Visualizing a Bosonic Symmetry Protected Topological Phase in an Interacting Fermion Model

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(Dated: October 21, 2016)

Symmetry protected topological (SPT) phases in free fermion and interacting bosonic systems have been classified, but the physical phenomena of interacting fermionic SPT phases have not been fully explored. Here, employing large-scale quantum Monte Carlo simulation, we investigate the edge physics of a bilayer Kane-Mele-Hubbard model with zigzag ribbon geometry. Our unbiased numerical results show that the fermion edge modes are gapped out by interaction, while the bosonic edge modes remain gapless at the (1 + 1)d boundary, before the bulk quantum phase transition to a topologically trivial phase. Therefore, finite fermion gaps both in the bulk and on the edge, together with the robust gapless bosonic edge modes, prove that our system becomes an emergent bosonic SPT phase at low energy, which is directly observed in an interacting fermion lattice model.

PACS numbers: 71.10.Fd, 71.27.+a, 73.43.-f

Introduction. Symmetry protected topological (SPT) phases are bulk gapped states with either gapless or degenerate edge excitations protected by symmetries. The SPT phases in free fermion systems, like topological insulators [1–5], acquire metallic edge states and have been fully classified [6, 7]. On the other hand, although bosonic SPT phases have been formally classified and constructed as well from group cohomology [8, 9] and field theories [10–13], there has been little study about realization of bosonic SPT states in condensed matter systems, except for the well-known one-dimensional Haldane phase that is realized in a spin-1 Heisenberg model [14, 15] and some proposals of realizing a two-dimensional bosonic SPT state in cold atom systems [16]. Using the same “flux-attachment” picture as Ref. 16, lattice models of bosonic integer quantum Hall states have been studied [17–21].

Recently it was proposed that instead of directly studying bosonic systems, the physics of bosonic SPT states can be mimicked by interacting fermionic systems, in the sense that its low energy physics is completely identical to bosonic SPT states [22]. For example, in an interacting fermion model on the AA-stacked bilayer Kane-Mele-Hubbard model, a bona fide interaction-driven topological phase transition has been studied in our previous papers [23–25]. A direct continuous quantum phase transition between a quantum spin Hall (QSH) phase and a topologically trivial Mott insulator was found via large-scale quantum Monte Carlo (QMC) simulations. At the critical point, only the bosonic spin and charge gaps are closed, while the bulk single-particle excitations remain open. This transition can be described by a (2+1)d O(4) nonlinear sigma model with a topological Θ-term [23, 24, 26]. However, as for the physics on the edge, although the field theory and renormalization group anal-

![FIG. 1.](color online) (a) Illustration of AA-stacked honeycomb ribbon ($L_{a_1} = 3$, $L_{a_2} = 3$) with periodic (open) boundary condition along the $a_1$ ($a_2$) direction. $a_1 = (1,0)$ and $a_2 = (1/2, \sqrt{3}/2)$ are the primitive translation vectors. $A_1$, $B_1$, $A_2$ and $B_2$ are the four sublattices within one unit cell. (b) J–Jz phase diagram of bilayer Kane-Mele-Hubbard model. The bosonic SPT (BSPT, red) and dimer Mott insulator (DMI, blue) phases are separated by a bulk transition. The dashed lines inside BSPT denote the J values, above which one can clearly see the exponential decay of the single-particle Green’s function at the boundary from our finite-size calculations. The relative range of such region becomes wider as Jz increases.
This conclusion and the second term represents the magnetic Ising (approximated) interaction $J_z$. When $J_z/t > 1$, it is perceivable that the gapless edge modes in the interacting QSH phase are hallmarks of SPTs, we perform the simulation with periodic (open) boundary condition along the $a_1$ ($a_2$) direction [see Fig. 1 (a)]. The main results unveil a substantial region ($\sim t$) of the bosonic SPT state before the bulk phase transition, while at the same time bosonic $O(4)$ correlation functions present a clear power-law decay.

