Topological obstructed atomic limit by annihilating Dirac fermions

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We show that annihilating a pair of Dirac fermions implies a topological transition from the critical semi-metallic phase to an Obstructed Atomic Limit (OAL) insulator phase instead of a trivial insulator. This is shown to happen because of branch cuts in the phase of the wave functions, leading to non trivial Zak phase along certain directions. To this end, we study their $Z_2$ invariant and also study the phase transition using Entanglement Entropy. We use low energy Hamiltonians and numerical result from model systems to show this effect. These transitions are observed in realistic materials including strained graphene and buckled honeycomb group-V (Sb/As).

I. INTRODUCTION

There has been a slew of progress in the past years improving our understanding of topological phases. This has extended the possibility of having topologically non-trivial systems which were previously restricted to internal symmetries[1], to systems that are protected by crystalline symmetries[2,3]. Many new possibilities of Symmetry Protected Topological phases (SPT) were realized including multi-pole insulators[4], fragile insulators[5] and boundary obstructed topological phases[6]. Ref. [9] showed that by combining crystalline symmetries with underlying orbital symmetries, one can obtain a class of topologically non-trivial insulators called “Obstructed Atomic Limit” (OAL) insulators which are distinct from trivial “Atomic Insulators” (AI). OAL insulators are systems where Wannier Charge Centers (WCC) of the occupied band manifold are exponentially localized on Wyckoff positions that are distinct from the atomic positions. They thus cannot be adiabatically connected to a phase where the WCC are located at the atomic positions. This results in a dimerized insulating state.

These phases of matter often lead to charge fractionalization in co-dimensions $\geq 1$ because of the filling anomaly[10]. This may, in general, lead to extrinsic Higher Order Topologically Insulators (HOTT)[11, 12] i.e., systems where the occurrence of zero-energy corner states or gap-less hinge modes may depend on properties/symmetries of the boundary.

Meanwhile, Dirac systems are the classic example of a symmetry-protected gap-less topological phase. These are systems which have topological charge around nodal points stabilized by having Time Reversal Symmetry (TRS) along with a spatial symmetry. Apart from the ubiquitous example of graphene, we have recently shown that a slightly buckled honeycomb monolayer of As and Sb have Dirac nodes, protected by a $C_2$ twofold rotation and located along high symmetry lines, which can move along these line and annihilate in pairs[13]. There can also be states where the nodes are located on a general point in the Brillouin zone (BZ)[14].

These unpinned Dirac nodes can be gapped out without breaking TRS and the crystal symmetry protecting them by annihilating them in pairs of opposite topological charges at the Time Reversal Invariant Momenta (TRIM). There have been various artificial systems where this kind of merging has been observed, including the honeycomb Fermi gas[15, 16], in microwave experimental systems[17], and mechanical graphene[18]. It has also been shown that electronic 2D graphene[19], $\alpha$-(BEDT-TTF)$_2$I$_3$[20], phosphorene[21] also have this feature upon applying strain. More recently, we showed that 2D group-V buckled honeycomb systems (Sb,As) undergo the same transitions[13, 22] and interestingly we found that they undergo two different merging transitions.

In this paper, we show that topological Dirac semimetals necessarily undergo a transition to a topologically non-trivial OAL phase upon annihilating Dirac cones of opposite winding number. We start by looking at the low energy Hamiltonian describing the annihilation physics, after which we use the Zak phase to understand the topology of the system. We will then proceed to use symmetry indicators to find the topological classification and finally study the phases using the idea of Entanglement Entropy.
mirror/line invariant given by $\sigma$ by $\sigma_m$ing limit if $k$ Dirac point to move along
This symmetry is the key that protects and forces the $\sigma$ theory. (EE). Several examples are presented to illustrate the theory.

