Exotic Quantum Phase Transitions of \((2 + 1)d\) Dirac fermions

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Introduction

The interplay between topology and interactions can lead to very rich new physics. For bosonic systems, it is understood that strong interactions can lead to many symmetry protected topological (SPT) phases [1,2] that are fundamentally different from the standard Mott insulator and superfluid phases. In addition to producing various topological orders, for fermionic systems strong interactions can also reduce the classification of free fermion topological insulators and superconductors [3–11]. That is, interactions can drive free fermion topological superconductors to a trivial phase; namely the edge states of the free fermion topological superconductor can be gapped out without degeneracy by a symmetry preserving short range interactions without going through a bulk quantum phase transition. The most famous example is the \(^3\)He-B topological superconductor protected by time-reversal symmetry, whose boundary is described by a \((2 + 1)d\) Majorana fermion \(\chi\) with the Hamiltonian \(H = \int d^2x \chi^\dagger \left( i\sigma^1 \partial_x + i\sigma^2 \partial_y \right) \chi\). Without interactions, \(^3\)He-B has a \(\mathbb{Z}\) classification; therefore for arbitrary copies of \(^3\)He-B, its boundary remains gapless as long as time-reversal symmetry is preserved [12–14]. In other words any fermion-bilinear mass term \(\chi^\dagger \sigma^a \chi_b\) at the boundary would break the time-reversal symmetry. However, once interactions are turned on, the classification of \(^3\)He-B is reduced to \(\mathbb{Z}_{16}\); i.e., with 16 copies of \(^3\)He-B, its boundary can be gapped out by interactions while preserving the time-reversal symmetry [9,10]. In other words, the boundary is fully gapped by interactions with \(\langle \chi^\dagger \sigma^a \chi_b \rangle = 0\), for \(a, b = 1\ldots 16\).

Although the classification of interacting \(^3\)He-B has been understood, the following question remains: if the interactions are tuned continuously, can there be a direct second order quantum phase transition between the weakly interacting gapless boundary and the strongly interacting fully gapped nondegenerate boundary state? Even if such a second order phase transition exists, its field theory description is unknown because the standard field theory that describes a phase transition of interacting Dirac or Majorana fermions is the Gross-Neveu model [15], which corresponds to the order-disorder phase transition of a bosonic field \(\phi_{ab}\) that couples to a fermion bilinear mass operator: \(\phi_{ab} \chi^\dagger a \sigma^y \chi_b\) [39]. Therefore in the Gross-Neveu model, the gap of the Majorana fermion is induced by a nonzero expectation value of a fermion bilinear mass: \(\langle \chi^\dagger a \sigma^y \chi_b \rangle \neq 0\), which would break the time-reversal symmetry at the boundary of \(^3\)He-B.

In this paper we will demonstrate that such a novel direct second order transition indeed exists, which is fundamentally different from the standard Gross-Neveu theory. But instead of studying the boundary of a \(3d\) system (which is numerically challenging), we will just study a \(2d\) lattice model, whose low energy field theory is identical to the boundary of \(16\) copies of \(^3\)He-B, despite the difference in lattice regularization. We will demonstrate that in this \(2d\) lattice model there is indeed a direct second order quantum phase transition between \(16\) flavors of gapless \((2 + 1)d\) Majorana fermions (8 copies of Dirac fermions) and a fully gapped phase that does not break the symmetry of the lattice model. This shows that the fermion gap does not correspond to any fermion bilinear mass.

We will also study another exotic quantum phase transition between the weakly interacting quantum spin Hall (QSH) insulator with spin \(S^z\) conservation and spin Chern number 2, and the fully gapped and symmetric phase in the strong interaction limit mentioned in the previous paragraph. In the noninteracting limit, the phase transition between the topological insulator and trivial insulator is driven by closing the Dirac mass gap, which requires that the single particle excitation is gapless at the critical point. However, in this paper we demonstrate that, with interaction, at this quantum phase transition the spin and charge gap both close, while the single particle excitation remains gapped. Therefore, this quantum phase transition only involves bosonic degrees of freedom, which allows this quantum phase transition to be described by a bosonic field theory. We propose that the field theory for this transition is an...
The QSH insulator and the trivial phase correspond to $\pi < \Theta \leq 2\pi$ and $0 \leq \Theta < \pi$ respectively, while the quantum critical point corresponds to $\Theta = \pi$.

