Topological Superconductivity in Dirac Honeycomb Systems

Kyungmin Lee*, Tamagagna Hazra*, Mohit Randeria, and Nandini Trivedi
Department of Physics, Ohio State University, Columbus, Ohio 43210, USA

We examine superconducting states of gapped Dirac honeycomb systems and outline a novel route to topological superconductivity. We consider the Kane-Mele model and explore the effect of three different interactions – on-site attraction $U$, nearest-neighbor density-density attraction $V$ and nearest-neighbor antiferromagnetic exchange $J$ – within self-consistent Bogoliubov-deGennes theory. We find rich phase diagrams with several exotic phases, including two topological states with finite center-of-mass momentum pairing, one with and one without time-reversal invariance. We argue that the topological states emerge naturally from pairing within a Dirac cone, which is allowed only with $V$ and not with the other interactions. We also discuss the possible relevance of our results to transition metal dichalcogenides and to cold atom experiments.

I. INTRODUCTION

There has been considerable excitement about the search for topological superconductors in recent years. Signatures of topological superconductivity have been observed in one-dimensional chains with proximity-induced superconductivity [1, 2], chiral two-dimensional superconductor Sr$_2$RuO$_4$ [3, 4], and more recently in doped topological insulators with intrinsic superconductivity such as Cu$_4$Bi$_2$Se$_3$ [5] or Sn$_{1-x}$In$_x$Te [6].

Gapped Dirac electrons effectively describe the low energy physics of transition metal dichalcogenide (TMD) materials like MoS$_2$ and WS$_2$ [7], where superconductivity arises intrinsically below ~10K [8–10], though in this case it appears that these are trivial superconductors. Other TMD materials like 1T$'$-WTe$_2$ exhibit gapless edge states, suggesting that they are topological insulators [11]. These have also been reported to be superconducting [12, 13]. Whether they are topological, however, is still unclear.

Recently, magic angle twisted bilayer graphene [14] has emerged as a model system for understanding superconductivity in the strongly correlated regime. It has been shown [15–17] that, despite the concentration of charge density on a triangular lattice, the low energy physics is that of a Dirac honeycomb system.

With these motivations, we examine the superconducting states that emerge in the Kane-Mele model [18] as a result of various interactions. This is the archetypal model on a honeycomb lattice that exhibits a transition from a topological to a trivial insulator as a function of spin-orbit coupling [see Fig. 1]. What are the superconducting instabilities of this gapped Dirac system? Under what conditions do we get topological superconducting states? These are the primary questions we address in this paper.

We use self-consistent Bogoliubov-deGennes theory to map out the phase diagrams of the Kane-Mele model with three different types of interactions, and analyze the topological invariants associated with the resulting superconducting phases. With an on-site interaction, we always find a trivial s-wave superconductor, irrespective of whether the parent insulator is trivial or topological [see Fig. 2(a)].

Nearest-neighbor density-density attraction leads to a much richer phase diagram, with four exotic triplet states, all with finite center-of-mass momentum pairing [see Fig. 2(b)]. Two of these states are topological, a time-reversal symmetric helical superconductor and a chiral superconductor that breaks time-reversal. These topological states involve paring within the same Dirac cone, and are stabilized when the underlying band structure is close to the transition between the topological and the trivial insulating phases.

With antiferromagnetic nearest-neighbor interaction, we find exotic singlet states with broken rotation, translation and time-reversal symmetries, however, none of these states are topological [see Fig. 2(c)].

In the final section, we compare our results with previous theoretical works on superconductivity in transition metal dichalcogenides, and also comment on the implications of our results for cold atom experiments.

