Stability of line-node semimetals with strong Coulomb interactions and properties of the symmetry-broken state

Carlos Naya, Tommaso Bertolini, and Johan Carlström

Department of Physics, Stockholm University, 106 91 Stockholm, Sweden

(Dated: March 9, 2022)

We employ diagrammatic Monte Carlo simulations to establish criteria for the stability of line-node semimetals in the presence of Coulomb interactions. Our results indicate a phase transition to a chiral insulating state that occurs at a finite interaction threshold which we determine. We also compute the Landau levels for out-of-plane and in-plane magnetic fields in the symmetric and symmetry-broken phases. We find that the magnetic field couples to the chiral order parameter, implying that this degree of freedom can be manipulated in situ in experiments. Finally, we check the existence of edge states in the symmetry-broken phase. On the system’s boundary, we note that the metallic “drum-head” states that exist in the symmetric phase are gapped out. However, the symmetry-broken phase permits topological defects in the macroscopic order parameter in the form of domain walls, which host metallic “interface states.” These consist of line-like gap-closings that occur on the two-dimensional interfaces.

Topological semimetals exhibit a band structure that is gapped everywhere except at a few nodal points, where the bands meet. The topological nature of these protects them against perturbations and also gives rise to unique phenomena like the chiral anomaly—where nodal points act as sources and sinks of a spontaneous current—and Fermi arcs, which are direct manifestations of the bulk topology [1]. Applications of topological semimetals are thus far mainly as building blocks of information technology [2–4]. Several of these materials exhibit a large magnetoresistance effect [5] that may be exploited in magnetic field sensors [6], and spintronic devices [7].

In the search for new and technologically useful semimetals, symmetry-protected topological phases have emerged as an important platform that dramatically expands the types of nodal features realized in a material. Typically, this involves a combination of point group symmetries and explicitly broken time-reversal or inversion symmetry. The result is a wide class of band touching points that carry more than unit topological charge [8, 9] and may also involve multiple bands [10, 11] or have to be classified as line-nodes [12–18].

While the explicit reliance on symmetry significantly widens the scope of topological and semimetallic materials, it also has implications for the role of correlations in these: In tight-binding models of bilayer graphene, the dispersion is quadratic around the nodal points, yet the system develops a nematic instability at an infinitesimal interaction [19]. For multiple-charge Weyl nodes and line-node semimetals with contact interaction, renormalization group theory indicates instabilities at a finite threshold [20, 21]. This is also true for single-layer graphene, where actual material parameters are situated close to a chiral symmetry-breaking regime [22]. Thus, semimetallic phases that depend explicitly on symmetry may be susceptible to correlation effects that destroy the underlying symmetry.

Reliably predicting the parameter regimes where symmetry-protected topological phases remain stable faces several delicate problems. The absence of screening means that interactions are effectively long-ranged, leading to infrared divergencies. Furthermore, competition between correlation effects originating from different length scales is very likely. For example, in graphene, the long-range part of the interaction drives the system towards an asymptotically free Dirac liquid with divergent Fermi velocity as $T \to 0$, without causing any instabilities [23]. Thus, the renormalization of the dispersion occurring primarily at the infrared end increases the effective kinetic energy relative to the short-range part of the interaction, which is believed to drive the phase transition. Therefore, an accurate solution to this class of problems requires that all length scales are treated on an equal footing.

A type of symmetry-protected topological phase that has attracted considerable interest is the nodal-line semimetal. Predictions of this state has been made in TlTaSe$_2$ [15], CaAgP$_2$ [16] and Ca$_2$P$_2$ [17] and ZrSiS [24] based on reflection symmetry. In PbTaSe$_2$ it has also been confirmed by angle resolved photo emission spectroscopy [14]. Recently, the observations of strongly renormalized transport properties and Fermi velocity—as compared to DFT calculations—in ZrSiS was interpreted as an indication of a strongly correlated line-node semimetal [25].

In this work, we employ diagrammatic Monte Carlo simulations [26] to establish quantitative criteria for the stability of line-node semimetals in the presence of long-range interactions and also characterize the symmetry-broken phase which occurs for sufficiently strong coupling. We find evidence for a chiral insulator that supports metallic interfaces on domain walls that interpolate between different signs of the order parameter and can be manipulated in situ via an external field.

