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# Topological nematic phase in Dirac semi-metals

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We study the interaction effect in a three dimensional Dirac semimetal and find that two competing orders, charge-density-wave orders and nematic orders, can be induced to gap the Dirac points. Applying a magnetic field can further induce an instability towards forming these ordered phases. The charge density wave phase is similar as that of a Weyl semimetal while the nematic phase is unique for Dirac semimetals. Gapless zero modes are found in the vortex core formed by nematic order parameters, indicating the topological nature of nematic phases. The nematic phase can be observed experimentally using scanning tunnelling microscopy.

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Dirac semimetals are materials whose bulk valence and conduction bands touch only at certain discrete momenta, around which the low energy physics is described by gapless Dirac fermions with linear energy dispersion. The two-dimensional Dirac semimetal is realized in graphene and has been studied extensively. The three-dimensional Dirac semimetals were predicted to exist in Na<sub>3</sub>Bi and Cd<sub>3</sub>As<sub>2</sub> [1–3] and these predictions were confirmed in the recent angular resolved photon emission experiments [4, 5]. The three-dimensional Dirac semimetal contains multiple copies of Weyl fermions and thus, they can exhibit non-trivial topology. Different from Weyl semimetals, the gapless nature of Dirac semimetals requires the protection of crystalline symmetries. As a consequence, by breaking some of these symmetries, Dirac semimetals can be driven towards other exotic states such as Weyl semimetals [6–10] and axionic insulators [11, 12].

In this letter, we consider the mass generation of a three dimensional Dirac semimetal with two Dirac points protected by rotational symmetry, such as the one realized in Na<sub>3</sub>Bi. Three different complex mass terms will arise when interaction is included in the effective Hamiltonian of a three-dimensional Dirac semimetal Na<sub>3</sub>Bi. One complex mass is generated by charge density wave (CDW) that involves inter-Dirac-cone scattering and breaks translational symmetry. The other two complex masses come from nematic orders that break three-fold rotational symmetry ( $C_3$ ) by involving excitations with different spins but within a single Dirac point. Within the mean field approximation, we map the phase diagram and find that intra-Dirac-cone interaction can spontaneously break rotational symmetry and drive the system into topological nematic phases. Electron charge distribution is identified for nematic phases, which can be directly detected by scanning tunnelling microscope (STM). We further discuss localized states in topological defects as a consequence of topological nature of nematic

phases. We would like to emphasize that since gapless Dirac cones are protected by rotational symmetry, a gap opening by breaking rotation symmetry can lower the energy of a Dirac semi-metal. Thus, the presence of nematic phases is generic in rotational-symmetry protected Dirac semimetals.

Let us start by describing our model. The low energy physics of Na<sub>3</sub>Bi is well captured by the  $k \cdot p$  type of Hamiltonian density  $H_0(\mathbf{k})$  around the  $\Gamma$  point [2]

$$H_0(\mathbf{k}) = \begin{pmatrix} M(\mathbf{k}) & Ak_+ & 0 & 0 \\ Ak_- & -M(\mathbf{k}) & 0 & 0 \\ 0 & 0 & M(\mathbf{k}) & -Ak_- \\ 0 & 0 & -Ak_+ & -M(\mathbf{k}) \end{pmatrix} \quad (1)$$