II. KANE-MELE MODEL WITH INTERACTIONS

To study the pairing instability of a two-dimensional Dirac system across the topological phase transition between topological and trivial insulating phases, we take the Kane-Mele model as the underlying band structure [18]:

$$H_{KM} = -t \sum_{\langle i,j \rangle} \psi_i^\dagger \psi_j - \mu \sum_i \psi_i^\dagger \psi_i - i \lambda_{SO} \sum_{\langle i,j \rangle} v_{ij} \psi_i^\dagger \sigma_j^x \psi_j + m_{AB} \sum_i \zeta_i \psi_i^\dagger \psi_i$$

(1)

where $\psi_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$ is the electron creation operator at site $i$, and $\langle \cdots \rangle$ and $\langle \cdot, \cdot \rangle$ represent nearest-neighbor and next-nearest-neighbor pairs of sites. Here, $t$ is the nearest-neighbor hopping amplitude, $\mu$ the chemical potential, $\lambda_{SO}$ the strength of Ising spin-orbit coupling, with $v_{ij} = \text{sgn}(\hat{z} \cdot (\mathbf{v}_1 \times \mathbf{v}_2))$ where $\mathbf{v}_1$ and $\mathbf{v}_2$ are nearest-neighbor vectors that connect an electron hop from site $i$ to site $j$, and $m_{AB}$ the sublattice potential, with $\zeta_i = 1 (-1)$ if the site $i$ belongs to the sublattice $A$ ($B$).

**Symmetry and topology:** The topology of a non-interacting (or mean-field) Hamiltonian is character-
Interactions: The purpose of our calculation we have chosen the transition for all values of $x$ for the other Dirac cones remains constant at $E$. The mass of the Dirac cones in each valley being massless. The mass of the non-interacting Kane-Mele model defined in Eq. (1). The blue hexagon marks the $\Gamma$ point in the reduced Brillouin zone. The color of the curves indicate the sign of the Berry curvature: In each spin sector, the signs of the topological insulator phase. The color of the curves is varied between (c) $0 \leq x < 1/2$ in the trivial insulator phase, (d) $x = 1/2$ at the topological transition, and (e) $1/2 < x \leq 1$ in the topological insulator phase. The color of the curves indicates the sign of the Berry curvature at $K$ and $K'$ are opposite in the trivial phase, and the same in the topological phase. At the topological transition ($x = 1/2$), there is a single Dirac cone in each spin sector in the corresponding valley.

FIG. 1. (a) Honeycomb lattice on which the Hamiltonian in Eq. (1) is defined. The blue hexagon marks the $\sqrt{3} \times \sqrt{3}$ supercell used in our study, which allows pairing with finite center-of-mass crystal momentum $K$ and $K'$ of Cooper pairs in addition to $\Gamma$. (b) Brillouin zone of the honeycomb lattice. The inner blue hexagon represents the reduced Brillouin zone of the supercell; both $K$ and $K'$ defined for the original Brillouin zone are folded to the $\Gamma$ point in the reduced Brillouin zone. (c)-(e) Dispersions of the non-interacting Kane-Mele model defined in Eq. (1). The solid (dashed) curves show the dispersion of electrons with spin up (down). The parameter $x = 3\sqrt{3}l_{SO}/(m_{AB} + 3\sqrt{3}l_{SO})$ that represents the relative strength of the Ising spin-orbit coupling is varied between (c) $0 < x < 1/2$ in the trivial insulator phase, (d) $x = 1/2$ at the topological transition, and (e) $1/2 < x \leq 1$ in the topological insulator phase. The color of the curves indicate the sign of the Berry curvature: In each spin sector, the signs of the Berry curvature at $K$ and $K'$ are opposite in the trivial phase, and the same in the topological phase. At the topological transition ($x = 1/2$), there is a single Dirac cone in each spin sector in the corresponding valley.

Hamiltonian $H_{KM}$ with three different types of interactions: (1) attractive on-site interaction $-U \sum_i n_i c_i^\dagger c_i$, (2) attractive nearest-neighbor density-density interaction $-V \sum_{ij} n_i n_j$, or (3) antiferromagnetic nearest-neighbor Heisenberg interaction $-J \sum_{ij} \sigma_i \cdot \sigma_j$, where $n_i \equiv c_i^\dagger c_i$, $n_i \equiv \psi_i^\dagger \psi_i$, and $\sigma_i^\dagger \psi_i \sigma_i$ for $\mu = x, y, z$. In each case, we decouple the interaction in the pairing channel and find the Bogoliubov-de Gennes ground states. We have also numerically calculated the topological index in each phase corresponding to its symmetry.

