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Quantum Phase Transitions Between Bosonic Symmetry Protected Topological States Without Sign Problem: Nonlinear Sigma Model with a Topological Term

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(Dated: February 10, 2016)

We propose a series of simple $2d$ lattice interacting fermion models that we demonstrate at low energy describe bosonic symmetry protected topological (SPT) states and quantum phase transitions between them. This is because due to interaction the fermions are gapped both at the boundary of the SPT states and at the bulk quantum phase transition, thus these models at low energy can be described completely by bosonic degrees of freedom. We show that the bulk of these models is described by a $\mathrm{Sp}(N)$ principal chiral model with a topological Θ-term, whose boundary is described by a $\mathrm{Sp}(N)$ principal chiral model with a Wess-Zumino-Witten term at level-1. The quantum phase transition between SPT states in the bulk is tuned by a particular interaction term, which corresponds to tuning Θ in the field theory and the phase transition occurs at $\Theta = \pi$. The simplest version of these models with $N = 1$ is equivalent to the familiar $\mathrm{O}(4)$ nonlinear sigma model (NLSM) with a topological term, whose boundary is a $(1 + 1)d$ conformal field theory with central charge $c = 1$. After breaking the $\mathrm{O}(4)$ symmetry to its subgroups, this model can be viewed as bosonic SPT states with $\mathrm{U}(1)$, or Z_2 symmetries, etc. All these fermion models including the bulk quantum phase transitions can be simulated with determinant Quantum Monte Carlo method without the sign problem. Recent numerical results strongly suggest that the quantum disordered phase of the $\mathrm{O}(4)$ NLSM with precisely $\Theta = \pi$ is a stable $(2 + 1)d$ conformal field theory (CFT) with gapless bosonic modes.

I. INTRODUCTION

Unlike fermionic symmetry protected topological (SPT) states (or equivalently called topological insulators and topological superconductors), bosonic SPT states all require strong interaction, which makes it very difficult to analyze any generic model of bosonic SPT states. The original general Hamiltonians for bosonic SPT states proposed in Ref. 1,2 and the lattice models that describe the Z_2 SPT state[3,4] are exactly soluble, but they are artificial and only describe the fixed points of the SPT states. Most discussions of bosonic SPT states so far are based on effective field theories[5–7], and their exact relation to lattice models was not carefully explored yet.

Besides their special symmetry protected edge states, SPT states must also have special quantum phase transitions between each other (or from the trivial state). These transitions are clearly beyond the Ginzburg-Landau paradigm because no symmetry is spontaneously broken across the transition. In order to study bosonic SPT states more quantitatively, especially at the quantum phase transitions between bosonic SPT states, we need lattice models that can be tuned away from their fixed points, namely they are not soluble, but can be simulated reliably without sign problem. Several lattice models of bosons with statistical interactions[8–11] has been proposed and studied by various numerical techniques. In this paper, we propose a series of $2d$ lattice models built with interacting fermions instead of bosons. However, we argue that in the entire phase diagram the fermions never have to show up at low energy. First of all,

we demonstrate that the edge states (interface between SPT and trivial states) at the $(1 + 1)d$ boundary only contain gapless boson modes, while fermions are gapped by interaction. Then it is expected that at the bulk quantum phase transition between the SPT and the trivial states the fermions are also gapped while bosons are gapless, which can be understood in a simple Chalker-Coddington network construction of the bulk quantum phase transition[12]. Indeed, it was shown in an interacting bilayer quantum spin Hall model[13,14] that the quantum phase transition between the SPT and trivial states only involve gapless bosonic modes. Especially, the data in Ref. 14 strongly suggests that along a special $\mathrm{SO}(4)$ symmetric line of the model, the SPT-trivial quantum phase transition (which is described the $\mathrm{O}(4)$ nonlinear sigma model (NLSM) with $\Theta = \pi$) is a special $(2 + 1)d$ conformal field theory (CFT) that only involves bosonic fields, which is consistent with the conjectured renormalization group flow diagram in Ref. 15.

In this work, we will first review and further analyze the model used in Ref. 13,14. Then we demonstrate that this model can be generalized to a whole series of models with N times of fermion flavors, and we argue that the bulk is described by a $\mathrm{Sp}(N)$ principal chiral model with a topological $\Theta-$term, and by tuning one parameter this model can have a quantum phase transition between SPT and trivial state, which in the field theory occurs precisely at $\Theta = \pi$. In the SPT phase the boundary of this model is described by the $\mathrm{Sp}(N)_1$ CFT. Again all the fermion modes at the boundary are gapped out by interaction, and hence we expect the same happens

at the SPT-trivial transition in the bulk (based on the Chalk-Coddington construction[12]), which awaits further numerical confirmation. Implication of our results on the $2d$ boundary of $3d$ fermionic and bosonic SPT states will also be discussed.

II. BILAYER QUANTUM SPIN HALL INSULATOR

A. Bulk Theory

1. Model and Symmetry

In this section let us first review and also further analyze the model used in Ref. 13,14, which is an interacting bilayer quantum spin Hall insulator without sign problem. Let $c_{i\ell} = (c_{i\ell\uparrow}, c_{i\ell\downarrow})^{\mathsf{T}}$ be the spin-1/2 fermion doublet on site-i layer-ℓ. The free fermion part of the Hamiltonian for the bilayer QSH model is given by

$$H_{\text{band}} = -t \sum_{\langle ij \rangle, \ell} c_{i\ell}^{\dagger} c_{j\ell} + \sum_{\langle\langle ij \rangle\rangle, \ell} \mathrm{i}\lambda_{ij} c_{i\ell}^{\dagger} \sigma^z c_{j\ell} + H.c., \quad (1)$$

where t is the nearest neighbor hopping and $\lambda_{ij} = -\lambda_{ji}$ is the Kane-Mele spin-orbit coupling, as illustrated in Fig. 1. The layer index $\ell = 1, 2$ labels the two layers of QSH systems. Without any interaction, the free-fermion Hamiltonian H_{band} has a pretty high symmetry $\text{SO}(4) \times \text{SO}(3)$.[14] The symmetry will be most evident, if we rewrite the model in a new set of fermion basis (roughly by a particle-hole transformation of fermions in the second layer), defined by

$$f_{i\uparrow} \equiv \begin{pmatrix} f_{i\uparrow 1} \\ f_{i\uparrow 2} \end{pmatrix} = \begin{pmatrix} c_{i1\uparrow} \\ (-)^i c_{i2\uparrow}^{\dagger} \end{pmatrix},$$
$$f_{i\downarrow} \equiv \begin{pmatrix} f_{i\downarrow 1} \\ f_{i\downarrow 2} \end{pmatrix} = \begin{pmatrix} (-)^i c_{i1\downarrow} \\ c_{i2\downarrow}^{\dagger} \end{pmatrix}, \quad (2)$$

where $(-)^i = +/-$ on sublattice A/B respectively. In the new basis, the Hamiltonian H_{band} reads

$$H_{\text{band}} = \sum_{i,j,\sigma} (-)^{\sigma} f_{i\sigma}^{\dagger} (-t_{ij} + \mathrm{i}\lambda_{ij}) f_{j\sigma} + h.c., \quad (3)$$

where $(-)^{\sigma} = +/-$ for spin $\uparrow / \downarrow$ respectively. Here $t_{ij} = t$ for nearest neighboring sites i, j and $t_{ij} = 0$ otherwise.