II. PHASE DIAGRAM OF ANNIHILATING DIRAC CONES

It was shown by G. Montambaux et al. \[19\] that the low energy Hamiltonian close to the annihilation of two Dirac cones takes the universal form

$$H(k) = \left( d + \frac{k^2}{2m_x} \right) \sigma_x + p_y k_y \sigma_y$$ \hspace{1cm} (1)

Here $m_x, p_y$ controls the effective mass (along $k_x$) and velocity (along $k_y$) directions. Close to annihilation, the system takes massless and massive dispersion along the directions $k_y$ and $k_x$ respectively. It is clear that $H$ obeys Time Reversal Symmetry (TRS), implying $H(k) = H^*(-k)$, has inversion symmetry ($I$) given by $\sigma_x H(k) \sigma_x = H(-k)$ and chiral symmetry ($C$) described by $\sigma_y H(k) \sigma_x = -H(-k)$. Finally, the system also has a mirror/$C_2$ ($M$) symmetry that leaves the entire $k_y = 0$ line invariant given by $\sigma_x H(k_x, k_y) \sigma_x = H(k_x, -k_y)$. This symmetry is the key that protects and forces the Dirac point to move along $k_x$. It has been shown \[19\] that the ground state solution can either be in: (i) the semi-metallic limit with two sets of oppositely wound Dirac cones at $\pm \sqrt{-2m_x}d$ if $m_x d < 0$, or (ii) the insulating limit if $m_x d > 0$. We show that the phase diagram of this Hamiltonian is much richer, as seen in Figure 1 Phases I and III, which were previously thought to be trivial insulators, in fact, belong to the class of OAL insulators. Figure 1 shows the phase diagram of $H(k, m_x, d)$. Phases I (III) correspond to an insulating state in bulk without (with) boundary states in the co-dimension=1 system. II (IV) are semi-metallic systems with two Dirac cones and edge states propagating outside (in-between) in their co-dimension=1 system.

The difference between these phases are encoded in the phase of their complex eigenstates. The eigenstates of Eq(1) are given by $|\pm\rangle = \frac{1}{\sqrt{2}} (1, \pm e^{i\theta(k)})$ where

$$\theta(k) = \tan^{-1} \left( \frac{p_y k_y}{d + k^2/2m_x} \right)$$ \hspace{1cm} (2)

and $|--\rangle, |--\rangle$ correspond to the lower and higher eigenvalue, which are

$$E_{\pm} = \mp \sqrt{(d + k_x^2/2m_x)^2 + k_y^2 p_y^2}$$ \hspace{1cm} (3)

Figure 2 shows the phase at each $k$ plotted together with the eigenvalues (central insert). For Phase II, the left two panels show the phase of the ground state $|--\rangle$ (in a1) and the excited $|--\rangle$ (in a2). Note that for Phase IV, the excited state $|+-\rangle$ is shown in (a1) and the ground state $|--\rangle$ (in a2), but both correspond to $m_x d < 0$, corresponding to the dispersion of two Dirac cones of opposite winding number. Close to $\pm k_0 = \pm \sqrt{-2m_x d}$, Eq.(1) can be expanded to $H(k) = \pm \frac{k_0}{2m_x} k_x \sigma_x + p_y k_y \sigma_y$ using $k_x = \pm k_0 + q_x$. These phases of the complex eigenstates describe surfaces in $k$ space which are nothing but Riemann surfaces \[23\] when viewing the $k_x, k_y$ as the real and imaginary part of a complex number $z = k_x + ik_y$, or rather they represent one principal branch of the Riemann surface.

To understand the mechanism better, we consider a complex holomorphic function $f(z) = (z - k_0)^{-1} - (z^* + k_0)^{-1}$. In the phases II and IV (Figure 2) i.e. in the Dirac cone limit, the complex eigenstate phases of Eq. (1) are the same as the phases of $\pm f(z)$, with $+$ referring to the cases (a1), (a2) respectively. As seen from Figure 2, the excited and ground state wave functions of Phase II in the semi-metallic phase have a branch cut along the intervals $(-k_0, +k_0)$ and $(-\infty, -k_0) \cup (k_0, +\infty)$ respectively, just as the $f(z)$ function. The excited and ground state phases are related by a phase shift of $\pi$ and the choice of branch cut picked up by each eigenstate is determined by the sign of $m_x$ and $d$. In the limit $k_0 \to 0$
one reaches the insulating state. This completely detaches the Riemann surface of one of the eigenstates and connects it to the next branch. This results in extending the branch cut from \((-\infty, \infty)\) for one of the wave function and closing the branch cut on the other as seen in Figure 2 \((a) \rightarrow (b)\).

