomb plaquettes, with $m_{i,1} = I_e \hat{A}_h$ for one-quarter of the honeycomb plaquettes, and $m_{i,2} = -I_e \hat{A}_h/3$ for the rest. Similarly, one-quarter of the triangular plaquettes have $m_{t,1} = -I_e \hat{A}_t$, and the rest have $m_{t,2} = I_e \hat{A}_t/3$. Here, $I_e = -\frac{\pi}{2} \frac{2t_{iCDW}}{\hbar} \phi_0$ denotes the magnitude of the electric loop current. $\hat{A}_h,t,i$ is along $\hat{z}$, such that for $I_e > 0$, the current flows counter clockwise. And its magnitude is determined by the area of the honeycomb (h)
and triangular (t) plaquette. In unit of Bohr magneton \( \mu_B = \frac{e\hbar}{2m_e} \), we have \( m \sim I_c \mathcal{A} = -\frac{2t_1}{G_{\text{CDW}}} \phi_0 \mathcal{A} \mu_B \), where \( Ry = \frac{m_e e^4}{3\pi^2 \hbar^2} \approx 13.6eV \) is the Rydberg energy, \( r_b = \frac{4\pi e^2}{mc^2} \approx 5.29 \times 10^{-11}m \) is the Bohr radius. In \( I_c \), the factor \( \frac{2t_1}{G_{\text{CDW}}} \) is dimensionless and scales with the polarization bubble \( \approx \ln^2(\lambda \Lambda^2/T_c) \sim O(1) \), the order parameter (in unit of energy) at low temperature can be approximated as \( \phi_0 \sim k_BT_c \), where \( T_c \) is the transition temperature for iCDW order. This gives \( m_{t,1} \approx -0.047 \text{sgn}(\phi_0)\mu_B z, \) \( m_{e,1} \approx 0.008 \text{sgn}(\phi_0)\mu_B z, \) where we take \( 2t_1/G_{\text{CDW}} = 1 \). We also note that similar analysis has been done in the literature for cuprates \[67\] and iron-pnictides \[68\].

Next, we discuss the uniform magnetization induced by the iCDW order. On the symmetry ground, uniform magnetization requires iCDW order at all three momenta \( \mathbf{M} \) nonzero. Otherwise, the system is invariant under the anti-unitary symmetry composed of time reversal and translation, which forbids any uniform magnetization. In general, the magnetic field couples to the electrons through both the minimal coupling and the Zeeman coupling. Here, we consider the orbital magnetization contribution for the 3Q± iCDW order. Following \[69\], the orbital magnetization in terms of the Bloch wave function reads,

\[
\mathcal{M}^z_{\text{orb}} = \frac{e}{2\hbar} \sum_{n, q} \text{Im} \left[ (\partial_q u_{n,q}) \times (\epsilon_{n,q} - \hat{H}_{\text{MF}}(q)) |\partial_u u_{n,q}^*| \right] f_{n,q}.
\]

where \( \hat{H}_{\text{MF}}(q) \) is the mean field Hamiltonian one can infer from Eq. (8). \( f_{n,q} = f(\epsilon_{n,q} - \mu) \) is the equilibrium Fermi distribution function.

For simplicity, we consider the perfect nesting case when the Fermi energy in the disordered phase is at the van-hove point, this gives 1/3 filling in the patch model. When the 3Q iCDW order is present, the triple degenerate bands at the \( \mathbf{M} \) points are fully gapped, and only the lowest band is filled. Noting that the unit of the summand in Eq. (28) is \( \frac{\hbar^2}{m_e} \) (coming from the kinetic energy), for a filled band, the summand must be expressed as a function of the only dimensionless parameter in the expression, which reads \( \hat{\epsilon} = \hbar^2 q^2/(2m_e) \), i.e. the summand (after averaging over the angular direction in \( \mathbf{q} \)) must be expressed as \( \sim \frac{\hbar^2}{2m_e} \mathcal{F}(\hat{\epsilon}) \). This means physically that for electrons within an energy of order the gap \( \phi \), the typical orbital moment is an order one fraction of a Bohr magneton.

The orbital magnetization can be expressed as

\[
\mathcal{M}^z_{\text{orb}} = \frac{e\hbar}{2m_e} N \frac{\phi_0}{\hbar^2/(2m_e\alpha_0^2)} \frac{\sqrt{3}}{2\pi} \int_0^\Lambda d\hat{\epsilon} \mathcal{F}(\hat{\epsilon})
\]

\[
= N\mu_B \frac{\phi_0}{Ry} \left( \frac{a_0}{a_b} \right)^2 \frac{\sqrt{3}}{2\pi} I_F,
\]

where \( N \) is the number of unit cells, \( I_F = \int_0^\Lambda d\hat{\epsilon} \mathcal{F}(\hat{\epsilon}) \) is the value of the integral, which is bounded and can be computed numerically as \( I_F \approx -0.87 \). Again approximating \( \phi_0 \sim k_BT_c \), the orbital magnetization per unit cell is \( M^z_{\text{orb}}/N \sim -0.017 \text{sgn}(\phi_0)\mu_B \).

This orbital magnetization is small but the smallness is primarily due to the small number of electrons within the region near the energy gap. As remarked above, for a typical electron within this region, the orbital moment is a substantial fraction of \( \mu_B \). This suggests that the iCDW state may be favored by the application of a magnetic field.

