Stable Flatbands, Topology, and Superconductivity of Magic Honeycomb Networks

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We propose a new principle to realize flatbands which are robust in real materials, based on a network superstructure of one-dimensional segments. This mechanism is naturally realized in the nearly commensurate charge-density wave of 1T-TaS₂ with the honeycomb network of conducting domain walls, and the resulting flatband can naturally explain the enhanced superconductivity. We also show that corner states, which are a hallmark of the higher-order topological insulators, appear in the network superstructure.

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Band theory of electrons has gone through a renaissance in recent years, especially concerning its topological nature [1,2]. Band structures are also an important starting point to understand strongly correlated systems. In particular, when the Fermi level lies in a flatband, the correlation effects become dominant, leading to many interesting physics including superconductivity and magnetism. A few theoretical principles to realize flatbands are known, most notably the chiral (sublattice) symmetry and an imbalance between the number of sublattice sites [3,4]. However, once further nearest-neighbor hoppings, which generally exist in real materials, are included, the chiral symmetry is lost and the flatbands in the simplified model acquire a substantial curvature. This is a major reason why it has been difficult to realize flatbands in real materials and observe resulting strong correlation effects experimentally, with few exceptions [5–7].

In this Letter, we propose a novel general principle to realize flatbands based on a network of one-dimensional segments. The resulting flatbands are protected by the combination of crystal and time-reversal symmetries, and are robust even in the presence of the further neighbor hoppings, as long as the effective hopping range is shorter than the segment length. We argue that this mechanism is naturally realized in the nearly commensurate charge-density wave (NC-CDW) phase of 1T-TaS₂, in which the domain walls play the role of the one-dimensional metallic segments [8]. The robust flatbands ensured by the new principle give a natural explanation of the observed superconductivity, which is strongly reminiscent of the moiré physics [5–7] of twisted bilayer graphene. Moreover, the network superstructure can also lead to corner states, i.e., a higher-order topological insulator.

Experimentally, 1T-TaS₂ has a rich phase diagram of CDW orders [9] and superconductivity (SC) [10–12], which are accessible by tuning temperature, pressure, and doping. There are three distinct regimes: commensurate CDW (C-CDW), NC-CDW, and incommensurate CDW. The C-CDW phase has a long-ranged charge ordering and appears at the lowest temperature with the ambient pressure. This state is the correlation-driven Mott insulator [13–15]. When the C-CDW ordering is slightly suppressed by pressure or doping, then the domain walls appear in between the locally charge-ordered domains, i.e., it enters into the NC-CDW state. If the pressure or doping increase further, the SC emerges from this NC-CDW state. Note that a similar phase diagram is obtained in another CDW material, namely, 1T-TiSe₂ [16]. This suggests that the NC-CDW [10–12,16,17] is somehow essential for realizing SC in these CDW materials though how this actually happens has been unclear. We will point out that a honeycomb network of metallic domain walls in the NC-CDW phase [8,18,19] hosts a series of robust flatbands ensured by the new principle, giving a natural explanation for the observed SC.

1. Model and flatbands: A recent STM study [8] combined with DFT calculation provided an unprecedented detail of the electronic structure of the network, where the metallic nature of the domain walls and trijunctions is clearly exposed. Similar structure emerges in, e.g., helium mixture absorbed to graphite [20]. Here we consider a minimal tight-binding model, which consists of the low-energy modes inside the domain walls; see Fig. 1(a).

$$H_0 = -t_0 \sum_{\langle r,r' \rangle} c_{r,\sigma}^\dagger c_{r',\sigma} - t_J \sum_{\{r,r'\} \in J} c_{r,\sigma}^\dagger c_{r',\sigma} + \text{H.c.}, \quad (1)$$

FIG. 1. (a) Network of 1D metals. In Eq. (1), only the sites along the straight blue lines are included. The other sites represent the insulating domain sites. The gray line represents the unit cell. (b) The states inside the flatbands. Blue and red colored regions have the opposite signs and a destructive interference appears for any hopping shorter than the link length (e.g., l). (c) Band structure of Eq. (1). (d) Band structure including the domain sites.