**MODEL**

We consider the case of a single nodal line with a bare Fermi velocity of $v^0_f$ running along the $z$-axis

$$H_0(k) = v^0_f k_{xy} \cdot \sigma,$$  

(1)
with an interaction of the form
\[ V(k) = \frac{\alpha}{k^2 + \lambda^{-2}}. \]  
(2)

Here, \( \lambda \) is a fictitious screening length introduced to regularize the series, and we are thus principally interested in the limit \( \lambda \to \infty \). We consider a cylindrical domain given by
\[ |k_z| \leq \Lambda, \quad \sqrt{k_x^2 + k_y^2} \leq \Lambda, \]  
(3)

where \( \Lambda \) is the ultra violet cutoff. Because of a scale invariance associated with the linear dispersion, the only relevant length scale in the low-temperature limit is the ratio of the UV cutoff and the inverse screening length \( \Lambda/\lambda^{-1} \). To see this, we may choose a temperature and energy scale where the temperature is unity by rewriting the partition function
\[ z(\beta, H) = z(1, \beta H). \]  
This gives a bare Greens function
\[ \frac{1}{i\omega - \beta H_0(k)} = G_0(\omega, \beta k), \quad \omega = (2n + 1)\pi, \]  
(4)

where we have exploited the linearity of \( H_0 \) in \( k \). Diagrammatic corrections to the Greens function take the form
\[ \delta G(\omega, \beta k) = \prod_{n=1}^{N} d\beta k_n \prod_{j=1}^{N} \beta V(k_j) \prod_{l=1}^{2N+1} G_0(\omega_l, \beta k_l), \]  
(5)

where \( N \) is the expansion order. If we introduce a change of scale \( k' = \beta k \) we obtain
\[ \delta G(\omega, k') = \prod_{n=1}^{N} d\beta k'_n \prod_{j=1}^{N} \beta V(k'_j) \prod_{l=1}^{2N+1} G_0(\omega_l, k'_l). \]  
(6)

For a screened Coulomb interaction in \( D = 3 \) we find
\[ \beta^{-D} \frac{\alpha}{k'^2/\lambda^2 + \lambda^{-2}} = \frac{\alpha}{k^2 + \lambda^2\lambda^{-2}}. \]  
(7)

The UV cutoff changes scales as \( \Lambda \to \beta \Lambda \), giving
\[ G(\omega, \beta k, \lambda^{-1}, \Lambda) = G(\omega, 1, k', \beta \Lambda^{-1}, \beta \Lambda), \]  
(8)

which is characterized by the ratio \( \Lambda/\lambda^{-1} \) in the limit \( \beta \to \infty \).

In the perturbative regime, the nodal line \( 1 \) is protected by a symmetry due to being odd under an orthonormal map \( k \to -k \). The implication of this symmetry is that on the \( k_z \)-axis, the Greens function must have a pole at zero energy as long as the series expansion remains convergent [27]. Correspondingly, destroying the semimetallic phase requires breaking this symmetry. In a diagrammatic framework, this phase transition can be identified via a divergent susceptibility with respect to a symmetry-breaking perturbation.

**CONTACT INTERACTION**

For contact interaction, the self-consistent Fock theory can be solved analytically due to translation invariance in momentum space. Specifically, the self-energy satisfies the relation
\[ \Sigma(\omega_n, k) = \frac{1}{\beta} \sum_n \int \frac{d^3q}{(2\pi)^3} V(q-k) G_0^{-1}(\omega_n, q) \Sigma(\omega_n, q), \]  
(9)

Here, it should be noted that at the level of Fock theory, \( \Sigma \) is independent of frequency, and thus de facto takes the form of a correction to the effective dispersion. Furthermore, contact interaction does not renormalize the Fermi velocity since \( H_0(k) \) is an odd function. Since the self energy is translation invariant, it must therefore take the form \( \Sigma(k) = \Delta \sigma_z \). Inserting this self-energy in (9) and summing over frequency, we obtain
\[ \Sigma(k) = \Delta \sigma_z = \int \frac{d^3q}{(2\pi)^3} \frac{H_0(q)}{2\sqrt{(v_f^0 q_y)^2 + \Delta^2}} \times \tanh(\frac{\beta(\sqrt{(v_f^0 q_y)^2 + \Delta^2})}{2}). \]  
(10)

where the integral of \( H_0 \) over \( k \) vanishes. Thus, Eq. (10) provides a self-consistent equation for \( \Delta \) as a function of the coupling strength, whose solutions will provide the gap parameter in this regime. Solutions for which \( \Delta \) is finite correspond to a symmetry-broken state, while the symmetric phase is characterized by a vanishing gap. In the low-temperature limit, and for a cylindrical domain (3) with \( \Lambda = 1 \), the integral (10) provides an algebraic expression for the gap of the form
\[ \eta \frac{\Delta}{v_f^0} = \left( \frac{1 + \frac{\Delta^2}{v_f^0}}{\eta} \right) - 1 = 0. \]  
(11)

where we have introduced \( \eta = \alpha(2\pi)^{-2} \). Equation (11) predicts a critical coupling strength \( \eta_c/v_f^0 = 2 \), see Fig. 1. Above this threshold, the gap is given by
\[ \frac{\Delta}{v_f^0} = \frac{\eta}{4v_f^0} - \frac{v_f^0}{\eta}. \]  
(12)

The onset of chiral a phase at a finite interaction strength is consistent with results from renormalization group theory for contact interaction [21].