**Model Hamiltonian**

The Hamiltonian we study is an interacting spin-1/2 fermion system defined on a bilayer honeycomb lattice (Fig. 1):

$$H = T + T' + W$$

$$T = -t \sum_{\langle ij \rangle} \sum_{\ell, s} (c_{i\ell s}^\dagger c_{j\ell s} + h.c.)$$

$$T' = i\lambda \sum_{\langle\langle ij\rangle\rangle} \sum_{\ell} \nu_{ij} c_{i\ell}^\dagger \sigma^z c_{j\ell}$$

$$W = \frac{U}{2} \sum_{i, \ell} (n_{i\ell} - 1)^2$$

$$+ J \sum_i \left[ S_{i1} \cdot S_{i2} + \frac{1}{4} (n_{i1} - 1)(n_{i2} - 1) - \frac{1}{4} \right]$$

where $s = \uparrow, \downarrow$ and $\ell = 1, 2$ denote the spin and layer index. $T + T'$ and $W$ are the noninteracting and interacting (respectively) parts of the Hamiltonian. We will set $t = 1$ as the energy unit throughout this paper. We also define $n_{i\ell} = n_{i\ell \uparrow} + n_{i\ell \downarrow}$, $S_{i\ell}^\mu = \frac{1}{2} c_{i\ell \sigma}^\dagger \sigma^\mu c_{i\ell}$, and $n_{i\ell s} = c_{i\ell s}^\dagger c_{i\ell s}$. $(\langle ij \rangle)$ stands for a next-nearest-neighbor lattice link. $\nu_{ij} = \pm 1$ depending on whether the hopping path defined by the nearest-neighbor bonds connecting sites $i$ and $j$ bends to the right or to the left. With only the $T$ term, the low energy limit of this model is described by 8 flavors of $(2+1)d$ massless Dirac fermions (or 16 Majorana fermions) in its Brillouin zone. In the noninteracting limit, i.e., $U = J = 0$, a nonzero $\lambda$ will cause the $T'$ term to gap out $T$ and drive the system into a QSH phase with spin Chern number $C_s = 2$ (to be defined later in Eq. (3)). The $U$ term in $W$ is a Hubbard repulsion while the $J$ term consists of an antiferromagnetic Heisenberg spin interaction between the two layers and a density-density interaction. In this paper we will fix $J/U = 2$. Then in the strong interacting limit the ground state is a trivial gapped phase that respects all the symmetry:

$$|\Psi\rangle = \prod_i (c_{i1\uparrow}^\dagger c_{i2\downarrow} - c_{i1\downarrow}^\dagger c_{i2\uparrow}) |0\rangle.$$  (2)

The phase diagram of this model is depicted in Fig. 2.

**FIG. 1:** The bilayer honeycomb lattice. In each layer, $t$ and $\lambda$ are the nearest- and next-nearest-neighbor hopping. The Hubbard interaction $U$ acts on each site, and the Heisenberg interaction $J$ acts across the layers.

**FIG. 2:** (Color online.) A schematic phase diagram of the bilayer honeycomb model. The red line is the phase boundary between the two QSH phases of opposite spin Chern numbers $C = \pm 2$ (colored yellow/green), where both the single particle and the spin/charge gaps are closed. The blue line is the phase boundary between the QSH phase $\Theta = \pm 2\pi$ and the trivial gapped phase $\Theta = 0$, where the single particle gap remains open but the spin/charge gaps are closed. $U_c$ is the tricritical point, above which the spin Chern number changes inside the trivial phase (without gap closing) through the dashed line, also see Fig. 3.

**Phases and Excitation Gaps**

Before we present our results for the 2d model, we will first consider a 1d system composed of two coupled chains. In this 1d system, $T'$ becomes

$$T'_1 = -\frac{\lambda}{2} \sum_{i, \ell, s} (-1)^i (c_{i+1, \ell, s}^\dagger c_{i, \ell, s} + h.c.)$$  (3)

In the noninteracting limit, $\lambda < 0$ corresponds to 4 copies of the Su-Schrieffer-Heeger model of polyacetylene or 8 copies of the Kitaev’s 1d topological superconductor with a nontrivial boundary state, while $\lambda > 0$ corresponds to a trivial state. We are interested in connecting the $\lambda < 0$ SPT phase to the $\lambda > 0$ trivial phase without a phase transition. (This demonstrates the already known fact that $\lambda < 0$ and $\lambda > 0$ are actually in the same phase under interaction.) Fidkowski and Kitaev demonstrated how to do this in one dimension using an interaction term which corresponds to $W$ but with a simpler $J$ term: $+JS_{i,1} \cdot S_{i,2}$. We modify
Fidkowski and Kitaev’s interaction term slightly so that it can be simulated by quantum Monte Carlo (QMC) without a sign problem [17]. This modification will not change the qualitative results of the model.

Our results are depicted in Fig. 4(a) and Fig. 4(b). With $\lambda = 0$, the system is gapped out immediately with infinitesimal interaction, because as was computed explicitly, the four fermion term is marginally relevant at $\lambda = 0$. The gap we measure scales exponentially with $1/U$, which is consistent with the renormalization group calculation. With finite $\lambda$, there is no phase transition at finite $U$, see Fig. 4(b); namely the entire phase diagram of this 1d system is one trivially gapped phase except for the isolated gapless point $\lambda = U = J = 0$.