The QMC method employed here is the projective auxiliary-field quantum Monte Carlo approach [30, 31]. It is a zero-temperature version of the determinantal QMC algorithm. The specific implementation of the QMC method on the model in Eq. (1) is presented in Ref. [24]. The projection parameter is chosen at $\Theta = 50/t$ and the Trotter slice $\Delta \tau = 0.05/t$. Since the gapless edge modes are hallmarks of SPTs, we perform the simulation with periodic (open) boundary condition along the $a_1$ ($a_2$) direction [see Fig. 1 (a)]. The effective action for the interacting edge modes reads

$$ S = \int d\tau dx \frac{1}{4\pi} (\partial_x \phi^\dagger K \partial_x \phi + \partial_x \phi^\dagger V \partial_x \phi) - \lambda \cos(l_0^g \phi), $$

$$ K = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, V = v_0 \begin{pmatrix} 1 & -g & g \\ -g & 1 & 0 \\ g & 0 & 1 \end{pmatrix}, $$

where $g = J_z/(4\pi v_0 - J_z)$, $u = (J_z + J)/4\pi v_0 - J_z$ and $v_0$ is the bare velocity of the edge modes. $\lambda \propto J$ is the backscattering term induced by the interlayer Heisenberg interaction with the corresponding edge vector $l_0^g = (1, -1, -1, 1)^T$. The scaling dimension of $\cos(l_0^g \phi)$ is

$$ \Delta_0 = \frac{2(1 - u - 2g)}{(1 - u)^2 - 4g^2}. $$

Without the Ising interaction $J_z$ (i.e. $g \to 0$), the operator $\cos(l_0^g \phi)$ is marginal from the scaling dimension.
Δ0 = 2. Further renormalization group (RG) analysis[27] shows that the term λ cos(ℏ₀φ) is marginally relevant, meaning that the fermionic edge modes of the non-interacting QSH state are unstable to the interaction J. As long as J is turned on, the boundary fermions will be gapped out by the interaction, leaving only bosonic edge modes described by the spin $c_{i1}^\dagger c_{i1} - c_{2i}^\dagger c_{2i}$ and charge $c_{11}^\dagger c_{21} - c_{1L}^\dagger c_{1T}$ fluctuations. However, due to the marginal nature of RG flow, the boundary fermion gap could be very small for small J, which is hard to resolve in our finite-size numerical study. The positive $J_z$ interaction (i.e., $g > 0$) helps to boost the RG flow by reducing the scaling dimension $Δ_0$ according to Eq. (3), such that J becomes relevant and the gap in the single-particle (fermionic) spectrum can be observed in numerics for smaller J as well. In the following, we will show that with moderate interaction J, the QSH edge modes indeed become bosonic at low energy, resembling the key feature of BSPT states. The interaction $J_z$ will help to enhance the fermion gap and make the BSPT edge modes more prominent in a finite-size system.

**Numerical results.** Figures 2 (a) and (b) show the single-particle Green’s function $G'_{ij} = \langle \Psi | c_{i\sigma}^\dagger c_{j\sigma} | \Psi \rangle / \langle \Psi | \Psi \rangle$ along the edge as a function of $J/t$, at $J_z/t = 0$ and 1, respectively. $|\Psi\rangle \propto e^{-\Theta H/2} |\Psi_T\rangle$ is the ground state wave function projected from a trial wave function $|\Psi_T\rangle$ [24]. We see a clear exponential decay before the bulk transition at $J_z/t \approx 3.73$ (for $J_z/t = 0$) and $J_z/t \approx 2.7$ (for $J_z/t = 1$). The exponential decay of edge single-particle Green’s function at $J < J_c$ indicates that fermions are no longer gapless at the boundary between our model system and a topologically trivial one (such as vacuum).

![Figure 2](image1.png)  
![Figure 3](image2.png)

To rule out the possible finite-size effect, we employ several different ribbon geometries in the QMC calculations. From Fig. 3 (a), it is hard to determine whether the edge single-particle Green’s function will exponentially decay in the thermodynamic limit when $J/t = 2.5$, $J_z/t = 0$ because of the strong finite-size effect. However, when $J/t = 2.75$, $J_z/t = 0$, we see a clear exponential decay no matter if $L_{a_1}$ and $L_{a_2}$ are even or odd, large or small, and the single-particle Green’s function has a clear trend to truly exponential decay in the thermodynamic limit.