Figure 1. **Self-consistent solution for the gap** with contact interactions, as a function of the rescaled coupling strength \( \eta \). A second order transition is established at \( \eta_c/v_f^0 = 2 \).
The frequency-independent part of the self-energy can be written in terms of the chiral order parameter as follows. First, we note that the metric parts of the self-energy result from competition between the symmetric and antisymmetric components of very fragile meta-stable symmetric solutions that likely exist but never reach the critical coupling, we observe a family of extremely small or relatively large symmetry-breaking terms, respectively. For most parameter regimes, these result in identical solutions. However, at low temperatures and for a coupling strength that is slightly larger than the critical coupling, we observe a family of solutions with energy bands that are translation invariant in the z-direction. Furthermore, we assume a symmetry of the self-energy

$$ e^{-i\phi} \Sigma^{\pm}(\omega, k) e^{i\phi} = \Sigma(\omega, R^z k) $$

where \( R^z \) represents a rotation around the z-axis by \( \phi \).

The results from the diagrammatic Monte Carlo simulations are summarized in Fig. 2. For most parameter ranges, the order parameter scales approximately as \( O \sim (\eta/\nu_f)^2 \), prompting us to plot the square root. The solutions correspond to different values of \( \gamma \), which controls the model parameters according to (15). As we progressively decrease the temperature and increase the screening length, the order parameter saturates to a single line which depends only on \( \eta/\nu_f \), indicating that the chiral order exhibits a well-defined IR limit at zero temperature. The presented data corresponds to a first and second-order expansion.

In Fig. 3 we see the critical coupling strength as a function of \( \gamma \), extracted from the data presented in Fig. 2. The critical point saturates to \( \eta_f/\nu_f^0 = 0.45 \pm 0.1 \). The correction from first to second order falls within the error bars, indicating that this problem is very well captured by self-consistent Fock theory. This is consistent with previous applications of diagrammatic techniques to semimetallic systems: In Weyl semimetals, the correction to the Greens function is almost entirely contained in the frequency-independent part of the self-energy, leading to the emergence of virtually free fermions [33]. In graphene, at least the long-range part of the interaction drives the system towards an asymptotically free Dirac liquid [23], while for short-range interactions, the convergence of the series has been demonstrated analytically up to a finite threshold [34]. Most likely, this results from the exponential suppression of diagram topologies that involve excitation of the background in semimetals.

**LANDAU LEVELS AND MAGNETIC RESPONSE**

To compute the Landau levels arising when the line-node is placed in a magnetic field, we consider a dispersion of the form (1) and take the Fermi velocity to be unity. This gives

$$ H(k) = k_x \sigma_x + k_y \sigma_y = \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix}, $$

with energy bands

$$ \varepsilon_{\pm} = \pm \sqrt{k_x^2 + k_y^2}. $$

Thus, the nodal line runs along the z-axis \((0, 0, k_z)\).
Since we consider an infinitely long nodal line, we assume a component, prompting us to define an order parameter of the metric parts of the self energy respectively (see also discussion slightly larger than the critical coupling, we observe a family of very fragile meta-stable symmetric solutions that likely result from competition between the symmetric and antisymmetric parts of the energies). The chiral symmetry-breaking is generated by the frequency-independent part of the self energy can be written as

\[ \eta \equiv \sqrt{\frac{O}{v_f^0}} \]

O. We then rewrite the integral over \( k \) as

\[ \int \frac{d^2k}{(2\pi)^2} \Rightarrow \int \frac{d^2k}{v_f^0} \]

representing a rotation around the \( e \). A stochastic summation of the expansions

\[ (2) \]

result from competition between the symmetric and antisymmetric interactions. For larger values of \( \gamma \), the solutions collapse onto a single line indicating that the chiral order remains convergent in the infrared limit.

**Figure 2.** The chiral order parameter \( O \) as a function of the interaction strength \( \eta \) in units of the bare Fermi velocity for Fock theory (a), and second-order theory (b). Note that we display the square root of the order parameter since it is approximately quadratic in \( \eta \) over most parameter ranges. Here, the screening parameter is \( \lambda^{-1} = 10^{-2} \times 2^{-\gamma} \), while \( \beta v_f^0 = 10^2 \times 2^\gamma \) so that the solutions correspond to progressively lower temperatures and longer screening lengths. For larger values of \( \gamma \), the solutions collapse onto a single line indicating that the chiral order remains convergent in the infrared limit.