The SO(4) symmetry rotates the following fermion bilinear operators $\boldsymbol{N}_i = (N_i^0, N_i^1, N_i^2, N_i^3)$ as an O(4) vector:

$$\boldsymbol{N}_i = f_{i\downarrow}^{\dagger} (\tau^0, \mathrm{i}\tau^1, \mathrm{i}\tau^2, \mathrm{i}\tau^3) f_{i\uparrow} + h.c., \quad (4)$$

where $\tau^{0,1,2,3}$ are Pauli matrices acting on the f-fermion doublets. The SO(4) group is naturally factorized to $\text{SU}(2)_{\uparrow} \times \text{SU}(2)_{\downarrow}$ as right and left isoclinic rotations, under which the fermions transform as $f_{i\sigma} \to U_{\sigma} f_{i\sigma}$ with $U_{\sigma} \in \text{SU}(2)_{\sigma}$ for $\sigma = \uparrow, \downarrow$. It is straight-forward to see
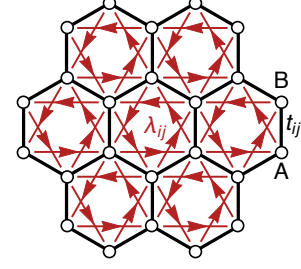

FIG. 1: Honeycomb lattice with the nearest neighboring hopping t_{ij} and the 2nd nearest neighboring hopping λ_{ij}. $\lambda_{ij} = -\lambda_{ji} = \lambda$ if i follows the bound orientation to j. The lattice can be divided into A and B sublattices.

the band Hamiltonian H_{band} in Eq. (3) is invariant under both $\text{SU}(2)_{\uparrow}$ and $\text{SU}(2)_{\downarrow}$, and hence SO(4) symmetric. On the other hand, the SO(3) symmetry rotates another set of fermion bilinear operators $\boldsymbol{M}_i = (M_i^1, M_i^2, M_i^3)$ as an O(3) vector. Let $M_i^{\pm} = M_i^1 \pm \mathrm{i}M_i^2$, the definition of $\boldsymbol{M}_i$ follows from

$$M_i^- = \sum_{\sigma} f_{i\sigma}^{\mathsf{T}} \mathrm{i}\tau^2 f_{i\sigma}, \quad M_i^3 = (-)^i \sum_{\sigma} (-)^{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma}, \quad (5)$$

and $M_i^+ = (M_i^-)^{\dagger}$. This also defines an SU(2) symmetry of the f-fermions, denoted as $\text{SU}(2)_M$. The SU(2) generators are given by $\boldsymbol{Q} = \sum_i \boldsymbol{Q}_i$ with $Q_i^a = \frac{1}{2\mathrm{i}} \epsilon_{abc} M_i^b M_i^c$. Let $Q_i^{\pm} = Q_i^1 \pm \mathrm{i}Q_i^2$, the $\text{SU}(2)_M$ generators can be explicitly written as

$$Q_i^- = (-)^i \sum_{\sigma} (-)^{\sigma} f_{i\sigma}^{\mathsf{T}} \mathrm{i}\tau^2 f_{i\sigma},$$
$$Q_i^3 = \sum_{\sigma} (f_{i\sigma}^{\dagger} f_{i\sigma} - 1). \quad (6)$$

The physical meaning of Q^3 is the total number of f-fermions away from half-filling, which is obviously conserved. It can be further checked that $[H_{\text{band}}, \boldsymbol{Q}] = 0$, so the model is indeed $\text{SU}(2)_M \simeq \text{SO}(3)$ symmetric. Therefore on the free-fermion level, the bilayer QSH model has the $\text{SO}(4) \times \text{SO}(3) \simeq \text{SU}(2)_{\uparrow} \times \text{SU}(2)_{\downarrow} \times \text{SU}(2)_M$ symmetry.

In terms of the original fermion $c_{i\ell} = (c_{i\ell\uparrow}, c_{i\ell\downarrow})^{\mathsf{T}}$, the O(4) vector $\boldsymbol{N}_i$ and the O(3) vector $\boldsymbol{M}_i$ have simple physical interpretations. They correspond to the following fermion bilinear orders,[13,14]

$$\text{SDW:} \ \boldsymbol{S}_i = (N_i^0, N_i^3, M_i^3) = \sum_{\ell} (-)^{i+\ell} c_{i\ell}^{\dagger} \boldsymbol{\sigma} c_{i\ell},$$
$$\text{SC:} \ \Delta_i = N_i^2 + \mathrm{i}N_i^1 = 2c_{i1}^{\mathsf{T}} \mathrm{i}\sigma^y c_{i2}, \quad (7)$$
$$\text{Exciton:} \ D_i = M_i^1 + \mathrm{i}M_i^2 = -2(-)^i c_{i1}^{\dagger} c_{i2}.$$

The spin density wave (SDW) is an antiferromagnet both between the sublattices and across the layers, the super-conductivity (SC) is an inter-layer spin-singlet s-wave pairing, and the exciton condensation is an inter-layer

particle-hole pairing with opposite phase between the sublattices. The SO(4) symmetry rotates the SDW-XY and the SC order parameters, and the SO(3) symmetry rotates the exciton and the SDW-Z order parameters. In the original fermion basis, the SO(3) $\simeq$ SU(2)$_M$ generators read

$$Q_i^- = -2c_{i2}^\dagger \sigma^z c_{i1}, \; Q_i^3 = \sum_\ell (-)^\ell c_{i\ell}^\dagger c_{i\ell}. \qquad (8)$$

So the SU(2)$_M$ symmetry rotates the original c-fermions across the layers, and Q^3 is the charge difference between the layers. Because the layers are identical to each other in the bilayer QSH model Eq. (1), the SU(2)$_M$ symmetry is manifest.

2. Phase Diagram

A generic four-fermion interaction that preserves the SO(4) × SO(3) symmetry takes the form of

$$H_{\text{int}} = -\sum_{i,j} \left(J_{ij} \boldsymbol{N}_i \cdot \boldsymbol{N}_j + U_{ij} \boldsymbol{M}_i \cdot \boldsymbol{M}_j \right), \qquad (9)$$

where $\boldsymbol{N}_i$ and $\boldsymbol{M}_i$ are fermion bilinear operators defined in Eq. (4) and Eq. (5) respectively. To simplify, we consider the nearest neighboring coupling $J_{ij} = J\delta_{\langle ij \rangle}$ of O(4) vectors, and the on-site interaction $U_{ij} = U\delta_{ij}$ of O(3) vectors. Then the full Hamiltonian of the interacting bilayer QSH model reads

$$H = \sum_{i,j,\sigma} (-)^\sigma f_{i\sigma}^\dagger (-t_{ij} + i\lambda_{ij}) f_{j\sigma} + h.c.$$
$$- J\sum_{\langle ij \rangle} \boldsymbol{N}_i \cdot \boldsymbol{N}_j - U\sum_i \boldsymbol{M}_i \cdot \boldsymbol{M}_i. \qquad (10)$$

Or in terms of the original c-fermion,

$$H = H_{\text{band}} + H_{\text{int}},$$
$$H_{\text{band}} = -t\sum_{\langle ij \rangle, \ell} c_{i\ell}^\dagger c_{j\ell} + \sum_{\langle\langle ij \rangle\rangle, \ell} i\lambda_{ij} c_{i\ell}^\dagger \sigma^z c_{j\ell} + H.c.,$$
$$H_{\text{int}} = -J\sum_{\langle ij \rangle} \tfrac{1}{2}(S_i^+ S_j^- + \Delta_i^\dagger \Delta_j + h.c.) \qquad (11)$$
$$- U\sum_i \left(\tfrac{1}{2}(D_i^\dagger D_i + D_i D_i^\dagger) + S_i^z S_i^z \right),$$

where $S_i^\pm = S_i^x \pm iS_i^y$ and $\boldsymbol{S}_i, \Delta_i, D_i$ are c-fermion bilinear operators defined in Eq. (7).

A schematic phase diagram of the model is shown in Fig. 2. In the weak interaction limit when both J and U are small, the model is an SO(4) bosonic SPT phase. In the next subsection we will demonstrate that the interaction gaps out the fermion modes of the boundary states of the quantum spin Hall insulator, which leaves the boundary only a CFT with central charge $c = 1$ and
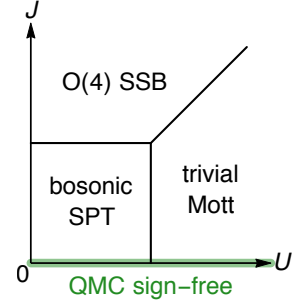

FIG. 2: A schematic phase diagram of the interacting bilayer QSH model.

exact SO(4) symmetry. The boundary precisely corresponds an $(1 + 1)d$ O(4) NLSM with a Wess-Zumino-Witten (WZW) term at level $k = 1$.

