Weyl semimetal with strong long-range Coulomb interactions

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Abstract. We theoretically study the stability of a Weyl semimetal against strong long-range Coulomb interactions. We consider a lattice model for a time-reversal symmetry broken Weyl semimetal with two nodes, and take into account the $1/r$ Coulomb interactions between the bulk electrons. Based on the U(1) lattice gauge theory, we investigate the system from the strong coupling limit. It is shown that spatial inversion (parity) symmetry of the system is spontaneously broken in the strong coupling limit, and a Weyl semimetal with broken time-reversal and inversion symmetries, which is different from the noninteracting one, survives in the strong coupling limit.

1. Introduction
Weyl semimetals have attracted much attention recently as a novel topological phase of matter. Weyl semimetals have three-dimensional (3D) gapless linear dispersions near the band touching points, the Weyl nodes. The low-energy effective Hamiltonian near the Weyl nodes is described by the Weyl Hamiltonian $\mathcal{H}(k) = \pm v_F k \cdot \sigma$ with $\pm$ denoting the chirality, $v_F$ being the Fermi velocity, and $\sigma_i \ (i = 1, 2, 3)$ being the Pauli matrices [1, 2]. Breaking of at least time-reversal or spatial inversion symmetry is required to realize Weyl semimetal phases [3, 4]. Topological nature of Weyl semimetals is understood by the fact that each Weyl node can be regarded as a “monopole” with its charge given by chirality [5], and by the anomalous Hall effect originating from the theta term [6, 7, 8]. Further, single Weyl node cannot be gapped out, since all the three Pauli matrices are used. The bulk energy gap opens only if pairs of Weyl nodes with opposite chirality meet and annihilate each other. From this topological property, it is expected that Weyl semimetals are stable against perturbations.

In this paper, we focus on the stability of a time-reversal symmetry broken Weyl semimetal with two nodes against strong $1/r$ long-range Coulomb interactions. This is because screening effects are expected to be weak in Dirac fermion systems due to the vanishing density of states near the Fermi level. As a powerful non-perturbative method which enables us to treat strong $1/r$ Coulomb interactions properly, we employ the U(1) lattice gauge theory. Based on the U(1) lattice gauge theory with the mean-field approximation, we analyze the system from the strong coupling limit.

2. Theoretical Model
Let us consider a lattice model that describes a time-reversal symmetry broken Weyl semimetal with two nodes separated in momentum space. Theoretically, such a situation can be realized by
two orbitals, and eigenvalues of the Hamiltonian (1) is easily obtained as ferromagnetic coupling between the bulk electrons and magnetic impurities [10]. The energy near the Fermi level $E_F = 0$ touch at two points (Weyl nodes). Note that we have set $v_F = 1$.

the case where magnetic impurities are doped to a 3D topological insulator. The noninteracting single-particle Hamiltonian is given by

$$
\mathcal{H}_0(\mathbf{k}) = v_F \sum_{j=1}^3 \alpha_j \sin k_j + m(\mathbf{k})\alpha_4 + b\Sigma_3, \tag{1}
$$

where $v_F$ is the Fermi velocity, and $m(\mathbf{k}) = m_0 + r \sum_{j=1}^3 (1 - \cos k_j)$. The Hamiltonian (1) with $b = 0$ and $0 > m_0/r > -2$ is known as the effective Hamiltonian for 3D topological insulators such as Bi$_2$Se$_3$ [9]. The matrices $\alpha_n$ and $\Sigma_3$ are given by the Dirac representation:

$$
\alpha_j = \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix}, \quad \alpha_4 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \Sigma_3 = \begin{bmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{bmatrix}, \tag{2}
$$

with $\sigma_j$ being the Pauli matrices. The spinor of the Hamiltonian (1) is written in the basis of $\psi_\mathbf{k} = [c_{\mathbf{k}+\uparrow}, c_{\mathbf{k}+\downarrow}, c_{\mathbf{k}-\uparrow}, c_{\mathbf{k}-\downarrow}]^T$, where $c$ is the annihilation operator of an electron, $+,-$ denote two orbitals, and $\uparrow (\downarrow)$ denotes up-(down)-spin. Then we see that the term $b\Sigma_3$ describes a ferromagnetic coupling between the bulk electrons and magnetic impurities [10]. The energy eigenvalues of the Hamiltonian (1) is easily obtained as

$$
E(\mathbf{k}) = \pm \sqrt{v_F^2 (\sin k_1^2 + \sin k_2^2)} + \sqrt{v_F^2 \sin k_3^2 + m(\mathbf{k})^2 \pm b}^2. \tag{3}
$$