To quantify the topology, one can calculate the Zak phase\([21][25]\) along the \(j^{th}\) direction, which for each band \(n\) is given by
\[
\gamma_n^j = -i \int_0^{2\pi} \langle u_{nk} | \frac{\partial}{\partial k} | u_{nk} \rangle dk
\]
where \(|u_{nk}\rangle\) is the lattice-periodic part of the wavefunction of \(n^{th}\) band. We can also write this in terms of the Wannier Charge Centers (WCC), \(x_n^i\), defined by
\[
\gamma^i = 2\pi x_n^i
\]
and the total Zak phase is
\[
\gamma = \sum_n \gamma_n^j
\]
It is easy to see that the Zak phase along a given direction becomes necessarily non-vanishing when it crosses through a phase discontinuity. This can happen when the phase continues to the next complex branch by having a branch cut as we discussed above.

From the previous discussion, \(\gamma_n^j(k_x) = 0\) everywhere except for the points passing through the branch cut. For example, in the semi-metallic case, based on the values of \(m\) and \(d\), one gets a non trivial Zak phase either inside or outside the Dirac cones. Once the parameters are tuned to reach either of the insulating phases I/III, one obtains a Zak phase of \(\pi\) or \(0\) at all values of \(k_x\). Non-trivial Zak phase along this direction indicates a non trivial 1D topology along this path which results in a surface spectrum in co-dimension \(\geq 1\). It should be noted that although the existence of surface states in the OAL limit is topologically guaranteed, the protection is not. The protection stems from the underlying symmetry of the surface termination\([26]\).

Analogous to the Su–Schrieffer–Heeger (SSH) model\([27]\), the effect of non trivial Zak phase can be captured using the symmetry indicators at the high symmetry points. For the present case of a Dirac annihilating system, we start by looking at the different symmetry groups that are preserved throughout the BZ. A band crossing at a generic point along high symmetry line \((l)\) is protected by a symmetry \(g \in G_l\) (\(G_l\) is the little group along \(l\)) which is preserved throughout the high symmetry line. Hence, the only way to gap this kind of system is to annihilate the opposite winding band crossing points with each other at a TRIM High Symmetry Point (HSP) \((P)\). This point would have a higher symmetry with \(g \in G_l \subset G_P\). Before the annihilation at the HSP, the bands are made up of two distinct irreducible representations (irreps), say \(A, B\) and along the high symmetry line, by \(a\) and \(b\). Because of compatibility, \(a\) and \(b\) need to have different parity eigenvalue given by \(+, -\). Another way to see this is to realize that, at the transition point occurring at the HSP, the two bands have a massless dispersion along one direction and thus need to have different inversion eigenvalue in order for the bands to be degenerate.

This parity switching is not accidental and is deeply connected to the Zak phase (or polarization) of the system. For an inversion symmetric system, one can re-write the Zak phase along a given direction \(i\) connecting \(X_1\) and \(Y_i\) by \(\pi x_i\) \([26][20]\) where \(x_i\) is
\[
(-1)^{\chi_i} = \prod_{j \in \text{occ.}} \frac{\eta_j(X_i)}{\eta_j(Y_i)}
\]
\[\eta_j(X_i)\] is the parity eigenvalue of the \(j^{th}\) band at \(X_i\). Here, \(\chi_i\) is a quantized \(\mathbb{Z}_2\) invariant. The derivation of the invariant using the sewing matrix theory is given in Appendix A. It is trivial to see that one can construct a \(\mathbb{Z}_2\) invariant \(\zeta\) given by
\[
(-1)^{\zeta} = \prod_{j \in \text{occ.}} \eta_j(\Gamma)\eta_j(X_1)\eta_j(M)\eta_j(X_2),
\]
which distinguishes between Phase I/III (gapped) and II/IV (gapless).