To couple the system to an external magnetic field, we introduce the displacement of the momentum \( k \) by the vector potential \( A \):

\[ k \rightarrow k' = k + A. \]  

\[ (21) \]

First, we consider a magnetic field along the z-direction, i.e., \( B = Bz \). Working in the axial gauge, the vector potential reads \( A = (-By/2, Bx/2, 0) \), so that we can define the ladder operators in terms of the new momenta

\[ a = \frac{k_x - ik_y}{\sqrt{2B}}, \quad a^\dagger = \frac{k_x + ik_y}{\sqrt{2B}}. \]  

\[ (22) \]

**Figure 3.** Critical coupling strength \( \eta_c \) in units of the bare Fermi velocity \( v_f^0 \) for progressively lower temperatures and longer screening lengths, parameterized as \( \lambda^{-1} = 10^{-2} \times 2^{-\gamma} \), and \( \beta v_f^0 = 10^2 \times 2^\gamma \). For \( \gamma \geq 3 \) we estimate the critical coupling to \( \eta_c/v_f^0 = 0.45 \pm 0.01 \). The corrections at second order are not discernible at this accuracy.

which allows us to write the Hamiltonian in the form

\[ H = \begin{pmatrix} 0 & \sqrt{2Ba}^\dagger \\ \sqrt{2Ba} & 0 \end{pmatrix}. \]  

\[ (23) \]

The Landau levels can be easily found from the eigenequation \( H \Phi = E \Phi \). For \( \Phi = (|\phi_1\rangle, |\phi_2\rangle)^T \), we obtain the two equations

\[ \sqrt{2Ba}^\dagger |\phi_1\rangle = E |\phi_1\rangle, \]  

\[ (24) \]

\[ \sqrt{2Ba} |\phi_2\rangle = E |\phi_2\rangle, \]  

\[ (25) \]

and, by inserting the first equation into the second, we arrive at

\[ 2Ba^\dagger a |\phi_2\rangle = E^2 |\phi_2\rangle, \]  

\[ (26) \]

which describes a harmonic oscillator with

\[ E = \pm \sqrt{2Bn}, \quad |\phi_2\rangle = c |n\rangle, \quad n = 0, 1, 2, \cdots \in \mathbb{N}, \]  

\[ (27) \]

where \( c \) is a normalization constant. Then, for \( |\phi_1\rangle \) we have

\[ |\phi_1\rangle = \pm |n-1\rangle. \]  

\[ (28) \]

Therefore, for a magnetic field in the z-direction, the Landau levels are given by

\[ E_\pm = \pm \sqrt{2Bn}, \]  

\[ (29) \]

with eigenstates

\[ \Phi_\pm = c \left( \frac{\pm |n-1\rangle}{|n\rangle} \right). \]  

\[ (30) \]
monic so that standard recipes for extracting the Landau levels second. By using the commutator 
\[ [a, a^\dagger] = 1 \]
expressed in this language, the Hamiltonian (19) takes the form
\[ H = \begin{pmatrix} k_x - i\sqrt{\frac{B}{2}}(a + a^\dagger) & 0 \\ 0 & k_x + i\sqrt{\frac{B}{2}}(a + a^\dagger) \end{pmatrix} \].

From the eigenequation \( H\Phi = E\Phi \), we obtain for \( |\phi_1\rangle \) and \(|\phi_2\rangle\)
\[ \begin{align*} 
  k_x - i\sqrt{\frac{B}{2}}(a + a^\dagger) |\phi_2\rangle & = E|\phi_1\rangle, \\
  k_x + i\sqrt{\frac{B}{2}}(a + a^\dagger) |\phi_1\rangle & = E|\phi_2\rangle.
\end{align*} \]

As before, we can take the first equation and plug it into the second. By using the commutator \([a, a^\dagger] = 1\), we finally arrive at
\[ \begin{align*} 
  k_x^2 + \frac{B}{2}(a^2 + (a^\dagger)^2 + 2a^\dagger a + 1) |\phi_2\rangle & = E^2 |\phi_2\rangle. \tag{35}
\end{align*} \]
Solving the equation (35) is complicated by the presence of terms of the form \( \sim a^2 \) and \( \sim (a^\dagger)^2 \), which render it anharmonic so that standard recipes for extracting the Landau levels are not applicable. For this reason, we adopt the Bargmann representation [36–38], which has been widely used in this scenario. Notably, this technique was applied to an anharmonic oscillator with a quartic potential [39] and the two-mode squeeze harmonic oscillator and the \( k \)-th-order harmonic generation [40]. In this representation, the ladder operators are related to a complex variable \( z \) according to
\[ a^\dagger = z, \quad a = \frac{d}{dz} \] \[ \tag{36} \]
whilst the wave function is a holomorphic function of \( z \) only, namely,
\[ |\phi_1\rangle = \varphi_1(z), \quad |\phi_2\rangle = \varphi_2(z). \tag{37} \]
Expressed in this formalism, Eq. (35) takes the form
\[ \frac{B}{2} \varphi_2'' + Bz\varphi' + \left[ \frac{B}{2}(z^2 + 1) + k_x^2 \right] \varphi_2 = E^2 \varphi_2, \tag{38} \]
where we have used the notation \( \varphi'_2 = \frac{d\varphi_2}{dz} \) and \( \varphi''_2 = \frac{d^2\varphi_2}{dz^2} \).