where the second sum over $\{r, r'\} \in J$ runs over the sites around the junctions J and $t_J \leq t_0$. Here σ represents the spin and the sum over it is assumed. The spin rotational symmetry is also assumed for simplicity. The model also has time-reversal symmetry $\mathcal{T}$, and crystalline D_6 symmetry, which are the symmetries observed in the STM experiment of 1T-TaS₂ [8]. Diagonalizing Eq. (1), we find a cascade of flatbands, Dirac and quadratic band crossings; see Fig. 1(c). On top of this, a three-component spin-1 Dirac fermion [21] can appear when $t_J/t_0 \rightarrow 0$. The number of the flatbands is proportional to the number of the sites between the junctions. The topological band crossings are protected by symmetries. On the other hand, the flat dispersion cannot be generally protected because it requires infinitely many parameters to be tuned. Hence, they are generically fragile, e.g., against the second neighbor hoppings [22]. Despite of the fragile nature, flatbands are an ideal stage to realize correlation-dominated physics, such as ferromagnetism, and thus have been studied vigorously [33]. A well-known mechanism which gives rise to flatbands is an imbalance between sublattice sites in bipartite lattices. This was applied [3] to hyperhoneycomb systems which have some similarities with the systems we study in this Letter. However, such flatbands can be generically removed by inclusion of short-ranged further neighbor hoppings, which exist in real materials.

Remarkably, our flatbands from the network defy this standard phenomenology and are stable against D_6 -symmetric local perturbations. For example, addition of the third-neighbor hoppings t_3 near the nodes do not disperse the flatbands. We can even include the insulating

electronic states from the domain area (described by H_{dom}); see Fig. 1(a). The full Hamiltonian is now $H = H_0 + H_{\text{dom}} + H_{\text{coup}}$, with

$$H_{\text{coup}} = -t_d \sum_{\langle r, r' \rangle} c_{r, \sigma}^\dagger d_{r', \sigma} + \text{H.c.},$$

where $c_{r, \sigma}$ ($d_{r, \sigma}$) electrons belong to the network (to the domains). Here H_{dom} is described by the band insulator which has the two energy-split states per site and the different sites are connected by the small hopping t_d [Fig. 1(a)]. From the perturbative reasoning, we expect that this model includes all the possible symmetric local perturbations. Notably, the flatbands and overall band shapes remain almost intact inside the gap [Fig. 1(d)]. This result implies that in NC-CDW 1T-TaS₂, even if the bulk bands from the domain region are included, flatbands inside the gap are almost intact. Finally, the flatbands survive [22] against the Rashba spin-orbit coupling. Such stability is absent for other networks [22]. In passing, we note that this is consistent with our previous phenomenological approach; see Ref. [22].

To explain the unusual stability, we look into the structure of the wave functions inside the flatbands. We find that those wave functions vanish at the junctions [22]. Hence, when the low-energy modes are entirely from the network and only the nearest neighbor hoppings are included, i.e., $t_J = 0$ in Eq. (1), the wave function is a standing wave $\psi(l)$ [Fig. 1(b)]. From such standing waves, we can construct a set of localized states [34] which consist of the flatbands: we consider a linear combination around the honeycomb plaquette with a sign oscillation, i.e., $\Psi \sim \sum_a (-1)^a \psi(l)$ for $a \in \{1, 2, \dots, 6\}$ labeling the six links around the plaquette; see Fig. 1(b). Then we see that this state cannot disperse into the neighboring plaquettes because of the destructive interference. Such destructive interference persists as far as the hopping distance is shorter than the length of the wire. Finally, the intrawire further neighbor terms do not alter this conclusion because they affect only the energy and intrawire structure of the standing waves [22]. This illustrates the importance of the symmetry and the locality on the stability of the flatbands. We can also understand that the cascade of the flatbands *must* appear because there are many standing wave solutions per wire [35].