The possible parity changes at four HSP in an example 2D Brillouin zone are illustrated in Fig. 3(a). Starting with phase I, we have all the eigenvalues trivially equal to each other. Without any parity inversion, this gapped system is in the “trivial OAL” limit with no edge states. For Phase III, we have 2 constitutive inversions that have happened leading to a gap being opened up. These configurations along with \([3]\) can be used to determine whether edge states exist along each direction. For example, in the first configuration of Phase III shown in Figure 3(a2), we have \(\Gamma = X_1 = -1\) while \(X_2 = M = +1\), leading to non-trivial winding throughout the BZ where cut along \(b_1\) which again leads to non-trivial Zak phase throughout the system and thus an edge state. Distinguishing Phase II and IV turns out to be more subtle and requires knowledge about the position of gapless crossing as shown in Figure 3(b)/(c). For example, \(\Gamma = M = X_2 = +1\) and \(X_1 = -1\) can correspond to both Phase II or IV depending on the position of the Dirac cone which is shown as a black cross either along \(M - X_1\) in Phase IV or along \(\Gamma - X_1\) in Phase II.

Figure 3(b1) shows one such configuration of parities which can be created by two crossing scenarios. In (b1), we have created a symmetry protected crossing along \(X_1 - M\) which changes the parity at \(X_1\). This creates a non trivial Zak phase along \(\Gamma - X_1\), the effect of which can be seen on the corresponding 1D edge states when projected onto the \(b_2\) direction and thus leads us to phase IV. The band structure of this 1D system is schematically shown in (b3). This is in contrast to the cut along the \(b_1\) direction, where one would just see the Dirac crossing projected onto \(X_1\).

The same configuration shown in (b1) can be devised from a protected crossing along \(\Gamma - X_1\) which is shown in (c1). This now creates a non-trivial Zak phase along \(X_1 - M\). Following the same procedure, the resulting edge states are shown in (c2) (phase II) and (c3). One could move this protected crossing along \(X_1 - \Gamma\) and annihilate them at \(\Gamma\) which in-turn switches the parity at \(\Gamma\). This leads us to a configuration given by \((\Gamma, X_1, M, X_2) = (-, -, +, +)\) which results in phase III.
FIG. 3: (a) Possible combinations of parity eigenvalues for different phases. (b)/(c) Distinguishing phase II and IV based on position of Dirac cone and corresponding edge states. (b1)/(c1) shows the possible positions of Dirac crossing for the same parity arrangement. (b2)/(c2) show their respective 1 dimensional band structure when the system is cut along $b_2$ direction while (b3)/(c3) shows the same edge spectrum when cut along $b_1$ direction.

where now there is a non trivial Zak phase along both $X_1 - M$ and $\Gamma - X_2$. Similarly, annihilating the Dirac crossing at $X_1$ instead of $\Gamma$ leads to a switch in parity at $X_1$ resulting in a trivial phase i.e. phase I.

III. PHASE TRANSITIONS AND ENTANGLEMENT ENTROPY

A key concept relating the different phases described above is that of dimerization which can be probed using entanglement. Entanglement has been used to understand topological phases of various systems, including QSHI [28], Chern insulators [29] and topological insulators [30–32] and recently even for higher order topological systems [33] and topological phase transitions [34] in such systems. This is done by calculating the entanglement spectrum (ES) of the system.

Given a ground state wavefunction of a system $\Psi_{GS}$, one can spatially separate it into two parts $A$ and $B$. Then the entanglement spectrum is the eigen-spectrum of the the correlation matrix

$$C_{ij}^A = \text{Tr} (\rho_A c_i^A c_j^\dagger)$$

where $c_i^A/c_i^\dagger$ are the annihilation/creation operators and the density matrix $\rho_A$ restricts them to the $A$-part of the system, for sites $\in A$. The entanglement eigen-spectrum $\xi$ of $C$, for our system cut along $\vec{a}$, is dependent on $k_\perp$ for a cut of the system along $k_{||}$, where $\perp$ and $||$ are defined with r.t $\vec{a}$. In the thermodynamic limit, most of the eigenvalues lie exponentially close to 0 and 1 [36] while a value of $\frac{1}{2}$ captures the physics of the maximally entangled zero mode.