The trivial solution consists of a combination of two exponentials does not correspond to the Landau levels, and the energy \( E \) still appears as an arbitrary constant. To extract the nontrivial solutions, we need to introduce a change of variables of the form
\[ \varphi_2(z) = e^{-z^2/2} \psi_2(z). \tag{39} \]
The differential equation then takes the form
\[ \psi_2'' + \omega^2 \psi_2 = 0, \quad \text{with} \quad \omega^2 = \frac{2}{B}(k_x^2 - E^2). \tag{40} \]
The trivial solution consisting of a combination of two exponentials does not correspond to the Landau levels, and the energy \( E \) still appears as an arbitrary constant. To extract the nontrivial solutions, we need to introduce a change of variables of the form
\[ \rho = e^z \Rightarrow z = \ln \rho \tag{41} \]
which finally transforms the equation for \( \psi_2 \) into
\[ \rho^2 \frac{d^2\psi_2}{d\rho^2} + \rho \frac{d\psi_2}{d\rho} + \omega^2 \psi_2 = 0. \tag{42} \]
Now, we may find solutions of this equation as a polynomial in \( \rho \) of degree \( n \) by considering
\[ \psi_2(\rho) = \sum_{i=0}^{n} f_i \rho^i. \tag{43} \]
Plugging this into the equation we obtain an expression in terms of the coefficients of the expansion \( f_i \),
\[ \omega^2 f_0 + (1 + \omega^2) f_1 \rho + \sum_{i=2}^{n} (i^2 + \omega^2) f_i \rho^i = 0. \tag{44} \]
where $\psi$ wave function component

Since our assumption of a polynomial of degree $n$ implies $f_n \neq 0$, it trivially follows that $n^2 + \omega^2 = 0$, giving Landau levels with an energy

$$E_{\pm} = \pm \sqrt{\frac{1}{2} n^2 B + k_z^2},$$

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)

(45)
The Landau levels are given by

\[ E_{\pm} = \pm \sqrt{\frac{1}{2} \hbar^2 B + k_x^2 + \Delta^2}, \]

with the wave function components

\[ \phi_{1,\pm}(z) = \frac{c}{E_{\pm} - \Delta} \left( k_x - i \sqrt{\frac{B}{2 \hbar}} \right) e^{i n z^2/2}, \]
\[ \phi_2(z) = c e^{i n z^2/2}, \]

where \( c \) is a normalization constant.

In the symmetry-broken phase, the system becomes gapped, with Landau levels situated at finite energies, as seen in Fig. 7. The levels closest to the Fermi surface attain a gap of \( |\Delta| \) which is thus independent of the chirality.

### INTERFACE STATES

In the symmetric phase, the line-node semimetals exhibit metallic drum-head surface states [15], which are generalizations of the Fermi arcs that occur in the Weyl semimetals [1]. These states are stabilized by a combination of topology and symmetry in the sense that the states are topologically protected in a subspace generated by the symmetry. Once this symmetry is spontaneously broken, the lines are gapped out, and the edge states are no longer protected.

However, the symmetry-broken phase permits domain walls that interpolate between regions of different chirality, on which the symmetry-breaking term \( \Delta \) changes sign. This opens the possibility for metallic interface states that are bound to these topological defects. To model this scenario, we consider a domain wall described by

\[ \Delta = \Delta(y) = \begin{cases} 
\Delta_+, & y > 0 \\
\Delta_-, & y < 0 \\
0, & y = 0
\end{cases}, \]

where \( \Delta_+ > 0 \) and \( \Delta_- < 0 \) are constants.

To identify the interface states, we apply an analytical approach based on trial functions that has been applied to Fermi arcs within Weyl semimetals in semi-infinite systems [41, 42]. Since \( \Delta(y) \) is translation invariant in the \( \hat{x} \) and \( \hat{z} \) directions but not along \( \hat{y} \), it follows that \( k_x \) and \( k_z \) are good quantum numbers while \( k_y \) is not. Hence, we conduct the substitution \( k_y \to -i \partial_y \), which transforms the perturbed Hamiltonian into

\[ H(k_x, -i \partial_y, k_z, y) = k_x \sigma_x - i \partial_y \sigma_y + \Delta(y) \sigma_z. \]

Next, we introduce a trial wave function of the form

\[ \Psi(x, y, z) = \psi_\lambda(x, z) = \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} e^{-i \lambda y|x, z}. \]

Therefore, our problem is reduced to the eigenequation

\[ H(k_x, -i \partial_y, k_z, y) \Psi = E \Psi, \]

with a continuity condition at \( y = 0 \). The secular equation, \( \det[H(k_x, -i \partial_y, k_z, y) - E] = 0 \), may be used to find the possible values of \( \lambda \), namely,

\[ \lambda = \pm \sqrt{k_x^2 + \Delta^2 - E^2}. \]

