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Chiral anomaly, charge density waves, and axion strings from Weyl semimetals

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We study dynamical instability and chiral symmetry breaking in three-dimensional Weyl semimetals, which turns Weyl semimetals into "axion insulators." Charge density waves (CDWs) are found to be the natural consequence of chiral symmetry breaking. The phase mode of this charge density wave state is identified as the axion, which couples to an electromagnetic field in the topological $\theta\mathbf{E}\cdot\mathbf{B}$ term. One of our main results is that "axion strings" can be realized as the (screw or edge) dislocations in the charge density wave, which provides a simple physical picture for the elusive axion strings. These axion strings carry gapless chiral modes, therefore they have important implications for dissipationless transport properties of Weyl semimetals with broken symmetry.

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Introduction. Topological insulators are among the most recent active research fields in condensed matter physics.[1–3] Among the remarkable aspects of topological insulators is the ubiquitous role played by Dirac fermions. In fact, most of the recently discovered topological insulators can be regarded as massive Dirac fermion systems with lattice regularization.[3] When the mass vanishes, we have massless Dirac fermions, which are two copies of a Weyl fermion with opposite chiralities. The Dirac fermions, which obey the Dirac equation, are described by spinors with four components, while the Weyl fermions are two-component fermions described by the following simple Weyl equation,

$$\pm v_F \boldsymbol{\sigma}\cdot\mathbf{k}\psi = E\psi, \tag{1}$$

where $\pm$ is referred as chirality ($+$ for left handed, $-$ for right handed), and v_F is the Fermi velocity. Since the Dirac fermion can be decomposed into two copies of the Weyl fermion, the latter is a more elementary building block. In fact, it is our current understanding of nature that elementary fermions such as quarks and electrons fall into the Weyl fermion framework because the left-handed and right-handed fermions carry different gauge charges in the standard model of particle physics.[4]

It is worth noting that in writing down Eq. (1) we have assumed that the two "Weyl points," at which the energy gap closes, are both located at $\mathbf{k} = 0$. In the particle physics context, this assumption seems to be natural, however, in condensed matter physics, without imposing symmetry constraints such as time reversal symmetry and inversion symmetry, Weyl points are generally located at different points in the momentum space. This fact has interesting consequences for Weyl fermion systems with broken symmetry, as we will show in this Rapid Communication.

Although the Weyl fermion plays a crucial role in the description of elementary fermions in nature, it has been studied in the condensed matter context only very recently.[5–23] Weyl semimetals in three dimensions (3D) are analogous to graphene[24] in two dimensions (2D) in the sense that both are described in terms of gapless fermions with approximately linear dispersion, but the 3D Weyl semimetals are richer in that they are more closely related to various fundamental phenomena such as the chiral anomaly.[11,12,23] Unlike topological insulators, whose transport is dominated by topologically protected surface states, in the Weyl semimetal the bulk transport is most important. Their unique semimetallic behaviors in 3D can be potentially engineered for the semiconductor industry.

The interaction effect plays a fundamental role in the dynamics of Weyl fermions. One possibility is the pairing interaction which leads to superconducting instability. Qi, Hughes, and Zhang's Fermi surface topological invariant[25] implies that if the pairing amplitudes have opposite sign for Weyl points with opposite chirality, topological superconductors are obtained. Another consequence of the interaction, which we will focus on in this Rapid Communication, is spontaneous chiral symmetry breaking. Chiral symmetry breaking is the phenomenon of the spontaneous generation of an effective mass of Weyl fermions, namely, a pairing between the fermions (electrons) and antifermions (holes) with different chiralities. Due to the chiral anomaly, the Goldstone mode θ is coupled to the electromagnetic field as $\theta\mathbf{E}\cdot\mathbf{B}$, therefore, this Goldstone mode is an "axion."[26–29]

In this Rapid Communication, we focus on chiral symmetry breaking in Weyl semimetal and axion strings in a condensed matter context, which have features that are absent in particle physics. We would like to mention that an axion string can be realized on the surface of topological insulators with a magnetic domain wall,[30] and axionic dynamics has been studied in topological magnetic insulators.[31,32] Here we study a route to axionic dynamics through chiral symmetry breaking induced by the interaction effect. The resultant states are charge density wave (CDW) states, which are experimentally observable. One of our main results is that the (screw or edge) dislocations of CDWs are exactly the "axion strings," which are important topological defects carrying gapless chiral modes. In these chiral modes electrons move solely in one direction without backscattering. In particle physics, axion strings have interesting cosmological implications such as the gravitational lenses effect,[33] but observable evidences are elusive. Axion strings in condensed matter systems have the advantage that they are much easier to detect. In the Weyl semimetal studied here, axion strings have important effects on the transport properties since they provide chiral modes supporting dissipatonless transport.