$$S = \int \mathrm{d}\tau \mathrm{d}x \mathrm{d}u \, \frac{1}{2g}(\partial_\mu \boldsymbol{n})^2 + \frac{ik}{2\pi}\epsilon_{abcd}n^a \partial_\tau n^b \partial_x n^c \partial_u n^d, \qquad (12)$$

where $\boldsymbol{n} = (n^0, n^1, n^2, n^3)$ transforms like a vector under O(4). Based on this boundary theory, we can conclude that the bulk theory is a $(2 + 1)d$ O(4) NLSM with a Θ-term at Θ = 2π:

$$S = \int \mathrm{d}\tau \mathrm{d}^2x \, \frac{1}{2g}(\partial_\mu \boldsymbol{n})^2 + \frac{i\Theta}{2\pi^2}\epsilon_{abcd}n^a \partial_\tau n^b \partial_x n^c \partial_y n^d, \qquad (13)$$

where the coupling strength g is controlled by J. The relation between g and J is indirectly inferred from their physical consequences. A large J in Eq. (10) will favor the ferromagnetic long-range order of $\boldsymbol{N}_i$, which breaks the O(4) symmetry spontaneously. A small g in Eq. (13) will suppress the fluctuation of $\partial_\nu \boldsymbol{n}$ and stabilize the long-range order of $\boldsymbol{n}$, which also breaks the O(4) symmetry. Thus we identify the small g limit with the large J limit, which both correspond to the spontaneous symmetry broken (SSB) phase. Reversely in the large g (small J) limit, the model Eq. (13) is in the O(4) symmetric disordered phase with a topological Θ-term, which describes the $2d$ bosonic SPT phase.[6,7,16] The field theories, either on the boundary Eq. (12) or in the bulk Eq. (13), can also be derive by coupling the fermions to a bosonic O(4) vector field $\boldsymbol{n}_i$ via

$$H_{\text{cp}} = -\sum_i \boldsymbol{n}_i \cdot \boldsymbol{N}_i, \qquad (14)$$

where $\boldsymbol{N}_i$ are fermion bilinear operators in Eq. (4). Integrating out the fermions,[17] will generate the bosonic theories mentioned above.

Another way to connect the bilayer QSH insulator to the bosonic SPT state is to consider the fermions as partons of the O(4) vector field $\boldsymbol{N}_i$ under the constraint $\boldsymbol{Q}_i = 0$, which amounts to gauging the SU(2)$_M$ symmetry. After the fermions are confined by the SU(2)$_M$ gauge field, the remaining bulk degrees of freedom will be

purely bosonic. The gauge theory argument along this line has been discussed in Ref. 18, arriving at the conclusion that the bilayer QSH state precisely becomes a bosonic SPT state under gauge confinement. After coupling the fermions to dynamical gauge fields, it is equivalent to view the fermions as "slave fermions", which is an approach taken in Ref. 16,19,20. However in this work, we will use interactions to gap out the fermions instead of confining the fermions by gauge fluctuations.

Now we consider the effect of the on-site interaction U. Large enough U will drive the system to a featureless Mott insulator (no symmetry breaking and topologically trivial) as indicated in Fig. 2. At first glance, this seems counterintuitive because one may expect the interaction Hamiltonian $H_U = -U\boldsymbol{M}_i \cdot \boldsymbol{M}_i$ to favor a mean-field ground state with $\langle \boldsymbol{M}_i \rangle \neq 0$ on each site, which would then break the SO(3) symmetry spontaneously. However such mean-field state is not an eigenstate of the Hamiltonian H_U and hence not the true ground state. Take the mean-field states $|M_i^3 = \pm 2\rangle$ for example (where ± 2 are the maximal/minimal eigenvalues of the M_i^3 operator). Because $(M_i^1)^2 + (M_i^2)^2$ does not commute with M_i^3, the states $|M_i^3 = \pm 2\rangle$ must be mixed to produce the true on-site ground state: $|M_i^3 = +2\rangle + |M_i^3 = -2\rangle$, which is actually an SO(4) × SO(3) *singlet state*. Although the expectation value of the O(3) vector $\langle \boldsymbol{M}_i \rangle = 0$ vanishes in the singlet state, $\langle \boldsymbol{M}_i \cdot \boldsymbol{M}_i \rangle$ is not zero, so that the Hamiltonian H_U does gain energy from the singlet state. The singlet state has the energy $-12U$ (per site), which is lower than the energy of any mean-field state. By exact diagonalization of the on-site interaction H_U, it can be verified that the singlet state is the unique on-site ground state and is gapped from all excited states by the energy of the order $\sim U$.

Therefore in the large U limit, the model has an unique and fully-gapped ground state, which is the direct product of on-site SO(4) × SO(3) singlets

$$|\text{GS}\rangle = \prod_i M_i^+ |0\rangle_f = \prod_i (f_{i\uparrow2}^\dagger f_{i\uparrow1}^\dagger + f_{i\downarrow2}^\dagger f_{i\downarrow1}^\dagger)|0\rangle_f, \quad (15)$$

where $|0\rangle_f$ denotes the zero fermion state of f-fermions. One can see $M_i^+|0\rangle_f$ is just another way of writing the singlet state $|M_i^3 = +2\rangle + |M_i^3 = -2\rangle$, given $M_i^3 \sim f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow}$. In the original c-fermion basis, the ground state reads

$$|\text{GS}\rangle = \prod_i \Delta_i^\dagger |0\rangle_c = \prod_i (c_{i1\downarrow}^\dagger c_{i2\uparrow}^\dagger - c_{i1\uparrow}^\dagger c_{i2\downarrow}^\dagger)|0\rangle_c, \quad (16)$$

where $|0\rangle_c$ denotes the zero fermion state of c-fermions. Because the ground state is unique and fully gapped, it should be stable against all local perturbations, and can be considered as a representative state that controls the whole trivial Mott phase.

The symmetry property of the ground state is most obvious in the f-fermion basis. It is easy to see that the ground state $|\text{GS}\rangle$ in Eq. (15) is invariant under SU(2)$_\uparrow$ × SU(2)$_\downarrow$, because $f_{i\sigma2}^\dagger f_{i\sigma1}^\dagger$ is the SU(2)$_\sigma$ singlet operator and $|0\rangle_f$ is also SU(2)$_\sigma$ invariant (for both

$\sigma = \uparrow, \downarrow$). The SU(2)$_M$ symmetry can be verified by showing $\boldsymbol{Q}|\text{GS}\rangle = 0$. Since $|\text{GS}\rangle$ is at half-filling, $Q^3|\text{GS}\rangle = 0$. Then by definition, $[Q_i^a, M_j^b] = 2\mathrm{i}\epsilon^{abc}\delta_{ij}M_i^c$, thus $Q_i^- M_i^+ = M_i^+ Q_i^- - 4M_i^3$, so

$$Q_i^-|\text{GS}\rangle = \prod_{j \neq i} M_j^+ (M_i^+ Q_i^- - 4M_i^3)|0\rangle_f = 0. \quad (17)$$

Because $Q_i^- \sim (-)^\sigma f_{i\sigma}^\mathsf{T} \mathrm{i}\tau^2 f_{i\sigma}$ only contains fermion annihilation operators and $M_i^3 \sim (-)^\sigma f_{i\sigma}^\dagger f_{i\sigma}$ is a sum of number operators, both of them quench the fermion vacuum state $|0\rangle_f$, therefore $Q^-|\text{GS}\rangle = \sum_i Q_i^-|\text{GS}\rangle = 0$. In conclusion, the large-U ground state preserves the full SU(2)$_\uparrow$ × SU(2)$_\downarrow$ × SU(2)$_M \simeq$ SO(4) × SO(3) symmetry.

In the trivial Mott phase, both the fermionic and bosonic excitations are gapped. In the large U limit, the single particle gap is $9U$, the O(3) vector gap is $8U$ and the O(4) vector gap is $12U$. The O(4) vector gap can be soften by the inter-site coupling J. When the gap is soften to zero, the O(4) boson will condense and the system will enter the SSB phase. So we expect the order-disorder transition to happen at $J \sim U$ in the strong interaction limit.

The most interesting feature of this model is the topological transition between the bosonic SPT phase and the trivial Mott phase. Previous numerical study[14] shows that with the exact SO(4) symmetry described in this section, there can be a direct continuous transition between the bosonic SPT phase and the trivial Mott phase, where the gap of bosonic modes $\boldsymbol{N}$ closes, while the fermion gap remains open. Thus we expect this phase transition can be described by Eq. (13). The phase diagram and the renormalization group flow of Eq. (13) was studied in Ref. 15. In the large g (small J) regime, the bosonic SPT phase corresponds to $\pi < \Theta \leq 2\pi$ controlled by the stable fixed point $\Theta = 2\pi$, and the trivial Mott phase corresponds to $0 \leq \Theta < \pi$ controlled by the stable fixed point $\Theta = 0$. The two phases are separated by the quantum phase transition at $\Theta = \pi$, which in general can be either first order or continuous, while numerical results in Ref. 14 demonstrates that this transition is continuous, which implies that the disordered phase of Eq. 13 with $\Theta = \pi$ is a $(2+1)d$ CFT. The stability of this CFT against perturbations that break the SO(4) symmetry needs further studies.