We consider therefore how an rCDW state may be converted into an iCDW state by such a field, assuming the energy of the iCDW state is not too much higher than that of the rCDW in zero field. For simplicity we consider low temperature, where the above estimate is valid (near \( T_c \), the orbital magnetization will be proportional to \( \phi^3 \), and greatly suppressed). In general, a magnetic field breaks time-reversal, so will always induce some iCDW component if the rCDW is present. We thus take \( \Delta_0 = N_a + i\phi_0 = |\Delta|e^{i\theta} \) (assuming a 3Q+ state), and express the energy in terms of \( |\Delta| \) and \( \theta \). A simplified form for the energy density is

\[
\mathcal{E} = -m|\Delta|^2 (1 + \lambda \cos \theta) - \mu h m|\Delta| \sin \theta,
\]

where \( m \) is the mass scale for the saddle points, \( h \) is the magnetic field (in the \( z \) direction), \( \mu \) is a typical orbital moment for the iCDW electrons, and is a fraction of \( \mu_B \). The first term is the condensation energy of the CDW, and the second term is the dipole energy associated with the orbital magnetization. The parameter \( \lambda > 0 \) describes the energetic preference for rCDW over iCDW order in zero field (as well as the preference for 3Q+ over 3Q- order). When the competition between the two is close, \( \lambda \ll 1 \). Minimizing over \( \theta \), we obtain

\[
\tan \theta = \frac{\mu h}{\lambda |\Delta|}.
\]

We see that the rCDW smoothly evolves into an iCDW with applied field, and this occurs on a scale which can be a small fraction of the gap, if \( \lambda \ll 1 \). We note that the energy density in Eq. (30) is simplified, and does not capture topological physics relevant to the perfect nesting situation when the system is doped exactly to the saddle point filling. In this case, the system is a trivial insulator for \( \theta = 0 \), and a Chern insulator for \( \theta = \pi/2 \), and hence there must be a topological transition, associated gap closing, and non-analyticity of the energy at some intermediate angle. However, we expect this distinction to be washed out away from perfect nesting and for generic filling.

VI. SUMMARY

In this paper, we have discussed various mechanisms to induce charge density wave order in kagomé metals,
motivated by experiments on the AV$_3$Sb$_5$ materials. We began with a g-ology description based on a continuum saddle point model, which is quite general to two dimension-mental materials with hexagonal symmetry, and was originally introduced in the context of doped graphene in Ref.[46]. We extended the renormalization group analysis of this problem to the general case, i.e. with both repulsive and attractive bare interactions, and showed that several distinct density wave and superconducting insta-bilities are possible, depending upon parameters. We also showed that the attractive bare interactions may come from coupling of electrons to optical phonons, which induces attraction in certain channels ($g_l$) and lowers the phonon energy. The latter effect may be relevant to the phonon softening observed in ab-initio calculations [70].

Our focus then turned to charge density wave order at the vectors $M_0$, which correspond both to the locations of the saddle points in the Brillouin zone and the spanning vectors between them. They are half reciprocal lattice vectors and reside at the centers of the zone faces. We applied a mean field theory to the real charge density wave (rCDW) states of the continuum interacting model, and found isotropic 3Q± as well as nematic 1Q rCDW states occur and may be tuned by chemical potential. We also carried out a Landau theory analysis of the rCDW orders (and a detailed derivation of the Landau theory coefficients from the continuum model) which shows that when this is the leading instability, the above states are the only ones that occur with a high degree of generality. Next, we considered the alternate cases of a 3Q imaginary charge density wave (iCDW) – actually a state of circulating currents, i.e. orbital moments – and a spin density wave (rSDW), which are competing instabilities with the same wavevectors. We showed that both iCDW and rSDW can induce rCDW order, though in both cases the charge density order is then not the primary order parameter. Finally, we detailed a number of extensions and implications of the analysis to derive explicit charge and current patterns, three dimensional ordered states, critical properties, and orbital magnetization of the 3Q iCDW state.

What are the specific implications of these results for the AV$_3$Sb$_5$ materials? Three distinct compounds, with A=K,Cs,Rb, have been studied to our knowledge. All are known to show rCDW order for which the projection of the order parameter onto the 2d kagomé plane is of the 3Q $M_0$ type. A key question is whether the rCDW is the primary order parameter, or whether it is secondary and induced, as discussed above, by either an iCDW or rSDW order. Notably, both the iCDW and rSDW orders break time-reversal symmetry, and hence should be detectable via their induced local magnetic moments through e.g. muon spin resonance or neutron scattering. To our knowledge, there is no direct evidence of time-reversal breaking from any measurement in zero magnetic field (and there is some counter-evidence from muon spin resonance on KV$_3$Sb$_5$[26]). This does not definitively exclude states with very small moments, as indeed may be expected in the iCDW case (c.f. Sec. V D).

The discussion of three-dimensional order in Sec. V B1 provides some more clear diagnostics. There, we showed that the iCDW is expected to display identical induced rCDW order in all layers, i.e. the z-component of the rCDW ordering wavevector should be zero. By contrast, a pure rCDW is consistent with $k_z = 0, \pm \frac{1}{2}, \pm \frac{1}{3}, \frac{1}{4}$. Moreover, rCDW states with $k_z \neq 0$ should show “nematic” C$_3$ rotational symmetry breaking at the surface, due to the three-dimensional coupling, which again is not expected in the iCDW states.