Finite COM momentum pairs: Since the low-energy electronic degrees of freedom lie at valleys near $K$ and $K'$ [see Fig. 1], we also allow pairing of two electrons from the same valley. To incorporate such pairing with Cooper pairs having finite center-of-mass momentum $2K \equiv K'$ or $2K' \equiv K$, we use a supercell with 6 sites [see Fig. 1(a)], whose reduced Brillouin zone folds the $K$ and $K'$ to $\Gamma$ [see Fig. 1(b)]. This introduces 6 on-site pairing order parameters and 36 nearest-neighbor pairing order parameters. We then minimize the ground state energy within this exhaustive parameter space.

III. VARIOUS SUPERCONDUCTING PHASES AND THEIR TOPOLOGY

On-site attraction $U$: In the Kane-Mele model at $\mu = 0$ with on-site attractive interaction $U$, we find three different phases as shown in Fig. 2(a). Away from $x = 1/2$, the system stays an insulator for weak interaction due to the finite band gap: Its topological property is completely determined by the underlying band structure parametrized by $x$. For strong enough interaction, we find a uniform $s$-wave spin-singlet superconducting phase. Since the pairing leaves the $\mathcal{T}$-symmetry intact, the Bogoliubov-de Gennes Hamiltonian is in the class DIII, with a $Z_2$ topological index $\nu = 0$ or 1, defined analogously to the $Z_2$ topological index $\nu$ of class AII topological insulator, but in terms of the Bogoliubov quasiparticles in Nambu space. The superconducting state that arises from either the topological insulator or the trivial insulator is a trivial superconductor with $\bar{\nu} = 0$. This can be understood in the following way: The insulating phase can be seen as a $\mathcal{T}$-invariant superconductor with zero pair potential. Such “superconducting state” is trivial since $\bar{\nu} = 2\nu = 0$ (mod 2) independent of $\nu$; (the factor of two is due to the particle-hole redundancy of Nambu spinors). Thus it is natural that the $s$-wave pairing state that arises out of the insulating phase, regardless of whether it is topological or trivial, is a trivial superconducting state, and is guaranteed to be trivial near a continuous transition.

Nearest-neighbor attraction $V$: With attractive nearest-neighbor density-density interaction $V$, we find a much richer phase diagram shown in Fig. 2(b). (We have implicitly assumed the presence of long range Coulomb repulsion to prevent phase separation at stronger interac-
The results are summarized in Tab. I. We find four distinct superconducting phases, all of which are always chosen from the A sublattice, \( S_z \) conservation rather than the full SU(2) spin rotation symmetry, it is more convenient to decompose the spin-triplet channels into spin-singlet and three spin-triplet pairing states. Near \( x = 0 \) we find “trivial nematic singlet SC” that is \( T \)-invariant and breaks the \( C_3 \) rotation symmetry of the system. Near \( x = 1 \) we find “trivial chiral singlet SC”, which is \( T \)-breaking with pairing in the spin-singlet channel.

FIG. 2. Phase diagrams of Kane-Mele model in Eq. (1) as functions of the tuning parameter \( x = \frac{3\sqrt{3}\lambda_{SO}}{(m_{AB} + 3\sqrt{3}\lambda_{SO})} \) which interpolates between the trivial and topological insulating band structures, with three different types of interactions: on-site attractive interaction \( U \), nearest-neighbor attractive density-density interaction \( V \), and nearest-neighbor antiferromagnetic Heisenberg interaction \( J \). Solid lines mark continuous (topological) phase transitions, and the dotted lines mark first order transitions. (a) With \( U \), we find an s-wave pairing state that is topologically trivial. (b) With \( V \), we find more exotic pairing states, two of which are topological: The green region near \( x = 1/2 \) is a topological helical superconductor. (c) With \( J \), we find two distinct topologically trivial singlet pairing states. Near \( x = 0 \) we find “trivial nematic singlet SC” that is \( T \)-invariant, and breaks the \( C_3 \) rotation symmetry of the system. Near \( x = 1 \) we find “trivial chiral singlet SC”, which is \( T \)-breaking with pairing in the spin-singlet channel.