3. Sign-Free QMC Simulation

In this subsection we show that the whole $J = 0$ line in the phase diagram Fig. 2 can be simulated by determinant QMC without fermion sign problem. Along the $J = 0$ line, the interacting bilayer QSH model in Eq. (10) admits sign-free QMC simulations. We perform Hubbard-Stratonovich (HS) decomposition of the on-site interaction in the O(3) vector channel by introducing the O(3) auxiliary field $\boldsymbol{m}_i$, such that $-U\boldsymbol{M}_i^2 \rightarrow -\boldsymbol{m}_i \cdot \boldsymbol{M}_i + \frac{1}{4U}\boldsymbol{m}_i^2$. The partition function is a sum of

the Boltzmann weight $W[\boldsymbol{m}_i(\tau)]$ over spacetime configurations of the auxiliary field $\boldsymbol{m}_i(\tau)$,

$$
\begin{aligned}
Z &= \sum_{[\boldsymbol{m}_i(\tau)]} W[\boldsymbol{m}_i(\tau)], \\
W[\boldsymbol{m}_i(\tau)] &= \mathrm{Tr} \prod_\tau e^{-\Delta\tau H[\boldsymbol{m}_i(\tau)]},
\end{aligned}
\tag{18}
$$

where $H[\boldsymbol{m}_i]$ is a fermion bilinear Hamiltonian as a functional of $\boldsymbol{m}_i$,

$$
H[\boldsymbol{m}_i] = H_{\mathrm{band}} + \sum_i \left(-\boldsymbol{m}_i \cdot \boldsymbol{M}_i + \frac{1}{4U}\boldsymbol{m}_i^2 \right). \tag{19}
$$

It can be verified that the Hamiltonian $H[\boldsymbol{m}_i]$ has the following time-reversal symmetry $\mathcal{T}$ for all configurations of $\boldsymbol{m}_i$.

$$
\mathcal{T}: \begin{cases} f_{i\uparrow} \to \mathcal{K}\mathrm{i}f_{i\downarrow}^\dagger \\ f_{i\downarrow} \to \mathcal{K}\mathrm{i}f_{i\uparrow}^\dagger \end{cases}, \begin{cases} f_{i\uparrow}^\dagger \to \mathcal{K}(-\mathrm{i})f_{i\downarrow} \\ f_{i\downarrow}^\dagger \to \mathcal{K}(-\mathrm{i})f_{i\uparrow} \end{cases}, \tag{20}
$$

where $\mathcal{K}$ is the complex conjugation operator. According to Ref. 21–23, the time-reversal symmetry ensures the weight $W[\boldsymbol{m}_i]$ to be positive definite, which allows QMC simulations without the fermion sign problem.

However when $J \neq 0$, we are not aware of any sign-free QMC simulation scheme that also preserves the SO(4) symmetry. The most straight-forward HS decomposition of the J-term interaction is in the O(4) vector channel, as done in Eq. (14). However it suffers from the fermion sign problem. Because the fermion sign structure of the weight $W[\boldsymbol{n}_i(\tau)]$ must match the bosonic SPT sign structure described by the topological Θ-term in Eq. (13), which requires each O(4) skyrmion in the spacetime configuration of $\boldsymbol{n}$ to be associated with a minus sign. Such sign structure is a defining feature of the bosonic SPT phase, and can not be avoided. It turns out that other HS decompositions in the fermion hopping/pairing channels do not eliminate the sign problem either.

Nevertheless if we are allowed to break the SO(4) symmetry, we can introduce the inter-site correlation of $\boldsymbol{N}$ field without spoiling the sign-free QMC. Because as long as the time reversal symmetry in Eq. (20) is preserved, the Boltzmann weight will be positive definite. Among the four components of the vector $\boldsymbol{N}$, only N^0 is time-reversal odd (i.e. $\mathcal{T}: N^0 \to -N^0$), and the remaining components $N^{1,2,3}$ are time-reversal even (i.e. $\mathcal{T}: N^{1,2,3} \to N^{1,2,3}$). Hence the following decomposition is time reversal symmetric,

$$
H[\boldsymbol{m}_i, \boldsymbol{n}_i] = H[\boldsymbol{m}_i] + \sum_i \sum_{a=1,2,3} n_i^a N_i^a + \cdots, \tag{21}
$$

which will result in positive definite weight $W[\boldsymbol{m}_i, \boldsymbol{n}_i]$. Therefore it is possible to explore the entire J-U phase diagram like Fig. 2, if we lower the SO(4) symmetry to its SO(3), U(1) or Z_2 subgroups.

B. Boundary Theory

1. One-Loop RG

On the free-fermion level, the helical edge modes of the bilayer QSH model is described by

$$
H_{\mathrm{bdy}} = \int \mathrm{d}x (\psi_L^\dagger \mathrm{i}\partial_x \psi_L - \psi_R^\dagger \mathrm{i}\partial_x \psi_R), \tag{22}
$$

where ψ_L (ψ_R) is the left (right) moving edge mode associated to $f_\uparrow$ ($f_\downarrow$). Both of them are complex fermion doublets,

$$
\psi_L = \begin{pmatrix} \psi_{L1} \\ \psi_{L2} \end{pmatrix}, \psi_R = \begin{pmatrix} \psi_{R1} \\ \psi_{R2} \end{pmatrix}. \tag{23}
$$

The SO(4) symmetry is factorized to $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ acting on ψ_L and ψ_R respectively. On symmetry ground, the most generic $\mathrm{SO}(4) \times \mathrm{SO}(3)$ invariant interaction that can be induced on the boundary takes the form of

$$
H_{\mathrm{int}} = \int \mathrm{d}x (\lambda_J \boldsymbol{N} \cdot \boldsymbol{N} + \lambda_U \boldsymbol{M} \cdot \boldsymbol{M}), \tag{24}
$$

where the O(4) vector $\boldsymbol{N}$ follows from Eq. (4) as

$$
\boldsymbol{N} = \psi_R^\dagger (\tau^0, \mathrm{i}\tau^1, \mathrm{i}\tau^2, \mathrm{i}\tau^3)\psi_L + h.c., \tag{25}
$$

and the O(3) vector $\boldsymbol{M}$ follows from Eq. (5) as

$$
M^- = \sum_{\sigma=L,R} \psi_\sigma^\intercal \mathrm{i}\tau^2 \psi_\sigma, \quad M^3 = \sum_{\sigma=L,R} (-)^\sigma \psi_\sigma^\dagger \psi_\sigma. \tag{26}
$$

Along the $J = 0$ line, we expect $\lambda_J \to 0$ and $\lambda_U < 0$ at the UV scale. To facilitate the analysis, we split the $\lambda_U \boldsymbol{M} \cdot \boldsymbol{M}$ interaction into the in-plane $H_\pm$ and out-of-plane H_3 terms, and rearrange the interaction as

$$
\begin{aligned}
H_{\mathrm{int}} &= \int \mathrm{d}x (\lambda_\pm H_\pm + \lambda_3 H_3 + \lambda_0 H_0), \\
H_\pm &= \tfrac{1}{2}(M^+ M^- + M^- M^+), \\
H_3 &= M^3 M^3, \\
H_0 &= \tfrac{1}{3}\boldsymbol{M} \cdot \boldsymbol{M} - \tfrac{1}{6}\boldsymbol{N} \cdot \boldsymbol{N} + \tfrac{2}{3} \\
&= \sum_{\sigma=L,R} (\psi_\sigma^\dagger \psi_\sigma - 1)^2.
\end{aligned}
\tag{27}
$$

Here the SO(3) symmetry is allowed to be broken if $\lambda_\pm \neq \lambda_3$. However we will show that the anisotropy is irrelevant under RG. The one-loop RG equations are

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\ell}\lambda_\pm &= -\tfrac{4}{3}\lambda_\pm \lambda_3, \\
\frac{\mathrm{d}}{\mathrm{d}\ell}\lambda_3 &= -\tfrac{4}{3}\lambda_\pm^2, \\
\frac{\mathrm{d}}{\mathrm{d}\ell}\lambda_0 &= \tfrac{4}{3}\lambda_\pm^2 + \tfrac{8}{3}\lambda_\pm \lambda_3.
\end{aligned}
\tag{28}
$$

At the free-fermion fixed point, $\lambda_\pm$ is always a marginally relevant perturbation, regardless of its initial sign. The interaction will flow towards the $(\lambda_\pm, \lambda_3, \lambda_0) \to$

$(-1, -1, +3)$ direction if $\lambda_\pm < 0$, or towards the $(\lambda_\pm, \lambda_3, \lambda_0) \to (+1, -1, -1)$ direction if $\lambda_\pm > 0$. The fixed-point interaction will take the following form

$$H_{\text{int}} = \int dx \big(-4\lambda_\pm (\psi_{R1}^\dagger \psi_{R2}^\dagger \psi_{L1} \psi_{L2} + h.c.) \\ - 2\lambda_3 (\psi_R^\dagger \psi_R - 1)(\psi_L^\dagger \psi_L - 1) \big). \tag{29}$$

with $\lambda_3 < 0$ and $\lambda_\pm = \pm \lambda_3$. In both cases, the SO(3) symmetry is restored under the RG flow. At the RG fixed point, the interaction is expected to gap out fluctuations of the O(3) vector $\boldsymbol{M}$ on the boundary. Since $\boldsymbol{M}$ is a collective mode of fermions, so the fermions must also be gapped out by the interaction on the boundary.