up to the second order in  $k$ , where  $M(\mathbf{k}) = M_0 - M_1 k_z^2 - M_2(k_x^2 + k_y^2)$ . The bases here are  $|s, \uparrow\rangle, |p_+, \uparrow\rangle, |s, \downarrow\rangle, |p_-, \downarrow\rangle$ , where for a basis  $|\alpha, \sigma\rangle$ ,  $\alpha = s, p_{\pm}$  is the orbital index and  $\sigma = \uparrow, \downarrow$  is the spin index. The above bases are also denoted as  $|\frac{1}{2}\rangle, |\frac{3}{2}\rangle, |-\frac{1}{2}\rangle, |-\frac{3}{2}\rangle$  based on the total angular momentum of each state.  $M_0, M_1, M_2$  and  $A$  are material dependent parameters. The part of  $H_0(\mathbf{k})$  that is proportional to the identity is not important and has been neglected. The energy dispersion is  $E(\mathbf{k}) = \pm\sqrt{M^2(\mathbf{k}) + A^2 k_+ k_-}$  and two gapless points are located at  $K_i = (0, 0, (-1)^i \sqrt{M_0/M_1})$ , with  $i \in \{1, 2\}$ . The low energy effective Hamiltonian around  $K_1$  and  $K_2$  can be expanded from (1), and it is given by  $\tilde{H}_0 = \sum_{\mathbf{k}} \Psi^\dagger(k) \tilde{H}_0 \Psi(k)$  in the second quantized language, where

$$\begin{aligned} \Psi(k) &= (c_{k,1,s,\uparrow}, c_{k,1,p,\uparrow}, c_{k,1,s,\downarrow}, c_{k,1,p,\downarrow}, \\ &\quad c_{k,2,s,\uparrow}, c_{k,2,p,\uparrow}, c_{k,2,s,\downarrow}, c_{k,2,p,\downarrow})^T, \\ \tilde{H}_0 &= Ak_x \alpha_0 \otimes \Gamma_3 - Ak_y \alpha_0 \otimes \Gamma_4 + m(k_z) \alpha_3 \otimes \Gamma_5 (2) \end{aligned}$$

$\mathbf{k} = (k_x, k_y, k_z)$  is the momentum relative to the Dirac points  $K_i$ ,  $m(k_z) = -2\sqrt{M_0 M_1} k_z$  and  $c_{k,i,a,\sigma}^\dagger$  creates an electron with  $a$  orbital and spin  $\sigma$  at  $K_i + k$ . We also

denote  $c_{k,i,p\pm,\sigma}$  as  $c_{k,i,p,\sigma}$  for brevity.  $\vec{\sigma}, \vec{\tau}, \vec{\alpha}$  are Pauli matrices characterizing spin, orbital and valley degree of freedoms.  $\Gamma$  matrices are defined as  $\Gamma_{1,2,3} = \sigma_{1,2,3} \otimes \tau_1$ ,  $\Gamma_4 = \sigma_0 \otimes \tau_2$  and  $\Gamma_5 = \sigma_0 \otimes \tau_3$ . It is easy to see that they obey Clifford algebra  $\{\Gamma_i, \Gamma_j\} = 2\delta_{i,j}$ .

We note that  $\hat{H}_0$  is the minimal model for Dirac semimetals with time reversal (TR) symmetry and inversion symmetry. To describe the effective Dirac behavior of electrons near  $K_i$ , we keep only the linear terms in  $k$ . It should be emphasized that including other higher order off-diagonal terms cannot open a gap at  $K_1$  and  $K_2$  since two degenerate states transform differently under three-fold rotational symmetry.

The fermionic field operator  $\Psi$  can be thought of as four copies of Weyl fermions, two with left-handed chiralities and the other two right-handed. Here, we focus on the case with charge conservation and thus, the mass terms can only be formed by interactions of two Weyl fermions with opposite chiralities and therefore, there are two possible mass terms. The first one comes from two Weyl fermions with opposite chiralities at different momenta ( $K_1$  and  $K_2$ ). This term breaks translational symmetry and corresponds to CDWs. Such a term can also be found in Weyl semimetals and is responsible for axion insulator phases [11–13]. Since Dirac semimetals can be viewed as two copies of Weyl semimetals that conserve TR symmetry, the gapped phase due to CDWs should also be thought of as two copies of axion insulator phases which are related to each other by TR symmetry. The second mass term couples two Weyl fermions at the same momentum ( $K_1$  or  $K_2$ ). Since the gapless nature of Dirac semimetals at a fixed momentum is protected by  $C_3$  symmetry, it is natural to expect this mass term to break rotation symmetry but preserves translational symmetry. This corresponds to a nematic phase. Therefore, these mass terms should be generated by the following order parameters:

$$\begin{aligned} \text{CDW} : D_{\alpha,\beta,\sigma} &= \langle c_{k,1,\alpha,\sigma}^\dagger c_{k,2,\beta,\sigma} \rangle, \\ \text{nematic} : N_{\alpha,\beta,K_i} &= \langle c_{k,i,\alpha,\uparrow}^\dagger c_{k,i,\beta,\downarrow} \rangle. \end{aligned} \quad (3)$$