Requiring the wave function to vanish at \( y \to \pm \infty \), we need to separate the two regions of different chirality into \( \Psi_+ \) for \( y > 0 \) and \( \Psi_- \) for \( y < 0 \). Then, we obtain

\[ \Psi_+ = c_+ \psi_{\lambda+} |x, z\rangle = c_+ \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} e^{\lambda y|x, z}, \]
\[ \Psi_- = c_- \psi_{\lambda-} |x, z\rangle = c_- \begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} e^{-\lambda y|x, z}, \]
where $c_{\pm}$ are constants whilst
\[ \lambda_{\pm} = \mp \sqrt{k_x^2 + \Delta_y^2 - E^2}. \] (67)

On the other hand, for the eigenstates, there are two possible sets of spinors $\psi^\pm = (\psi_x^\pm, \psi_y^\pm)^T$:
\[ \psi^\pm = \left( \frac{\lambda_{\pm} - k_x}{\Delta_y} \right) \text{ and } \psi^\mp = \left( \frac{\Delta_y + E}{\lambda_{\pm} + k_x} \right). \] (68)

Imposing that the solution is continuous at $y = 0$ we obtain
\[ c_+ \psi_+(y = 0, E) = c_- \psi_-(y = 0, E), \] (69)
or equivalently,
\[ c_+ \psi^+ - c_- \psi^- = 0. \] (70)

Thus, the condition (70) gives us a system of two equations with two unknowns, $c_+$ and $c_-$. Hence, to have a nontrivial solution, it is necessary that
\[ \det[\psi^+ - \psi^-] = 0. \] (71)

Imposing this condition on the eigenvectors defined by Eq. (68) and using Eq. (60) we find
\[ -(\lambda_+ - k_x)E + (\lambda_- - k_x)E = 0, \] (72)
\[ (\lambda_+ + k_x)E - (\lambda_- + k_x)E = 0, \] (73)
which reduces to
\[ \lambda_+ = \lambda_- = 0 \quad \Rightarrow \quad E = \pm k_x. \] (74)

Therefore, we obtain two localized states proximate to the interface $y = 0$ given by the wave functions
\[ \Psi_{\pm}(E = -k_x) = c_{\pm} \left( -\Delta_y - k_x \over \Delta_y + k_x \right) e^{-\Delta_y y} |x,z\rangle, \] (75)
\[ \Psi_{\pm}(E = k_x) = c_{\pm} \left( -\Delta_y + k_x \over \Delta_y + k_x \right) e^{-\Delta_y y} |x,z\rangle, \] (76)
where $c_{\pm}$ is the normalization. At $k_x = 0$ these meet at the Fermi level, implying a metallic interface state in the form of a line-node that is exponentially localized to the domain wall.

To solve the problem of interface states on a domain wall for a more realistic gap $\Delta$ which is continuous in $y$, it is generally necessary to apply numerical methods since the analytical technique introduced above cannot be applied when the gap has an explicit dependence on $y$. To obtain a numerically tractable problem in this scenario, we first conduct an inverse Fourier transform on $y$ and consider a finite system that can be diagonalized to find the possible surface states. For this purpose, we consider a Hamiltonian which is periodic in $k_y$ instead of its continuum equivalent:
\[ H = \sin k_x \sigma_x + \sin k_y \sigma_y, \] (77)

Explicitly writing the creation and annihilation operators, we find
\[ H = \sum_k \left[ \sin k_x (a_k^\dagger b_k + b_k^\dagger a_k) + i \sin k_y (a_k^\dagger b_k + b_k^\dagger a_k) \right]. \] (78)

The inverse Fourier transforms along the $\hat{y}$ direction takes the form
\[ a_k = \frac{1}{\sqrt{M}} \sum_j e^{-ik_y j} a_{k,j}, \quad b_k = \frac{1}{\sqrt{M}} \sum_j e^{-ik_y j} b_{k,j}, \] (79)
where $M$ corresponds to the number of layers in the $\hat{y}$ direction, $j$ is the layer index, and $k_{||}$ denotes the momentum parallel to the (010) surface. Thus, we obtain
\[ H = \sum_{k,j} \left[ \sin k_x c_{k,j}^\dagger \sigma_x c_{k,j} - \frac{i}{2} c_{k,j}^\dagger \sigma_y c_{k,j+1} \right. \] (80)
\[ + \left. \frac{i}{2} c_{k,j+1}^\dagger \sigma_y c_{k,j} \right], \] (81)
where we have defined
\[ c_{k,j} = (a_{k,j}, b_{k,j})^T. \] (82)

In this case, the symmetry breaking contribution to the full Hamiltonian may be written as
\[ H_{\Delta} = \sum_{k,j} \Delta(j) c_{k,j}^\dagger \sigma_x c_{k,j}, \] (83)
where the dependence on $y$ is translated into the layer label $j$. As before, we are interested in a perturbation $\Delta(j)$ that changes sign at $y = 0$. We consider the scenarios of both an even or odd number of layers. In the latter case we take $j_0 = \frac{1}{2}(M + 1)$ so that the middle layer $j_0$ corresponds to $y = 0$, implying that $\Delta$ vanishes at $y = 0$. We consider a linear perturbation ranging from $-\Delta_0$ to $+\Delta_0$, with $\Delta_0 > 0$ that is given by
\[ \Delta(j) = 2 \frac{j - \frac{1}{2}}{M - 1} \Delta_0 - \Delta_0. \] (84)