Several experimental papers are directly related to the above aspects of the CDW order. X-ray scattering found Bragg peaks associated with three-dimensional CDW order with $k_z = 1/2$ in RbV$_3$Sb$_5$, CsV$_3$Sb$_5$ in Ref.[22], $k_z = 1/4$ in CsV$_3$Sb$_5$ in Ref.[27]. Ref.[24] measured an in-plane shift of the order in the top two layers of CsV$_3$Sb$_5$ across a step edge using STM, indicating $k_z > 0$. These observations are consistent with primary rCDW order. Ref.[36] measured a “nematic” (i.e. C$_3$ symmetric) dependence of the c-axis resistivity in CsV$_3$Sb$_5$ on an in-plane magnetic field in the normal (but CDW) state up to about 60K, 2/3 of the critical temperature. Such behavior would be expected below the CDW $T_c$ for any rCDW except the “screw” state with $k_z = 1/3$. The STM study in Ref. [20] notes differences in the intensities of the three charge order wavevector peaks in KV$_3$Sb$_5$. This reference concludes that the three intensities are all unequal, and denote this as a “chiral” charge order. To our eyes, their Fourier transform STM data (Fig.3abc of Ref.[20]) is better described by two strong and approximately equal intensities and one weaker one, which is consistent with our theory of inter-layer coupling. A very recent paper reports the latter type of anisotropy in independent STM measurements of KV$_3$Sb$_5$ [71].

While the above evidence seems to favor primary rCDW order, iCDW or SDW states might be realized in some situations, e.g. as competing orders that appear at lower temperatures or induced through applied fields. Indeed the early observation of large anomalous Hall effect[72] in KV$_3$Sb$_5$ motivated several later works to promote the possibility of an iCDW (recently similar behavior was observed in CsV$_3$Sb$_5$[38]). As discussed in Sec. V D, the 3Q iCDW does indeed macroscopically break time-reversal and is accompanied by a uniform orbital moment and a large Berry curvature in the vicinity of the saddle points, which should induce an anomalous Hall effect. We discussed how, if iCDW order is only slightly higher in energy than rCDW, the iCDW can be induced by modest applied fields, which may provide a possible explanation of Ref.[72]. Further study of the anomalous Hall effect and its correlation with other measurements is however needed to test this possibility.

While this manuscript was in preparation, several theore-tical works appeared discussing density wave order in these materials. Ref. [73] evaluated the mean field ground state energies for multiple density wave orders. Ref.[74] considered a single orbital extended Hubbard model on
the kagome lattice, and within mean field theory found dominant iCDW order. Ref.[75] discusses a coupled mean field theory of spin and charge orders and Chern bands in a continuum saddle point model similar to the one used here and postulates a complex CDW state in the AV materials with three unequal magnitudes of CDW at the three $M_\alpha$ wavevectors.

In this paper, we have focused on density wave order, which is clearly the dominant instability in the AV materials. However, the superconductivity occurring at lower temperature is of considerable interest as well. Since it occurs within the density wave ordered state, the understanding of the latter should be important for developing a theory of superconductivity in this family.

ACKNOWLEDGMENTS

We acknowledge useful discussions with Stephen Wilson, Brenden Ortiz, Sam Teicher, and Ilija Zeljkovic. L.B. is supported by BES Award DE-SC0020305. M.Y. is supported in part by the Gordon and Betty Moore Foundation through Grant GBMF8690 to UCSB and by the National Science Foundation under Grant No. NSF PHY-1748958. T.P. was supported by the National Science Foundation through Enabling Quantum Leap: Convergent Accelerated Discovery Foundries for Quantum Materials Science, Engineering and Information (Q-AMASE-i) award number DMR-1906325.