Now let us move on to the honeycomb lattice. It is well-known that a weak short range interaction is irrelevant for a massless $(2 + 1)d$ Dirac/Majorana fermion, which implies that the interaction can gap out the fermion only when it is strong enough. Thus along the $\lambda = 0$ axis in Fig. 2, a semimetal-insulator phase transition is expected at finite $U/t$. Indeed, our numerical results suggest that with increasing $U/t$, there is one continuous phase transition at finite $U_c/t \sim 1$ where the single particle gap opens up gradually from zero, and the single particle gap increases monotonically afterwards. In the large $U/t$ limit, this model is exactly soluble, and the ground state is a trivial direct product of on-site spin singlets between the two layers as in Eq. (2). Therefore in the large $U/t$ limit this gapped phase does not correspond to any fermion quadratic mass term. But it is still possible that some other symmetry breaking order parameters may emerge for intermediate $U/t$. To verify that this is not the case, we performed a mean field analysis where we focus on the order parameters that minimize the energy of the interaction term at the mean field level. The details of this mean field analysis are presented in the Mean-Field Energy of Order Parameters appendix. We identify three order parameters that could potentially minimize the interaction energy: the antiferromagnetic order, the interlayer spin singlet Cooper pairing, and the interlayer exciton excitation. But our numerical results demonstrate that none of these order parameters emerge and stabilize in the entire phase diagram. Thus we conclude that there is indeed a continuous quantum phase transition between the gapless Dirac/Majorana fermion phase in the weak interacting limit and the fully gapped symmetric trivial phase in the strong interaction limit. Since the quantum phase transition is continuous, there must be a field theory description for this phase transition. Although the exact form of this field theory is unknown, it must be fundamentally different from the
FIG. 5: Single particle gap, spin gap (gap for spin-1 excitation), and charge gap (gap for charge-2 excitation) on the bilayer honeycomb lattice with \( J/U = 2 \). (a) When \( \lambda = 0 \), there is a single continuous phase transition from a semimetal to a trivial insulator at \( U_c \approx 1 \), whose field theory also describes the phase transition of the boundary of 16 copies of the \(^3\)He-B phase. (b) When \( \lambda = 0.25 \), only the spin and charge gap close at the continuous phase transition from an SPT to a trivial insulator (which is at \( U_c \approx 1.5 \) for \( \lambda = 0.25 \)). We propose that this phase transition is described by a bosonic O(4) nonlinear sigma model field theory with a \( \Theta \)-term [Eq. (5)]. These gaps are calculated as explained in the Gap Calculation Methods appendix. This involves calculating gaps in finite systems of sizes up to 9x9 unit cells (with 4 sites each) and extrapolating to the infinite size limit. Error bars on all figures denote one standard deviation (i.e. \( \approx 68\% \) confidence).

standard Gross-Neveu model. The same field theory must be applicable to the interaction driven mass gap at the boundary of 16 copies of the \(^3\)He-B phase.

Now let us consider the case with finite \( \lambda \). In the noninteracting limit, a finite \( \lambda \) term will drive the system into a quantum spin Hall insulator with spin Chern number \( C_s = 2 \); i.e. the Chern number for spin-up (spin-down) fermion is \( +2 \) (\( -2 \)) (see Eq. (6) for definition). Because our system has \( S^z \) conservation, this state is still a nontrivial topological insulator with stable boundary states. While increasing \( U/t \), there must be a quantum phase transition between this topological insulator and the strongly coupled trivial gapped state (blue line in the phase diagram Fig. 2). In the noninteracting limit, the transition between a topological insulator and trivial insulator is driven by closing the Dirac fermion gap. In Fig. 5(b) we can see that there is indeed a quantum phase transition at finite \( U/t \); but at this quantum critical point the single particle gap does not close, while our data suggests that the gaps for the inplane antiferromagnetic spin order parameter \( \vec{N} x \sim (-1)^{i+i} c_1^\dagger c_1 \sigma^x c_1 \), \( \vec{N} y \sim (-1)^{i+i} c_1^\dagger c_1 \sigma^y c_1 \) and interlayer spin singlet Cooper pair \( \Delta \sim c_1^\dagger \sigma^y c_{1,2} \) (referred to as the spin and the charge gaps respectively) both vanish at the critical point. This implies that in the low energy limit this quantum phase transition only involves bosonic degrees of freedom, allowing the fermionic excitations to be integrated out from the field theory.