The exponential decay of single-particle Green’s function at the boundary in the thermodynamic limit indicates that the gapless fermion edge mode in the non-interacting case is gapped out by the interlayer exchange interaction. Hence the fermion excitations have a gap both in the bulk and on the edge [24]. However, as shown in our edge analysis, the system can still be non-trivial in
FIG. 4. (Color online) The log-log plot of equal-time two-particle $O(4)$ vector correlation function at the boundary for (a) $J_z/t = 0$ and (b) $J_z/t = 1$. Both panels show the power-law decay behaviors before the bulk topological phase transition at $J_z/t$.

the bosonic sector \[27\]. To see this, we calculate the XY spin (SDW-XY) correlation function and superconducting pairing (SC) correlation function at the boundary. According to the analysis in Ref. \[27\], we define them as

$$N_{AA}^{+}(r_j - r_i) = \frac{1}{2}\left[S^+_{A_1 A_2}(r_j - r_i) - S^+_{A_1 A_2}(r_j - r_i)\right]$$

$$\Delta_{AA}(r_j - r_i) = \langle \hat{\Delta}_{A_1 A_2} \hat{\Delta}_{A_1 A_2} \rangle \langle \Psi | \Psi \rangle$$ \[4\]

where $S^+_{m n}(r_j - r_i) = \langle \Psi | \frac{1}{2}(S^+_i S^-_j + S^-_i S^+_j) | \Psi \rangle / \langle \Psi | \Psi \rangle$, $m, n = A_1, A_2$ denote the $A$ sublattice sites in the first and second layer. $i$ and $j$ label the unit cells. $\hat{S}^+_i$ is the spin flip operator and $\hat{\Delta}_{A_1 A_2}$ is the interlayer singlet creation operator. Figures 4 (a) and (b) show the SDW-XY correlation function at the boundary as a function of $J_z/t$. Before the bulk quantum phase transition, they all show the power-law decay at $J < J_c$. Due to the $SO(4)$ symmetry, the SDW-XY and SC correlation functions are exactly the same because they rotate into each other \[24, 27\]. So the physical bosonic boundary modes are simply the SDW-XY and SC fluctuations on the boundary.

Turning on an extra on-site Hubbard interaction $U \sum_n (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 1)^2$ (see Sec. VII in the Supplemental Material \[29\] for the $U/t$ path chosen in the bulk phase diagram) to our original model Eq. (1) would break the $O(4)$ symmetry, and change the scaling dimension of the spin and Cooper pair operators. According to the bosonization analysis in Ref. \[27\], the spin and pairing $O(4)$ bosonic modes always have power-law correlation, with $N_{AA}^{+}(r) \propto |r|^{-\alpha}$ and $\Delta_{AA}(r) \propto |r|^{-\beta}$. $\alpha$ and $\beta$ depend on the Luttinger parameters, but their product remains a universal constant: $\alpha \beta = 1$. This is due to the fact that, spin and charge are a pair of conjugate variables at the boundary, which is a physical consequence of the SPT state in the bulk. This prediction is confirmed in our simulation. In Fig. 5, at $J_z/t = 2.75$ and $J_z/t = 0$. The inset shows the extracted Luttinger parameters as a function of $U/t$.

**Discussion.** In this paper, we have performed QMC simulation for a proposed interacting lattice fermion model, and explicitly demonstrated that this system shows a bosonic SPT state, in the sense that the boundary has gapless bosonic modes, but no gapless fermionic modes under interaction. Recently it was also proposed that the same physics can be realized in an AB stacking bilayer graphene under a strong out-of-plane magnetic field and Coulomb interaction \[32\]. Our model, though technically different, should belong to the same topological class, and it has the advantage of being sign problem free for QMC simulation. Unbiased information of such a strongly correlated system, including transport and spectral properties, can be obtained from QMC simulation, and quantitative comparison with the up-coming experiments is hence made possible.

The numerical calculations were carried out at the National Supercomputer Center in Guangzhou on the Tianhe-2 platform. Z.Y.M acknowledges the support from the Ministry of Science and Technology (MOST) of...
China under Grant No. 2016YFA0300502, the National Natural Science Foundation of China (NSFC Grants No. 11421092 and No. 11574359), as well as the National Thousand-Young-Talents Program of China. C.X. and Y.Z.Y. are supported by the David and Lucile Packard Foundation and NSF Grant No. DMR-1151208. T.Y. and N.K. are supported by JSPS KAKENHI No. 15H05855. H.Q.W., Y.Y.H., and Z.Y.L. acknowledge support from the NSFC Grants No. 11474356 and No. 91421304 and Special Program for Applied Research on Super Computation of the NSFC-Guangdong Joint Fund (the second phase).