On the other hand, possible mass terms should then anti-commute with  $\hat{H}_0$  and there are only six of such terms:  $\alpha_0 \otimes \Gamma_1$ ,  $\alpha_0 \otimes \Gamma_2$ ,  $\alpha_1 \otimes \Gamma_5$ ,  $\alpha_2 \otimes \Gamma_5$ ,  $\alpha_3 \otimes \Gamma_1$ ,  $\alpha_3 \otimes \Gamma_2$ . Based on the above analysis, we identify all possible mass terms and introduce

$$\begin{aligned} N_{s,p,1}^* &= N_{p,s,1}^* = \Delta_1 + \Delta_2, \\ N_{s,p,2}^* &= N_{p,s,2}^* = \Delta_1 - \Delta_2, \\ D_{s,s,\uparrow}^* &= D_{s,s,\downarrow}^* = -D_{p,p,\uparrow}^* = -D_{p,p,\downarrow}^* = \Delta_3, \end{aligned} \quad (4)$$

where  $\Delta_j$ 's are generally complex:  $\Delta_j = |\Delta_j|e^{i\theta_j}$  ( $j \in 1, 2, 3$ ).

To dynamically generate these mass terms, we consider an effective interaction between different species of Dirac

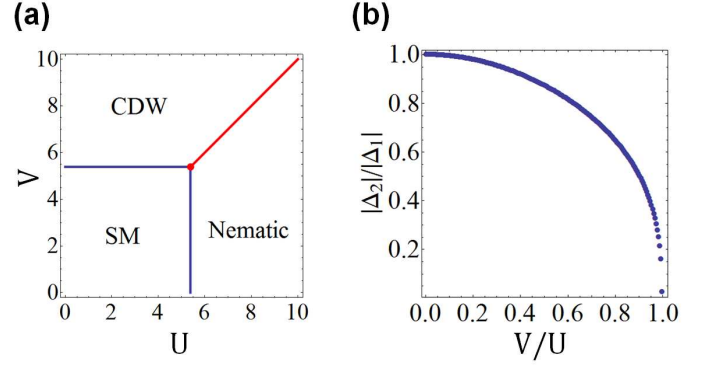


FIG. 1. (a) Phase diagram of interacting 3D Dirac semimetal  $\text{Na}_3\text{Bi}$ . (b) In the nematic phase, the ratio between  $\Delta_2$  and  $\Delta_1$  is plotted as a function of  $V/U$ .

fermions as given by

$$\hat{H}_{int} = U \sum_k \sum_i \rho_i(k) \rho_i(k) + V \sum_k \sum_{i \neq j} \rho_i(k) \rho_j(k), \quad (5)$$

where  $\rho_i = \sum_{\alpha,\sigma} c_{k,i,\alpha,\sigma}^\dagger c_{k,i,\alpha,\sigma}$  are the density operators. Here, the  $U$  term describes the interaction between two electrons near one momentum  $K_i$  while  $V$  term describes that of electrons between  $K_1$  and  $K_2$ . This effective interaction can be obtained from the Coulomb interaction, as shown in the Supplementary Materials [14].