Close to the quantum critical point, we can define a four component unit vector \( \mathbf{n} \) with \( n^2 = 1 \), which couples to the fermions as follows:

\[
n_1 \vec{N} x + n_2 \vec{N} y + n_3 \text{Re}(\Delta) + n_4 \text{Im}(\Delta).
\]

(4)

We propose that the phase diagram for \( \lambda \neq 0 \) can be described by the following effective bosonic field theory:

\[
S = \int d^2x dr \frac{1}{g} (\partial_\mu \mathbf{n})^2 + \frac{i\Theta}{\Omega_3} \epsilon_{abcd} n^a \partial_x n^b \partial_y n^c \partial_i n^d, \quad (5)
\]

where \( \Omega_3 = 2\pi^2 \) is the volume of a three dimensional sphere with unit radius. The field theory Eq. (5) can be derived using the same method as Ref. [18] after integrating out the fermions. The phase diagram and renormalization group flow of the \((1 + 1)d\) analogue of Eq. (5) were calculated explicitly in Ref. [19,21]; and it was demonstrated that the entire phase \( 0 \leq \Theta < \pi \) is controlled by the fixed point \( \Theta = 0 \), while the entire phase \( \pi < \Theta \leq 2\pi \) will flow to the fixed point \( \Theta = 2\pi \). \( \Theta = \pi \) is the phase transition between the two phases.

The phase diagram of Eq. (5) was studied in Ref. [22], and again in the disordered phases (phases with large \( g \)) \( \Theta = \pi \) is the quantum phase transition between the two phases with \( 0 \leq \Theta < \pi \) and \( \pi < \Theta < 2\pi \).

In Eq. (5), the fixed point \( \Theta = 2\pi \) describes a bosonic symmetry protected topological (SPT) state with \( \mathbb{U}(1) \times \mathbb{U}(1) \) symmetry [23], where the two \( \mathbb{U}(1) \) symmetries correspond to charge and \( S^z \) conservation respectively. The boundary of Eq. (5) with \( \Theta = 2\pi \) is a \((1 + 1)d\) O(4) NLSM with a Wess-Zumino-Witten term at level \( k = 1 \), which corresponds to a \((1 + 1)d\) conformal field theory. In the bulk theory we can define two bosonic rotor fields \( b_1 \sim n_1 + i n_2 \) and \( b_2 \sim n_3 + i n_4 \). \( b_1 \) and \( b_2 \) carry spin-1 and charge-2 respectively. The fixed point \( \Theta = 2\pi \) in Eq. (5) implies that a vortex of \((n_3, n_4)\) \((2\pi\)-vortex of \( b_2 \), also \( \pi \)-flux seen by the fermions)
carries one $b_1$ boson; namely a $\pi$-flux for fermions carries spin $S^z = 1$, which is precisely consistent with the QSH insulator with spin Chern number 2 [24, 25]. Thus the fixed point $\Theta = 2\pi$ has all the key properties of the QSH insulator phase. At the fixed point $\Theta = 0$, the boundary of Eq. (5) is trivial. The phase transition between the quantum spin Hall insulator and the trivial state can be driven by tuning the parameter $\Theta$, where the quantum critical point corresponds to $\Theta = \pi$.

**Spin Chern Number and Green’s Function**

Having mapped out the phase boundaries in the phase diagram, let us discuss the topological properties of the various phases. The gapped ground states of the bilayer honeycomb model in Eq. (1) belong to the fermion SPT phases protected by both the charge and the spin U(1) symmetries, which is $\mathbb{Z}$ classified (even with interaction). With this classification, each SPT state is characterized by a quantized topological number, the spin Chern number, in analogy to the TKNN integer for integer quantum Hall states, which can be constructed by the following fermion Green’s function [26, 33] as

$$C_s = \frac{1}{4\pi^2} \int d^3k e^{i\omega \lambda} \text{Tr} [-\sigma^z G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\lambda G^{-1}],$$

where $\sigma^z$ is the spin $S^z$ matrix, $G(k) = -\langle c_k c_k^\dagger \rangle$ is the fermion Green’s function in the frequency and momentum space $k = (i\omega, k)$ with $i\omega$ being the Matsubara frequency, and $\partial_\mu$ here stands for $\partial / \partial k_\mu$. In the non-interacting limit, the physical meaning of the spin Chern number is associated to the spin Hall conductance $\sigma^\text{spin}_H = C_s e / 2\pi$. Nevertheless, the formula Eq. (6) is still well-defined for interacting systems, as long as we use the full interacting fermion Green’s function [26, 27, 30–33]. However for interacting systems, the spin Chern number no longer necessarily corresponds to the spin Hall response.

