

Sublattice modulated superconductivity in the kagome Hubbard model

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We identify a superconducting order featuring spatial pair modulations on the kagome lattice subject to on-site Hubbard U and nearest-neighbor V interactions. Within our functional renormalization group analysis, this state appears with a concomitant d -wave superconducting (SC) instability at zero lattice momentum, where it distinguishes itself through *intra-unit-cell modulations* of the pairing function thus breaking the discrete space group symmetry. The relative weight of the sublattice modulated superconductor (SMS) and d -wave SC is influenced by the absolute interaction strength and coupling ratio V/U . Parametrically adjacent to this domain at weak coupling, we find an intra-unit-cell modulated vestigial charge density wave and an s -wave SC instability. Our study provides a microscopic setting and thorough description of this novel SMS arising within a translation symmetry broken background.

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I. INTRODUCTION

Superconducting (SC) order beyond spatially uniform pairing is a longstanding area of condensed matter research [1]. The idea of a pair density wave (PDW), i.e., spatially varying electron pairing manifesting either as finite-range fluctuations or long-range order, has attained significant attention in the context of high- T_c cuprates [2]. There, intriguing phenomena such as Fermi arcs or layer decoupling find a rather intuitive explanation from the viewpoint of a PDW reference state. Most recently, PDWs have surfaced in experimental signatures for a plethora of material classes such as kagome metals, transition-metal dichalcogenides, heavy-fermion compound UTe_2 , and pnictides [3–7], evoking a universality of the PDW state in correlated electron systems. As tempting and rich as the principal phenomenology might be, the microscopic evidence for a PDW state still is rather poor. Spatially modulated SC pairing has only been rigorously accessed in the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) scenario of subjecting weak-coupling spin-singlet SC to a magnetic field [8,9]. Without an external field, there is no generic weak-coupling solution featuring Cooper pairs at finite lattice momentum. Therefore, the majority of previous attempts had to resort to effective mean-field treatments either through postulating

finite-range bare pair hopping [10] or analyzing higher-order terms of Ginzburg-Landau expansions [11–13]. It is then usually a matter of nonuniversal parameter choice whether one finds a PDW as competing order to uniform SC and charge density wave (CDW), or as a, possibly fluctuating, high-temperature mother state yielding vestigial SC and CDW order at lower temperature [1]. It is thus of central interest to identify a microscopic approach to correlated electron systems that realizes a PDW state [14].

The functional renormalization group (FRG) [15,16] suggests itself as a natural method to access ordering instabilities at and beyond weak coupling. Even though it lacks an analytical control parameter which is the archetypal challenge for any order at intermediate coupling, the FRG treats all bilinear fermionic orders on equal footing and allows for a smooth interpolation to the weak-coupling limit by reducing the interaction strength. FRG calculations were demonstrated to adequately describe even intricate phase diagrams of multiorbital/multisublattice correlated electron systems such as iron pnictides [17,18]. As a guiding motif for our study of spatially modulated superconductors we identify the non-trivial sublattice structure of experimentally observed PDW materials. This suggests the $U - V$ kagome Hubbard model (KHM), where U and V denote the on-site and nearest-neighbor (NN) electronic repulsion on the kagome lattice, respectively, as a blueprint to examine the sublattice structure of the low-energy fluctuations and its imprint on emergent exotic electronic orders [19,20]. In particular, the geometry of

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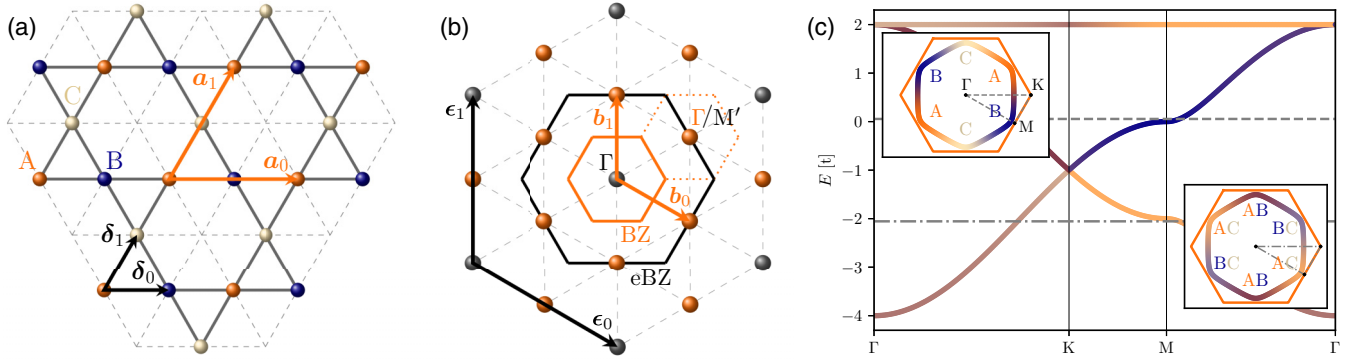