Dynamical chiral symmetry breaking. We consider the simplest model for dynamical chiral symmetry breaking, which nevertheless captures the most salient physical consequences.

First let us present the free part H_0 of the Hamiltonian. The four-band model studied here is a simplified version of the model of Weyl semimetal given in Refs. 7 and 12. We have $H_0 = c^\dagger h c$ with

$$h = v_F \sum_{i=1}^{3} \Gamma^i(-i\partial_i - eA_i - q_i\Gamma) - eA_0, \tag{2}$$

where we have defined the Dirac matrices $\Gamma^\mu(\mu = 0,1,2,3)$ satisfying $\{\Gamma^\mu,\Gamma^\nu\} = 2\delta^{\mu\nu}$, Γ is the chirality operator with the properties $\Gamma^2 = 1$ and $[\Gamma,\Gamma^i] = 0$,[34] A_μ is the external electromagnetic potential, and $\mathbf{q} = (q_1,q_2,q_3)$ is a vector that shifts the gapless points away from $\mathbf{k} = 0$. The simplest choices of the Dirac matrices are $\Gamma = \tau^3 \otimes 1$ and $\Gamma^i = \tau^3 \otimes \sigma^i (i = 1,2,3)$. The low energy modes from the left-hand $(\Gamma = +1)$ chirality are described by $h_+(k) \approx v_F \boldsymbol{\Gamma} \cdot (\mathbf{k} - \mathbf{q}) = v_F \boldsymbol{\sigma} \cdot (\mathbf{k} - \mathbf{q})$ near $\mathbf{k} = \mathbf{q}$. Similarly, there is a Weyl point at $-\mathbf{q}$ for the right-handed $(\Gamma = -1)$ chirality. The low energy dynamics is dominated by these two Weyl points located at $\mathbf{Q}_1 = \mathbf{q}$ and $\mathbf{Q}_2 = -\mathbf{q}$, respectively, with

$$h_\pm(k) = \pm v_F \boldsymbol{\sigma} \cdot (\mathbf{k} - \mathbf{Q}_i), \tag{3}$$

where the prefactor ± 1 is the chirality. For later convenience let us define two operators $\tau^\pm = \tau^1 \pm i\tau^2$ with the property $\{\tau^\pm,\Gamma\} = 0$.

Now we would like to investigate the effects of the four-fermion interaction in Weyl semimetals. Let us write down the effective action in the imaginary time as

$$S = \int d\tau d\mathbf{r} \left\{ c_\mathbf{r}^\dagger [\partial_\tau + h + m^*(\mathbf{r})\tau^+ + m(\mathbf{r})\tau^-] c_\mathbf{r} + \frac{|m(\mathbf{r})|^2}{g} \right\}, \tag{4}$$

in which we have written the interaction in terms of the auxiliary field $m(\mathbf{r})$, which can be integrated out to give the four-fermion interaction $-g(c_\mathbf{r}^\dagger \tau^+ c_\mathbf{r})(c_\mathbf{r}^\dagger \tau^- c_\mathbf{r})$.

It usually happens that a dynamically generated energy gap can lower the ground state energy of a nominally gapless system. Let us investigate such a possibility of condensation $\langle m(\mathbf{r}) \rangle \neq 0$. Since the low energy dynamics is dominated by the two Weyl points, let us write down the expansion $c_\mathbf{r} = e^{i\mathbf{Q}_1\mathbf{r}} c_{L,\mathbf{r}} + e^{i\mathbf{Q}_2\mathbf{r}} c_{R,\mathbf{r}} + \cdots$, where $c_{R/L}$ are cut off in the momentum space at Λ, i.e., $c_{L/R,\mathbf{r}} = \sum_{|\mathbf{p}|<\Lambda} e^{i\mathbf{p}\mathbf{r}} c_{L/R,\mathbf{p}} + \cdots$, and the "$\cdots$" terms are high energy modes with $|\mathbf{p}| > \Lambda$. At the mean-field level we have $m(\mathbf{r}) = -g\langle c_\mathbf{r}^\dagger \tau^+ c_\mathbf{r} \rangle = -ge^{-i\mathbf{Q}\mathbf{r}} \langle c_L^\dagger \tau^+ c_R \rangle$, where we have defined $\mathbf{Q} = \mathbf{Q}_1 - \mathbf{Q}_2 = 2\mathbf{q}$. We note that $\langle c_L^\dagger \tau^+ c_R \rangle$ is a "slow" field whose characteristic momentum is small compared to $|\mathbf{Q}|$.