2. Abelian Bosonization

In the following, we will use the Abelian bosonization to show that the interaction indeed gaps out the fermion mode, and drive the boundary into a $SU(2)_1$ CFT. The boundary fermions in Eq. (23) can be written as

$$\psi_{\sigma\alpha} = \frac{\kappa_{\sigma\alpha}}{\sqrt{2\pi a}} e^{i\phi_{\sigma\alpha}} \quad \sigma = L, R, \; \alpha = 1, 2, \tag{30}$$

where a is a short distance cut-off and $\kappa_{\sigma\alpha}$ is the Klein factor that ensures the anticommutation of the fermion operators. The helical edge modes in Eq. (22) can be bosonized to a Luttinger liquid (LL)

$$S_{\text{LL}} = \int d\tau dx \frac{1}{4\pi} (\partial_x \phi^\intercal K \partial_\tau \phi + \partial_x \phi^\intercal V \partial_x \phi), \tag{31}$$

where $\phi = (\phi_{L1}, \phi_{L2}, \phi_{R1}, \phi_{R2})^\intercal$, and the density fluctuations are given by $\psi_{\sigma\alpha}^\dagger \psi_{\sigma\alpha} = \frac{1}{2\pi}(-)^\sigma \partial_x \phi_{\sigma\alpha}$. The K matrix reads

$$K = \begin{pmatrix} +1 & & & \\ & +1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}. \tag{32}$$

The V matrix is an identity matrix at the free-fermion fixed point, and will be modified under interactions.

Under the RG flow, forward scatterings become irrelevant, and the fixed point interaction only contains umklapp and backward scatterings as in Eq. (29). In terms of the bosonized degrees of freedom ϕ,

$$H_{\text{int}} = \int dx \frac{g_3}{2\pi} \sum_{\alpha,\beta} \partial_x \phi_{L\alpha} \partial_x \phi_{R\beta} - 8\lambda_\pm \cos(l_0^\intercal \phi), \tag{33}$$

where $g_3 = \lambda_3/\pi$ and the vector $l_0 = (1, 1, -1, -1)^\intercal$. So the full boundary theory reads

$$S = S_{\text{LL}} - 8\lambda_\pm \int d\tau dx \cos(l_0^\intercal \phi), \tag{34}$$

with the V matrix given by

$$V = \begin{pmatrix} 1 & 0 & g_3 & g_3 \\ 0 & 1 & g_3 & g_3 \\ g_3 & g_3 & 1 & 0 \\ g_3 & g_3 & 0 & 1 \end{pmatrix}. \tag{35}$$

So the scaling dimension of $\cos(l_0^\intercal \phi)$ is

$$\Delta_0 = 2\sqrt{\frac{1 + 2g_3}{1 - 2g_3}}. \tag{36}$$

For small λ_3, $\Delta_0 \simeq 2 + 4\lambda_3/\pi$ (recall that $g_3 = \lambda_3/\pi$). The gapping term $\cos(l_0^\intercal \phi)$ is marginal ($\Delta_0 = 2$) at the free-fermion fixed point $\lambda_3 = 0$, and will become relevant ($\Delta_0 < 2$) if $\lambda_3 < 0$.

Although we started from a rather specific fixed point interaction in Eq. (29), the resulting boundary theory in Eq. (34) is of the generic form which is compatible with symmetry requirements. The SO(4) × SO(3) $\simeq$ SU(2)$_L$ × SU(2)$_R$ × SU(2)$_M$ symmetry action is not transparent in the Abelian bosonization, nevertheless its U(1)$_L$ × U(1)$_R$ × U(1)$_M$ subgroup is clear:

$$\begin{aligned} \text{U(1)}_L &: \psi_L \to e^{i\alpha_L \tau^3} \psi_L, \\ \text{U(1)}_R &: \psi_R \to e^{i\alpha_R \tau^3} \psi_R, \\ \text{U(1)}_M &: \psi_{L/R} \to e^{i\alpha_M} \psi_{L/R}. \end{aligned} \tag{37}$$

Correspondingly the ϕ field is transformed as follows

$$\phi \to \phi + \begin{pmatrix} 1 & 0 & 1 \\ -1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_L \\ \alpha_R \\ \alpha_M \end{pmatrix}. \tag{38}$$

Therefore $-8\lambda_\pm \cos(l_0^\intercal \phi)$ is the most relevant symmetry-preserving cosine term that can be added to the action. The O(4) vector $\boldsymbol{N}$ are linearly recombinations of the following fermion bilinear operators (and their conjugates)

$$\begin{aligned} \psi_{R1}^\dagger \psi_{L1} = e^{il_1^\intercal \phi}, \quad l_1^\intercal = (1, 0, -1, 0); \\ \psi_{R1}^\dagger \psi_{L2} = e^{il_2^\intercal \phi}, \quad l_2^\intercal = (0, 1, -1, 0); \\ \psi_{R2}^\dagger \psi_{L1} = e^{il_3^\intercal \phi}, \quad l_3^\intercal = (1, 0, 0, -1); \\ \psi_{R2}^\dagger \psi_{L2} = e^{il_4^\intercal \phi}, \quad l_4^\intercal = (0, 1, 0, -1). \end{aligned} \tag{39}$$

They transform under U(1)$_L$ × U(1)$_R$ but not U(1)$_M$. These operators $e^{il_a^\intercal \phi}$ ($a = 1, 2, 3, 4$) all have the same scaling dimension

$$\Delta_a = \frac{-2g_3}{1 - 2g_3 - \sqrt{1 - 4g_3^2}}. \tag{40}$$

At the free-fermion fixed point, $-8\lambda_\pm \cos(l_0^\intercal \phi)$ is a marginal perturbation, meaning that it is sitting right at a KT transition point. So any finite $\lambda_\pm$ will render the cosine term relevant, regardless of the sign of $\lambda_\pm$, as shown in Fig. 3. The RG equation near KT transition is given by

$$\begin{aligned} \tfrac{d}{d\ell} \lambda_\pm &\sim (2 - \Delta_0) \lambda_\pm, \\ \tfrac{d}{d\ell} \Delta_0^{-1} &\sim \lambda_\pm^2. \end{aligned} \tag{41}$$

Plugging in Eq. (36) for Δ_0 and expanding around $\lambda_3 \to 0$, we arrive at $\frac{d}{d\ell} \lambda_\pm \sim -\lambda_\pm \lambda_3$, $\frac{d}{d\ell} \lambda_3 \sim -\lambda_\pm^2$, consistent with Eq. (28), therefore the $\lambda_\pm$ term is marginally relevant.
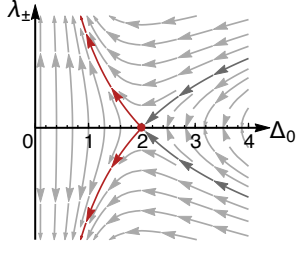
FIG. 3: RG flow near the KT transition point. The free-fermion fixed point $(\Delta_0, \lambda_\pm) = (2, 0)$ is marked out by a red point. The red arrows illustrate the RG flow after small $\lambda_\pm$ perturbation.