FIG. 3. Real-space patterns of the pairing order parameters that we find with nearest-neighbor attractive density-density interaction. A bond between sites \( i \) and \( j \) represents pair potential \( \Delta_{ij} \) of the “topological helical triplet SC”, which is \( \sim \Phi_{ij} \), and \( d_{ij} \) of the “p-Kekule SC”, which is \( \sim \Phi_{ij}^{K} \). The color of a bond marks the phase of the order parameter, which is also indicated \( 1, -1, \omega, \text{and } \omega^2 \) on the bonds. Since both \( \Delta_{ij} \) and \( d_{ij} \) are antisymmetric under \( i \leftrightarrow j \), we choose a convention for the phases: \( i \) is always chosen from the A sublattice, and \( j \) from the B sublattice.

TABLE I. Summary of the superconducting phases in Fig. 2(b) found with attractive nearest-neighbor density-density interaction \( V \).

| superconducting phase | \( \{\psi, \Delta_{ij}, d_{ij}, \Delta_{ij}'\} \) | \( T \)-sym. topo. index |
|-----------------------|---------------------------------|------------------------|
| top. helical triplet  | \( \Delta_{ij} \sim \Phi_{ij}^K \) | Yes \( \bar{\nu} = 1 \) |
| triv. p-Kekule triplet| \( d_{ij} \sim \Phi_{ij}^K \) | Yes \( \bar{\nu} = 0 \) |
| top. chiral triplet   | \( \Delta_{ij} \sim \Phi_{ij}^K \) | \( \bar{\nu} = 0 \) |
| (or its \( T \)-partner) | \( d_{ij} \sim \Phi_{ij}^K \) | \( \bar{\nu} = 1 \) |

where \( \sigma^\mu \) for \( \mu = 0, x, y, z \) are the identity and the Pauli matrices in spin space. Since, however, the Hamiltonian \( H_{KM} \) only has a \( U(1) \) spin rotation symmetry related to the \( S_z \) conservation rather than the full SU(2) spin rotation symmetry, it is more convenient to decompose the pairing channels into \( \psi \) (Cooper pairs with spin \( S = 0 \)), \( \Delta_{\uparrow} \) \( (S = 1, S_z = 1) \), \( d^x \) \( (S = 1, S_z = 0) \), and \( \Delta_{\downarrow} \) \( (S = 1, S_z = -1) \). We find four distinct superconducting phases, all of which have \( \Delta \) purely in the spin-triplet channel (with \( \psi_{ij} = 0 \)). The results are summarized in Tab. I.
**Topological helical SC:** Around $x = 1/2$ at weaker interaction strength, we find a $T$-invariant topological ($\tilde{\nu} = 1$) pairing state which we dub “topological helical spin-triplet superconductor” [green region in Fig. 2(b)]. The pairing in this state is in the equal-spin channel ($\Delta_{i\uparrow}, \Delta_{i\downarrow} \neq 0$), with finite momentum Cooper pairs, as indicated by the real-space pattern of $\Delta_{i\uparrow,j\uparrow}$ shown in Fig. 3(a), which goes as $\Delta_{i\uparrow,j\uparrow} \sim \Phi^K$, where $\Phi^K_{ij} = e^{iK(x_1-x_2)}$, for $i$ in sublattice A and $j$ in sublattice B. $\Phi^K$ represents pairing with center-of-mass momentum $2Q$. The translation symmetry of the lattice, however, is not broken since the magnitude of the pair potential is uniform across all unitcells and only the phase modulates.