We expect the flatbands to be removed either by long-ranged direct hopping across the domains or by breaking symmetries. Indeed, we can show [22] that the flatbands are lifted when the symmetries are broken, or when such long-ranged hoppings [e.g., t_f in Fig. 1(b)] are included. This means that, for the NC-CDW state of 1T-TaS₂, we need a sizable hopping between the two sites apart by $\sim \mathcal{O}(80)$ Å [8] to remove the flatbands, which is not realistic. This explains why the dispersion of the “flatbands” are very small but still finite when the domain sites are included. When the time-reversal symmetry is broken, the band

touchings are gapped out and it results in dispersive Chern bands [22], which is a natural platform for fractionalization [36].

For 1T-TaS₂, we constructed a tight-binding model in the Supplemental Material [22], which fits reasonably well with DFT + *U* calculation on the domain wall. The tight-binding parameters scale as $1/d^5$ [23], where *d* is the distance between the atomic sites. From this, we find that the cascade of the flatbands emerges [22]. Next, we comment on the effect [37–40] of the interlayer coupling. The interlayer interaction has been suggested to be important in 1T-TaS₂. However, we remark that there are plenty of experimental data and theory [8,15] suggesting that the main physics is essentially 2D. For example, the resistivity along the *c* axis is much larger, e.g., by 500 times [41], than the intralayer resistivity [41,42] and anisotropic 2D charge transfer is observed for the NC-CDW state [43]. Further, the SC *T_c* is almost insensitive to the pressure [10] and not much affected under the dimensional reduction [11]. Based on these, we focus on the 2D physics here.

2. Superconducting states: Having established the stability of the flatbands, we now discuss the many-body physics when the Fermi level is near one of the flatbands. Such a system is unstable toward various particle-hole and particle-particle channels. However, guided by experiments, we mainly focus on superconductivity in this Letter.

First, we perform the simplest BCS mean-field theory with the phenomenological interaction

$$H_{\text{int}} = U \sum_{\mathbf{r}} n_{\mathbf{r}}^2 + V \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} n_{\mathbf{r}} n_{\mathbf{r}'} \quad (2)$$

Projecting to the BCS channel, we obtain [22]

$$H_{\text{int}} \rightarrow H_{\text{BCS}} = \sum_{l \in \mathbb{Z}} g_l \sum_{\mathbf{p}, \mathbf{k}} \hat{\Delta}_{l, \mathbf{p}}^\dagger \cdot \hat{\Delta}_{l, \mathbf{k}}, \quad (3)$$

where g_l is the interaction strength along the pairing channel of the angular momentum *l*, which we compute numerically. $\hat{\Delta}_{l, \mathbf{p}}$ is the corresponding pairing order parameter. Note that, within the mean-field decomposition of Eq. (2), only the spin-singlet sector appears. Below we consider only the *s*-wave and (*d* + *id*)-wave pairing channels, i.e., g_0 and $g_2 = g_{-2}$ of Eq. (3). Higher angular momentum pairing channels ($|l| > 2$) will belong to the same representations of *s*- or (*d* ± *id*)-wave pairing channels in the honeycomb symmetry. The magic of the flatbands appears when the gap equation is solved.

$$\frac{1}{g_l} \sim \int_{\text{BZ}} \frac{d^2 k |F_l(\mathbf{k})|^2}{\sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |F_l(\mathbf{k}) \Delta_l|^2}} \sim \frac{1}{|\Delta_l|},$$

where $F_l(\mathbf{k})$ is the form factor [22], e.g., $F_2(\mathbf{k}) \rightarrow (k_x + ik_y)^2$ for $|\mathbf{k}| \ll 1$ and $\epsilon_{\mathbf{k}} = \mu$. Hence, the gap is linearly enhanced, i.e., $|\Delta_l| \sim |g_l|$ (if $g_l < 0$), instead of the standard

FIG. 2. (a) Phase diagram. “s-wave” represents an *s*-wave SC, and “FM” (“NM”) represent ferromagnetic (normal metal) state. The green region is a (*d* + *id*)-wave SC. (b) Pictorial representation of the model for the higher-order topology. Here $|t| < |g|$ supports the 0D state at the junctions and the corner at the boundary. The gray line represents the unit cell. (c) Density distribution of four in-gap modes of (d). (d) Energy eigenvalues for a single unit cell with open boundary condition for $t/g = 0.1$.