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Supplemental material: Visualizing a Bosonic Symmetry Protected Topological Phase in an Interacting Fermion Model

I. $J_z/t = 2$ RESULTS

Fig. S1 shows the single-particle Green’s function and SDW-XY correlation function at the ribbon edge as a function of interlayer $J/t$ interaction when $J_z/t = 2$. The bulk quantum critical point is obtained from energy curves and SDW-XY magnetic structure factors which will be shown in the following section. The $J_z/t = 2$ case shares the similar behavior as the $J_z/t = 0$ and 1 cases. The single-particle Green’s function at the ribbon edge shows the exponential decay before the bulk quantum phase transition, while the SDW-XY correlation function still decays as a power-law behavior.

![FIG. S1. Single-particle Green’s function (a) and SDW-XY correlation function (b) at the ribbon edge as a function of $J/t$ when $J_z/t = 2$.](image)

II. MAGNETIC ORDERS

The Ising-like $J_z$ term in our Hamiltonian can be decompose into the following three terms,

$$-\frac{J_z}{4}\sum_i [(\hat{n}_{1i\uparrow} - \hat{n}_{1i\downarrow}) - (\hat{n}_{2i\uparrow} - \hat{n}_{2i\downarrow})]^2 = -\frac{J_z}{4}\sum_i \hat{n}_{\xi i\sigma} + \frac{J_z}{2}\sum_i \hat{n}_{\xi i\uparrow}\hat{n}_{\xi i\downarrow} + 2J_z\sum_i \hat{S}^z_{1i}\hat{S}^z_{2i}$$

(S1)

The first term is the on-site potential term, the second term is the on-site Coulomb repulsive interaction and the third term is the Ising exchange interaction between two layer sites. When $J_z \gg J$, $J_z$ will drive the system into a Ising antiferromagnetic ordered (SDW-Z) state. We define the SDW-Z antiferromagnetic magnetic order along $z$ direction as follows

$$M^z_{A_i}(r_j - r_i) = S^z_{A_i}r_i, S^z_{A_i}r_j - S^z_{A_i}r_i, S^z_{A_i}r_j - S^z_{A_i}r_i + S^z_{A_i}r_j - S^z_{A_i}r_i$$

(S2)

From Fig. S2, there is no SDW-XY and SDW-Z magnetic orders (and no time-reversal symmetry breaking) in the whole $J/t > 0$ parameter regime when $J_z/t \leq 2.0$. However, when $J_z/t = 3.0$, SDW-Z order emerges in the middle of $J/t$ parameter region.

III. ENERGY CURVES

We plot the expectation values of four parts of the Hamiltonian in Fig. S3 as a function of $J/t$ for different $J_z/t$ values. From the inflection point of the energy curves and magnetic structure factor shown in Fig. S2, we can obtain the approximate bulk quantum phase transition points without calculating the energy gaps.
Fig. S2. SDW-XY (a,c) and SDW-Z (b, d) structure factor as a function of $J/t$ and linear system size $L$ for $J_z/t = 2$ and $J_z/t = 3$. There is no SDW-Z magnetic order when $J_z/t \leq 2$ in the whole $J/t$ regime. Around the bulk quantum phase transition critical point (QCP), SDW-XY structure factor shows a power-law increasing tendency with system size $L$, however, the power-law increasing exponent is less than 2 which means no SDW-XY magnetic order will develop around the QCP in the thermodynamic limit.

Fig. S3. Ground state energy per site as a function of $J/t$ when $J_z/t = 1$ and 2. The linear system size used here is $L = 15$. Combined with Fig. S2, we can get the phase diagram which is shown in Fig.1 (b) in the main text.

IV. OTHER MATRIX ELEMENTS OF EDGE GREEN’S FUNCTION AND O(4) CORRELATION FUNCTION

In the main text, we only show the Green function between $A_1$ sublattice and $B_1$ sublattice in the same layer along the ribbon edge, i.e., an off-diagonal term of the edge Green’s function matrix. Here, we present that the diagonal parts of Green function matrix also show similar behavior as the off-diagonal part.

Fig. S4 shows the trace of single-particle Green’s function matrix $\text{Tr}G^i = G^{i}_{A_1A_1} + G^i_{A_2A_2} + G^i_{B_1B_1} + G^i_{B_2B_2}$ at the ribbon edge as a function of $J/t$ when $J_z/t = 0$. The diagonal part of single-particle Green’s function at the edge also shows the exponential decay before the bulk quantum phase transition.