The Weyl nodes appear where the wave vector $\mathbf{k}$ satisfies the condition $b^2 = |m_0 + r \sum_{j=1}^3 (1 - \cos k_j)|^2 + v_F^2 \sin^2 k_3$ and $\sin k_1 = \sin k_2 = 0$. $k_1$ and $k_2$ can take the value 0 or $\pi$. In this study, we set $|m_0|$ small to restrict the existence of the Weyl nodes on the $(k_1,k_2) = (0,0)$ line. The $k_3$ dependence of the energy spectrum (3) for some values of $b$ is shown in Fig. 1.

Next we take into account the $1/r$ long-range Coulomb interactions between the bulk electrons, by introducing a scalar potential $A_0$. This procedure enables us to describe the system by the U(1) lattice gauge theory. The Euclidean action of the system is then given by [11]

$$
S = S_F^{(0)} + (m_0 + 3r + r_r) \sum_n \bar{\psi}_n \psi_n + b \sum_n \bar{\psi}_n \gamma_0 \Sigma_3 \psi_n + S_G, \tag{4}
$$

where $S_F^{(0)}$ is the fermionic part without the mass term

$$
S_F^{(0)} = - \sum_n \left[ \bar{\psi}_n P_0^- U_{n,0} \psi_{n+0} + \bar{\psi}_{n+0} P_0^+ U_{n,0}^\dagger \psi_n \right] - \sum_{n,j} \left[ \bar{\psi}_n P_j^\dagger \psi_{n-j} + \bar{\psi}_{n+j} P_j \psi_n \right]. \tag{5}
$$
and $S_G$ is the pure U(1) gauge part

$$S_G = \beta \sum_n \sum_{\mu > \nu} \left[ 1 - \frac{1}{2} \left( U_{n,\mu} U_{n+\mu,\nu} U_{n+\nu,\mu} U_{n,\nu}^\dagger + \text{H.c.} \right) \right]. \tag{6}$$

Here $\bar{\psi} = \psi_0^\dagger \gamma_0$, $n = (n_0, n_1, n_2, n_3)$ denotes a spacetime lattice site on a 4D hypercubic lattice, $\mu$ denotes the unit vector along the $\mu$ direction, and $P_{\mu}^\pm = (r_{\mu} \pm \gamma_{\mu})/2$ with $r_0 = r_T$ and $r_1 = r_2 = r_3 = r$. $U_{n,\mu}$ are the U(1) link variables with $U_{n,0} = 1$ and $U_{n,0} = e^{iA_{0,n}} (-\pi \leq A_{0,n} \leq \pi)$. Note that we have rewritten the scalar potential $A_{0,n}$ as $eA_{0,n}/v_F \rightarrow A_{0,n}$ with $e$ the electric charge. Taking the noninteracting limit ($A_{0,n} \rightarrow 0$) in the action (4), we obtain the Hamiltonian (1). $r_T$ is introduced to eliminate fermion doublers resulting from the lattice regularization of the timelike action.

The parameter $\beta$ which represents the strength of $1/r$ Coulomb interactions is given by

$$\beta = \frac{v_F \epsilon}{e^2} = \frac{v_F \epsilon}{4\pi \alpha c}, \tag{7}$$

where $\epsilon$ is the dielectric constant of the system, $c$ is the speed of light in vacuum, and $\alpha (\simeq 1/137)$ is the fine-structure constant. Here note that $v_F/c \sim 10^{-3}$ in condensed matter. Namely, small Fermi velocity makes the $1/r$ Coulomb interactions effectively strong. In the following, we consider the case with $\beta \ll 1$, i.e., the case with small dielectric constant.