Using $\xi_i(k_\perp)$, one can define the entanglement entropy (EE) as

$$S = - \int_{BZ} dk_\perp \sum_i [\xi_i(k_\perp) \log \xi_i(k_\perp) + (1 - \xi_i(k_\perp)) \log (1 - \xi_i(k_\perp))]$$

$S$ measures the mean degree of entanglement between the given spatial split with value ranging from 0 to 1 with 1 being maximally entangled. One can see from the co-dimension=1 spectrum that the phases II, IV would have contribution to entangled states for some values of $k_\perp$, while III would be maximally entangled throughout the BZ. From Eq.(7), this results in

$$S_\alpha = \begin{cases} 0 & \alpha = I \\ 0 < S_\alpha < 1 & \alpha \in \{II, IV\} \\ 1 & \alpha = III \end{cases}$$

As an example to illustrate the entanglement spectrum, we pick strained anisotropic graphene. The details of that model are explained in Sec. IV C. In Fig. 4(a) we show the entanglement entropy $S$ for anisotropic graphene along four paths moving between the different phases. These changes are obtained by linearly varying
FIG. 4: (a) Entanglement entropy $S$ through the path shown in the inset for strained graphene (b) $\partial S$ (black) and $\partial^2 S$ (red) for the corresponding path in (a) ($S$ is shown in the background as a dashed line for clarity). (c) $S$ and (d) $\partial S$ throughout the parameter space for strained graphene, black and white lines in left and right panel show the transition points from semi-metal to insulator in bulk.

IV. EXAMPLES

In this section, we show various model systems where these phases can be observed. IV A illustrates the transition in 1D while IV B and IV C introduces 2D systems.

A. 1D Example

We start by looking at the 1D SSH system given by

$$\mathcal{H}_{SSH} = (t_1 + t_2 \cos(k)) \sigma_x + t_2 \sin(k) \sigma_y$$

(9)

This system, at half filling is metallic for $t_1 - t_2 = \delta = 0$ with a Dirac dispersion and has an insulating phase on either side of the $\delta$. Based on the sign of $\delta$ the system can either be in OAL or not and this choice precisely describes if the system dimerizes within or outside the unit-cell. This system thus undergoes a phase transition from I to III when crossing the origin at $\delta = 0$. This can be seen by expanding $\mathcal{H}_{SSH}$ near the vicinity of the Dirac point, where it reduces to $(t_1 - t_2) \sigma_x + t_2 k \sigma_y$ which is nothing but the projection of (1) onto the $k_y$ axis. This can also be seen by computing the entanglement entropy, where one sees a first order divergence with $\delta$ being the order parameter as shown in Figure 5. This is similar to the transition seen in Sec. III from phase I to III.

FIG. 5: $S$ (green) and $\partial_\delta S$ (red) for $\mathcal{H}_{SSH}$

Though this is not an example of moving annihilation where the Dirac fermions move in k-space as a function of tuning parameters, this annihilation happens by mixing Dirac fermions from the 1$^{st}$ BZ and 2$^{nd}$ BZ by doubling a single atom unit cell and folding the BZ.

B. 2D Example: criss-crossed SSH

Moving to 2D, we here present a simple model in which we can move the Dirac points. It is a simple extension of the SSH model that we dub criss-crossed SSH or CC-SSH and is shown in Figure 6 (left), which indicates the hopping integrals between sites used in the model.

Because of the bipartite nature of the CCSSH model, the Hamiltonian can be written:

$$\mathcal{H}(\mathbf{k}) = h_x(\mathbf{k}) \sigma_x + h_y(\mathbf{k}) \sigma_y$$

(10)

where

$$h_x(\mathbf{k}) = t_1 + t_2 \cos(k_y) + 2t_x \cos(k_x)$$

(11a)

$$h_y(\mathbf{k}) = t_2 \sin(k_y)$$

(11b)

Eq (11a) is almost identical to the SSH Hamiltonian but with an added $t_x$ interaction that is patterned in
a criss-crossed fashion. It is easy to see that the system has Time Reversal Symmetry (TRS) giving us \( \mathcal{H}(k) = \mathcal{H}(-k) \), has inversion symmetry (\( \mathcal{I} \)) given by \( \sigma_z \mathcal{H}(k) \sigma_x = \mathcal{H}(-k) \) and chiral symmetry (\( \mathcal{C} \)) as \( \sigma_x \mathcal{H}(k) \sigma_x = -\mathcal{H}(k) \). Finally, the system also has a Mirror/\( C_2 \) (\( \mathcal{M} \)) symmetry that leaves the \( k_y = 0 \) line invariant and is given by \( \sigma_y \mathcal{H}(k_x, k_y) \sigma_y = \mathcal{H}(k_x, -k_y) \).