[1] M. Imada, A. Fujimori, and Y. Tokura, Metal-insulator transitions, Rev. Mod. Phys. 70, 1039 (1998).
[2] J. Ngai, F. Walker, and C. Ahn, Correlated oxide physics and electronics, Annual Review of Materials Research 44, 1 (2014). https://doi.org/10.1146/annurev-matsci-070813-113248.
[3] D. C. Johnston, The puzzle of high temperature superconductivity in layered iron pnictides and chalcogenides, Advances in Physics 59, 803 (2010), https://doi.org/10.1080/00018732.2010.513480.
[4] D. J. Scalapino, A common thread: The pairing interaction for unconventional superconductors, Rev. Mod. Phys. 84, 1383 (2012).
[5] M. Sato and Y. Ando, Topological superconductors: a review, Reports on Progress in Physics 80, 076501 (2017).
[6] A. W. Tsen, R. Hovden, D. Wang, Y. D. Kim, J. Okamoto, K. A. Spoth, Y. Liu, W. Lu, Y. Sun, J. C. Hone, L. F. Kourkoutis, P. Kim, and A. N. Pasupathy, Structure and control of charge density waves in two-dimensional It-tas2, Proceedings of the National Academy of Sciences 112, 15054 (2015), https://www.pnas.org/content/112/49/15054.full.pdf.
[7] L. Ye, M. Kang, J. Liu, F. Von Cube, C. R. Wicker, T. Suzuki, C. Joziwak, A. Bostwick, E. Rotenberg, D. C. Bell, et al., Massive dirac fermions in a ferromagnetic kagome metal, Nature 555, 638 (2018).
[8] I. R. Fisher, L. Degiorgi, and Z. X. Shen, In-plane electronic anisotropy of underdoped “122” Fe-arsenide superconductors revealed by measurements of detwinned single crystals, Reports on Progress in Physics 74, 124506 (2011).
[9] Y. Sato, S. Kasahara, H. Murayama, Y. Kasahara, E. G. Moon, T. Nishizaki, T. Loew, J. Porras, B. Keimer, T. Shibaiuchi, and Y. Matsuda, Thermodynamic evidence for a nematic phase transition at the onset of the pseudogap in yb2cu3o7, Nature Physics 13, 1074 (2017).
[10] C. M. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. E. Ruckenstein, Phenomenology of the normal state of cu-o high-temperature superconductors, Phys. Rev. Lett. 63, 1996 (1989).
[11] G. R. Stewart, Non-fermi-liquid behavior in d- and f-electron metals, Rev. Mod. Phys. 73, 797 (2001).
[12] O. Gunnarsson, M. Calandra, and J. E. Han, Colloquium: Saturation of electrical resistivity, Rev. Mod. Phys. 75, 1085 (2003).
[13] C. M. Varma, Colloquium: Linear in temperature resistivity and associated mysteries including high temperature superconductivity, Rev. Mod. Phys. 92, 031001 (2020).
[14] A. Chubukov, Pairing mechanism in Fe-based superconductors, Annual Review of Condensed Matter Physics 3, 57 (2012), https://doi.org/10.1146/annurev-conmatphys-020911-125055.
[15] Q. Si, R. Yu, and E. Abrahams, High-temperature superconductivity in iron pnictides and chalcogenides, Nature Reviews Materials 1, 16017 (2016).
[16] K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R. A. Dilanian, and T. Sasaki, Superconductivity in two-dimensional coo2 layers, Nature 422, 53 (2003).
[17] M. L. Foo, Y. Wang, S. Watauchi, H. W. Zandbergen, T. He, R. J. Cava, and N. P. Ong, Charge ordering, commensurability, and metallicity in the phase diagram of the layered na3coo2, Phys. Rev. Lett. 92, 247001 (2004).
[18] J. D. Jorgensen, M. Avdeev, D. G. Hinks, J. C. Burley, and S. Short, Crystal structure of the sodium cobaltate deuterate superconductor na3coo2-4zd3o (x \approx \frac{1}{2}), Phys. Rev. B 68, 214517 (2003).
[19] B. R. Ortiz, L. C. Gomes, J. R. Morey, M. Winiarski, M. Bordelon, J. S. Mangum, I. W. Oswald, J. A. Rodriguez-Rivera, J. R. Neilson, S. D. Wilson, et al., New kagome prototype materials: discovery of kv3sb5, RbV3sb5, and CsV3sb5, Physical Review Materials 3, 094407 (2019).
[20] Y.-X. Jiang, J.-X. Yin, M. M. Denner, N. Shumiya, B. R. Ortiz, J. He, X. Liu, S. S. Zhang, G. Chang, I. Belopolski, Q. Zhang, M. S. Hossain, T. A. Cochran, D. Multer, M. Litskevich, Z.-J. Cheng, X. P. Yang, Z. Guguchia, G. Xu, Z. Wang, T. Neupert, S. D. Wilson, and M. Z. Hasan, Discovery of topological charge order in kagome superconductor kv3sb5 (2020), arXiv:2012.15709 [cond-mat.supr-con].
[21] H. Zhao, H. Li, B. R. Ortiz, S. M. L. Teicher, T. Park, M. Ye, Z. Wang, L. Balents, S. D. Wilson, and I. Zeljkovic, Cascade of correlated electron states in a kagome superconductor CsV3Sb5, arXiv e-prints , arXiv:2103.03118 (2021), arXiv:2103.03118 [cond-mat.supr-con].
[22] H. X. Li, T. T. Zhang, Y. Y. Pai, C. Marvinyin, A. Said, T. Yilmaz, Q. Yin, C. Gong, Z. Tu, E. Vescovo, R. G. Moore, S. Murakami, H. C. Lei, H. N. Lee, B. Lawrie, and H. Miao, Observation of Unconventional Charge Density Wave without Acoustic Phonon Anomaly in Kagome Superconductors AV3Sb5 (A=Rb,Cs), arXiv e-prints , arXiv:2103.09769 (2021), arXiv:2103.09769 [cond-mat.supr-con].

[23] E. Uykur, B. R. Ortiz, S. D. Wilson, M. Dressel, and A. A. Tsirlin, Optical detection of charge-density-wave instability in the non-magnetic kagome metal KV3Sb5 as determined by muon spin spectroscopy, Jour-
to the mott state: From condensed-matter systems to superfluidity in optical lattices, Annals of Physics 324, 1452 (2009), July 2009 Special Issue.

[46] R. Nandkishore, L. Levitov, and A. Chubukov, Chiral superconductivity from repulsive interactions in doped graphene, Nature Physics 8, 158 (2012).

[47] R. Nandkishore, G.-W. Chern, and A. V. Chubukov, Itinerant Half-Metal Spin-Density-Wave State on the Hexagonal Lattice, Physical Review Letters 108, 227204 (2012).

[48] R. Nandkishore and A. V. Chubukov, Interplay of superconductivity and spin-density-wave order in doped graphene, Physical Review B 86, 115426 (2012).

[49] Y.-P. Lin and R. M. Nandkishore, Chiral twist on the high-Tc phase diagram in moiré heterostructures, Phys. Rev. B 100, 085136 (2019).

[50] D. V. Chichinadze, L. Classen, and A. V. Chubukov, Nematic superconductivity in twisted bilayer graphene, Phys. Rev. B 101, 224513 (2020).

[51] D. V. Chichinadze, L. Classen, and A. V. Chubukov, Valley magnetism, nematicity, and density wave order in twisted bilayer graphene, Phys. Rev. B 102, 125120 (2020).

[52] L. Classen, A. V. Chubukov, C. Honerkamp, and M. M. Scherer, Competing orders at higher-order van hove points, Phys. Rev. B 102, 125141 (2020).

[53] Y.-P. Lin and R. M. Nandkishore, Parquet renormalization group analysis of weak-coupling instabilities with multiple high-order van hove points inside the brillouin zone, Phys. Rev. B 102, 245122 (2020).