The full Hamiltonian can then be treated within the mean field approximation (see the Supplementary Materials [14] for details), the free energy at zero temperature is then given by

$$F = H_{MF} - \sum_{E_k \in \text{occupied}} E_k(|\Delta_1|, |\Delta_2|, |\Delta_3|, \theta), \quad (6)$$

Here  $E_k$  is the excitation spectrum in the mean field level, whose detailed expression is shown in the Supplementary Materials [14].  $\theta = \theta_1 - \theta_2$  represents the phase difference between the two nematic order parameters. To minimize the free energy, a state where  $\theta = \frac{\pi}{2}$  is favored. We establish self-consistency equations to map the phase diagram in Fig. 1(a). The semimetallic phase is relatively stable under weak interaction because the density of states vanishes at Dirac points. As the interaction strength exceeds critical value  $U_c$  ( $V_c$ ), the system develops a gap. In the large  $U$  ( $V$ ) limit, the system favors nematic (CDW) ordering. Starting from the bi-critical point  $(U_c, V_c)$ , the system will go across a first-order phase transition at the  $U = V$  line between the CDW and nematic phases.

The ordered phase of CDW is similar to that in Weyl semimetals, the physical consequence of which has been discussed in details in [11–13]. For our system, the CDW is along the  $k_z$  direction with the wave vector  $\mathbf{Q} = 2\sqrt{M_0/M_1}\hat{z}$ , which can be in principle observed in an STM. Chiral modes have been proposed to exist at the dislocation line of Weyl semimetals, but since our

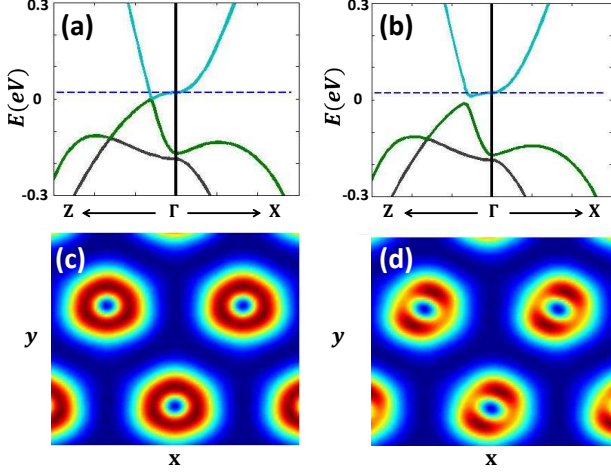


FIG. 2. The energy dispersion from realistic  $k \cdot p$  theory and LDOS for one Bi layer. (a) and (c) are for free semimetal, while (b) and (d) are for the interacting case. In the LDOS plot, red (blue) color represent a large (small) LDOS.

TR invariant system is a copy of two Weyl semimetals, we have two copies of chiral modes that are TR partners and thus, our system exhibits helical modes.

What is really unique in the Dirac semimetals is the nematic phase. This nematic phase is actually a superposition of two inequivalent nematic orders  $\Delta_1$  and  $\Delta_2$  with a phase difference of  $\frac{\pi}{2}$ . By applying TR operation  $\Theta = \alpha_1 \otimes i\sigma_2 \otimes \tau_0$ , we find  $\Delta_1$  breaks TR symmetry while  $\Delta_2$  preserves TR symmetry. In Fig. 1 (b), the co-existence of two nematic orders is numerically confirmed. As the ratio  $V/U$  increases from 0 to 1, we find that the ratio  $\Delta_2/\Delta_1$  decreases from 1 to 0. This indicates that the system spontaneously breaks TR symmetry in the nematic phase. Next, we will discuss several physical phenomena of nematic phases, which can be observed in experiments.