For an even number of layers, the gap function $\Delta$ given by (84) does not vanish anywhere since there is no center layer. In Fig. 8 we display the corresponding energy dispersion for the different states with $\Delta_0 = 1$ and a total number of layers $M = 51$, as a function of $k_x$ (note that the solution is independent of $k_z$). The states plotted in red exhibit a gap-closing point at $k_x = n\pi$, implying that a line node is present. To establish the spatial extent of the nodal states, we introduce the following metric
\[ \Pi(j) = \frac{|\psi_j|^2}{\Psi^\dagger \Psi}, \] (85)
where $\Psi = (\psi_1, \psi_2, \ldots, \psi_j, \ldots, \psi_M)^T$ is the wave function of the state. The metric (85) is shown in Fig. 9, revealing that the metallic interface state is exponentially localized to the center layer $j_0$. 
Figure 8. Metallic interface states situated at a domain wall that interpolates between different signs on the chiral order parameter. The energy levels correspond to a system with 51 layers in the $\hat{y}$-direction with a linear symmetry-breaking term given by Eq. (84). The red lines correspond to a family of solutions that are exponentially localized to the middle layer that exhibits a line node at $k_x = 0$.

Figure 9. Exponentially localized interface states. The blue curve presents the spatial extent of the localized states as defined by the metric (85). The red curve represents a fit of the form (86), displaying excellent agreement.

One may note that, after the introduction of $\Delta(j)$, the system is gapped in every layer but the one corresponding to $j_0$, where $\Delta(j_0) = 0$. It should therefore be expected that the interface states fall off as

$$\frac{1}{c_0} e^{-\Delta(j)(j-j_0)}, \tag{86}$$

where $c_0$ is a normalization constant. The red curve in Fig. 9 shows a fit of the form (86) with $c_0$ as a free parameter, revealing that there is an excellent agreement. The result for an even number of layers was found to be indistinguishable from the case of an odd number implying that the metallic interface states do not depend on details of the domain wall.

### SUMMARY

In conclusion, we have examined the stability of line-node semimetals in the presence of Coulomb interactions and found a chiral instability occurring at a finite interaction strength. The chiral order parameter exhibits a well-defined behavior in the limit of an infinite screening length despite the presence of infrared divergencies in this problem. By computing the Landau levels, we observe that an out-of-plane magnetic field couples to the chiral order parameter, implying that this degree of freedom can be controlled in experiments. While the drum-head edge states associated with line-node semimetals vanish in the chiral phase, we observe metallic interface-states in this regime, which exist on domain walls interpolating between regions of different chirality. These domain walls could conceivably be trapped on a sample with a concave geometry in experiments.

This work was supported by the Swedish Research Council (VR) through grant 2018-03882 and Stiftelsen Olle Engkvist via grant 204-0185. Computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at the National Supercomputer Centre in Linköping, Sweden. J. C. would like to thank Lars Fritz for important input and discussions.

[1] S. Jia, S.-Y. Xu, and M. Z. Hasan, Nature Materials 15, 1140 (2016).
[2] A.-Q. Wang, X.-G. Ye, D.-P. Yu, and Z.-M. Liao, ACS Nano 14, 3755 (2020).
[3] J. Ma, Q. Gu, Y. Liu, J. Lai, P. Yu, X. Zhao, Z. Liu, J.-H. Chen, J. Feng, and D. Sun, Nature Materials 18, 476 (2019).
[4] W. Han, Y. Otani, and S. Maekawa, npj Quantum Materials 3, 27 (2018).
[5] N. Kumar, Y. Sun, N. Xu, K. Manna, M. Yao, V. Süss, I. Leermakers, O. Young, T. Fürster, M. Schmidt, H. Borrmann, B. Yan, U. Zeitler, M. Shi, C. Felser, and C. Shekhar, Nature Communications 8, 1642 (2017).
[6] Y. Wang, E. Liu, H. Liu, Y. Pan, L. Zhang, J. Zeng, Y. Fu, M. Wang, K. Xu, Z. Huang, Z. Wang, H.-Z. Lu, D. Xing, B. Wang, X. Wan, and F. Miao, Nature Communications 7, 13142 (2016).
[7] Y. Sun, Y. Zhang, C. Felser, and B. Yan, Phys. Rev. Lett. 117, 146403 (2016).
[8] B. Singh, G. Chang, T.-R. Chang, S.-M. Huang, C. Su, M.-C. Lin, H. Lin, and A. Bansil, Scientific Reports 8, 10540 (2018).
[9] C. Fang, M. J. Gilbert, X. Dai, and B. A. Bernevig, Phys. Rev. Lett. 108, 266802 (2012).
[10] B. Bradley, J. Cano, Z. Wang, M. G. Vergniory, C. Felser, R. J. Cava, and B. A. Bernevig, Science 353 (2016), 10.1126/science.aaf5037.
[11] P. Tang, Q. Zhou, and S.-C. Zhang, Phys. Rev. Lett. 119, 206402 (2017).
[12] T. Bzdúšek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Solyanov, Nature 538, 75 (2016).
[13] T. czv Bzdúšek and M. Sigrist, Phys. Rev. B 96, 155105 (2017).
[14] G. Bian, T.-R. Chang, R. Sankar, S.-Y. Xu, H. Zheng, T. Neu- pert, C.-K. Chiu, S.-M. Huang, G. Chang, I. Belopolski, D. S.
Sanchez, M. Neupane, N. Alidoust, C. Liu, B. Wang, C.-C. Lee, H.-T. Jeng, C. Zhang, Z. Yuan, S. Jia, A. Bansil, F. Chou, H. Lin, and M. Z. Hasan, Nature Communications 7, 10556 (2016).