FIG. 1. Kagome fermiology and extended zone scheme. (a) Kagome lattice with sublattices A , B , and C along with the inter- ($\mathbf{a}_{0,1}$) and intra- ($\delta_{0,1}$) unit-cell vectors. (b) Fourier transform of the kagome lattice with the Brillouin zone (BZ) in orange and extended Brillouin zone (eBZ) in black. M' points in the eBZ coincide with the Γ point in the BZ. (c) The kagome band structure features a flat band and two dispersive bands which display a particular eigenstate sublattice distribution according to sublattice interference [21]. The p -type (m -type) van Hove fillings are symbolized by dashed (dashed-dotted) lines.

the KHM promotes sublattice interference (SI) [21], leading to pronounced nonlocal interactions and emergent NN pair hopping, which creates a propensity for PDW formation [22].

Moreover, the sublattice degree of freedom allows for a formation of intra-unit-cell modulated states. In analog to an intra-unit-cell modulated charge density wave we observe a superconducting state of equal pair modulation periodicity, that hence features similar phenomenology to a PDW. However, this state does not break an additional translation symmetry but rotational symmetry within the unit cell and hence surfaces as a $\mathbf{Q} = 0$ instability in the BZ. As this deviates from the common definition of PDW, we label the obtained instability sublattice modulated superconductor (SMS).

In this paper, we develop a theory for an SMS state observed within FRG calculations. Specifically, the state we find does not appear as a parasitic onset order to another electronic instability, but unfolds as part of the leading instability in the particle-particle (pp) channel descending from a pristine kagome metallic state. In terms of symmetry classification at the pp instability level, admixes with in-plane d -wave SC (d SC) in the E_2 irreducible representation of the hexagonal point group C_{6v} . The key to disentangle the SMS from the d SC contribution is the center of mass dependence of the condensate wave function in the triatomic unit-cell basis. Here, the SMS component exhibits intra-unit-cell modulations while the d SC component is uniform.

II. KAGOME HUBBARD MODEL (KHM)

We start from

$$H = t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} + \frac{V}{2} \sum_{\langle i,j \rangle; \sigma\sigma'} n_{i\sigma} n_{j\sigma'}, \quad (1)$$

where $c_{i\sigma}^\dagger, c_{i\sigma}$ denote electron creation and annihilation operators at site i with spin σ , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and t , U , and V denote the energy scales of hopping, on-site Hubbard, and NN repulsion, respectively. The kagome lattice depicted in Fig. 1(a) features a nonbipartite lattice of corner-sharing triangles, resulting in three sublattices A , B , and C as well

as Bravais lattice vectors $\mathbf{a}_0$ and $\mathbf{a}_1$. Alternatively, it can be interpreted as a charge density wave formation at $3/4$ filling of an underlying triangular lattice with halved unit-cell vectors δ_0 and δ_1 , where every fourth unoccupied site is projected out. In reciprocal space [Fig. 1(b)], this corresponds to the reduced (orange) and extended (black) Brillouin zone (BZ) spanned by the vectors $\mathbf{b}_{0,1}$ and $\boldsymbol{\epsilon}_{0,1}$ according to $\mathbf{b}_i^\top \mathbf{a}_j = \boldsymbol{\epsilon}_i^\top \boldsymbol{\delta}_j = 2\pi \delta_{ij}$. The three inequivalent van Hove points at the M points in the BZ epitomize a peculiar density of states of differing sublattice occupancy [pure p type at filling $n = 5/12$ for the upper and mixed m type ($n = 3/12$) for the lower van Hove level in Fig. 1(c)] [21,23], a generic feature of kagome metals which has been recently confirmed by angle-resolved photoemission spectroscopy (ARPES) [24,25]. For both m and p type, the mismatch of sublattice support for electronic eigenstates connected by van Hove point nesting triggers SI.