The first observable is the charge distribution. Since the mass term of nematic orders couples  $|\pm\frac{3}{2}\rangle$  to  $|\pm\frac{1}{2}\rangle$ , we expect the charge distribution in one unit-cell breaking three fold rotation. Since the charge distribution cannot be extracted from the effective Hamiltonian, we consider a more realistic  $k \cdot p$  Hamiltonian based on the first principles calculations. The method has been successfully applied to the construction of the effective Hamiltonian of topological insulator materials [15], and we only describe our procedure briefly here. The eigen wave functions at  $k = 0$  can be expanded in term of plane waves in the first principles calculations. Here, 36 bands are taken into account, denoted as  $|n\rangle$  ( $n = 1, 2, \dots, 36$ ). We act the crystal Hamiltonian with periodic potential on the basis and obtain the  $k \cdot p$  Hamiltonian  $H_{nm}^{kp} = (E_n + \frac{\hbar^2 k^2}{2m})\delta_{nm} + \frac{\hbar}{m} k \cdot p_{nm}$ , where  $E_n$  is the eigen-energy for the  $n$  band at  $k = 0$ ,  $m$  is electron mass

and  $p_{nm} = \langle n|p|m\rangle$  is the matrix element. We diagonalize this  $36 \times 36$  Hamiltonian and the energy dispersion is shown in Fig. 2(a), which qualitatively fits to that from the first principles calculations. In particular, a level crossing between conduction and valence bands, which corresponds to Dirac points, can be seen along the  $\Gamma - Z$  line. From the eigen wave functions, one can show that the conduction and valence bands indeed belong to the  $|\pm\frac{3}{2}\rangle$  and  $|\pm\frac{1}{2}\rangle$  states, respectively. Thus, these two states cannot be coupled to each other along the  $\Gamma - Z$  line. As discussed above, the interaction can introduce the coupling between these two states in the nematic phase. Therefore, we can add a constant coupling between the  $|\pm\frac{1}{2}\rangle$  and  $|\mp\frac{3}{2}\rangle$  states near the Fermi energy in our  $k \cdot p$  Hamiltonian, leading to a gap opening, as shown in Fig. 2(b). To show that the obtained states possess nematic orders, we calculate the local density of states (LDOS) in the  $x$ - $y$  plane for the Bi layer. As shown in Fig. 2(c), without interaction, the maxima of the LDOS (red color) appear as an isotropic ring around the position of Bi atoms, corresponding to the  $p_{\pm}$  orbitals of Bi atoms. The spatial distribution of LDOS respects three-fold rotation symmetry. After adding the coupling term between  $|\pm\frac{1}{2}\rangle$  and  $|\mp\frac{3}{2}\rangle$  states, the isotropic ring evolves into two peaks pointing a certain direction, thus breaking  $C_3$  rotation (see Fig. 2(d)). This corresponds exactly to the nematic phase. Such electron density distribution can be directly measured through STM.

The second phenomenon is the appearance of gapless modes in topological defects of the nematic phase, revealing the topological nature of this phase. Complex mass terms  $\Delta = |\Delta|e^{i\theta}$  in a Dirac system are highly non-trivial in the sense that their phases  $\theta$  are identified as dynamical axion fields, which will give rise to bulk axionic terms in the form of  $\theta\epsilon^{\mu\nu\rho\sigma}F_{\mu\nu}F_{\rho\sigma}$  [11, 12, 16–21]. In 2D Dirac systems, complex mass terms will show up as a  $U(1)$  or  $\mathbb{Z}_n$  vortex structure in both graphene [22, 23] and  $\pi$ -flux square lattice [24, 25] in the presence of interactions. As a consequence, zero modes will localize at the vortex centers carrying fractionalized charges. In 3D Weyl/Dirac systems, those zero modes extend to 1D chiral modes that go through the center of the vortices along the  $z$ -direction [11, 12]. These are known as axion strings. As is in the case of CDW, we expect a similar physics to occur in the vortex of nematic order parameters.