In the weak interaction regime, the spin Chern number for the bilayer QSH state is $C_s = \pm 2$, depending on the sign of $\lambda$. The two QSH phases are separated by a topological phase transition at $\lambda = 0$ (the red line in Fig. 2), where the single-particle gap closes, and the Green’s function develops poles at zero frequency and at the $K$ and $K'$ points in the Brillouin zone. Due to this singularity of the Green’s function, the spin Chern number is allowed to change across the gapless phase boundary. Above the critical point $U_c$, this phase transition is gapped out by interaction, but the spin Chern number still changes discontinuously across $\lambda = 0$, as proven in Ref. 34. The transition of the spin Chern number (dashed violet line in Fig. 2) hidden in the trivial gapped phase implies that the Green’s function must have zeros (instead of poles) at zero frequency. This is based on the observation that in Eq. (6) $G$ and $G^{-1}$ are interchangeable, so the spin Chern number can either change through the poles of $G$ or the zeros of $G$ (which are poles of $G^{-1}$) [34, 35]. When the fermions are gapped out by strong interaction, it is impossible to have poles of $G$ at zero frequency, so the spin Chern number can only change through the zeros of $G$.

The zeros of the Green’s function is a prominent property of the trivial gapped phase ($U > U_c$), in contrast to the poles along the topological phase boundary ($U < U_c$). It is found that both the poles and the zeros are located at the $K$ and $K'$ points in the Brillouin zone, and can be verified in our QMC simulation. Along the $\lambda = 0$ axis, the Green’s function at $K$ point $G(\omega, K)$ develops a pole as $\omega \to 0$ when $U < U_c$ [Fig. 3]; while it approaches zero when $U > U_c$ [Fig. 4]. In the strong interaction limit, Ref. 34 predicts that the Green’s function should follow the behavior $G(\omega, K) \approx \omega / (\omega^2 + \Delta^2)$ (where $\Delta \sim U$ is the typical scale of the quasi-particle gap), and in the zero frequency limit $G(\omega, K) \propto \omega$ approaches to zero linearly with $\omega$. Our numerical result matches all these
predictions quite well.

Summary —

In this work we demonstrate that there exist two novel continuous quantum phase transitions for 16 copies of \((2 + 1)d\) Majorana fermions, both cases are very different from the Standard Gross-Neveu model and Ginzburg-Landau theory. However, a controlled analytical field theory calculation for the critical exponents is not known yet; we will leave this to future studies.

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[42] In the original Gross-Neveu model introduced in Ref. 15, \(\phi_{ab}\) is always an identity matrix. Here we use a general-ized definition of the Gross-Neveu model.
[43] Eq. (3) has four flavors of complex fermions, which can be written as 8 flavors of Majorana fermion chains up to basis transformation, i.e. 8 copies of Kitaev’s 1d topological SC.

Mean-Field Energy of Order Parameters

In this appendix, we will investigate the order parameters that are favored at the mean-field level. Since our model only has on-site interactions, we will only consider on-site order parameters in this appendix.

We start from the free fermion limit. In momentum space, the fermion kinetic Hamiltonian takes the following form

\[
T + T' = \sum_k \sum_{\ell=1,2} \left[ c_{kA\ell}^\dagger \sigma^\ell \left( c_{kB\ell} \right) \sigma^\ell \right] \left( g(k) + f(k) \sigma^\ell \right) \left( f^\dagger(k) \sigma^\ell \right) \left( c_{kA\ell} \right) \left( c_{kB\ell}^\dagger \right),
\]  

(7)
where $A$ and $B$ label the sublattice sites in each unit cell, $g(k) = -2\lambda(\sin 3k_x - 2\sin \frac{\sqrt{3}k_x}{2} \cos \frac{3k_y}{2})$, and $f(k) = -t(e^{-ik_y} + 2e^{ik_y/2} \cos \frac{3k_x}{2})$. Let us first switch to the Majorana fermion basis

$$
\chi_k = \begin{bmatrix} K \\ K' \end{bmatrix} \otimes \begin{bmatrix} A \\ B \end{bmatrix} \otimes \frac{1}{2} \otimes \begin{bmatrix} \uparrow \\ \downarrow \end{bmatrix} \otimes \begin{bmatrix} \Re c_k \\ \Im c_k \end{bmatrix},
$$

(8)

then expand the kinetic Hamiltonian $T + T'$ around the $K = (+\frac{4\pi}{3\sqrt{3}}, 0)$ and $K' = (-\frac{4\pi}{3\sqrt{3}}, 0)$ points in the Brillouin zone,

$$
T + T' = \frac{1}{2} \sum_k \chi_k^\dagger (vk_x \sigma^{31000} + vk_y \sigma^{02002} + m \sigma^{33032}) \chi_k,
$$

(9)

where $\sigma^{ijk\cdots} = \sigma^i \otimes \sigma^j \otimes \sigma^k \otimes \cdots$ stands for the direct product of Pauli matrices, $v = 3t/2$, and $m = 3\sqrt{3}\lambda$. We consider all the fermion bilinear orders $\Delta_{\text{valferv}} = \chi^\dagger T^\text{valferv} \chi$ that can gap out the fermions at the $K$ and $K'$ points to gain a kinetic energy benefit, implying that $\sigma^\text{valferv}$ must be a $32 \times 32$ anti-symmetric matrix that anti-commutes with both $\sigma^{31000}$ and $\sigma^{02002}$. We found 136 such matrices that are qualified as the fermion mass terms.