This $T$-invariant superconducting state, whose non-trivial topology is characterized by the $\mathbb{Z}_2$ topological index $\tilde{\nu} = 1$, can be understood in terms of the Dirac dispersions at each valley. When $x \approx 1/2$, the low energy electronic degrees of freedom are spin-valley locked [see Fig. 1(d)]. The order parameters $\Delta_{i\uparrow,j\uparrow} \sim \Phi^K_{ij}$ and $\Delta_{i\downarrow,j\downarrow} \sim \Phi^{K'}_{ij}$, therefore represent pairing between two electrons of the same spin from the same valley, which can be written in momentum space as

$$\sum_{\mathbf{q}} \Delta_{K+\mathbf{q}} c^\dagger_{K+\mathbf{Q},i} c_{-K-\mathbf{Q},i} + \Delta_{K'} c^\dagger_{K',\mathbf{Q},i} c_{-K',\mathbf{Q},i} + \text{H.c.} \quad (3)$$

For small $\mathbf{q}$, $\Delta_{K+\mathbf{q}} = \Delta_K + O(q^2)$ with $\Delta_K \neq 0$. The finite momentum pair potential $\Delta_{K+\mathbf{q}}$ thus plays the role of “uniform s-wave” gap within the Dirac cone at the $K$ valley (and similarly $\Delta_{K'+\mathbf{q}}$ for the $K'$ valley), which effectively becomes $p_x \pm i p_y$ pairing in the band basis [22, 23]. This results in a non-zero Chern number $\hat{C} = \pm 1$ in each spin sector, leading to a non-trivial $\mathbb{Z}_2$ index $\tilde{\nu} = 1$.

**p-Kekule SC:** At $x = 1$ and nearby where the underlying band structure is in the topological insulator phase, we find a $T$-invariant trivial ($\tilde{\nu} = 0$) pairing state which we dub “p-Kekule triplet superconductor” [blue region in Fig. 2(b)]. The pairing in this state is in the opposite-spin spin-triplet channel ($d^z \neq 0$), and also has finite momentum Cooper pairs, forming the “p-Kekule” pattern in real-space [see Fig. 3(b)]. This phase was previously found by Tsuchiya et al. [24] who studied the same Hamiltonian in the $x = 1$ limit.

**Topological chiral SC:** In a thin region between the topological helical SC and the p-Kekule SC, we also find a $T$-breaking topological superconducting state with non-zero Chern number $\hat{C} = \pm 1$ [purple region in Fig. 2(b)]. We dub this state “topological chiral triplet superconductor”. In this state, one of the valleys develops equal-spin-pairing gap within the same cone, while the other valley develops an opposite-spin spin-triplet pairing gap across the two Dirac cones in the same valley. This results in a non-zero Chern number with contribution from only one of the spin species (and thus one valley due to spin-valley locking).

**Trivial $T$-breaking SC:** At $x \approx 0$ and at larger interaction strength, the system favors a pairing state which is $T$-breaking with a mixture of equal-spin and opposite-spin pairing channels [pink region in Fig. 2(b)]. This state, which we dubbed “trivial $T$-breaking triplet superconductor”, is distinct from the “topological chiral triplet superconductor”, and is topologically trivial ($\hat{C} = 0$).

**Antiferromagnetic Heisenberg exchange $J$:** With antiferromagnetic Heisenberg exchange $J$ between nearest neighboring sites, we find two distinct superconducting states as shown in Fig. 2(c). Both of these states are topologically trivial, but have exotic characteristics: The pairing state for $x \leq 1/2$ is dubbed “nematic singlet SC”, which is $T$-invariant but breaks rotation symmetry. The pairing state for $x \geq 1/2$, on the other hand, is dubbed “chiral singlet SC”, which is in the spin-singlet channel, yet is $T$-breaking and also breaks translation symmetry. The real-space patterns of the singlet order parameter $\psi_{ij}$ in these phases are shown in Fig. 4.

**Finite doping $\mu \neq 0$:** So far we have considered the band structure at half filling with $\mu = 0$, and found topological superconducting phases with $V$. Do these topological phases exist even when the underlying band structure is metallic? Figure 5 shows the phase diagram with $V$ at $\mu = t/4$. Note that $B_2 = t/2$, and therefore the metallic...
phase contains a single spin non-degenerate Fermi surface in each valley. We find superconducting phases with the same pair potential configurations as in the $\mu = 0$ phase diagram in Fig. 2(b), in addition to a metallic phase around $x = 1/2$. The topological indices of these states remain identical to the $\mu = 0$ case.