By applying in-plane vortex structures for the complex nematic order parameters, our system at fixed  $k_z$  can be directly mapped into previous 2D Dirac systems. Therefore, zero modes are expected to show up at both  $K_1$  and  $K_2$ . To verify this, a numerical calculation is performed in a layered 2D vortex configuration. We keep the periodicity in the  $z$  direction, while placing open boundary conditions in the  $x$ - $y$  plane. For simplicity, on a  $32 \times 32$  square lattice, we place a  $U(1)$  vortex-antivortex pair structure instead of the actual  $\mathbb{Z}_3$  vortices. We visual-

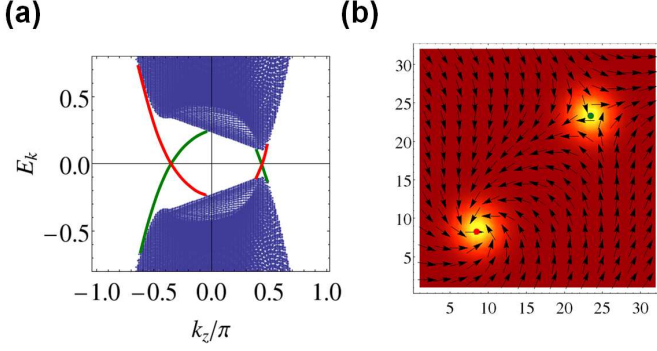


FIG. 3. (a) The fermionic spectrum in a  $U(1)$  vortex-antivortex configuration on a  $32 \times 32$  square lattice with open boundary conditions. We choose the following set of parameters:  $M_0 = -0.6$ ,  $M_1 = -0.3$ ,  $M_2 = -0.4$ ,  $A = 0.4$ ,  $|U||\Delta_1| = 0.25$ ,  $|U||\Delta_2| = 0.1$ . Gapless energy bands in red (green) are localized at the vortex (anti-vortex) center. (b) LDOS at  $E_F = 0$  is plotted which clearly shows zero modes are localized at vortex or antivortex center. The red (green) dot shows the location of a vortex (antivortex) center while yellow (red) color represent a large (small) LDOS.

ize these vortex structures in Fig. 3(b) by the arrow indicating phase information of following site-dependent order parameters [24]:

$$\begin{aligned}\tilde{\Delta}_1(x, y, k_z) &= |\Delta_1| \frac{(\omega - \omega_1)(\omega - \omega_2)^*}{|(\omega - \omega_1)(\omega - \omega_2)|}, \\ \tilde{\Delta}_2(x, y, k_z) &= k_z \frac{|\Delta_2|}{|\Delta_1|} \tilde{\Delta}_1(x, y, k_z).\end{aligned}\quad (7)$$

Here,  $\omega = x + iy$  is a complex coordinate and  $\omega_j = x_j + iy_j$  is the complex coordinate of vortex ( $j = 1$ ) or anti-vortex center ( $j = 2$ ). As shown in Fig. 3(a), the bulk dispersion is gapped while gapless modes penetrate the bulk gap twice at two different momenta. In Fig. 3(b), we plot the LDOS at  $E_F = 0$  together with vortex configurations in real space. It is confirmed that these modes are highly localized at the vortex (anti-vortex) center. The gapless nature of these modes relies on the fact that they are separated at different momenta, and requires the translational symmetry along the  $z$ -direction.

So far, we have discussed the effects of interaction in driving Dirac semimetals toward other phases. However, those phases along with their novel physical phenomena can only be realized under relatively strong interaction. To overcome this difficulty, one can apply a magnetic field along the  $z$  direction such that Landau levels emerge. Similar strategies have been applied to achieve quantum Hall ferromagnetism in graphene systems [26, 27], where spin orbital coupling (SOC) is almost absent. The strong SOC in Dirac semimetals, however, tends to tilt spins. As a result, CDW and nematic phases are more likely to be favored than ferromagnetism in Dirac semimetals. The Landau levels in Dirac semi-metals have been observed experimentally

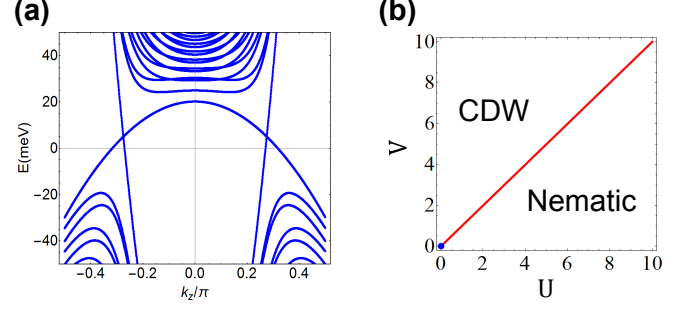


FIG. 4. (a) Landau level dispersion along  $k_z$  with magnetic field  $B = 10$  T. (b) Phase diagram of  $\text{Na}_3\text{Bi}$  under magnetic field and interaction.