In the momentum space the fermion matrix in Eq. (4) can be approximated by $M = -i\omega + v_F \tau^3 \boldsymbol{\sigma} \cdot \mathbf{p} + m^*(\mathbf{Q})\tau^+ + m(\mathbf{Q})\tau^-$ at low energy, therefore, we can obtain the gap equation

$$\frac{1}{2g} = \int \frac{d\omega d^3p}{(2\pi)^4} \frac{1}{\omega^2 + v_F^2 p^2 + |m|^2} \tag{5}$$

from the mean-field relation $m(\mathbf{r}) = -g\langle c_\mathbf{r}^\dagger \tau^+ c_\mathbf{r} \rangle$. The solution to Eq. (5) can be obtained as $\frac{1}{g_c} - \frac{1}{g} = \frac{1}{8\pi^2 v_F^3} |m|^2 \ln \frac{v_F^2 \Lambda^2 + |m|^2}{|m|^2}$, where $g_c = \frac{8\pi^2 v_F}{\Lambda^2}$. We have taken a Lorentz-invariant cutoff $|\mathbf{p}| < \Lambda, \omega < v_F \Lambda$ in the above calculation, but if we take the cutoff only for $|\mathbf{p}|$ but not for the ω, we can check that g_c takes the same value. Because we are concerned with the cases with $|m| \ll \Lambda$, the solution can be approximated by

$$\frac{1}{g_c} - \frac{1}{g} = \frac{1}{8\pi^2 v_F^3} |m|^2 \ln \frac{v_F^2 \Lambda^2}{|m|^2}, \tag{6}$$

which shows that dynamical symmetry breaking (or "exciton condensation") occurs only when the interaction is sufficiently strong $(g > g_c)$.

A qualitative understanding of g_c is simple. The kinetic energy per fermion is $E_K \sim v_F \Lambda$, while the interaction energy per fermion is $E_I \sim g\Lambda^3$, where Λ^3 accounts for the spatial density of Weyl fermions. To have chiral condensation, we must have $E_K \sim E_I$, or $g_c \sim v_F/\Lambda^2$. To satisfy this condition, larger E_I (stronger interaction) and smaller E_K (narrower bandwidth in Dirac dispersion) is favored.

Axion dynamics and topological theta term. We have above that when $g > g_c$, chiral symmetry is spontaneously broken. From a symmetry consideration, the Ginzburg-Landau effective action (omitting the chiral anomaly at this stage) of $m(\mathbf{r})$ can be expressed as

$$S_m = \int dt d\mathbf{r} \left[\frac{1}{2}\gamma \left(|\partial_t m'|^2 - v_a^2 |\partial_i m'|^2 \right) + \delta |m'|^2 + \eta |m'|^4 \right], \tag{7}$$

where $\gamma, v_a, \delta, \eta$ are phenomenological parameters, and $m' \equiv m e^{i\mathbf{Q}\cdot\mathbf{r}}$ is the "slow" field. In the symmetry breaking phase, $\delta < 0$ and $|m|$ develops a nonzero expectation value. The effective action S_m is invariant if we shift the phase of $m(\mathbf{r})$ by a spacetime-independent phase factor, but in fact this symmetry is broken by a chiral anomaly, which endows a topological theta term to the effective action, as we explain below. Let us first write $m(\mathbf{r}) = |m(\mathbf{r})| \exp[-i\mathbf{Q} \cdot \mathbf{r} - i\theta(\mathbf{r})]$. We can perform a chiral transformation $c(\mathbf{r}) \to c(\mathbf{r}) e^{-i(\mathbf{Q}\cdot\mathbf{r}+\theta)\Gamma/2}$, then $m(\mathbf{r}) \to m(\mathbf{r}) e^{i(\mathbf{Q}\cdot\mathbf{r}+\theta)}$. After this chiral transformation the phase of $m(\mathbf{r})$ is removed and $m(\mathbf{r})$ become real numbers, however, due to the fact that the fermion path integral measure is not invariant,[35] this chiral transformation generates an anomalous term $S_{\text{anomaly}} = \frac{e^2}{32\pi^2} \int dt d\mathbf{r} \epsilon^{\mu\nu\lambda\rho} (\mathbf{Q} \cdot \mathbf{r} + \theta) F_{\mu\nu} F_{\lambda\rho} = \frac{e^2}{4\pi^2} \int dt d\mathbf{r} (\mathbf{Q} \cdot \mathbf{r} + \theta) \mathbf{E} \cdot \mathbf{B}$, where we have used the natural unit $\hbar = c = 1$.