3. Possible Orders in the Strong Coupling Limit

In this section, we derive the effective action in the strong coupling limit $\beta = 0$, and then consider the possible orders in the strong coupling limit. The effective action up to arbitrary order in $\beta$ can be obtained by integrating out the variable $U_{n,0}$ as

$$Z = \int \mathcal{D}[\psi, \bar{\psi}, U_0] e^{-S} = \int \mathcal{D}[\psi, \bar{\psi}] e^{-S_{\text{eff}}} . \tag{8}$$

In the strong coupling limit $\beta = 0$, we only have to evaluate the integral $\int \mathcal{D}U_0 e^{-S_F^{(0)}} = \prod_n \int_{-\pi}^{\pi} \frac{dA_{0,n}}{2\pi} e^{-S_F^{(0)}}$, since $U_{n,0}$ is contained only in $S_F^{(0)}$. After a calculation, we obtain the effective action in the strong coupling limit given by

$$S_{\text{eff}} = -\sum_{n,j} \left[ \bar{\psi}_n P_j^+ \psi_{n+j} + \bar{\psi}_{n+j} P_j^+ \psi_n \right] + (m_0 + 3r + r_T) \sum_n \bar{\psi}_n \psi_n + b \sum_n \bar{\psi}_n \gamma_0 \Sigma_3 \psi_n + \sum_n \text{tr} \left[ N_n P_0^+ N_{n+0}^+ P_0^- \right], \tag{9}$$

where we have defined $(N_n)_{\alpha \beta} = \bar{\psi}_{n,\alpha} \psi_{n,\beta}$. The subscripts $\alpha$ and $\beta$ denote the component of the spinor.

Next we decouple the interaction term [the last term in Eq. (9)] to fermion bilinear form with the use of the mean-field approximation. We apply the extended Hubbard-Stratonovich transformation [12] to the trace of the product of two arbitrary matrices $A$ and $B$:

$$e^{\text{extr}AB} = \text{(const.)} \times \int \mathcal{D}[Q, Q'] \exp \left\{ -\kappa \left[ Q_{\alpha \beta} Q'_{\alpha \beta} - A_{\alpha \beta} Q'_{\alpha \beta} - B^T_{\alpha \gamma} Q'_{\beta \gamma} \right] \right\} , \tag{10}$$

where $\kappa$ is a positive constant, and the superscript $T$ denotes the transpose of a matrix. This integral is approximated by the saddle point values $Q_{\alpha \beta} = \langle B^T \rangle_{\beta \alpha}$ and $Q'_{\alpha \beta} = \langle A \rangle_{\beta \alpha}$. Then we should set $(\kappa, A, B) = (1, N_n P_0^+, -N_{n+0} P_0^-)$. 

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Table 1. Transformation properties under time-reversal $T$ and spatial inversion (parity) $P$ of 16 independent matrices consisting of $\alpha_\mu$ with $\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}1$ ($\mu, \nu = 1, 2, 3, 4, 5$).

| Matrices | $1$ | $\alpha_j$ | $\alpha_4$ | $\alpha_5$ | $\Sigma_j$ | $\Sigma'_j$ | $\Pi_j$ | $\Pi_0$ |
|----------|-----|-------------|-------------|-------------|-------------|-------------|--------|--------|
| Time-reversal $T$ | $+$ | $-$ | $+$ | $-$ | $+$ | $+$ | $-$ | $+$ |
| Inversion $P$ | $+$ | $-$ | $+$ | $-$ | $+$ | $+$ | $-$ | $-$ |

Here let us consider the resulting mean-field Hamiltonian. The mean-field action of the interaction term takes the form

$$\mathcal{H}(k) = \mathcal{H}_0(k) + \gamma_0\langle N_n \rangle$$

$$= \alpha_j \sin k_j + m(k)\alpha_4 + b\Sigma_3 + \gamma_0\langle N_n \rangle.$$  \hspace{1cm} (11)