From $l_0^\mathsf{T} K^{-1} l_0 = 0$, we know that $\cos(l_0^\mathsf{T}\phi)$ is a bosonic operator. So as $\lambda_\pm$ flows to infinity under RG, the field ϕ will be pinned by the cosine term to $l_0^\mathsf{T}\phi = 0 \mod 2\pi$. Any operator $O_l = e^{il^\mathsf{T}\phi}$ that does not commute with $\cos(l_0^\mathsf{T}\phi)$ (i.e. $l^\mathsf{T}K^{-1}l_0 \neq 0$) will be gapped out. Using this criterion, it is easy to check that all fermions are gapped out, and the $\mathrm{O}(4)$ vector operators $\boldsymbol{N}$ as in Eq. (39) remain gapless. Further more, $l_0^\mathsf{T}\phi = 0 \mod 2\pi$ implies that any charge vector l_a will be equivalent to $l_a + n l_0$ ($n \in \mathbb{Z}$). As a result, we establish the equivalences $l_1 \sim -l_4$ and $l_2 \sim -l_3$ among the $\mathrm{O}(4)$ operators. So under interactions, there are only two independent bosonic modes left on the boundary. Let us choose $l_1^\mathsf{T}\phi$ and $l_2^\mathsf{T}\phi$ as the bosonic boundary modes, the effective K matrix can be obtained from the projection $K_{\mathrm{eff}}^{-1} = P^\mathsf{T} K^{-1} P$ with $P = (l_1, l_2)$. The result is

$$K_{\mathrm{eff}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{42}$$

which exactly describes the bosonic SPT boundary.[5] According to Eq. (39), the physical meaning of the bosonic boundary modes are simply the SDW-XY and SC fluctuations on the boundary,

$$\begin{aligned} e^{il_1^\mathsf{T}\phi} &= \psi_{R1}^\dagger \psi_{L1} \sim N^0 - \mathrm{i}N^3 = S^-, \\ e^{il_2^\mathsf{T}\phi} &= \psi_{R1}^\dagger \psi_{L2} \sim N^2 - \mathrm{i}N^1 = \Delta^\dagger. \end{aligned} \tag{43}$$

Then the K_{eff} matrix describes the effect that each 2π vortex of the pairing field $\Delta^\dagger$ will trap a spin-1 excitation S^-. This corresponds to the spin Hall conductance $\sigma_{\mathrm{sH}} = 2$, consistent with the bilayer QSH state in the free-fermion limit.

As the gapping term $\cos(l_0^\mathsf{T}\phi)$ becomes relevant, its scaling dimension Δ_0 will flow to 0 as shown in Fig. 3. From Eq. (36), $\Delta_0 \to 0$ corresponds to $g_3 \to -1/2$. Substitute the fixed point $g_3 = -1/2$ to Eq. (40), we find $\Delta_a = 1/2$, meaning that the scaling dimensions of both the SDW-XY and SC boundary modes are modified to $1/2$ under the RG flow, which is consistent with the $\mathrm{SU}(2)_1$ CFT, and it is also described by the IR fixed point of the $\mathrm{O}(4)$ NLSM with WZW term at level $k = 1$,[24,25]

as we have claimed in Eq. (12),

$$S = \int \mathrm{d}\tau \mathrm{d}x \mathrm{d}u \, \frac{1}{2g}(\partial_\mu \boldsymbol{n})^2 + \frac{\mathrm{i}k}{2\pi}\epsilon_{abcd}n^a \partial_\tau n^b \partial_x n^c \partial_u n^d. \tag{44}$$

The $\mathrm{O}(4)$ vector field $\boldsymbol{n}$ couples to the fermion bilinear terms $\boldsymbol{N}$ via $H_{\mathrm{cp}} = -\sum_i \boldsymbol{n}_i \cdot \boldsymbol{N}_i$ as mentioned in Eq. (14), such that $\boldsymbol{n} \sim \boldsymbol{N}$ in terms of symmetry properties. Therefore according to Eq. (43), $\boldsymbol{n}$ is related to the bonsonization field ϕ via $n^0 - \mathrm{i}n^3 \sim e^{il_1^\mathsf{T}\phi}$ and $n^2 - \mathrm{i}n^1 \sim e^{il_2^\mathsf{T}\phi}$. Such a connection becomes more evident if we note that the WZW term requires each 2π soliton of $n^2 - \mathrm{i}n^1$ (winding of the complex field $n^2 - \mathrm{i}n^1$ along x by 2π phase) should carry one unite of charge that is conjugate to $n^0 - \mathrm{i}n^3$. This topological response is nothing but the commutation relation $[l_1^\mathsf{T}\phi(x_1), \partial_x l_2^\mathsf{T}\phi(x_2)] = 2\pi \mathrm{i}\delta(x_1 - x_2)$ in the canonical quantization language, as required by the K_{eff} matrix in Eq. (42). So the K_{eff} matrix and the WZW term describe the same topological phenomenon.

Similar Luttinger liquid analysis for the helical edge modes was carried out in Ref. 26 under a lower symmetry, where the boundary can be unstable towards spontaneous symmetry breaking. In that case, the boundary bosonic modes are gapped out by symmetry breaking, however the bulk state still corresponds to a bosonic SPT state.

In conclusion, the interaction we designed can gap out all the fermions on the boundary and change the scaling dimension of the bosonic modes to that of the CFT $\mathrm{SU}(2)_1$, so that the interacting bilayer QSH model has no low-energy fermion both in the bulk and on the boundary, i.e. it becomes a real bosonic SPT state. More importantly, the interaction $-U\sum_i \boldsymbol{M}_i \cdot \boldsymbol{M}_i$ admits sign-free QMC simulations, providing us powerful numerical tools to study the $\mathrm{O}(4)$ bosonic SPT phase and its transition to the trivial SPT phase. The fate of the boundary modes can also be investigated by QMC.

III. LARGE-N GENERALIZATION

A. Bulk Theory

1. Model and Symmetry

The bilayer QSH model can be generalized to $2N$ layers by simply making more identical copies. On each site i, we define $4N$ fermions $c_{i\ell\sigma}$ with the layer index $\ell = 1, 2, \cdots, 2N$ and the spin index $\sigma = \uparrow, \downarrow$. Consider the following interacting fermion model,

$$\begin{aligned} H &= H_{\mathrm{band}} + H_{\mathrm{int}} \\ H_{\mathrm{band}} &= -t \sum_{\langle ij \rangle, \ell} c_{i\ell}^\dagger c_{j\ell} + \sum_{\langle\langle ij \rangle\rangle, \ell} \mathrm{i}\lambda_{ij} c_{i\ell}^\dagger \sigma^z c_{j\ell} + H.c. \\ H_{\mathrm{int}} &= -U \sum_i \boldsymbol{M}_i \cdot \boldsymbol{M}_i, \end{aligned} \tag{45}$$

where $\boldsymbol{M}_i$ follows the similar definitions in Eq. (7) as

$$M_i^- = 2(-)^i \sum_{\ell \in \text{odd}} c_{i,\ell} c_{i,\ell+1}^\dagger, \quad M_i^3 = \sum_\ell (-)^{i+\ell} c_{i\ell}^\dagger \sigma^z c_{i\ell}.$$
(46)

Following a similar transformation as in Eq. (2), we can switch to the more convenient f-fermion basis. The band Hamiltonian still takes the same form as Eq. (3)

$$H_{\text{band}} = \sum_{i,j,\sigma} (-)^\sigma f_{i\sigma}^\dagger (-t_{ij} + \mathrm{i}\lambda_{ij}) f_{j\sigma} + h.c.,$$
(47)

but $f_{i\sigma}$ are now $\mathrm{Sp}(N)$ multiplets. The model has a $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow \times \mathrm{SU}(2)$ symmetry. The fermions transform as $f_{i\sigma} \to S_\sigma f_{i\sigma}$ with $S_\sigma \in \mathrm{Sp}(N)_\sigma$ for $\sigma = \uparrow, \downarrow$. For each spin σ, the symplectic form is defined by an antisymmetric real matrix J_σ, such that

$$S_\sigma^{\mathsf{T}} J_\sigma S_\sigma = J_\sigma \quad \text{with} \quad J_\sigma^{\mathsf{T}} = -J_\sigma.$$
(48)

The $\mathrm{SU}(2) \simeq \mathrm{SO}(3)$ symmetry rotates the fermion bilinear operators $\boldsymbol{M}_i = (M_i^1, M_i^2, M_i^3)$ as an O(3) vector. Let $M_i^\pm = M_i^1 \pm \mathrm{i}M_i^2$, the definition of $\boldsymbol{M}_i$ follows form

$$M_i^- = \sum_\sigma f_{i\sigma}^{\mathsf{T}} J_\sigma f_{i\sigma}, \quad M_i^3 = (-)^i \sum_\sigma (-)^\sigma f_{i\sigma}^\dagger f_{i\sigma}, \quad (49)$$

and $M_i^+ = (M_i^-)^\dagger$. The $\mathrm{SU}(2)$ generators are therefore defined as $\boldsymbol{Q} = \sum_i \boldsymbol{Q}_i$ with $Q_i^a = \frac{1}{2\mathrm{i}} \epsilon_{abc} M_i^b M_i^c$. Let $Q_i^\pm = Q_i^1 \pm \mathrm{i}Q_i^2$, we can write down the $\mathrm{SU}(2)$ charges on each site explicitly

$$\begin{aligned} Q_i^- &= (-)^i \sum_\sigma (-)^\sigma f_{i\sigma}^{\mathsf{T}} J_\sigma f_{i\sigma}, \\ Q_i^3 &= \sum_\sigma (f_{i\sigma}^\dagger f_{i\sigma} - N), \end{aligned}$$
(50)

and $Q_i^+ = (Q_i^-)^\dagger$. The 3rd component of the global $\mathrm{SU}(2)$ charge $Q^3 = \sum_i Q_i^3$ is the total number of f-fermions in the system (counted with respect to half-filling), which is obviously conserved by the Hamiltonian H_{band} in Eq. (47). It can be further verified that $Q^\pm$ are also conserved, as $[H_{\text{band}}, \boldsymbol{Q}] = 0$. Therefore the free fermion model H_{band} has the $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow \times \mathrm{SU}(2)$ symmetry.