Taking the above chiral anomaly into account, the fluctuations of θ is described by the following simple axionic effective action,

$$S_\theta = \frac{f_a^2}{2} \int dt d\mathbf{r} \left[(\partial_t \theta)^2 - v_a^2 (\partial_i \theta)^2 \right] + \frac{e^2}{4\pi^2} \int dt d\mathbf{r} (\mathbf{Q} \cdot \mathbf{r} + \theta) \mathbf{E} \cdot \mathbf{B}, \tag{8}$$

where the notation f_a $(\equiv \gamma|m|)$ is deliberately chosen because it is analogous to the pion decay constant f_π, namely, that f_a is the "axion decay constant." We can also define a normalized field $a = f_a \theta$ and put Eq. (8) into a more standard form,

$$S_a = \frac{1}{2} \int dt d\mathbf{r} \left[(\partial_t a)^2 - v_a^2 (\partial_i a)^2 \right] + \frac{e^2}{4\pi^2} \int dt d\mathbf{r} \left(\mathbf{Q} \cdot \mathbf{r} + \frac{a}{f_a} \right) \mathbf{E} \cdot \mathbf{B}. \tag{9}$$

There is an effective action analogous to the last term for pion-photon coupling in a high energy context, which is responsible for the famous two-photon decay of the neutral pion. The axion-photon coupling is proportional to $1/f_a \sim 1/(\gamma|m|)$, thus we have the counterintuitive conclusion that when the chiral condensation becomes weaker, the axion-photon coupling becomes stronger.

Various topological responses can be calculated from the effective action given in Eq. (8). Taking a derivative with respect to A_μ, we have the current

$$j^\mu = \frac{e^2}{8\pi^2}\epsilon^{\mu\nu\lambda\rho}(Q_\nu + \partial_\nu\theta)F_{\lambda\rho} = \frac{e^2}{8\pi^2}\epsilon^{\mu\nu\lambda\rho}\left(Q_\nu + \frac{\partial_\nu a}{f_a}\right)F_{\lambda\rho}. \tag{10}$$

Analogous topological responses have been studied in topological insulators,[30] in which the first term in absent. Let us consider the special case of a constant magnetic field $B_z\mathbf{z}$ along the $\mathbf{z}$ direction, and then the charge density given by Eq. (10) is

$$j^0 = \frac{e^2}{4\pi^2}(Q_z + \partial_z\theta)B_z = \frac{e^2}{4\pi^2}\left(Q_z + \frac{\partial_z a}{f_a}\right)B_z. \tag{11}$$

The first term here is readily understood as layered quantum Hall effects,[36] with a layer thickness $2\pi/|\mathbf{Q}|$. The second term can be understood as follows. Let us consider the case $\mathbf{Q} = 0$ for simplicity, and take $|m| = 0$ first. In a constant magnetic field $B_z\mathbf{z}$, the dispersions of Weyl fermions can be obtained as $E_n(p_z) = \pm v_F\sqrt{p_z^2 + 2eB_z n}$ with $n = 0,1,\ldots$. The two gapless modes are the $n = 0$ Landau levels with $E(p_z) = \pm v_F p_z$, where $\pm$ corresponds to left and right chirality, respectively. Now a mass term $m = |m|e^{i\theta}$ mixes the two counterpropagating [essentially one dimensional (1D)] modes and opens a gap. The 1D charge density can be obtained from the Goldstone-Wilczek formula[37] $j^0|_{1d} = \frac{1}{2\pi}\partial_z\theta$, therefore, the final result of the 3D charge density is $j^0 = (eB_z/2\pi)(\partial_z\theta/2\pi) = \frac{e^2}{4\pi^2}B_z\partial_z\theta$, where we have added the density of states $eB_z/2\pi$ of Landau levels. This is exactly the second term of Eq. (11).