Next we consider the interaction effect. Among the 136 potential orders, the interaction $W$ will select out the most favorable ones. To determine the most favorable orders, we calculate the mean-field (Hartree-Fock) energy of $W$ for the potential orders $\Delta_{\text{valferv}}$, s.t. the interaction term decomposes into that ordering channel as $W = w_{\text{valferv}}|\Delta_{\text{valferv}}|^2$ with the mean-field energy $w_{\text{valferv}}$. The orders that can gain an interaction energy benefit (i.e. $w_{\text{valferv}} < 0$ given $U, J > 0$) are concluded in Tab. I: the layer-antiferromagnetic spin density wave, the inter-layer exciton order, and the inter-layer spin-singlet pairing order. When $\lambda \neq 0$, the $\lambda$ term suppresses the exciton order and the $z$-component of the spin density wave. As a result, when $\lambda \neq 0$ we only consider the XY component of the Neel order and the pairing order, which exactly corresponds to the four component vector $n$ defined in Eq. (4).

| $w_{\text{valferv}}$ | $\Delta_{\text{valferv}}$ | physical meaning |
|----------------------|----------------------|------------------|
| $-(J + 2U)/4$        | $\Delta^{03112}$     | layer-antiferromagnetic s-wave spin density wave |
| $-J/2$               | $\Delta^{03102}$     | inter-layer s-wave exciton order |
| $-J/2$               | $\Delta^{10121}$     | inter-layer spin-singlet s-wave superconductivity |

**Green’s Function in Both Free and Strong Interacting Limits**

In this appendix, we will calculate the fermion Green’s function analytically in both the free and the strong interacting limits. Suppose that in the Majorana basis, the kinetic Hamiltonian takes the most general fermion bilinear form $T + T' = \sum_{a,b} iu_{ab} \chi_a \chi_b$, where $a \& b$ are the combined label of site, layer, spin, and particle-hole indices; and $\chi_a$ & $\chi_b$ are the corresponding Majorana fermion operators. The full Hamiltonian $H = T + T' + W$ also includes the interaction term $W = \sum_i \sum_{\alpha_k} w_{\alpha_1 \alpha_2 \alpha_3 \alpha_4} \chi_{\alpha_1} \chi_{\alpha_2} \chi_{\alpha_3} \chi_{\alpha_4}$, where $i$ labels the site and $\alpha_k$ labels the rest of the internal degrees of freedoms.

Consider the fermion Green’s function, which is defined as $G_{ab} = -\langle \chi_a \chi_b \rangle$. In the free fermion limit, the Green’s function can be simply obtained from the single-particle Hamiltonian via $(G^{-1})_{ab} = i\omega \delta_{ab} - iu_{ab}$. In momentum space (expanded around the $K$ and $K'$ points) and using the Majorana basis, the kinetic Hamiltonian reads (see the previous appendix section),

$$
T + T' = \frac{1}{2} \sum_k \chi_k^\dagger (vk_x \sigma^{31000} + vk_y \sigma^{02002} + m \sigma^{33032}) \chi_k.
$$

(10)

So in the free fermion limit, the Green’s function is

$$
G(i\omega, k) = (i\omega \sigma^{00000} - vk_x \sigma^{31000} - vk_y \sigma^{02002} - m \sigma^{33032})^{-1} = \frac{i\omega \sigma^{00000} + vk_x \sigma^{31000} + vk_y \sigma^{02002} + m \sigma^{33032}}{(i\omega)^2 - (v^2k^2 + m^2)},
$$

(11)
where $v = 3t/2$ and $m = 3\sqrt{3}\lambda$ are determined by the hopping parameters. While in the strong interacting limit, the Green’s function (at low frequency limit) has the form

$$G(i\omega, k) \simeq \frac{i\omega^{00000} + \sum_{n=0}^{\infty} g_n (v k_x \sigma^{31000} + v k_y \sigma^{02002} + m \sigma^{33032})^{2n+1}}{(i\omega)^2 - \Delta^2} + O(\omega^2)$$

where $g_n$ are coefficients and the single-particle gap $\Delta = U/2 + 3J/4$ is determined by the interaction parameters. In our QMC simulation, we set $J = 2U$, so $\Delta = 2U$ in the $U \to \infty$ limit. However for finite $U$ in our simulation, the single particle gap $\Delta$ should generally be softer ($\Delta < 2U$). As one can see, Eq. (12) has the same structure on the numerator as Eq. (11), so they should result in the same spin Chern number. It is also found that $g_0 = 0$ for our model; however, this does not affect the spin Chern number.