2. Realizing Bosonic SPT Phases

We propose that the following on-site interaction can turn the $2N$-layer QSH system into a $\mathrm{Sp}(N) \times \mathrm{Sp}(N)$ bosonic SPT state,

$$H_{\text{int}} = -U \sum_i \boldsymbol{M}_i \cdot \boldsymbol{M}_i.$$
(51)

This interaction preserves the $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow \times \mathrm{SU}(2)$ symmetry. Tuned by the interaction strength U, the model has two phases: in the weak interaction regime,

the model is in a $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow$ (bosonic) SPT phase. In the strong interaction regime, the model is in a trivial Mott phase.

In the next subsection we will show that the boundary states at the weakly interacting regime is the CFT $\mathrm{Sp}(N)_1$, without any gapless fermion mode. Thus the bulk theory is a $\mathrm{Sp}(N)$ principal chiral model with a $\Theta-$term at $\Theta = 2\pi$,

$$S = \int \mathrm{d}\tau \mathrm{d}^2 x \frac{1}{g} \mathrm{Tr}' \partial_\mu S^{-1} \partial_\mu S + \frac{\mathrm{i}\Theta}{24\pi^2} \epsilon^{\mu\nu\lambda} \mathrm{Tr}' \mathcal{A}_\mu \mathcal{A}_\nu \mathcal{A}_\lambda,$$
(52)

with $\mathcal{A}_\mu = S^{-1} \partial_\mu S$ for $S \in \mathrm{Sp}(N)$, which describes the $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow$ bosonic SPT phase.

In the strong interaction limit $U \to \infty$, the Hamiltonian is decoupled on each site. The on-site interaction $-U\boldsymbol{M}_i \cdot \boldsymbol{M}_i$ can be exact diagonalized. We found that the on-site ground state is unique. Its energy is $E_{\text{GS}} = -4N(N+2)U$ (per site), and its wave function is

$$|\mathrm{GS}_i\rangle = \sum_{q=0}^N \alpha_q (Q_i^+)^q (M_i^+)^{N-q} |0\rangle_f,$$
$$\text{with } \alpha_q = \begin{cases} \frac{1}{q+1}\binom{N}{q} & q \in \text{even}, \\ 0 & q \in \text{odd}, \end{cases}$$
(53)

where $\binom{N}{q} \equiv \frac{N!}{q!(N-q)!}$ is the binomial coefficient and $|0\rangle_f$ denotes the zero fermion state of f-fermions. So the ground state of the whole system is simply a direct product state of on-site ground states

$$|\mathrm{GS}\rangle = \prod_i |\mathrm{GS}_i\rangle.$$
(54)

It is easy to see that $|\mathrm{GS}_i\rangle$ is $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow$ symmetric, because Q_i^+, M_i^+ and $|0\rangle_f$ are all invariant under $\mathrm{Sp}(N)_\uparrow \times \mathrm{Sp}(N)_\downarrow$ transformations. One can further verify that $|\mathrm{GS}_i\rangle$ also preserves the $\mathrm{SU}(2)$ symmetry by checking that $\boldsymbol{Q}_i |\mathrm{GS}_i\rangle = 0$. Thus the ground state is fully symmetric. Upon the ground state, the single particle excitation energy is $(4N + 5)U$, the O(3) excitation energy is $8U$ and the $\mathrm{Sp}(N)$ excitation energy is $(8N + 4)U$. All the fermionic and bosonic excitations are gapped from the ground state. Therefore the ground state describes a trivial (featureless) Mott insulator. Because the ground state is unique and fully gapped, it should be stable against any local perturbation. So we expect a stable phase of the trivial Mott insulator in the large U regime.

On the field theory level, the trivial Mott phase corresponds to the $\Theta = 0$ fixed point of the $\mathrm{Sp}(N)$ principal chiral model in Eq. (52). If there is a single continuous transition between the small-U SPT phase and the large-U trivial Mott phase, it must be described by the $\mathrm{Sp}(N)$ principal chiral model at $\Theta = \pi$. The phase diagram and the possible criticality can be numerically studied by QMC without fermion sign problem. Because the interaction term can still be decoupled in the O(3) vector channel by introducing the auxiliary field $\boldsymbol{m}_i$ as in

Eq. (19). The resulting Hamiltonian $H[\boldsymbol{m}_i]$ still has the time-reversal symmetry in Eq. (20), which ensures the Boltzmann weight $W[\boldsymbol{m}_i(\tau)]$ to be positive definite for any configurations of the auxiliary field $\boldsymbol{m}_i(\tau)$.

B. Boundary Theory

1. One-Loop RG

Without interaction, the boundary of the $2N$-layer QSH insulator hosts $2N$ pairs of counter-propagating fermion modes. The edge mode chirality is locked to the fermion spin: all the $2N$ left (right) moving fermions are of $\uparrow$ ($\downarrow$) spin, forming a $\mathrm{Sp}(N)_{L(R)}$ multiplet, denoted by $\psi_{L(R)}$. Thus bulk operators can be mapped to the boundary simply by rewriting $\uparrow \to L$ and $\downarrow \to R$. The boundary theory takes the same form as Eq. (22), and is repeated here

$$H_{\mathrm{bdy}} = \int \mathrm{d}x(\psi_L^\dagger \mathrm{i}\partial_x \psi_L - \psi_R^\dagger \mathrm{i}\partial_x \psi_R). \tag{55}$$

On the boundary, the O(3) vector $\boldsymbol{M}$ follows from Eq. (49) as

$$M^- = \sum_\sigma \psi_\sigma^\intercal J_\sigma \psi_\sigma, \ M^3 = \sum_\sigma (-)^\sigma \psi_\sigma^\dagger \psi_\sigma; \tag{56}$$

and the SU(2) charge $\boldsymbol{Q}$ follows from Eq. (50) as

$$Q^- = \sum_\sigma (-)^\sigma \psi_\sigma^\intercal J_\sigma \psi_\sigma, \ Q^3 = \sum_\sigma (\psi_\sigma^\dagger \psi_\sigma - N). \tag{57}$$

The bulk interaction H_{int} in Eq. (51) will induce a short range interaction $H_{\mathrm{int}} = -U' \int \mathrm{d}x \boldsymbol{M} \cdot \boldsymbol{M}$ on the boundary at the UV scale. However under the RG flow, $\int \mathrm{d}x \boldsymbol{Q} \cdot \boldsymbol{Q}$ will be generated. In the $N = 1$ case, the $\boldsymbol{Q} \cdot \boldsymbol{Q}$ term reduces to a linear combination of the $\boldsymbol{M} \cdot \boldsymbol{M}$ and $\boldsymbol{N} \cdot \boldsymbol{N}$ terms, i.e. $\boldsymbol{Q} \cdot \boldsymbol{Q} = \boldsymbol{M} \cdot \boldsymbol{M} - \boldsymbol{N} \cdot \boldsymbol{N} + 4$, which has been included in Eq. (24). The one-loop RG analysis is similar for $N > 1$ cases. For the purpose of RG analysis, we start with the most generic $\mathrm{Sp}(N)_L \times \mathrm{Sp}(N)_R \times \mathrm{SU}(2)$ symmetric interaction as follows

$$H_{\mathrm{int}} = \int \mathrm{d}x(\lambda_M \boldsymbol{M} \cdot \boldsymbol{M} + \lambda_Q \boldsymbol{Q} \cdot \boldsymbol{Q}). \tag{58}$$