Phase of the charge density wave is the dynamical axion. Now we will show that chiral symmetry breaking leads to density waves, among which the CDW is the simplest. The charge density is given by

$$\rho_1(\mathbf{r}) = \langle c_\mathbf{r}^\dagger\tau^1 c_\mathbf{r}\rangle = -\frac{m(\mathbf{r}) + m^*(\mathbf{r})}{2g} = -\frac{|m|}{g}\cos(\mathbf{Q}\cdot\mathbf{r} + \theta), \tag{12}$$

and similarly $\rho_2(\mathbf{r}) = \langle c_\mathbf{r}^\dagger\tau^2 c_\mathbf{r}\rangle = i[m(\mathbf{r}) - m^*(\mathbf{r})]/2g = |m|\sin(\mathbf{Q}\cdot\mathbf{r} + \theta)/g$. Let us explain their physical consequences. In fact, they depend on the physical degree of freedom to which τ is referred. Let us take a simplest example, namely, that $\tau^3 = \pm 1$ refers to $(|A\rangle \pm |B\rangle)/\sqrt{2}$, where A,B refer to two inequivalent sites in a unit cell,[38] then $\tau^1 = \pm 1$ refers to the A/B site, thus $\rho_1 = \rho_A - \rho_B$ is the staggered CDW. If we look at the charge density on site A (or B), it shows an oscillation with wavelength $2\pi/|\mathbf{Q}|$. In more general cases, other density modulations, such as CDWs of more general types and spin density waves, can show up.

The natural question is how to experimentally detect the CDW. Apart from bulk measurements, it can also be detected by simpler surface measurements such as scanning tunneling microscopy (STM). Denoting the angle between the surface normal and $\mathbf{Q}$ as α, we can obtain the surface CDW wavelength as $\lambda_{2d} = \frac{2\pi}{|\mathbf{Q}||\sin\alpha|}$.

It is worth noting that the interaction effect and CDW was studied in 2D Dirac systems in Refs. 39–41. More recently, the interaction effect on the surface of weak topological insulators has been studied in Ref. 42, in which CDW also has important physical consequences. The relation to the chiral anomaly is absent in these studies because the systems considered there are in 2D, where the concept of chirality is lacking.

Dislocations in a charge density wave are axion strings. Let us turn to the central part of this Rapid Communication, namely, the identification of CDW dislocations as axion strings, which may provide a dissipatonless chiral transport channel in 3D bulk materials. An axion string l is a one-dimensional dislocation of the axion field, around which the axion field θ changes by 2π, namely, that

$$\int_C d\theta = 2\pi, \tag{13}$$

where C is a small contour enclosing l clockwise. Axion strings are closely related to chiral anomaly, as was studied long ago in the work by Callan and Harvey[43] in the particle physics context. In the Weyl semimetals studied by us, the axion strings have a clear geometrical picture because θ is exactly the phase of the CDW. More explicitly, suppose that $\mathbf{Q} = (Q_x,Q_y,Q_z) = (0,0,Q)$, then it follows from Eq. (12) that the peaks of the CDW are located at 2D planes (x,y,z_n) with

$$z_n = -\frac{\theta + 2\pi n}{Q}, \tag{14}$$

where $n =$ integer. When θ is shifted, the peak position z_n follows the shifting of θ. In fact, the shifting of z_n around the small loop C enclosing the axion string is readily obtained from Eq. (14) as

$$\int_C dz_n = -\frac{\int_C d\theta}{Q} = -\frac{2\pi}{Q}, \tag{15}$$

which is exactly the wavelength of the CDW. The Burgers vector of the axion string as a dislocation of the CDW is exactly $(0,0,-2\pi/Q)$. For a general CDW wave vector $\mathbf{Q}$, the Burgers vector is readily obtained as $-2\pi\mathbf{Q}/|\mathbf{Q}|^2$.

Let us refer to the orientation of the axion string l as $\hat{\mathbf{l}}$. According to the relative orientation of $\hat{\mathbf{l}}$ and $\mathbf{Q}$, the axion string appears as different types of dislocation. When $\hat{\mathbf{l}}$ is parallel with $\mathbf{Q}$, we have a screw dislocation [Fig. 1(a)], while when $\mathbf{Q}$ is perpendicular with $\hat{\mathbf{l}}$, we have an edge dislocation [Fig. 1(b)]. We would like to mention that the edge dislocation with chiral modes has been studied in Ref. 44. Weyl semimetals provide a natural route to realizing such interesting topological defects. In the cases of edge dislocation, the origin of the chiral modes is most clear, because we can think of them as the edge states of a 2D quantum Hall system, which is just the slice appearing as the "edge."