III. FRG INSTABILITY ANALYSIS

The FRG formulates an ultraviolet to infrared cut-off flow of the two-particle electronic vertex operator $V(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) c_{\mathbf{k}_4}^\dagger c_{\mathbf{k}_3}^\dagger c_{\mathbf{k}_2} c_{\mathbf{k}_1}$ as a set of differential equations, where the $\mathbf{k}_i$ denote lattice momenta. We employ the FRG in its truncated-unity (TU) approximation (TUFRG), where the vertex is separated into three different contributions according to their distinctive transfer momenta [26], which can be classified as two particle-hole (ph) and a single particle-particle (pp) channel. The complementary vertex momenta are expanded in plane-wave form factors $\phi_f(\mathbf{k}) = e^{i\mathbf{r}_f \cdot \mathbf{k}}$ via the Bravais lattice sites $\mathbf{r}_f = n\mathbf{a}_0 + m\mathbf{a}_1$, $n, m \in \mathbb{Z}$. For the KHM, any channel vertex function is specified by a 4-tuple of sublattice indices $\{o_i\}$, $i = 1, 2, 3, 4$, transfer momentum $\mathbf{Q}$, and two residual momenta which we expand into form factors according to

$$\mathcal{V}_{ff'}^{[o_i]}(\mathbf{Q}) = \int_{\text{BZ}} d\mathbf{k} d\mathbf{k}' V^{[o_i]}(\mathbf{Q}, \mathbf{k}, \mathbf{k}') \phi_f(\mathbf{k}) \bar{\phi}_{f'}(\mathbf{k}'). \quad (2)$$

Truncating the set of basis functions, and reflecting the locality of pp and ph pairs, this unitary expansion becomes approximate. We terminate the flow at an energy scale Λ_c , upon encountering a divergence in a vertex element indicating

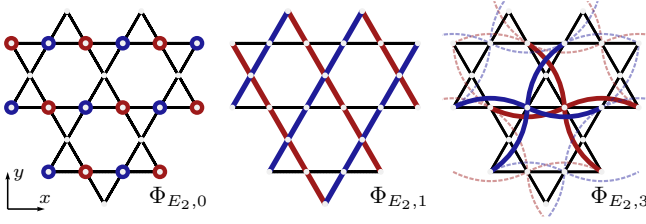


FIG. 2. Harmonics of the E_2 irrep with y -mirror eigenvalue -1 . We show the on-site ($\Phi_{E_2,0}$), first NN ($\Phi_{E_2,1}$), and third NN harmonic ($\Phi_{E_2,3}$). We skip the second NN due to its similarity to the first NN. Red/blue indicates a positive/negative value of the pair correlation Eq. (4) between connected sites.

a symmetry breaking phase transition. At this point, the effective vertex contains all higher-energy quantum fluctuations accessible within the FRG approach. For SC pairing at $\mathbf{Q} = 0$, the system's ground state is then obtained from the BCS gap equation which reduces to an eigenvalue problem

$$\lambda \Delta_{o_1 o_2}^f = \sum_{f' o_3 o_4} \mathcal{V}_{ff'}^{(o_i)}(0) \Delta_{o_3 o_4}^{f'} \quad (3)$$

at the onset of ordering. The functional form of the SC order parameter is thus given by the eigenstate $\Delta_{o_1 o_2}^f$ associated with the most negative eigenvalue λ . Exploiting the group symmetry constraints on Eq. (3) along Schur's lemma allows for a classification of $\Delta_{o_1 o_2}^f$ in terms of irreducible representations (irreps) of C_{6v} . Within our TUFGR analysis, we identify an extended region in the $U - V$ parameter space where $\mathbf{Q} = 0$ instabilities in the spin-singlet pp channel dominate, and the superconducting order parameter transforms according to the E_2 irrep.