At the $K$ (or $K'$) point, we set $k = 0$. Thus from the above results, we conclude that along the $\lambda = 0$ axis (s.t. $m = 0$) and below $U_c \sim 1.5$, the Green’s function shows a pole at zero frequency: $G(i\omega, K) \simeq 1/(i\omega)$ [Fig. 6(a)]; while above $U_c$, the Green’s function follows the behavior of $G(i\omega, K) \simeq (i\omega)/(\lambda^2 - \Delta^2)$ [Fig. 6(b)], where $\Delta$ is the quasi-particle gap. Away from the $\lambda = 0$ axis and at zero frequency, the Green’s function is expected to decay as $1/\lambda$ [Fig. 7] in the free fermion limit. Our numerical results are perfectly consistent with the predictions made above (see Fig. 6, Fig. 7).

**Continuous Symmetries**

In this appendix we study the continuous symmetries of our 2d model, which allow us to simplify our analysis. A summary is given in Tab. II. The symmetries of our model are easiest to understand in a Majorana basis, which was introduced in the Mean-Field Energy of Order Parameters appendix. In the exciton channel, interaction $W_i$ takes the form

$$W_i = 2^{-6} \sum_{\alpha=0,3} \sum_{\ell=0}^{3} \sum_{\psi=0,2} \left\{ \begin{array}{ll} +U & \ell = 0, 2 \\ -J/2 & \ell = 1, 3 \end{array} \right. \left( \chi_i^T \sigma^{\alpha\ell(0\psi)} \chi_i \right)^2 + \text{const}$$

Here there is no valley index on $\chi_{\alpha\ell\sigma\psi}$ since $\chi_i$ is written in real space:

$$\chi_i = \begin{bmatrix} A \\ B \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} \uparrow \\ \downarrow \end{bmatrix} \otimes \begin{bmatrix} \text{Re} \, c_i \\ \text{Im} \, c_i \end{bmatrix}$$

When $J/U = 2$ and $\lambda = 0$, this model has a $U(1) \times SO(5)$ symmetry generated by operators of the form $\sum_i \frac{1}{2} \chi_i^T T \chi_i$. 
where \( \Delta \) is the noninteracting part of our interacting Hamiltonian. As is typically done, we chose \( |t/\Theta| \) so that these order parameters transform like a vector under the above symmetries. The other six matrices will mix the spin density wave and exciton order parameters and conserve the charge difference between layers.

When \( J/U \neq 2 \) and \( \lambda = 0 \) the symmetry is \( U(1)^2 \times SU(2) \), which corresponds to separate \( U(1) \) charge conservation on each layer and \( SU(2) \) spin rotation. If \( J/U \neq 2 \) and \( \lambda \neq 0 \) then the \( SU(2) \) spin rotation symmetry reduces to a \( U(1) \) spin rotation symmetry about the \( z \) axis.

**QMC Methods**

The numerical results presented in this paper were calculated using projector quantum Monte Carlo (QMC), which is described in detail in Ref. [36]. Projector QMC is a kind of determinant QMC which focuses on the zero temperature ground states of nondegenerate fermion systems. Determinant QMC is a kind of auxiliary field QMC which uses a (usually discrete) Hubbard-Stratonovich transformation to decouple an interacting fermion Hamiltonian into a noninteracting Hamiltonian. All of these QMC methods are unbiased, controlled, and numerically exact numerical methods to calculate expectation values to arbitrary precision. Ground state expectation values are calculated from the imaginary time evolution of a trial wavefunction \( \langle \Psi_T \rangle \)

\[
\langle A \rangle = \lim_{\Theta \to \infty} \frac{\langle \Psi_T | e^{-\Theta H/2} A e^{-\Theta H/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-\Theta H} | \Psi_T \rangle} \quad (16)
\]

\( \Theta \) is a projection parameter which projects the trial wavefunction into the ground state. In practice, one must use a finite but large value for \( \Theta \). We chose to use \( \Theta = 64/t \) (where \( t \) is the hopping strength), which we found to be sufficient. As is typically done, we chose \( |\Psi_T| \) to be a Slater determinant in the ground state subspace of the noninteracting part of our interacting Hamiltonian \( (T + T' \text{ from Eq. (1)}) \).