exponential suppression $\sim \exp(-1/|g_l| \nu_l)$. Because there is no other scale, the mean-field energy of the SC is linear in g_l and so is the *T_c* [22]. Hence, the honeycomb network strongly enhances the SC *T_c*. The phase diagram for one flatband is in Fig. 2(a). Thus we conclude that, within the mean-field theory, the *s*-wave SC is strongly enhanced when *U* is attractive [44]. On the repulsive interaction side, the system exhibits ferromagnetism. While the repulsive *U* opens up a small window for the (*d* ± *id*)-channel pairing, the dominance of the *s*-wave SC is a characteristic feature of the present flatband system [22]. In passing, the BdG fermion spectrum is also computed [22].

Although the mean-field theory ignores the fluctuation, it is a good starting point for revealing possible phases and phase diagram. In fact, the mean-field theory qualitatively agrees with a rigorous result on flatband ferromagnetism [45] with a repulsive *U*, and our findings in this Letter are consistent with recent numerical studies in other flatband systems [44,46–48].

Let us comment on the interaction Eq. (2). The strong electron-phonon coupling in 1T-TaS₂ is known as the driving force for the formation of the CDW states [49]. However, after the formation of the CDW clusters through the electron-phonon coupling, the soft phonons are naturally hardened [50]. In particular, the domain wall in the NC-CDW state is also structurally reconstructed by forming its own CDW clusters from electron-phonon coupling [8], which will reduce the coupling more. Hence, we expect

that the electron-phonon coupling becomes inactive for the physics within the NC-CDW phase. Nevertheless, the phonon-electron interaction was essential in forming the parent CDW domains and the domain wall network, and hence its effect is already encoded the model Eq. (1). Next, it is well known that the coupling of electrons and (optical or gapped) phonons effectively plays the same role as the attractive U , which favors the s -wave SC [22]. This will effectively renormalize U in Eq. (2) toward negative. Hence, explicitly including the effects of these phonons does not alter the dominance of the s -wave SC [22]. On the other hand, the long-range Coulomb interaction will be efficiently screened due to the large density of states of flatbands and it will be rendered into a short-ranged interaction, which can be effectively encoded by Eq. (2).

It is instructive to consider the strong-coupling limit [51], where the interaction is bigger than the hopping integrals. For this, we start from the decoupled *strongly correlated* wires, each of which is described by a Tomonaga-Luttinger liquid (TLL)

$$H = \sum_{a,\sigma=c/s} \int dt \frac{v_\sigma}{2} \left[\frac{1}{K_\sigma} (\partial_t \theta_{a,\sigma})^2 + K_\sigma (\partial_t \phi_{a,\sigma})^2 \right],$$

where the Luttinger parameters $\{K_c, K_s\}$ capture the correlation nonperturbatively [52]. This is the correlated version of the scattering problem [8], which faithfully reproduced the band structures.

The two-dimensional SC can be preempted by the spin gap [52,53] in each wire. Once the spin gap forms, the low-energy physics of each wire is described by a single-component TLL of $\theta_{a,c}$ describing the fluctuating SC pairs [52]. Since the SC pair is bosonic, the junction of three TLLs at each vertex of the honeycomb network corresponds to the bosonic Y junction [54], rather than the fermionic one [55,56] where the fermion statistics plays an important role. When each wire has sufficient attraction, i.e., $K_c \leq 1$ [52], then the interwire coupling between the SC fluctuations, namely, the Josephson coupling J , becomes relevant [52]. Only interested in the pattern of the phases, we note that the problem is symmetrically equivalent to the XY model on the kagome lattice, while leaving the full quasi-1D treatment [53] to the future study

$$H_{\text{eff}} = J \sum_{\langle i,j \rangle} [e^{\sqrt{2}\pi i(\theta_{i,c} - \theta_{j,c})} + \text{H.c.}]. \quad (4)$$