Figure 6 shows the band structure for values of the \( t \)-parameters chosen ad-hoc to represent various phases mentioned in the main text along with \( \log(E_1 - E_2) \) to show the occurrence of unpinned Dirac points in the BZ. The values used are given in Table I. As always, because of Time Reversal Symmetry (TRS), we are guaranteed a Dirac cone of opposite winding number at \(-k\) for each \( k \). This system can be tuned to realize various phases taken in the text as shown in Figure 7 with \( t \)'s chosen to provide an example of the discussed phases. We show the bulk band structure with the Dirac cone and the gapped system along with the 1D band structure.

We now discuss Fig. 7 systematically. On the left we consider the chiral case, on the right, the changes due to breaking the chirality. On the left there are four panels each corresponding to the indicated phase. Within each panel, we show the bulk band structure at the top, followed by the band structure of a nanoribbon broken along one direction (second row, left) the full 2D band structure on a log-scale to identify the Dirac points (red) and finally, in the third row, the phases of the wave function plots. These branch cuts correspond to non trivial winding through their corresponding perpendicular \( k \).

Now let us look at this as a concrete example of the symmetry indicators used in the main text. Using our inversion matrix given by \( \sigma_x \), we can get the inversion eigen value of half filled system at TRIM points by computing \( \text{sgn}[t_1 + t_2 \cos(k_y) + 2t_x \cos(k_x)] \) for \( (k_x, k_y) = (\Gamma, X_1, M, X_2) = (0, 0), (0, \pi), (\pi, \pi), (\pi, 0) \). The values are shown in Table I. To make the transition clearer, we show in Figure 8 the dynamics of parity values close to trivial and non trivial transitions (Note the linear and quadratic dispersion at the transition point in the middle panels).

Next, we elucidate the role of chiral symmetry in the system. All the examples mentioned above respect chiral symmetry with \( \sigma_x \) being the chiral operator. This leads to the formed surface states being degenerate throughout the co-dimension \( \geq 1 \) system as seen on the left side of Figure 7. As it turns out, this is not a necessary condition for the surface protection. This can be easily seen by the fact that our invariants (and hence branch cuts) are unchanged with addition of a chiral breaking \( \sigma_z \) term and solely depends on \( \sigma_x \). To show this we explicitly break the chiral symmetry by adding a term such as \( 2t_x \cos(k_x) \sigma_z \). Figure 7(right) shows the surface spectrum where we have broken the chiral symmetry. It is easy to see that this does not nullify the existence of edge state, but rather breaks the degeneracy of the edge state that is guaranteed by chiral symmetry. This breaks it everywhere except at the point \( k = \pi(0) \) in case of an odd (even) chiral term as the term goes back to 0 giving back locally the chiral symmetry. Thus this leads to an interesting strong crystalline topological insulator state protected by inversion symmetry. This model is extremely similar to the example proposed by Ref.2.

C. Anisotropic Graphene

This system is shown in Figure 9(a) and the Hamiltonian is given by \( \mathcal{H} = h_x(k) \sigma_x + h_y(k) \sigma_y \) with

\[
\begin{align*}
   h_x(k) &= -\sum_{i=1}^{3} t_i \cos(\delta_i \cdot k) \\
   h_y(k) &= -\sum_{i=1}^{3} t_i \sin(\delta_i \cdot k)
\end{align*}
\]

where \( \delta_1 = \left( \frac{\sqrt{3}}{3}, 0 \right), \delta_2 = \left( -\frac{\sqrt{3}}{6}, \frac{1}{2} \right), \delta_3 = \left( -\frac{\sqrt{3}}{6}, -\frac{1}{2} \right) \) in Cartesian coordinates and \( t_i \) the anisotropic interac-
FIG. 7: (left) Bulk Band structure, Edge spectrum, \( \log(E_2 - E_1) \), and phase of \( \Psi_1 \) and \( \Psi_2 \) for phase I,II,III,IV given in text with parameters shown in Table I. (right) phase IV \( \rightarrow \) IVa and III \( \rightarrow \) IIIa upon breaking chiral symmetry but preserving inversion.