The one-loop RG equations are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\ell}\lambda_M &= -\tfrac{2}{3}(\lambda_M - \lambda_Q)^2, \\ \frac{\mathrm{d}}{\mathrm{d}\ell}\lambda_Q &= \tfrac{2}{3}(\lambda_M - \lambda_Q)^2. \end{aligned} \tag{59}$$

Therefore the interaction is marginally relevant when $\lambda_M < \lambda_Q$, and will follow towards the $(\lambda_M, \lambda_Q) \to (-1, +1)$ direction. The fixed point interaction is given by $\lambda_Q = -\lambda_M$ and $\lambda_M \to -\infty$,

$$\begin{aligned} H_{\mathrm{int}} =& \lambda_M(\boldsymbol{M} \cdot \boldsymbol{M} - \boldsymbol{Q} \cdot \boldsymbol{Q}) \\ =& 2\lambda_M\big((\psi_R^\intercal J_R \psi_R)^\dagger (\psi_L^\intercal J_L \psi_L) + h.c.\big) \\ &- 4\lambda_M(\psi_R^\dagger \psi_R - N)(\psi_L^\dagger \psi_L - N). \end{aligned} \tag{60}$$

The fixed point interaction only contains the left-right mixing terms. The interactions within the same chiral sector (forward scatterings) will only renormalize the mode velocity, and can be ignored. In the $N = 1$ case, Eq. (60) reduces to Eq. (29) by $\lambda_\pm = \lambda_3 = 2\lambda_M$ (at the fixed point).

2. CFT Analysis

For each chiral sector, we have the following decomposition of CFT:[27]

$$\mathrm{U}(2N)_1 \simeq \mathrm{O}(4N)_1 \simeq \mathrm{Sp}(N)_1 + \mathrm{SU}(2)_N. \tag{61}$$

This means the $\mathrm{U}(2N)_1$ or $\mathrm{O}(4N)_1$ CFT, which is described by $2N$ copies of free complex fermions or $4N$ copies of free Majorana fermions, can be decomposed into the direct sum of two interacting CFT: $\mathrm{Sp}(N)_1$ and $\mathrm{SU}(2)_N$. The validity of this equation can be seen from the central charges of these CFT:

$$c_{\mathrm{Sp}(N)_1} = \frac{N(2N+1)}{N+2}, \quad c_{\mathrm{SU}(2)_N} = \frac{3N}{N+2}, \tag{62}$$

the sum of these two gives $2N$, which is the central charge of $\mathrm{U}(2N)_1$ or $\mathrm{O}(4N)_1$.

Therefore the helical fermion CFT can be written in terms of $\mathrm{Sp}(N)$ and $\mathrm{SU}(2)$ current operators as

$$\begin{aligned} H_{\mathrm{bdy}} &= \int \mathrm{d}x \ (T_L + T_R), \\ T_\sigma =& :\psi_\sigma^\dagger \mathrm{i}\partial_x \psi_\sigma: \\ =& \frac{2\pi}{N+2}\big(J_{\mathrm{Sp}(N)_\sigma}^a J_{\mathrm{Sp}(N)_\sigma}^a + J_{\mathrm{SU}(2)_\sigma}^a J_{\mathrm{SU}(2)_\sigma}^a\big), \end{aligned} \tag{63}$$

where $\sigma = L, R$. The $\mathrm{Sp}(N)_\sigma$ current operators are given by

$$J_{\mathrm{Sp}(N)_\sigma}^a = :\psi_\sigma^\dagger A_\sigma^a \psi_\sigma:, \tag{64}$$

where A_σ^a ($a = 1, 2, \cdots, N(2N+1)$) are the $\mathrm{Sp}(N)_\sigma$ generators, which are properly normalized according to $\mathrm{Tr}\, A_\sigma^a A_\sigma^b = \frac{1}{2}\delta^{ab}$. The $\mathrm{SU}(2)_\sigma$ current operators are defined as

$$J_{\mathrm{SU}(2)_\sigma}^- = \tfrac{1}{2}(-)^\sigma :\psi_\sigma^\intercal J_\sigma \psi_\sigma:, J_{\mathrm{SU}(2)_\sigma}^3 = \tfrac{1}{2} :\psi_\sigma^\dagger \psi_\sigma:, \tag{65}$$

such that $J_{\mathrm{SU}(2)_\sigma}^{1(2)} = \mathrm{Re(Im)}J_{\mathrm{SU}(2)_\sigma}^-$. The current operators satisfy the Kac-Moody algebra

$$\begin{aligned} [J_{\mathrm{Sp}(N)_\sigma}^a(x), J_{\mathrm{Sp}(N)_\sigma}^b(y)] =& \mathrm{i}f_{\mathrm{Sp}(N)}^{abc} J_{\mathrm{Sp}(N)_\sigma}^c(x)\delta(x-y) \\ &+ (-)^\sigma \frac{\mathrm{i}\delta^{ab}}{4\pi}\delta'(x-y), \\ [J_{\mathrm{SU}(2)_\sigma}^a(x), J_{\mathrm{SU}(2)_\sigma}^b(y)] =& \mathrm{i}f_{\mathrm{SU}(2)}^{abc} J_{\mathrm{SU}(2)_\sigma}^c(x)\delta(x-y) \\ &+ N(-)^\sigma \frac{\mathrm{i}\delta^{ab}}{4\pi}\delta'(x-y), \end{aligned} \tag{66}$$

where $f_{\mathrm{Sp}(N)}$ and $f_{\mathrm{SU}(2)}$ are $\mathrm{Sp}(N)$ and $\mathrm{SU}(2)$ structure factors respectively.

The fixed point interaction H_{int} in Eq. (60) can be written exactly as a back-scattering term of the $\mathrm{SU}(2)$ currents

$$H_{\mathrm{int}} = -16\lambda_M J^a_{\mathrm{SU}(2)_R} J^a_{\mathrm{SU}(2)_L}, \tag{67}$$

because this term is marginally relevant, it will gap out the $\mathrm{SU}(2)_N \times \mathrm{SU}(2)_{-N}$ sector completely[28]. The boundary is left with the $\mathrm{Sp}(N)_1 \times \mathrm{Sp}(N)_{-1}$ modes only. The fermion modes at the boundary must also be gapped because the $\mathrm{SU}(2)_N$ sector as collective modes of the fermions are gapped. Hence indeed the interaction we design will drive the boundary of this system to a $\mathrm{Sp}(N)_1$ CFT, and the bulk of the SPT is described by Eq. 52.

IV. SUMMARY AND DISCUSSION

In this work, we designed a series of interacting fermion model with short-range interaction, and we demonstrated that these models can describe the quantum phase transition between a bosonic SPT state and a trivial Mott insulator state. These bosonic SPT states are described by a $\mathrm{Sp}(N)$ principal chiral model with a $\Theta-$term. These models can be reliably simulated using determinant QMC algorithm without sign problem. Our previous results[13,14] already suggest that this SPT-trivial transition is continuous, which corresponds to the case with $N = 1$.

The $\mathrm{Sp}(N)$ principal chiral model with $N = 1$, which is

also an O(4) NLSM was also used to describe the boundary of $3d$ bosonic SPT states[7,29]. But in those cases Θ is no longer a tuning parameter, because $\Theta = \pi$ is protected by the symmetry of the system, for instance time-reversal symmetry. Our results also suggest that if there is an exact SO(4) symmetry, the boundary of this SPT state could be a stable $(2+1)d$ CFT. But if the SO(4) symmetry is strongly broken down its subgroups, this CFT can be further driven into various topological orders as was discussed in Ref. 7,29.

Another interesting direction is to design a series of fermion models that would generate the $\mathrm{SU}(N)$ principal chiral model with a topological $\Theta-$term. This is a little difficult (though not impossible) to achieve using our method, because the interaction we designed in this paper is based on the $\mathrm{Sp}(N) \times \mathrm{Sp}(N)$ singlet vector $\boldsymbol{M}$, and because of the properties of the $\mathrm{Sp}(N)$ group, its singlet can still be a fermion bilinear operator, thus the interactions in our models are all four-fermion short range interaction. But if we want to generalize our idea to the $\mathrm{SU}(N)$ groups, it seems much higher order fermion interaction must be involved because two $\mathrm{SU}(N)$ fundamental fermions cannot form a $\mathrm{SU}(N)$ singlet in general. We will leave this to future study.

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