Gauging anomalous unitary operators

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Boundary theories of static bulk topological phases of matter are obstructed in the sense that they cannot be realized on their own as isolated systems. The obstruction can be quantified/characterized by quantum anomalies, in particular when there is a global symmetry. Similarly, topological Floquet evolutions can realize obstructed unitary operators at their boundaries. In this paper, we discuss the characterization of such obstructions by using quantum anomalies. As a particular example, we discuss time-reversal symmetric boundary unitary operators in one and two spatial dimensions, where the anomaly emerges as we gauge the so-called Kubo-Martin-Schwinger (KMS) symmetry. We also discuss mixed anomalies between particle number conserving U(1) symmetry and discrete symmetries, such as *C* and *CP*, for unitary operators in odd spatial dimensions that can be realized at the boundaries of topological Floquet systems in even spatial dimensions.

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I. INTRODUCTION

As the ground states of static, gapped Hamiltonians, unitary time-evolution operators of quantum many-body systems can be topologically distinct from each other or may exhibit topological properties. For example, time-evolution operators of periodically driven systems (Floquet systems) can give rise to Floquet Hamiltonians that are topological much the same way as static topological systems. Novel out-of-equilibrium phases of matter that do not have static counterparts can also be realized in such systems [1–7]. Floquet topological systems have been experimentally realized in synthetic systems, such as ultracold atoms, photonic, and phononic systems—see, for example, Refs. [8–11].

Similar to static topological phases, some Floquet unitaries are topological even in the absence of any symmetry, while others are topological in the presence of some symmetry, i.e., their topological properties (topological distinction) are protected by a symmetry. The examples of the former include those that support unidirectional quantum information flow at their boundaries, and are characterized by the chiral unitary index (GNVW index) [12–15]. On the other hand, bosonic Floquet systems in d spatial dimensions with a symmetry group G are classified by group cohomology $H^{d+1}(\tilde{G}, \mathrm{U}(1))$ where $\tilde{G} = G \times \mathbb{Z}$ or $G \rtimes \mathbb{Z}$ [16–19]. For noninteracting fermion systems, nontrivial topological Floquet unitaries in the ten Altland-Zirnbauer symmetry classes have been classified [20,21].

In static topological phases, it is known that a bulk-boundary correspondence holds. The boundary theory of a bulk topological phase is anomalous, in that it cannot be realized on its own as a local consistent theory. For example, on the boundary of a bulk symmetry-protected topological (SPT) phase protected by a global on-site symmetry, the symmetry cannot act purely locally (i.e., the symmetry action is neither on-site nor splittable); the boundary theory suffers from a 't Hooft anomaly. In general, quantum anomalies at the boundary go hand in hand with nontrivial bulk topology, and can be used as a diagnosis of the corresponding bulk. Such anomalies can often be detected by gauging, i.e., by subjecting the boundary theory to a background gauge field associated with the symmetry group [22–31]. One natural question is whether a similar formalism is applicable to Floquet topological phases.

In this paper, we discuss the anomalous (or topological) properties of unitary time-evolution operators that may appear on the boundary of topological Floquet unitary operators. In one-spatial dimension for bosonic systems, these unitaries (locality-preserving quantum cellular automata) can be expressed in terms of matrix-product unitaries [32–38]. We consider these unitaries in the presence of a global symmetry, including discrete symmetries, such as time-reversal, parity (reflection), charge-conjugation, and combinations thereof. In particular, we will develop gauging procedures, i.e., to introduce background gauge fields, to detect anomalous properties of these unitaries. As we will show, the boundary unitaries of topological Floquet systems suffer from quantum anomalies of discrete symmetries, similar to the boundary states appearing in static topological phases. The gauging procedure leads to explicit forms (formulas) of (many-body) topological invariants that can be used for arbitrary unitary operators with symmetries.

One convenient way to formulate our gauging procedure is to use the operator-state map (reviewed in Sec. II), and

regard unitary operators as short-range entangled states in the doubled Hilbert space, which may be viewed as unique ground states of some gapped Hamiltonians. We can then use tools from the physics of symmetry-protected topological phases to study the mapped states; we can follow the gauging procedure for static topological phases of matter. Section III is devoted to developing this idea. In particular, we will also establish the connection between the gauging procedure with temporal background gauge fields and the approach in Ref. [16] that deals with anomalous operator algebras appearing on boundaries of 1d topological Floquet systems. We will then generalize to incorporate spatial components of background gauge fields.

Also in Sec. III, we will discuss how we can gauge time-reversal symmetry. Specifically, as we will review in Sec. II, in the Schwinger-Keldysh formalism or in thermofield dynamics, time-reversal symmetry can be implemented as a unitary on-site $\mathbb{Z}_2$ symmetry—the so-called KMS (Kubo-Martin-Schwinger) symmetry [39–41]. This symmetry can be gauged in much the same way as unitary on-site symmetries in static topological phases of matter, in order to diagnose topological/anomalous properties of unitary operators.