IV. CLASSIFICATION OF THE E_2 pp INSTABILITY

A two-electron expectation value in the spin-singlet sector,

$$\langle c_{\mathbf{r}_i, \uparrow}^\dagger c_{\mathbf{r}_j, \downarrow}^\dagger - c_{\mathbf{r}_j, \uparrow}^\dagger c_{\mathbf{r}_i, \downarrow}^\dagger \rangle = \delta_{\mathbf{r}_i, \rho} \delta_{\mathbf{r}_j, \rho} \Phi(\mathbf{r}_i, \mathbf{r}_j), \quad (4)$$

is most conveniently described in terms of a center-of-mass coordinate (CMC) $\mathbf{R} = (\mathbf{r}_i + \mathbf{r}_j)/2$ and a relative coordinate (RC) $\mathbf{r} = \mathbf{r}_i - \mathbf{r}_j$. In the following, we denote the set of all lattice points by ρ and use ρ_o for points related to sublattice $o \in \{A, B, C\}$. We introduce $\mathbf{a}_2 = \mathbf{a}_1 - \mathbf{a}_0$ and $\delta_2 = \delta_1 - \delta_0$ for notational convenience. Since the kagome lattice is not of Bravais type, the directions of NN bonds depend on the sublattice. For each pairing distance, i.e., each value of the RC (on site, NN, etc.), the E_2 irrep is expanded in pairs of degenerate orthogonal states, characterized by even or odd transformation behavior under mirror symmetry along the y axis [26]. We order different E_2 candidate states by their RC length and constrain ourselves to the mirror-odd state as we present a graphical representation in Fig. 2. The on-site ($\mathbf{r} = 0$) pairing wave function reads

$$\Phi_{E_2,0}(\mathbf{R}, \mathbf{r}) = (\delta_{\mathbf{R}, \rho_A} - \delta_{\mathbf{R}, \rho_B}) \delta_{\mathbf{r}, 0}. \quad (5)$$

The absence of a lattice site at the point group's rotation center allows for such on-site pairing wave functions on any non-Bravais lattice. The trivial transformation property of the RC is complemented by a nontrivial CMC function due to the

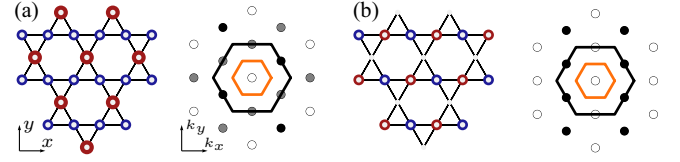


FIG. 3. Real-space representation of the two on-site pairing wave functions with E_2 symmetry and their Cooper pair momentum structure in the eBZ. Lighter shading corresponds to less intensity. Contrarily to the d SC pairing wave functions of Eq. (6), a finite Cooper pair momentum is revealed by the unfolding into the eBZ [26]. The depicted $\mathbf{Q}$ structure resembles the expected STM signature of the SMS state.

reduced site symmetry group of the $3c$ Wyckoff position. In contrast, the NN pairing state

$$\Phi_{E_2,1}(\mathbf{R}, \mathbf{r}) = \delta_{\mathbf{r}, \pm \delta_1} - \delta_{\mathbf{r}, \pm \delta_2} \quad (6)$$

features a trivial CMC dependence, and instead it is the RC that captures the E_2 transformation behavior. Whereas the second NN state is structurally equivalent [26] to the NN state, the third NN pairing reads

$$\begin{aligned} \Phi_{E_2,3}(\mathbf{R}, \mathbf{r}) = & \delta_{\mathbf{R}, \rho_B} \delta_{\mathbf{r}, \pm \mathbf{a}_0} - \delta_{\mathbf{R}, \rho_A} \delta_{\mathbf{r}, \pm \mathbf{a}_0} \\ & + \delta_{\mathbf{R}, \rho_C} (\delta_{\mathbf{r}, \pm \mathbf{a}_1} - \delta_{\mathbf{r}, \pm \mathbf{a}_2}). \end{aligned} \quad (7)$$

It cannot be decomposed into a product of solely CMC- and RC-dependent functions. This stems from two symmetry-inequivalent types of third NN on the kagome lattice due to the reduced C_{2v} site symmetry group, that yields the additional spatial CMC structure [26].