Depending on the sign of J , either the 2D s -wave or $(d \pm id)$ -wave SCs can emerge. When $J > 0$, then the so-called $\sqrt{3} \times \sqrt{3}$ order appears [57], which translates as the $(d \pm id)$ -SC. If $J < 0$, the conventional s -wave SC emerges. When the repulsive- U dominates the junction region and the region becomes Mott insulating [58], $J > 0$ can appear. From this strong-coupling limit, we can learn how the $2k_F$ -density wave of 1D wires competing with SC

is suppressed. For the generic filling of each wire, the momentum k_F will not be commensurate with the wire length L , i.e., $\phi_L = k_F L$ is not a rational number. This frustrates the phases of the density waves and thus their true two-dimensional order is strongly suppressed to develop. Because the density waves are the main competitors of the SC in one dimension, this gives a natural favor on the SC.

The domain wall states of 1T-TaS₂ presumably experience small correlation effect and the junction regions are quite metallic from the STM data [8]. Furthermore, no magnetism is observed in experiments, i.e., interaction is dominantly attractive. Furthermore, the SC in 1T-TaS₂ is experimentally observed for a broad range of the parameters [10,11]. When compared with Fig. 2(b), the SC is consistent with the s wave. These suggest that the SC state of 1T-TaS₂ is likely an s -wave SC.

3. Higher-order topology: When the filling per wire is commensurate, then the network can develop its own CDW order and become an insulator. We highlight here that the insulating network hosts an interesting possibility, namely, emergent corner states which are akin to those of the 2D higher-order topological insulators [24–26]. We illustrate this on the half-filled spinless fermion model, whose generalization to the spinful systems is straightforward. In such wires, the dimerization is expected, which manifests as the staggered nearest-neighbor hopping parameters; see Fig. 2(b). To clearly expose the corner states, we perform a finite-size calculation on a single unit cell of the network. In the spectrum Fig. 2(d), we see four in-gap modes, which are localized at the trijunction and the boundary Fig. 2(c). Those states are protected by crystal symmetries. We can also show that the above system similarly supports an in-gap mode at the corner of the edge. See Supplemental Material [22], where the junction of two gapped domain walls supports a corner mode protected by a reflection symmetry. Such 0D states protected by crystalline symmetries are the hallmarks of higher-order topology.

The above higher-order topology of gapped domain wall networks may be relevant to various materials with similar structures such as C-CDW 1T-TaS₂ [27] and twin boundary networks of MoSe₂ grown on MoS₂ [59]. Spectacularly, it has been noted [23,27] that the insulating domain walls of C-CDW 1T-TaS₂ have precisely the same structure as the dimerization, and they form junctions and networks. We believe that the confirmation of the higher-order topology in these systems will be an extremely interesting future problem, given that there is no concrete experimental demonstration of the 2D higher-order topology so far.

4. Conclusions: We considered the electronic structure of a conducting honeycomb network, where we uncovered the emergence of the cascade of the flatbands that are stable against various local perturbations. Compared to the previous studies [3,33,34,60–63], our work reveals that the

flatbands can emerge in much broader sets of the models beyond the models with chiral symmetry or only nearest-neighbor hopping terms. We also demonstrated that the domain wall network is an ideal place to find diverse topological band structures: topological band crossings, and higher-order corner states. We find that the robust flatbands and network geometry can explain the coexistence of SC and CDW states in the network materials, which goes beyond the previous Landau-Ginzburg theory [17], which is blind to the emergent electronics from the network.

The signature of the network and its role in SC can be detected in various experiments in 1T-TaS₂. First, the combination of our STM data, DFT calculation, [8] and the result of our current Letter already points strongly toward the existence of the flatbands. In particular, the scanning tunneling spectroscopy [8] showed that the band gap is filled, which again supports the emergence of cascade of band structures. In particular, one nearly flatband is observed right below the chemical potential in the currently available photoemission data [64–66] though further investigation will be desirable. Second, magnetotransport and oscillations can provide the information about the primary conducting and SC channels. They have been applied in the small twist-angle bilayer graphene [28,67] and textured superconducting states of 1T-TiSe₂ [16,17]. Also the flatbands show a few characteristic behaviors in thermodynamic quantities, which we summarize in the Supplemental Material [22]. It would be also interesting to perform numerical calculation on our network model with interactions, to confirm our predictions.

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