| Phase | \( t_x \) | \( t_1 \) | \( t_2 \) | \( t_c \) | \((\Gamma, X_1, M, X_2)\) |
|-------|---------|---------|---------|---------|-----------------|
| I     | -0.5    | 3.0     | 1.0     | 0       | (+,+,+,+)       |
| II    | 0.5     | 1.0     | 1.0     | 0       | (+,+,\,-,+)     |
| III   | -0.5    | 1.0     | 3.0     | 0       | (+,\,-,\,-,+)  |
| IV    | -0.5    | 1.0     | 1.0     | 0       | (+,\,-,+,+)     |
| IIIa  | -0.5    | 1.0     | 3.0     | 0.5     | (+,\,-,\,+)    |
| IVa   | -0.5    | 1.0     | 1.0     | 0.5     | (+,\,-,+,+)    |

TABLE I: Parameters used in Figure 7 along with \( \eta(k) \) \( \forall k \in \text{TRIM} \)

Note that for \( t_1 = t_2 = t_3 \) we are reduced to isotropic graphene. The well-known 2D band structure of that case is here shown in Figure 9 on the right of the top row. The color plot on a log-scale of the band structure as function of \( k \) in the \((k_x,k_y)\)plane clearly shows the location of the Dirac cones on the corners of the hexagonal Brillouin zone. Some of the important results regarding the entanglement entropy of this system were already shown in Sec. III. In that case we picked \( t_3 = 1 \) for simplicity although in this section we will consider more general choices of hopping parameters. It can be shown that
FIG. 8: Transition to OAL by annihilating Dirac points. + and − represents the parity eigenvalues (top) trivial phase (I) where the system annihilates the points at Γ (bottom) Non-trivial phase (I) where the system annihilates the points at $X_2$

for $t_3 = 1$ when the condition

$$|t_1 - 1| \leq |t_2| \leq |t_1| + 1$$

(14)

is satisfied, one is guaranteed to find Dirac points at $\pm k$ where $\pm k$ is the solution of

$$\cos (a_1 \cdot k) = \frac{1 - t_1^2 - t_2^2}{2t_1t_2}$$

$$\cos (a_2 \cdot k) = \frac{t_2^2 - t_1^2 - 1}{2t_1}$$

(15)

$$\cos ((a_1 - a_2) \cdot k) = \frac{t_2^2 - t_2^2 - 1}{2t_2}$$

where $a_1, a_2$ are the lattice vectors. More generally, the four band structure panels in Figure 9 show the finite width nanoribbon band structures of the model for different phases in the phase diagram as determined by the chosen hopping parameters, which are given in Table II.

**TABLE II: Parameters used in Figure 9**

| Phase | $t_1$ | $t_2$ | $t_3$ |
|-------|-------|-------|-------|
| I     | 1     | 1     | 3     |
| II    | -1    | 1     | 1     |
| III   | 1     | 3     | -1    |
| IV    | 1     | 3     | -1    |

In Sec. III the path chosen for the entanglement entropy is an interpolation between the lines connecting these parameter values in hyper-parameter space. Once again, one can easily verify the validity of the symmetry indicator by calculating the inversion eigenvalue at $\Gamma, X_1, M, X_2$ marked in the figure. Similarly, the annihilation transition in a honeycomb lattice made up of $p_x - p_y - p_z$ is observed when one buckles the honeycomb lattice by moving from $D_{6h}$ to $D_{3d}$ where one still gets movable Dirac points preserved by $C_2$ symmetry which has two annihilation transitions at $C_2$ symmetry which leads to the phase III.

**V. CONCLUSION**

We have shown that the annihilation of Dirac fermions, which can be described by a universal Hamiltonian leads to non-trivially gapped systems. The annihilation dynamics has a rich phase diagram with phases distinguishable by the path dependent Zak phase. We showed that two of the phases correspond to the Obstructed Atomic Limit insulators while the other two are semi-metallic. These phases have vastly different ground state wave functions in the corresponding co-dimension $\geq 1$ system. We showed the effect of transitions between these phases on their entanglement entropy. These transitions can be realized in realistic systems like 2D buckled honeycomb Sb or As, strained graphene, as well as in artificial systems. Moreover, since this is a universal property of an-
nihilation, with the recent extension of atomic obstruction to superconductors,[39] this should in principle also be applicable for more exotic 2D superconducting Dirac systems.[40]

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Appendix A: Zak Quantization