Note that $\gamma_0 = \alpha_4$. In Dirac fermion systems, the most general form of $\gamma_0\langle N_n \rangle$ is written in terms of 16 independent matrices which consist of $\alpha_\mu$. Such 16 matrices are given explicitly by $1$ (the identity matrix), $\alpha_\mu\ (\mu = 1, 2, 3, 4, 5)$, and $\alpha_\mu\alpha_\nu = -\frac{i}{2}[\alpha_\mu, \alpha_\nu]$ ($\mu < \nu$). The matrices $1$ and $\alpha_\mu$ are trivial. Let us closely look at the 10 matrices $\alpha_\mu\alpha_\nu$. In the Dirac representation, they are written explicitly as [11]

$$\Sigma_j \equiv \alpha_{ik}\epsilon_{ikj} = \begin{bmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{bmatrix}, \quad \Sigma'_j \equiv \alpha_j5 = \begin{bmatrix} \sigma_j & 0 \\ 0 & -\sigma_j \end{bmatrix},$$

$$\Pi_j \equiv \alpha_j4 = \begin{bmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{bmatrix}, \quad \Pi_0 \equiv \alpha_{45} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$  \hspace{1cm} (12)

where $j = 1, 2, 3$. Note that these are Hermitian matrices. It is easily shown that $\Sigma_j$ and $\Sigma'_j$ are odd under time-reversal but even under parity:

$$T\Sigma_jT^{-1} = T\Sigma'_jT^{-1} = -1, \quad P\Sigma_jP^{-1} = P\Sigma'_jP^{-1} = +1,$$  \hspace{1cm} (13)

where the time-reversal and parity operators are given by $T = 1 \otimes (-i\sigma_2)K$ ($K$ is a complex conjugation operator) and $P = \sigma_3 \otimes 1$, respectively. On the other hand, $\Pi_j$ are even under time-reversal but odd under parity:

$$T\Pi_jT^{-1} = +1, \quad P\Pi_jP^{-1} = -1.$$  \hspace{1cm} (14)

The properties of the 16 matrices are summarized in Table 1.

Let us consider the effects of the term $\gamma_0\langle N_n \rangle$. From Eq. (11), we can see the followings. First, the identity matrix shifts the energy level, and $\alpha_j\ (j = 1, 2, 3)$ shifts the location of the Weyl nodes. Second, the term $\Sigma_3$ is contained in the noninteracting Hamiltonian. As mentioned before, $b\Sigma_3$ is regarded as the ferromagnetic coupling between the bulk electrons and magnetic impurities. Then the terms $\Sigma_j\ (j = 1, 2, 3)$ can be neglected. Third, the terms $\Sigma'_j$ can be regarded as a kind of “antiferromagnetic” order, as is understood from its explicit form. Namely, the spins at the two orbitals point to opposite directions to each other. Here note that the spinor of the Hamiltonian is written in the basis of $\psi_k = [c_{k+\uparrow}, c_{k+\downarrow}, c_{k-\downarrow}, c_{k-\uparrow}]^T$. Thus the terms $\Sigma'_j\ (j = 1, 2, 3)$ can also be neglected. To summarize, we only have to take into account the terms $\alpha_4, \alpha_5, \Pi_\mu\ (\mu = 0, 1, 2, 3)$ as the possible orders. Here note that $\alpha_4$ modifies the mass of Dirac fermions $m_0$. Namely, the presence of $\alpha_4$ means the renormalization of the mass of Dirac fermions.
4. Free Energy in the Strong Coupling Limit

To obtain the ground state in the strong coupling limit $\beta = 0$, we need to derive the free energies for each instability at zero temperature. The free energies are derived from the usual formula $\mathcal{F} = -\frac{\mathcal{Z}}{\mathcal{V}} \ln \mathcal{Z}$ with $T$ and $\mathcal{V}$ being the temperature and volume of the system, respectively. The partition function $\mathcal{Z}$ is calculated by the Grassmann integral formula $\mathcal{Z} = \int \mathcal{D}[\psi, \bar{\psi}] e^{-\mathcal{H}_\text{total}} = \det \mathcal{M}$. As was shown in the previous section, we need to obtain the free energies for the $a_\alpha$ and $\Pi_\mu$ ($\mu = 0, 1, 2, 3$) instabilities. In what follows, we show the explicit expression of the free energy for the $\Pi_1$ (and $\Pi_2$) instability. Here note that these two instabilities are degenerate, since there is a spin degree of freedom in the $xy$-plane.