[54] A. T. Zheleznyak, V. M. Yakovenko, and I. E. Dzyaloshinskii, Parquet solution for a flat fermi surface, Phys. Rev. B 55, 3200 (1997).

[55] W. Metzner, C. Castellani, and C. D. Castro, Fermi systems with strong forward scattering, Advances in Physics 47, 317 (1998), https://doi.org/10.1080/000187398243528.

[56] A. V. Chubukov, D. V. Efremov, and I. Eremin, Magnetism, superconductivity, and pairing symmetry in iron-based superconductors, Phys. Rev. B 78, 134512 (2008).

[57] A. Chubukov, Renormalization group analysis of competing orders and the pairing symmetry in fe-based superconductors, Physica C: Superconductivity 469, 640 (2009), superconductivity in Iron-Pnictides.

[58] S. M. Teicher, (private communication).

[59] G. F. Koster, Properties of the thirty-two point groups (M.I.T. Press, Cambridge, Mass., 1963).

[60] N. Furukawa, T. M. Rice, and M. Salanhofer, Truncation of a Two-Dimensional Fermi Surface due to Quasiparticle Gap Formation at the Saddle Points, Physical Review Letters 81, 3195 (1998).

[61] H.-H. Lin, L. Balents, and M. P. A. Fisher, n-chain hubbard model in weak coupling, Phys. Rev. B 56, 6569 (1997).

[62] L. Balents and M. P. Fisher, Weak-coupling phase diagram of the two-chain hubbard model, Physical Review B 53, 12133 (1996).

[63] J. L. Cardy, M. Nauenberg, and D. Scalapino, Scaling theory of the potts-model multicritical point, Physical Review B 22, 2560 (1980).

[64] M. Schick, Application of the heisenberg model with cubic anisotropy to phase transitions on surfaces, Surface Science 125, 94 (1983).

[65] J. Manuel Carmona, A. Pelissetto, and E. Vicari, n-component ginzburg-landau hamiltonian with cubic anisotropy: A six-loop study, Phys. Rev. B 61, 15136 (2000).

[66] J. D. Jackson, Classical electrodynamics; 2nd ed. (Wiley, New York, NY, 1999).

[67] S. Lederer and S. A. Kivelson, Observable nmr signal from circulating current order in ybco, Phys. Rev. B 85, 155130 (2012).

[68] M. Klug, J. Kang, R. M. Fernandes, and J. Schmalian, Orbital loop currents in iron-based superconductors, Phys. Rev. B 97, 155130 (2018).

[69] J. Shi, G. Vignale, D. Xiao, and Q. Niu, Quantum theory of orbital magnetization and its generalization to interacting systems, Physical Review Letters 99, 10.1103/physrevlett.99.197202 (2007).

[70] H. Tan, Y. Liu, Z. Wang, and B. Yan, Charge density waves and electronic properties of superconducting kagome metals, arXiv e-prints , arXiv:2103.06325 (2021), arXiv:2103.06325 [cond-mat.supr-con].

[71] H. Li, H. Zhao, B. R. Ortiz, T. Park, M. Ye, L. Balents, Z. Wang, S. D. Wilson, and I. Zeljkovic, Rotation symmetry breaking in the normal state of a kagome superconductor KV3Sb5 (2021).

[72] S.-Y. Yang, Y. Wang, B. R. Ortiz, D. Liu, J. Gayles, E. Derunova, R. Gonzalez-Hernandez, L. Smekal, Y. Chen, S. S. Parkin, et al., Anomalous, anomalous Hall effect in the layered, Kagome, Dirac semimetal KV3Sb5, arXiv preprint arXiv:1912.12288 (2019).

[73] X. Feng, K. Jiang, Z. Wang, and J. Hu, Chiral flux phase in the kagome superconductor av3s5b5 (2021), arXiv:2103.07097 [cond-mat.supr-con].

[74] M. M. Denner, R. Thomale, and T. Neupert, Analysis of charge order in the kagome metal av3s5b5 (α =k,rb,cs) (2021), arXiv:2103.14045 [cond-mat.str-el].

[75] Y.-P. Lin and R. M. Nandkishore, Complex charge density waves at van hove singularity on hexagonal lattices: Haldane-model phase diagram and potential realization in kagome metals AV3Sb5 (2021), arXiv:2104.02725 [cond-mat.str-el].

[76] Dresselhaus, Mildred S. and Dresselhaus, Gene, Jorio, Ado, Group Theory: Application to the Physics of Condensed Matter (Springer, 2008).

[77] J. W. Milnor, Morse theory, 5th ed., Annals of mathematics studies No. 51 (Princeton Univ. Press, Princeton, NJ, 1973).

APPENDIX

A: Irreducible representations at Ms

As shown in Fig. 2, there are two saddle points at Ms. The little co-group at Ms is D2h, and the irreps of the two saddle points at Ms are Γ1 and Γ3. The convention used here is the one used in Ref. [59], and the orientation of the two symmetry axes are shown in Fig. 1(a).