IV. DISCUSSION AND OUTLOOK

To summarize, we have derived the phase diagram of the Kane-Mele model across its trivial-insulator-to-topological-insulator transition, with various interactions using the Bogoliubov-de Gennes framework. With attractive on-site interaction $U$, we find trivial s-wave superconductivity as expected. With nearest-neighbor interactions, both the attractive density-density interaction $V$, and the antiferromagnetic Heisenberg exchange $J$, we find exotic superconducting phases with finite Cooper-pair momentum. Especially with $V$, we find two distinct topological superconducting phases, one $T$-invariant and one $T$-breaking, near the trivial-insulator-to-topological-insulator transition, where one pair of the Dirac cones become gapless.

While the models we have solved are specific, the broad lessons we have learned are applicable to a broader class of phenomena. The central thrust of this work is to understand the conditions under which we get topological superconductivity in a Dirac system. Through our study of the Kane-Mele model, we have identified two crucial ingredients for obtaining a topological superconductor. First, there needs to be pairing within a Dirac cone [22, 25], with a pair potential that is uniform near the Dirac cone. Second, such pairing must manifest on a single time-reversed pair of non-degenerate Dirac cones for $T$-invariant helical SC. This corresponds to “topological helical triplet SC” in Fig. 2(b) that is characterized by a $Z_2$ topological index $\tilde{\nu} = 1$. If the pairing potential is non-zero only on one Dirac cone, we have a chiral superconductor characterized by a non-zero Chern number $\tilde{C}$. This corresponds to the purple region in Fig. 2(b), which is $T$-breaking.

A single time-reversed pair of spin-polarized Dirac cones appears naturally at the topological transition of the Kane-Mele model at $x = 1/2$. Pairing internal to each of these Dirac cones is necessarily between equal-spin electrons. It is only with nearest-neighbor density-density attraction that the equal-spin pairing channel is allowed. Both on-site attraction and AF Heisenberg exchange enable pairing in the singlet channel, we therefore find no topological superconductivity with these interactions.

Thus far, the search for topological superconductivity has been driven largely by one theme: break $T$ and get effectively spinless fermions, and then induce (effective) p-wave pairing between them. This originates from work by Kitaev in 1D [26] and $T$-breaking is central to this quest. One of the strengths of the work presented here is a paradigm for 2D topological superconductivity in presence of $T$-invariance and an explicit demonstration in the context of the Kane-Mele model.

We expect that the theoretical phase diagrams and general principles for topological superconductivity that we have unearthed from simple models are relevant for the low energy physics of monolayer TMD materials, like MoS$_2$, WS$_2$, WTe$_2$ and also for cold atoms.

Pairing in the TMD materials has hitherto been studied without incorporating the full effect of the honeycomb lattice [27, 28], ignoring the Dirac physics and the $\pi$ Berry phase around the valley. Yuan et al. [27] considered on-site and nearest-neighbour attraction on a triangular lattice, and found $T$-breaking topological superconductivity only in the presence of Rashba spin-orbit coupling. We note that the phases discussed there are, in principle, included in our mean-field study and turn out to be energetically less favored than the finite momentum paired states that we encounter. Hsu et al. [28] used renormalization group analysis to explore the leading instability of one spin-polarized circular Fermi surface at $K$ and $K'$ with on-site repulsive interactions. They found several degenerate paired states: an interpocket chiral SC, an intrapocket chiral SC and an intrapocket helical SC similar to our topological helical triplet SC phase.

Our results also have direct implications for the development of superconductivity in the spinless Haldane model in the presence of interactions, which are naturally of the nearest-neighbor density-density form. As we shall discuss elsewhere, we find that in this case the ground state is a topological superconductor with a Chern number of $\tilde{C} = \pm 1$. We note that the Haldane model has been experimentally realized with ultracold atoms [29] and there are proposals to engineer near-neighbor interactions [30].

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