We assume that $\langle N_n \rangle = -\sigma \mathbf{1} + \rho_1 \gamma_0 \Pi_1$. With the use of the extended Hubbard-Stratonovich transformation [Eq. (10)], the mean-field decoupling of the interaction term is done to be

$$e^{-\sum_n \text{tr} [N_n P_0^+ N_{n+\delta} P_0]} \sim \exp \left\{ -\sum_n \left[ (1 - r^2) \sigma^2 + (1 + r^2) \rho_1^2 + \bar{\psi}_n \Gamma \psi_n \right] \right\},$$

(15)

where $\Gamma = \frac{1}{2} [(1 - r^2) \sigma + (\gamma_0 \Pi_1)^T (1 + r^2) \rho_1]$. Substituting Eq. (15) into Eq. (9) and doing the Fourier transform, we obtain the effective action in terms of $\sigma$ and $\rho_1$ as

$$S_{\text{eff}}(\sigma, \rho_1) = \frac{1}{T} \left[ (1 - r^2) \sigma^2 + (1 + r^2) \rho_1^2 \right] + \sum_k \bar{\psi}_k \mathcal{M}(k; \sigma, \rho_1) \psi_k.$$

(16)

By calculating the determinant of $\mathcal{M}$, the free energy is obtained as [11]

$$\mathcal{F}(\sigma, \rho_1) = (1 - r^2) \sigma^2 + (1 + r^2) \rho_1^2 + \int_{-\pi}^{\pi} \frac{d^3 k}{(2\pi)^3} \ln \left\{ \frac{I(k, b, \bar{\rho}_1) I(k, -b, -\bar{\rho}_1) - J(k, b, \bar{\rho}_1)}{\bar{m}(k) + r_1^2 - b^2} \right\},$$

(17)

where $\bar{\rho}_1 = \frac{1}{2} (1 + r^2) \rho_1$ and $\bar{m}(k) = m_0 + \frac{1}{2} (1 - r^2) \sigma + r \sum_j (1 - \cos k_j)$. Two functions $I(k, b, \bar{\rho}_1)$ and $J(k, b, \bar{\rho}_1)$ are given by $I(k, b, \bar{\rho}_1) = [\bar{m}(k) + r_1 - b] \times \{ [\bar{m}(k) + r_1] + b \} + \{ \bar{m}(k) + r_1 + b \} \times \{ \bar{m}(k) + r_1 + b \}$ and $J(k, b, \bar{\rho}_1) = 4 \sin^2 k_3 \{ (\bar{\rho}_1 [\bar{m}(k) + r_1] + 2 \sin k_2) b^2 + b^2 \sin^2 k_1 \}$. The ground state is determined by the stationary condition $\partial \mathcal{F}(\sigma, \rho_1) / \partial \sigma = \partial \mathcal{F}(\sigma, \rho_1) / \partial \rho_1 = 0$.

5. Numerical Results

It is found that the $a_\alpha$, $\Pi_0$, and $\Pi_3$ instabilities do not appear in the strong coupling limit $\beta = 0$, and that the $\Pi_1$ (or $\Pi_2$) order is realized as the ground state in the strong coupling limit. Namely, spatial inversion symmetry is spontaneously broken in the strong coupling limit. The $b$ dependences of $\sigma$ and $\rho_1$ are shown in Fig. 2(a). It can be seen that the bandgap renormalization by $\sigma$ and the inversion symmetry breaking by $\rho_1$ occur simultaneously.