Now, we explain the one-to-one correspondence between the Brillouin zone patches, Ms, and the vanadium sites, Vα. Consider how Bloch states formed from s-orbitals placed on the vanadium sites (V1, V2, V3) transform at Ms. A s-orbital Bloch wave on V1 transforms as the irrep Γ1. On the other hand, s-orbitals placed on
V₂, V₃ form a reducible representation that can be decomposed into the Γ₂ + Γ₄ irreps. Notice that the irrep of the s-orbital on V₁ is even under inversion, but the irreps of the s-orbitals on the V₂, V₃ sites are odd under inversion. Since d-orbitals are even under inversion, this means that Bloch states formed from d-orbitals at V₁ must be even under inversion, but Bloch states formed from d-orbitals on V₂, V₃ must be odd under inversion. The saddle points at M₁ are even under inversion; therefore only the d-orbitals on the V₁ site contribute to the saddle point at M₁. Using a three-fold rotation, it is easy to see that at M₂, M₃, the contribution to the bands must come from d-orbitals on the V₂, V₃ sites respectively. Hence, there is an one-to-one correspondence between the Brillouin zone patches, M₁, and the vanadium sites, V₄. Away from M₁, d-orbitals on V₂, V₃ can start mixing with the saddle point bands, but we assume these contributions are small sufficiently close to M₁.

B: Microscopic mechanism of attractive fermion interaction

Generally, pure electronic interactions, i.e. the screened coulomb repulsion, give rise to repulsive interactions between patch fermions, which favor SDW rather than CDW instabilities. Indeed, the RG phase diagram (Fig. 4) suggests that attraction in the g₁(0) or g₃(0) channels is likely necessary to stabilize CDW order. Here, we show that the electron-optical phonon interaction may renormalize g₁(0) or g₃(0), and lead to attraction in these channels. Specifically, we define g₁(0) = g₁(0) + δg₁(0), where δg₁(0) is the bare interaction due to screened coulomb repulsion, and compute the renormalization δg₁(0).

Consider the standard coupling of electron density with an optical phonon. Because g₁(g₃) transfers spin (charge) between saddle points, these two interactions cannot be generated from coupling to a zone center phonon. Instead, both δg₁(0) and δg₃(0) require coupling with to a phonon at momentum M. Conversely, δg₂(0) and δg₄(0) are generated from coupling with a zone center phonon. A recent ab-initio calculation and experiment suggest softening of a breathing phonon mode at the fermion bilinear at momentum M₁ from the patch fermions should be in either the Γ₁⁺ or Γ₃⁺ irrep of D₂h, with,

\[ \Lambda_{Γ₁⁺} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \Lambda_{Γ₃⁺} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \]  

(B3)

Similarly, the representation of optical phonon modes at M₁ in irrep Γ₁⁺, Γ₃⁺ can be identified using [76],

\[ Γ_{oph} = Γ_{equiv} × Γ_{vec}, \]  

(B4)

where Γ_{equiv} is the equivalence representation for the kagome lattice sites at M, Γ_{vec} is the representation for lattice displacement, the same as that for a 3d vector. The Γ_{oph,1} irrep comes from either Γ_{equiv,2} × Γ_{vec,2} or Γ_{equiv,4} × Γ_{vec,4} optical phonon modes. While the Γ_{oph,3} irrep comes from either Γ_{equiv,2} × Γ_{vec,4} or Γ_{equiv,4} × Γ_{vec,2} optical phonon modes. For example, both the “star of David” and the “inverse star of David” breathing phonon mode studied in Ref. [70] comes from the Γ_{oph,1} = Γ_{equiv,2} × Γ_{vec,2} optical phonon mode related by reversing the sign of the lattice displacement field.

The effective four-fermion interaction renormalized by \( \mathcal{H}_{el–oph} \) reads,

\[ \delta \mathcal{H}_{eff} = \sum_{q, q', Γ, α} \mathcal{V}_Γ \left( \Psi_{q}^† \Lambda_{Γ, α} \Psi_q \right) \left( \Psi_{q'}^† \Lambda_{Γ, α}^† \Psi_{q'} \right), \]  

(B5)

where \( \mathcal{V}_Γ = g^2 D_Γ(M₁, Ω_n = 0) = -\frac{2g^2}{ω_{Γ, k}} < 0 \), with \( ω_{Γ, k} \) the phonon spectrum, \( D_Γ(k, Ω_n) = \frac{2g^2}{(ω_{Γ, k})^2 - ω_{Γ, k}^2} \) the phonon propagator. This gives finally,

\[ \delta g₁(0) = \mathcal{V}_{Γ₁⁺} + \mathcal{V}_{Γ₃⁺}, \]

\[ \delta g₃(0) = \mathcal{V}_{Γ₁⁺} - \mathcal{V}_{Γ₃⁺}. \]  

(B6)

It is straightforward to see that \( \delta g₁(0) < 0 \) while the sign of \( \delta g₃(0) \) depends on the relative strength of \( \mathcal{V}_{Γ₁⁺} \) and \( \mathcal{V}_{Γ₃⁺} \). As a result, all three fixed point solutions may be approached when the electron-phonon interaction is taken into account.
Experimentally, one may test for the significance of electron-phonon coupling by probing the effect on the phonons. In particular, the coupling $H_{\text{el-ph}}$ also renormalizes the phonon spectrum, and lowers the optical phonon gap. Indeed, the phonon gap for $u_{1,1}^+, u_{1,3}^+$ are lowered by $\delta m_{\text{oph}} = \langle y^2 \Pi_{\text{ph}}(M) \rangle$, which may lead to a Peierls structural transition when the renormalized phonon spectrum becomes gapless at $M$.

Does the CDW order observed in the kagomé materials come from electronic or structural instabilities? While the full answer to this question requires knowledge of the microscopic details and self-consistent analysis of the electron-phonon coupled system, we note that the four-fermion interaction can be significantly enhanced in the electron-phonon coupled system, we note that the four-fermion interaction can be significantly enhanced in the RG flow near the fixed point. Moreover, in the weak coupling limit, as $g_{\text{el-ph}}^{(0)}$ is weak, a moderate electron-phonon interaction could alter the sign of the bare fermion interaction, and lead to CDW ordering due to an electronic instability.