V. SMS WAVE FUNCTION

Two candidate states may belong to the same irrep and yet trace back to entirely different physical origins. For the A_1 pairing irrep on the square lattice, this has been extensively discussed in the context of $s_{\pm}$ - vs s_{++} -wave SC in iron pnictides [27,28]. For the kagome lattice, the fundamentally different nature of the E_2 form factors becomes apparent upon disentangling the spatial information encoded in CMC and RC, respectively. The Cooper pair wave function of typical zero momentum SCs features a uniform CMC dependence, while the RC encodes the transformation behavior of the associated irrep. Eq. (5), however, describes a scenario where the typical roles of CMC and RC are interchanged. It obeys $\sum_{\mathbf{R}} \Phi(\mathbf{R}, \mathbf{r}) = 0$, which is a characteristic of PDW-type pairing [29]. The key point to appreciate here is that despite the $\mathbf{Q} = 0$ channel, *spatially modulated contributions can be distinguished from homogeneous ones within the multisite unit cell*. This is the essential difference between the SMS and d SC contributions to an E_2 pp instability in the KHM.

Restoring the full real-space information previously encoded in the sublattice indices of the triatomic basis by transferring the SMS state of Eq. (5) to the extended BZ shown in Fig. 3 reveals finite momentum Cooper pairing, that can be directly attributed to a generalized version of the structure factor experimentally accessible in scanning tunneling microscopy (STM) measurements [for details, cf. Supplemental Material (SM) [26]]: By locally probing the differential

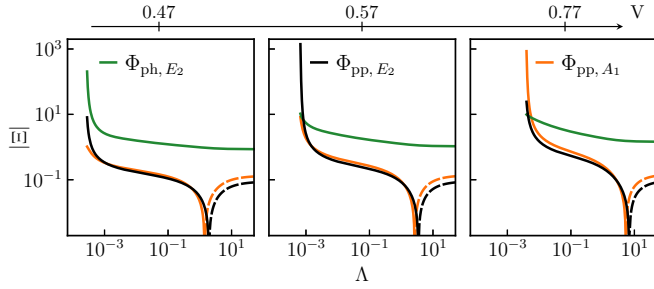


FIG. 4. FRG vertex analysis for $U/t = 0.14$ and $0.47 < V/t < 0.77$ as a function of the energy cutoff Λ . E_2 CDW (Φ_{ph, E_2} , green), SMS E_2 pp order (Φ_{pp, E_2} , black), and SC A_1 pp (Φ_{pp, A_1} , orange) compete for the leading instability. Attractive (repulsive) expectation values $|\Xi|$ of the leading instabilities at Λ_c are indicated by solid (dashed) lines [26].

conductance via the Josephson tunneling signal of a superconducting STM tip, the SC gap can be monitored with high spatial resolution. The Fourier transform of the pairing gap maps exhibits peaks at the wave vectors associated with the Cooper pair modulation, that can be matched with the peak structure in Fig. 3. This allows for a clear experimental distinction between the proposed SMS state and uniform SC pairing [30–34].

VI. SMS PHASE DOMAIN

Within our TUGRG analysis of the KHM, the E_2 pp instability domain is governed by intrasublattice pairing, i.e., the eigenstates of Eq. (3) are described by a linear combination of $\Phi_{E_2,0}$ and $\Phi_{E_2,3}$ [26]. This allows to identify the E_2 pp instability as a SMS. Such states were previously found, yet not adequately appreciated in the kagome phase diagram of Refs. [20,35]. The intrasublattice pairing tendency can be understood from the viewpoint of SI: Under the RG, effects of U are suppressed while V grows [22], making intersublattice pairing less favourable. This trend also manifests in the fact that the SMS instability at small U/t is parametrically framed by an E_2 -type CDW and an A_1 -type, i.e., s -wave SC (Fig. 4) at p -type van Hove filling.

The SMS state emerges as interstitial order via competing interaction processes projected into the pairing channel: U drives nonlocal spin fluctuations; V , by contrast, generates charge fluctuations entering the Cooper channel as on-site attractive interactions [36]. In Fig. 4, we illustrate the generic scenario of competing instabilities generated by this interplay of local and nonlocal interactions by comparing FRG flows for varying bare values $0.47 < V < 0.77$ at fixed $U = 0.14$, i.e., located in the weak-coupling domain. Both SMS-type and s -wave SC channels are initially repulsive (dashed lines) and subsequently turn attractive (solid lines) through the RG flow. Remarkably, the adjacent CDW features the same irrep and intrasublattice modulation as the SMS phase, suggesting vestigial symmetry-type restoration at the phase transition. In previous contexts, PDW fluctuations were similarly found to predominantly occur around phase transitions between a density wave phase and SC pairing, where a variety of competing and/or cooperative orders arise at