Let us consider the single-particle mean-field Hamiltonian in the phase with the $\Pi_1$ order, which is given by

$$\mathcal{H}_{\text{MF}}(k) = \alpha_j \sin k_j + \bar{m}(k) \alpha_4 + b \Sigma_3 + \rho_1 \Pi_1.$$

(18)

We can obtain the energy spectrum analytically as

$$E(k) = \pm \left\{ s^2(k) + [\bar{m}(k)]^2 + b^2 + \rho_1^2 \pm 2 \sqrt{[\bar{m}(k) - \rho_1 \sin k_2]^2 + (b^2 + \rho_1^2) \sin^2 k_3} \right\}^{1/2},$$

(19)

where $s^2(k) = \sum_{i=1}^{3} \sin^2 k_i$. Substituting the obtained values of $\sigma$ and $\rho_1$ into Eq. (19), it is found that the Weyl semimetal phase with broken time-reversal and inversion symmetries exists in the strong coupling limit. The Weyl semimetal phase in the strong coupling limit has two Weyl nodes, as in the noninteracting phase. However, due to the inversion symmetry breaking, the two Weyl nodes do not appear on the $k_3$ axis but appear on the $k_2$-$k_3$ plane. The phase diagram in the strong coupling limit is shown in Fig. 2(b). For comparison, the phase diagram in the noninteracting limit ($\beta = \infty$), which is obtained from Eq. (3), is shown in Fig. 2(c).
Figure 2. (a) $b$ dependences of $\sigma$ and $\rho_1$ in the strong coupling limit $\beta = 0$. (b) Phase diagram in the strong coupling limit. PTI and PT-broken Weyl semimetal represent the insulator with broken time-reversal and spatial inversion (parity) symmetries, and the Weyl semimetal with broken time-reversal and inversion symmetries, respectively. These phases are characterized by nonzero $\rho_1$. (c) Phase diagram in the noninteracting limit ($\beta = \infty$). MTI, T-broken Weyl semimetal, and AHI represent the magnetic topological insulator, the Weyl semimetal with broken time-reversal symmetry, and the anomalous Hall insulator, respectively. In the above three figures, parameters are set to be $m_0 = -0.6$, $r = 1$ and $r_\sigma = 0.5$.

6. Discussions and Summary
Here it should be noted that no symmetry is spontaneously broken in the strong coupling limit when $b = 0$. As mentioned in Sec. 2, the system with $b = 0$ represents 3D topological insulators of Bi$_2$Se$_3$ family. Therefore, in this study, it was also shown that 3D topological insulators of Bi$_2$Se$_3$ family are also stable against strong $1/r$ Coulomb interactions.

In the noninteracting limit, the phase boundaries where the Weyl semimetal phase appears and disappears are determined by the analytical condition such that $b = |m_0|$ and $b = 2r + m_0$. In the strong coupling limit, we determined the phase boundaries by plotting Eq. (19) numerically, and found that they can be approximated by $b \simeq |m_{\text{eff}}|$ and $b \simeq 2r + m_{\text{eff}}$ with $m_{\text{eff}} = m_0 + \frac{1}{2}(1 - r_\sigma^2)\sigma$. Note that $\sigma > 0$ and $r_\sigma \leq 1$. The condition $r_\sigma \leq 1$ comes from the reflection positivity of lattice gauge theories with Wilson fermions [13]. Then it can be said that the broadening of the Weyl semimetal phase, i.e., the stabilization of the Weyl semimetal phase, in the presence of $1/r$ Coulomb interactions is due to the bandgap renormalization.

In summary, we have studied the effects of strong $1/r$ long-range Coulomb interactions in a time-reversal symmetry broken Weyl semimetal. In the mean-field decoupling process of the interaction term in the strong coupling limit, we have taken into account all the possible 16 instabilities allowed in our model. It was found that spatial inversion (parity) symmetry of the system is spontaneously broken in the strong coupling limit. Nevertheless, the Weyl semimetal phase with broken time-reversal and inversion symmetries, which is different from the noninteracting phase, survives in the strong coupling limit.

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