C: Solutions of the rCDW mean-field theory

Here, we discuss the possible solutions of the rCDW mean-field theory. The free energy of the system as a function of the rCDW vector, $N = (N_1, N_2, N_3)$, has a tetrahedral point group symmetry, $T_d$. For fixed $|N| = N_0$, rCDW vectors can be categorized into different classes corresponding to the Wyckoff positions of $T_d$. In particular, there are three distinct rCDW classes that correspond to high symmetry points where the rCDW free energy must have a critical point on the $|N| = N_0$ surface. They are the $3Q+$, $3Q-$, and $1Q$ classes defined as rCDW states with the directions,

- $3Q+$: $\{(111), (1\bar{1}\bar{1}), (\bar{1}1\bar{1}), (\bar{1}\bar{1}1)\}$,
- $3Q-$: $\{((111), (1\bar{1}\bar{1}), (\bar{1}1\bar{1}), (\bar{1}\bar{1}1)\}$,
- $1Q$: $\{(\pm100), (0\pm10), (00\pm1)\}$.

Configurations in each class are related by $T_d$ symmetry. The critical points of the $3Q\pm$ must correspond to either a maxima or minima. This is because these directions coincide with the three-fold symmetry axes of $T_d$, so the curvature of the free energy around these points must have the same sign in all directions. The same cannot be said for the $1Q$ class which coincides with the two-fold axes of $T_d$, so points in the $1Q$ directions can either be saddle points or maxima/minima.

For $|N| = N_0$, the free energy is a smooth function defined on a sphere. Morse theory tells us that for such a function, the critical points must satisfy the following constraint, i.e. the number of maxima ($n_{\text{max}}$), minima ($n_{\text{min}}$), and saddle points ($n_{\text{sp}}$) must satisfy,

$$n_{\text{max}} + n_{\text{min}} - n_{\text{sp}} = \chi = 2,$$

(C1)

where $\chi = 2$ is the Euler characteristic of the sphere [77]. If we assume that the $3Q\pm$ and $1Q$ classes are the only critical points of the free energy, Eq. (C1) is satisfied if the $1Q$ class corresponds to a saddle point since there are 8 directions in the $3Q\pm$ classes and 6 directions in the $1Q$ class. Other solutions to Eq. (C1) require additional critical points on the sphere. Points on the sphere other than the high symmetry points listed above can be categorized using Wyckoff positions. For $T_d$, there are two types of low symmetry Wyckoff positions which we label $c, d$ with degeneracies $n_c = 12, n_d = 24$. It is straightforward to see that the simplest way to satisfy Eq. (C1) and include a low symmetry critical point is if there is a saddle point at the Wyckoff positions $c$ or alternatively, if there is a minimum/maximum at Wyckoff position $c$ and a saddle point at Wyckoff position $d$. In addition to the cases listed above, pairs of saddle points and maxima/minima can be added to both types of low symmetry Wyckoff positions while still satisfying Eq. (C1). However, we assume that cases with a large degeneracy of critical points are not physically relevant since they can only come from high-order terms with large powers of $N$ that are irrelevant at low energies, and correspond to highly oscillatory functions on the sphere. Therefore, given this assumption, the cases where the maxima/minima are only at the $3Q\pm$ or $1Q$ positions are expected and the solution to the rCDW mean-field theory should be in one of those directions.

A similar analysis can be extended to other order parameters. The iCDW and rSDW order parameters have a cubic point group symmetry, $O_h$, because they are odd under time-reversal symmetry unlike the rCDW order parameters. Therefore, the rCDW states in the $3Q+$ and $3Q-$ classes are related under time-reversal symmetry. Hence, for iCDW and rSDW, the the $3Q+$ and $3Q-$ classes are subsets of the larger $3Q$ class which is defined as the union of the $3Q\pm$ classes.

D: Landau theory coefficients

The coefficients, $K_1, K_2, K_3, K_4$, of the Landau theory defined in Eq. (12) are

$$K_1(T, \mu) = \frac{1}{2\Lambda^2} \int_{-\Lambda}^{\Lambda} \frac{d^2q}{(2\pi)^2} \frac{f(\varepsilon_2(q) - \mu) - f(\varepsilon_3(q) - \mu)}{\varepsilon_2(q) - \varepsilon_3(q)},$$

$$K_2(T, \mu) = -\frac{1}{2\Lambda^2} \int_{-\Lambda}^{\Lambda} \frac{d^2q}{(2\pi)^2} \left( \frac{f(\varepsilon_1(q) - \mu)}{\varepsilon_1(q) - \varepsilon_2(q) (\varepsilon_1(q) - \varepsilon_3(q))} \right).$$

(D1)
where \( f(\varepsilon) = 1/(\exp(\varepsilon/T) + 1) \) is the Fermi-Dirac function. These integrals can be evaluated asymptotically in the limit \( \mu, k_b T \ll a \Lambda^2, b \Lambda^2 \). If we assume perfect nesting, the patch dispersions take the form,

\[
\begin{align*}
\varepsilon_1(q) &= \frac{3t}{4} \left( 3q_x^2 - q_y^2 \right), \\
\varepsilon_2(q) &= \frac{3t}{4} 2q_y \left( q_y + \sqrt{3}q_x \right), \\
\varepsilon_3(q) &= \frac{3t}{4} 2q_y \left( q_y - \sqrt{3}q_x \right),
\end{align*}
\]

where \( t > 0 \). Given this definition, the asymptotic expressions of \( K_2, K_3, K_4 \) in the limit \( \mu, k_b T \ll t \Lambda^2 \) are