[15] G. Bian, T.-R. Chang, H. Zheng, S. Velury, S.-Y. Xu, T. Neupert, C.-K. Chiu, S.-M. Huang, D. S. Sanchez, I. Belopolski, N. Alidoust, P.-J. Chen, G. Chang, A. Bansil, H.-T. Jeng, H. Lin, and M. Z. Hasan, Phys. Rev. B 93, 121113 (2016).

[16] A. Yamakage, Y. Yamakawa, Y. Tanaka, and Y. Okamoto, Journal of the Physical Society of Japan 85, 013708 (2016), https://doi.org/10.7566/JPSJ.85.013708.

[17] L. S. Xie, L. M. Schoop, E. M. Seibel, Q. D. Gibson, W. Xie, and R. J. Cava, APL Materials 3, 083602 (2015), https://doi.org/10.1063/1.4926545.

[18] S. Kobayashi, Y. Yamakawa, A. Yamakage, T. Inohara, Y. Okamoto, and Y. Tanaka, Physical Review B 95 (2017), 10.1103/physrevb.95.245208.

[19] O. Vafek and K. Yang, Phys. Rev. B 81, 041401 (2010).

[20] B. Roy, P. Goswami, and V. Jurićić, Phys. Rev. B 95, 201102 (2017).

[21] B. Roy, Phys. Rev. B 96, 041113 (2017).

[22] M. V. Ulybyshev, P. V. Buividovich, M. I. Katnsnelson, and M. I. Polikarpov, Phys. Rev. Lett. 111, 056801 (2013).

[23] I. S. Tupitsyn and N. V. Proko'ev, Phys. Rev. Lett. 118, 026403 (2017).

[24] L. M. Schoop, M. N. Ali, C. Straßer, A. Topp, A. Varykhalov, D. Marchenko, V. Duppel, S. S. P. Parkin, B. V. Lotsch, and C. R. Ast, Nature Communications 7, 11696 (2016).

[25] Y. Shao, A. N. Rudenko, J. Hu, Z. Sun, Y. Zhu, S. Moon, A. J. Millis, S. Yuan, A. I. Lichtenstein, D. Smirnov, Z. Q. Mao, M. I. Katnsnelson, and D. N. Basov, Nature Physics 16, 636 (2020).

[26] K. Van Houcke, E. Kozik, N. Proko'ev, and B. Svistunov, Physics Procedia 6, 95 (2010).

[27] J. Carlström and E. J. Bergholtz, Physical Review B 97 (2018), 10.1103/physrevb.97.161102.

[28] R. Rossi, Phys. Rev. Lett. 119, 045701 (2017).

[29] R. Rossi, N. Proko'ev, B. Svistunov, K. V. Houcke, and F. Werner, EPL (Europhysics Letters) 118, 10004 (2017).

[30] J. Carlström, Phys. Rev. B 103, 195147 (2021).

[31] A. L. Fetter and J. D. Walecka, Quantum theory of many-particle systems (Dover Publications, 1971).

[32] J. Carlström, Phys. Rev. B 97, 075119 (2018).

[33] J. Carlström and E. J. Bergholtz, Phys. Rev. B 98, 241102 (2018).

[34] A. Giuliani and V. Mastropietro, Phys. Rev. B 79, 201403 (2009).

[35] V. Bargmann, Rev. Mod. Phys. 34, 829 (1962).

[36] V. Bargmann, Commun. Prue Appl. Math. 14, 187 (1961).

[37] V. Bargmann, Commun. Prue Appl. Math. 20, 1 (1967).

[38] F. T. Hioe and E. W. Montroll, Journal of Mathematical Physics 16, 1945 (1975), https://doi.org/10.1063/1.522747.

[39] Y.-Z. Zhang, Journal of Physics A: Mathematical and Theoretical 46, 455302 (2013).

[40] S.-B. Zhang, H.-Z. Lu, and S.-Q. Shen, New Journal of Physics 18, 053039 (2016).

[41] T. Ojanen, Phys. Rev. B 87, 245112 (2013).