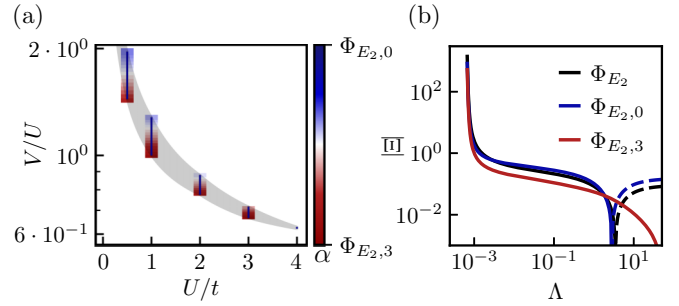


FIG. 5. (a) Admixture ratio α of $\Phi_{E_2,0}$ (blue) (5) and $\Phi_{E_2,3}$ (red) (7) for the E_2 pp domain at p -type van Hove filling ($n = 5/12$). (b) Expectation value of the leading eigenstate at Λ_c (black), $\Phi_{E_2,0}$, and $\Phi_{E_2,3}$. Negative (positive) values are indicated by solid (dashed) lines.

intermediate-coupling strength [1]. Any weak-coupling theory of PDW has hitherto relied on fine-tuned fermiology [37]. Here, however, we find that the SMS prevails beyond p -type van Hove filling whenever intra-unit-cell modulations become competitive to homogeneous pairing functions due to SI.

The competition of interaction processes is directly reflected in the pairing wave functions overlap with $\Phi_{E_2,0}$ and $\Phi_{E_2,3}$ [26] and their relative weight α , which is depicted in Fig. 5(a) for the SMS regime at p -type van Hove filling. Doping slightly away from this point significantly increases the SMS region, e.g., by a factor of ≈ 2.5 for $U = 3$ at $n = 1.01 \times 5/12$. The third NN state $\Phi_{E_2,3}$ does not suffer an energy penalty from U in (1) and thus promotes attractive pairing channel already at bare coupling [Fig. 5(b)]. Analogous to the previous discussion, V -driven intra-unit-cell charge fluctuations yield an on-site attraction of Cooper pairs through the RG flow [20]. The on-site contribution $\Phi_{E_2,0}$ to SMS increases with V , and eventually drives the system into an s -wave SC.

VII. CONCLUSION AND OUTLOOK

Our findings emphasize the fundamental role of the sublattice texture on the Fermi surface in a microscopic theory of spatially modulated pairing, a motif also shared among the different PDW candidates [37–39]. The new type of sublattice modulated SC instability we find for the KHM model is facilitated by the nontrivial basis in the unit cell. This allows spatial modulations of the Cooper pair wave function, while still exploiting the Cooper logarithm of a $\mathbf{Q} = 0$ pairing instability as the main driver for the symmetry breaking transition. This establishes the proposed type of SMS as a generic instability of a Fermi liquid with sublattice degrees of freedom and may explain the broad range of materials exhibiting PDW phenomenology. The breaking of rotational symmetry instead of translational symmetry by intra-unit-cell modulations of the SC order parameter finds a direct correspondence for magnetically ordered systems in the new field of altermagnetism [40,41]. Viewing the kagome lattice as a fictitious $3/4$ filling CDW of an underlying triangular lattice [Fig. 1(a)], we recover the expected intertwined character of PDW: The kagome-CDW at $2\delta_{1,0}$ comes along with a $2\delta_{1,0}$ PDW competing with d SC. This motif carries over to SC

within the 2×2 charge order in 135 kagome compounds [3,38]: Spatially modulated intra-unit-cell SC can arise within the enlarged 2×2 unit cell in the charge ordered phase without an additional translation symmetry breaking imposed by the SC transition. Within the SMS phase, experimental signatures of a PDW-like reciprocal Josephson effect can still be observed [42–44]. To target experimentally observed PDW states in kagome compounds such as the roton density wave reported for CsV_3Sb_5 within the charge order domain [3], the methodological shortcoming to surmount in the future is to continue the FRG flow throughout the preceding charge ordered phases [45].

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