A Trotter decomposition is then applied to the numerator of Eq. (16) to separate the exponents into three parts:

\[
e^{-\Theta H/2} = \left[ e^{-\Delta_T (T+T')} e^{-\Delta_T H_U} e^{-\Delta_T H_J} \right]^{N_T} + O(\Delta_T)^2
\]

where \( \Delta_T = \Theta/2N_T \), \( H_U \) is the \( U \) term of \( H \), and \( H_J \) is the \( J \) term of \( H \) [Eq. (1)]. In our simulations we used \( N_T \approx \sqrt{N_{\text{sweeps}}} \) so that the systematic errors due to the Trotter decomposition remain negligible compared to the statistical error resulting from the finite number of Monte Carlo sweeps performed: \( N_{\text{sweeps}} \). A sweep has occurred after all field variables have been given the chance to update. We used between 64 and 4096 sweeps for the results shown here. All observables have been checked against exact diagonalization simulations on small lattices. The statistical error due to the finite number of sweeps is shown on all plots as error bars which denote one standard error.
deviation (i.e. ≈ 68% confidence). A Hubbard-Stratonovich transformation is then applied to the interacting fermion problem to transform it into a free fermion problem at the expense of adding (discrete) bosonic variables. We used the same Hubbard-Stratonovich as introduced in [17]. The imaginary numbers due to the Kane-Mele $\lambda$ term are dealt with as described in [37].

Gap Calculation Methods

In this appendix we discuss in more detail how the gaps in Fig.4 and 5 are calculated. (We use the same approach that was used in Ref. [38].) First, we measure the rate of exponential decay in imaginary time of correlation functions for various order parameters [Fig.8]. (QMC is very efficient at making this measurement.) This decay has the form $\langle Q^\dagger Q \rangle \sim e^{-\tau \Delta + c}$ for large separations in imaginary time (i.e. $\tau \gg \Delta^{-1}$) where $\Delta$ is the energy gap associated with the order parameter $Q$. We then extrapolate the finite system size gaps $\Delta$ to the gap for a system with infinite size [Fig.9].
Topological Number Calculation Methods

In this appendix we describe how the topological numbers displayed in Fig. 3 are calculated from the Greens function. In one dimension, the topological number can be written as

$$N = \frac{1}{2\pi i} \int d\mathbf{k} \text{Tr} \left[ \Sigma \partial \mathbf{k} G^{-1} \right]$$

(17)

where $G = G(i\omega = 0, \mathbf{k})$ is the zero frequency Greens function and $\Sigma = \sigma^{300}$ in the basis

$$c_i = \left[ \begin{array}{c} A \\ B \\ \text{sublattice} \\ \text{layer} \\ \text{spin} \end{array} \right] \otimes \left[ \begin{array}{c} 1 \\ \text{layer} \end{array} \right] \otimes \left[ \begin{array}{c} \uparrow \end{array} \right]$$

(18)

To calculate this number using DQMC, we first measure the zero frequency Greens function $G(i\omega = 0)_k$ at the discrete (due to the finite lattice) momenta $k$. We then promote $G(i\omega = 0)_k$ to a continuous function $G(i\omega = 0, \mathbf{k})$ via interpolation. For example, one could choose a linear interpolation

$$G(i\omega = 0, \mathbf{k}) = \frac{k_2 - k}{k_2 - k_1} G(i\omega = 0)_{k_1} + \frac{k - k_1}{k_2 - k_1} G(i\omega = 0)_{k_2}$$

(19)

where $k_1$ and $k_2$ are the nearest discrete momenta to the continuous momentum $k$. The choice of interpolation method will not affect the topological number as long as the the lattice is large enough to sample enough momenta. This is because $N$ is a topological number and therefore insensitive to local perturbations. (Imagine calculating the winding number of a circle around the origin by approximating the circle as a polygon.) Once $G(i\omega = 0, \mathbf{k})$ has been attained via interpolation, it can be inserted into the equation for $N$ [Eq. (17)] to attain the topological number via numerical integration.
In two dimensions, the topological number can be written as

\[ C_s = \frac{1}{48\pi^2} \int d\omega d^2k e^{i\omega\rho} \text{Tr}[\Sigma G\partial_\mu G^{-1} G\partial_\nu G^{-1} G\partial_\rho G^{-1}] \] (20)

where \( G = G(i\omega, k) \) is the Greens function and \( \Sigma = -\sigma^{03} \) in the same basis as above. Now, we measure \( G(i\omega, k) \) at discrete Matsubara frequency \( \omega \) and discrete momenta \( k \) and then interpolate it to \( G(i\omega, k) \). However, the measured \( G(i\omega, k) \) is only reliable up to \( \omega \sim 2\pi N_\tau / \Theta \). Since \( G(i\omega, k) \) is expected to approach zero for large \( \omega \), we choose to let our interpolation approach zero at a finite \( \omega \sim 2\pi N_\tau / \Theta \) and remain at zero for larger \( \omega \). Again, this will not affect the calculated topological number as long as \( N_\tau / \Theta \) is sufficiently large. Finally, \( G(i\omega, k) \) is inserted into the equation for \( C_s \) [Eq. (20)] using numerical integration.