In the presence of inversion symmetry, one can calculate the quantized polarization/Zak phase by looking at the parity eigenvalue at the TRIM points[41]. With the Berry connection defined as \( \mathbf{A}_{ij}(k) = -i \langle u_i(k) | \partial_{k_i} | u_j(k) \rangle \), the polarization along the \( i \)th direction is defined as

\[
\begin{align*}
P_i &= \frac{1}{2\pi} \sum_{j=1}^{\text{occ}} \int_{-\pi}^{\pi} dk_1 dk_2 \mathbf{A}_{ij}^i(k) \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_1 dk_2 \text{Tr} \left[ \mathbf{A}_{ij}^i(k) \right]
\end{align*}
\]

Now we use the fact that we have a symmetry that leaves a line in \( k \) space invariant (as our Dirac point moves to annihilate). Without loss of generality, we call it mirror symmetry (although it could be a twofold rotation \( C_2 \) as well) and we denote the mirror operator by \( M \) (and \( \mathcal{M} \) in \( k \) space), we construct the sewing matrix \( \mathbf{B}_M \) as

\[
(B_M)_{ij}(k) := \langle u_i(Mk) | \mathcal{M} | u_j(k) \rangle
\]

Applying the mirror operation to (A1b) we get

\[
P_i = \frac{1}{2} \chi_i
\]

Where \( \chi_i = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk_1 dk_2 \text{Tr} \left[ (B_M)^i(\mathbf{M}) \partial_{k_i} B_M(k) \right] \).

Since \( (B_M)^i \) is unitary, we can rewrite

\[
\text{Tr} \left[ (B_M)^i \partial_{k_i} B_M(k) \right] = \partial_{k_i} \log(\det[(B_M)^i(k)])
\]

Using the fact \( \partial_{k_i} \log(\det[(B_M)^i(k_1, 0)]) = \partial_{k_i} \log(\det[(B_M)^i(-k_1, 0)]) \), we can now calculate the winding number of the sewing matrix along direction \( k_1 \) at \( k_2 = 0 \)

\[
\chi_1^{(i)} = \frac{i}{2\pi} \int_{-\pi}^{\pi} dk_1 \partial_{k_1} \log(\det[B_M(k_1, 0)])
\]

The last step is trivial when one notices that the eigenvalue of the \( \mathcal{M} \) operator is \( \pm 1 \) and thus \( \det[B_M(k)] = 1 \) means that we have \( \chi_i \) is constant under \( k_2 \) over a smooth gauge[42]. (A5d) is true \( \forall k_2 \). This can be rewritten to get us back to the equation in the main paper given by

\[
\prod_{j \in \text{occ.}} \eta_j(k).
\]

Finally as \( \chi_i \) is constant under \( k_2 \) over a smooth gauge, (A5d) is true \( \forall k_2 \). This can be rewritten to get us back to the equation in the main paper given by

\[
\ln(e^{-i\pi\chi_i}) = \ln \prod_{n \in \text{occ.}} \frac{\eta_n(X_i)}{\eta_n(\Gamma)}
\]

The same procedure can be used to obtain \( \chi_2 \).

As noted in Ref.[22] this can be seen intuitively too as follows. In the presence of Mirror/\( C_2 \) symmetry, we have \( \mathcal{M}H(k_x, k_y)\mathcal{M} = H(-k_x, k_y) \). It is easy to check that at TRIM points both inversion and \( \mathcal{M} \) symmetry map back the \( k \)-points to itself and thus they both make a good quantum number for the system at TRIM points. This means that we have \( |H(k_i)|, \mathcal{M}/\mathcal{T} = 0 \forall k_i \in \text{TRIM} \), thus as described in the main text, when the Dirac points meet at one of these TRIM points, they exchange their
parity eigenvalue creating an inversion or lack thereof. This entire proof, though it was here given specifically for 2D systems, can be generalized for 3D systems and indeed gives more interesting results as one can have two kinds of symmetries that cause protected semimetals: 1) line-invariant symmetries i.e. symmetries that leave a line in k-space invariant (e.g. $C_2$), or, 2) plane invariant symmetries (e.g. Mirror) and thus one could have nodal loops closing in and Dirac/Weyl semimetals annihilating. Further work to study these systems is needed.

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