[28–32]. Even though the higher Landau levels of  $\text{Na}_3\text{Bi}$  are gapped, the lowest Landau levels (LLs) are gapless at  $K_i$  ( $i = 1, 2$ ), see Fig. 4. We identify this degeneracy to be a crossing between  $|s, \uparrow\rangle$  and  $|p, \downarrow\rangle$  states, which is protected from developing a gap by  $C_3$  symmetry along (001) axis. To describe the low energy physics of the gapless LLLs, we define a four-component spinor,  $\Psi^\dagger = (c_{k,1,s,\uparrow}^\dagger, c_{k,1,p,\downarrow}^\dagger, c_{k,2,s,\uparrow}^\dagger, c_{k,2,p,\downarrow}^\dagger)$ . Mass terms in Eq. (4) are reduced to: (1) Density Wave:  $D_1 = D_{s,s,\uparrow}$ ,  $D_2 = D_{p,p,\downarrow}$ . (2) Nematic:  $N_1 = N_{s,p,K_1}$ ,  $N_2 = N_{s,p,K_2}$ . Through a similar mean field analysis (see the Supplementary Materials), the free energy at zero temperature is given by  $F = H_{MF} - \sum_i \sum_{k_z} \sqrt{m(k_z)^2 + \xi_i}$  where  $m(k_z) = -2\sqrt{M_1(M_0 - \frac{M_2}{l^2})}k_z$ .  $\xi_{1,2}$  are functions of order parameters  $D_{1,2}$  and  $N_{1,2}$ , whose detailed expressions are explicitly shown in the Supplementary Materials [14].

By minimizing the free energy, we obtain the phase diagram as shown in Fig. 4(b). Instability happens for arbitrarily weak repulsive interaction [12, 13] and as one tunes the interaction to go across  $V/U = 1$ , the system undergoes a phase transition from a CDW phase to a nematic phase or vice versa. Let us focus on the nematic regime ( $D_{1,2} = 0$ ) and the corresponding self-consistent equations can be solved analytically. As is shown in the Supplementary Materials [14], the critical temperature that characterizes a phase transition from semi-metallic phase to the nematic phase is

$$T_c = \frac{2e^\gamma v_f \Lambda}{\pi k_B} e^{-\frac{v_f \Lambda}{U} \frac{\hbar}{eBS}} \quad (8)$$

where  $\Lambda$  is the momentum cut-off and  $v_f = |\frac{m(k_z)}{k_z}|$  is the Fermi velocity.  $\gamma = 0.577\dots$  is the Euler constant and  $k_B$  is the Boltzmann constant. We have considered a sample with a finite area  $S$  in the  $x$ - $y$  plane. When  $T < T_c$ , non-zero nematic ordering will always be formed for arbitrary  $U$ . In the zero temperature limit, the magnitude of order parameter can be solved [14, 33]:  $|N_1| \approx \frac{2v_f \Lambda}{U} e^{-\frac{2\pi v_f \Lambda}{U} \frac{\hbar}{eBS}}$ . This expression indicates that a larger energy gap will show up for a larger magnetic

field. This instability under magnetic fields is a direct result of the finite Landau level degeneracy. This suggests the necessary condition for the instability is that the cyclotron length is much smaller than the sample size. In the Supplementary Materials [14], we further discuss the existing experiments studying LLs of Dirac semimetals, and predict possible evidence of nematic phases in STM measurements of Landau levels.

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