There are chiral modes propagating along the axion strings,[43] therefore, axion strings may serve as unique transport

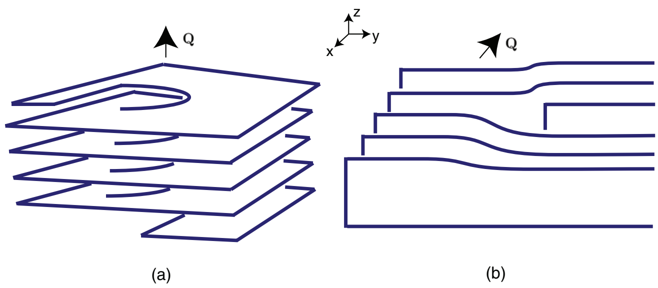

FIG. 1. (Color online) Axion strings as dislocations of a charge density wave. (a) Screw dislocation. (b) Edge dislocation. The delineated sheets are the peaks of the CDW. In both (a) and (b), the axion string is along the **z** direction. The Burgers vector is parallel to the axion string in (a), while it is perpendicular to it in (b).

channels in 3D materials with axionic dynamics. Such chiral modes carry a dissipationless current just as the quantum Hall edge and quantum anomalous Hall edge states, but the former are distinct in that they are buried in 3D bulk.

It is worth mentioning that dislocations in topological materials have also been studied in Ref. 45, but we would like to emphasize several prominent differences between the axion strings studied here and the dislocation lines in weak topological insulators studied in Ref. 45. First, in Ref. 45 the dislocations carrying gapless modes are indeed dislocations of the crystal lattice, while in our work the crystal lattice remains intact, and axion strings are just dislocations of the CDW. Second, the gapless modes studied in Ref. 45 are helical modes, which are unstable towards backscattering if time reversal symmetry is broken, while the gapless modes living on the axion strings studied here are robust chiral modes. It is also worth noting that in Ref. 12 line dislocation with chiral modes was studied, but the CDW is absent there, and more importantly, the bulk is also gapless there and the coupling between the dislocation mode and bulk mode can induce dissipation.

To conclude this part, we remark that the formation of axion strings in Weyl semimetals can be triggered by rapidly lowering the temperature from $T > T_c$ to $T < T_c$, where T_c is the critical temperature of chiral condensation (Kibble-Zurek mechanism).

Discussions and conclusions. We have studied dynamical chiral symmetry breaking and topological responses in Weyl semimetals. We have adopted a simple four-fermion interaction to simplify formulas. In more realistic models g is replaced by $g(\mathbf{Q})$. We note that an attractive interaction $-g(\mathbf{Q}) < 0$ at momentum $\mathbf{Q}$ is needed for chiral symmetry breaking. The values of $g(\mathbf{Q})$ for various materials depend on the material details, which is beyond the scope of this Rapid Communication. It is useful to mention that an effectively attractive electron-electron interaction can appear at some special momenta commensurate with the reciprocal lattice. Such an electron-lattice coupling effect is responsible for the Peierls transitions in 1D systems, and we expect that dynamical chiral symmetry breaking may also occur in 3D by this mechanism if $2\pi/|\mathbf{Q}|$ is commensurate with the crystal lattice. In this case chiral symmetry breaking can be thought of as generalized Peierls transitions, which induce dimerization, trimerization, etc.

Our model provides a geometrical picture of axion, which manifests itself as the phase of the CDW. One of our main results is the identification of axion strings as CDW (edge or screw) dislocations, which has no analog in particle physics. The axion strings have 1D robust chiral modes along them, which have great potential applications if the chiral symmetry breaking (exciton condensation) of a Weyl fermion is realized in experiment. Here we studied the general cases with $\mathbf{Q} \neq 0$. When $\mathbf{Q} = 0$ there is no CDW associated with chiral symmetry breaking, but the axion strings do exist and have an important implication for 3D transport properties.

Note added. Recently we became aware of a related work[46] on symmetry breaking in a Weyl semimetal by Zyuzin and Burkov, though CDW and axion strings were not studied. Due to the nonzero density of states considered in their work, the gap equation is also different from ours.

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