\[
K_2 \approx -\frac{16}{\pi^2 t \Lambda^2 k_b T} H_2(\mu/k_b T),
\]

where \( H_2, H_3, H_4 \) are the integral functions,

\[
\begin{align*}
H_2(z) &= \int_0^\infty dx \int_0^{x/\sqrt{3}} dy \left( \frac{F(\tilde{\varepsilon}_1(x, y) - z)}{\tilde{\varepsilon}_1(x, y) - \tilde{\varepsilon}_2(x, y)} \right) \\
H_3(z) &= \int_0^\infty dx \int_0^{x/\sqrt{3}} dy \left( \frac{F(\tilde{\varepsilon}_2(x, y) - z)}{\tilde{\varepsilon}_2(x, y) - \tilde{\varepsilon}_3(x, y)} \right) \\
H_4(z) &= \int_0^\infty dv \left( \frac{-F(v - z) + F(-v - z)}{v^3} + \frac{F'(v - z) + F'(-v - z)}{z^2} \right).
\end{align*}
\]

In the equations above, \( F(x) = 1/(e^x + 1) \), and \( \tilde{\varepsilon}_1(x, y) = 3x^2 - y^2, \tilde{\varepsilon}_2(x, y) = 2y(y + \sqrt{3}x), \tilde{\varepsilon}_3(x, y) = 2y(y - \sqrt{3}x) \). The expression holds for arbitrary ratios of \( \mu/k_b T \). The values of the \( H_2, H_3, H_4 \) when \( \mu \ll k_b T \) are

\[
\begin{align*}
H_2(0) &= 0.039571, \\
H_3(0) &= 0.014216, \\
H_4(0) &= 0.213139.
\end{align*}
\]

\( H_2, H_3, H_4 \) each change sign once at the following values:

\[
\begin{align*}
z_{0.2} &= 2.14268, \\
z_{0.3} &= 4.05161, \\
z_{0.4} &= 1.91067.
\end{align*}
\]

The expression for \( K_1 \) can be evaluated asymptotically when \( \mu \ll k_b T \):

\[
K_1 \approx -\frac{1}{6\sqrt{3} \pi^2 t \Lambda^2} \left( \ln(t \Lambda^2/k_b T)^2 + 2 \ln 3 \ln(t \Lambda^2/k_b T) \right).
\]

For \( \mu \ll T \), \( K_3 - 2K_4 \) which determines whether the quartic term of the rCDW Landau theory prefers a 3Q+
or 3Q− configuration is

\[ K_3 - 2K_4 \approx \frac{1}{\pi^2 t \Lambda^2 (k_B T)^2} \left( \frac{8H_3(0)}{3} - \frac{H_4(0)}{12 \sqrt{3}} \ln(t \Lambda^2 / k_B T) \right) \]  

(D21)

Therefore, \( K_3 - 2K_4 < 0 \) when

\[ \frac{\mu}{t \Lambda^2} \ll \frac{k_B T}{t \Lambda^2} < \exp \left( -32 \sqrt{3} \frac{H_3(0)}{H_4(0)} \right) \approx 0.0248. \]  

(D22)

E: Derivation of Eq. (22): the current operator

Here, we show more details to obtain the bond current operator, which is defined from the continuity equation of charge density. If we define the charge density at site \( r_\alpha \) as \( \hat{n}_{r_\alpha} = -e d_{r_\alpha}^\dagger d_{r_\alpha} \), the lattice version of the continuity equation reads,

\[ \frac{d \hat{n}_{r_\alpha}}{dt} + \sum_{r_\alpha \rightarrow r_\alpha'} \hat{j}_{r_\alpha r_\alpha'} = 0. \]  

(E1)

The expression for \( \hat{j} \) can be obtained from the equation of motion of \( \hat{n}_{r_\alpha} \) which reads,

\[ \frac{d \hat{n}_{r_\alpha}}{dt} = -\frac{i}{\hbar} \left[ \hat{n}_{r_\alpha}, \hat{H} \right] = -\frac{i}{\hbar} \left[ \hat{n}_{r_\alpha}, \hat{H}_0 \right] + \ldots \]  

(E2)

where \( ... \) denotes contribution from \( [\hat{n}_{r_\alpha}, \hat{H}_1] \), which only possibly contribute at \( O(\phi^2) \) to the bond-current order parameter \( \langle \hat{j} \rangle \). On the other hand, as only odd power in \( \phi \) term breaks time reversal symmetry, we conclude that \( \hat{H}_1 \) should not contribute to the bond-current order parameter at the mean field level. Therefore, only the contribution from \( \hat{H}_0 \) is considered. The NN bond order requires NN hopping term in \( \hat{H}_0 \). Noting,

\[ [\hat{n}_{r_\alpha}, \hat{H}_0] = \left[ \hat{n}_{r_\alpha}, t_1 \sum_{\langle r_{\alpha'}, r_{\alpha''} \rangle} d_{r_{\alpha'}}^\dagger d_{r_{\alpha''}} + e_{\alpha''} + d_{r_{\alpha'}} + e_{\alpha''} d_{r_{\alpha''}} \right] \]

\[ \approx \hat{n}_{r_\alpha}, t_1 \sum_{\alpha \neq \beta} \left( d_{r_{\alpha}}^\dagger d_{r_{\alpha} + e_{\beta}} - d_{r_{\alpha} + e_{\beta}}^\dagger d_{r_{\alpha}} \right), \]  

(E3)

where the second line comes from the fact that the commutator is nonzero only for bond satisfying \( r_\alpha = r_{\alpha'} \) or \( r_\alpha = r_{\alpha'} + e_\beta \), we find Eq. (22) in the main text.