For the SDW-XY correlation matrix, we have show the $|N^+_{AA}|$ (with combined elements) in the main text. Here, we also show you the power-law decay of $|N^+_{BB}|$ and $|S^+_{A_1B_1}|$ before the bulk quantum phase transition in Fig. S5,
FIG. S4. The trace of single-particle Green’s function matrix at the ribbon edge as a function of $J/t$ when $J_z/t = 0$.

where $N_{BB}^{+−}$ defines as

$$N_{BB}^{+−}(r_j - r_i) = \frac{1}{2} [S_{B_1B_1}^{±}(r_j - r_i) - S_{B_1B_2}^{±}(r_j - r_i) - S_{B_2B_1}^{±}(r_j - r_i) + S_{B_2B_2}^{±}(r_j - r_i)].$$  \hspace{1cm} (S3)

FIG. S5. The SDW-XY correlation functions $|N_{BB}^{+−}|$ and $|S_{A_1B_1}^{+−}|$ at the ribbon edge as a function of $J/t$ when $J_z/t = 0$.

V. FINITE-SIZE EFFECTS

In the main text, we mainly use the $L_{a_1} = 27, L_{a_2} = 9$ system size in the PQMC calculations. Here, we show that $L_{a_2} = 9$, which is the width of the ribbon, is large enough to obtain thermodynamic limit behavior. As shown in Fig. S6, when we increase the $L_{a_2}$ from 5 to 11, little change both in the single-particle Green’s function as well as two-particle bosonic correlation function, can be observed.

VI. STRANGE CORRELATOR

Apart from creating a physical spatial edge to study the edge physics, we can also calculate the strange correlator to reflect the physical edge between two topological distinct many-body ground state wave functions [33, 34].

$$C(r, r') = \frac{\langle \Omega | \hat{\phi}(r) \hat{\phi}(r') | \Psi \rangle}{\langle \Omega | \Psi \rangle}$$  \hspace{1cm} (S4)

we can define the single-particle strange correlator and spin strange correlator by replacing the bra state with a topological trivial state $\langle \Omega \rangle$ in Eq. (4) in the main text. The single-particle strange correlator also shows an exponential
(b) and the power-law decay of edge SDW-XY correlation function in Fig. 5 in the main text, we show in Fig. S8 (a) is also a bosonic SPT phase.

decay before the bulk quantum phase transition while the spin strange correlator remains power-law decay, indicating the interacting QSH phase $|\Psi\rangle$ is topologically distinct from the trivial phase $|\Omega\rangle$, and there exist gapless bosonic modes at the spatial interface between two systems.

FIG. S7. single-particle strange correlator and SDW-XY strange correlator as a function of $J/t$ when $J_s/t = 0$.

FIG. S6. The single-particle Green’s function and SDW-XY correlation function at the ribbon edge change little when we increase $L_{a_2}$ from 5 to 11. The insets show the $y$-axis values of the right-most points as a function of ribbon width $L_{a_2}$.

VII. ON-SITE $U$ INTERACTION

The phase diagram of bilayer KMH model with on-site $U \sum (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 1)^2$ interaction and inter-layer $J$ interaction is shown in Fig. S8 (a). The phase boundaries are obtained from the bosonic gap closing as well as the nonzero magnetic order parameter in our previous paper Ref. [24]. Based on the exponential decay of edge single-particle Green’s function in Fig. S8 (b) and the power-law decay of edge SDW-XY correlation function in Fig. 5 in the main text, we conclude that the quantum spin Hall phase with finite interaction $U$ and $J$ which is shown in Fig. S8 (a) is also a bosonic SPT phase.
FIG. S8. (a) Phase Diagram of bilayer KMH model with on-site $U$ interaction and inter-layer $J$ interaction. The red line shows the vertical phase path we used in Fig. 5 in the main text. The exponential decay of single-particle Green’s function at the ribbon edge indicates that fermions are still gapped when $U/t$ is increased at $J/t = 2.75$. 

(b) 

$log(g_{\alpha\beta}(r_1-r_2))$ vs $log(r_1-r_2)$ for different values of $U/t$. 

\[ \lambda/t=0.2, J/t=0, J/t=2.75 \]