We will apply the gauging procedure to diagnose anomalous (topological) properties of matrix product unitaries (Sec. IV), and boundary unitaries of Floquet Majorana fermion systems (Sec. V). For the case of 1d Majorana unitaries (realized at the boundaries of 2d Floquet topological unitaries), the model of our interest can be constructed by combining two copies of the Majorana fermion model with opposite chiralities discussed in Ref. [14]. We will also discuss 2d time-reversal symmetric Majorana unitaries that can be realized on the boundary of 3d bulk topological Floquet unitaries. Gauging the KMS symmetry reveals the $\mathbb{Z}_8$ classification of these unitaries.

In Sec. VI, we will consider the boundary unitatires of Floquet topological systems of charged fermions. Namely, there is a U(1) charge Q which commutes with these unitaries, $e^{i\theta Q}Ue^{-i\theta Q} = U$ ($\theta \in [0, 2\pi]$). The examples include the 1d boundary unitary of 2d Floquet topological Anderson insulators [12,42–46]. As shown in [46] the 1d boundary unitaries suffer from a mixed anomaly between U(1) and particle-hole symmetry. In this paper, we extend this analysis to higher-dimensional examples, and show that the anomalies are characterized by the Chern-Simons forms. The situation is analogous to the dimensional hierarchy of topological response theories of topological insulators discussed in Refs. [22,47]. However, the difference from the case of static topological phases is that the Chern-Simons forms for the anomalous boundary unitaries are written solely in terms of spatial components of the U(1) gauge field. We note that spatial Chern-Simons terms also appear in the topological quantum field theory description of non-Hermtian topological systems [48]. Finally, we also construct many-body topological invariants that can extract the Chern-Simons forms.

II. THE OPERATOR-STATE MAP AND THE KMS CONDITION

In this section, we will go through the ingredients of the operator-state map and the KMS condition that are necessary for our analysis of unitary operators [49,50].

A. The operator-state map

a. The reference state. We begin by reviewing some essential points of the operator-state map, which maps operators acting on a Hilbert space $\mathcal{H}$ to the corresponding states in the doubled Hilbert space $\mathcal{H}\otimes\mathcal{H}$—see below. In broader contexts, one can apply the channel-state map (the Choi-Jamiołkowski isomorphism) to arbitrary quantum channels (trace-preserving completely positive map), and associate them with quantum states (density matrices) in the doubled Hilbert space.

We start from the identity operator $I = \sum_i |i\rangle\langle i|$, and normalize it as $\Omega = \sum_i |i\rangle\langle i|/\sqrt{\mathcal{N}}$ so that $\mathrm{Tr}\,[\Omega^\dagger\Omega] = 1$. Here, $\mathcal{N} = \dim\mathcal{H} = \mathrm{Tr}\,I$ is the dimension of the Hilbert space. By "flipping" the bras in Ω, we define a "reference state," a maximally entangled state in the doubled Hilbert space $\mathcal{H}\otimes\mathcal{H}^*$:

$$|\Omega\rangle\!\rangle \equiv (1/\sqrt{\mathcal{N}})\sum_i |i\rangle\otimes|i\rangle^*. \tag{1}$$

Here, $|i\rangle^* = K|i\rangle$ transforms as a conjugate representation where K is complex conjugation. Under a unitary transformation V acting on $\mathcal{H}$, $|i\rangle$ and $|i\rangle^*$ transform complementarily as

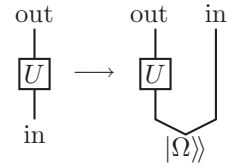
$$\begin{aligned} |i\rangle &\to V|i\rangle = \left(\sum_j |j\rangle\langle j|\right)V|i\rangle = \sum_j |j\rangle V_{ji}, \\ |i\rangle^* &\to KVK^{-1}K|i\rangle = KV|i\rangle = \sum_j |j\rangle^* V^*_{ji}, \end{aligned} \tag{2}$$

i.e., $|i\rangle$ and $|i\rangle^*$ transform as the fundamental and antifundamental representations of $U(\mathcal{N})$, respectively. We refer to these two Hilbert spaces as "out" and "in" Hilbert spaces. Like the operator Ω, which is invariant under a unitary transformation on $\mathcal{H}$, $\Omega \to V\Omega V^\dagger = \sqrt{\mathcal{N}}^{-1}\sum_i V|i\rangle\langle i|V^\dagger = \Omega$, the reference state $|\Omega\rangle\!\rangle$ enjoys the invariance under (2). The point here is that we consider the product of two representations that are conjugate to each other. The resulting product representation always includes a singlet representation. (While we use complex conjugation K here to pair up two Hilbert spaces, in later examples, we will consider a physical antiunitary symmetry operation, such as time reversal or time reversal combined with a unitary symmetry, such as CT, to define conjugate kets.)

b. The operator-state map. We can now introduce the operator-state map using the reference state $|\Omega\rangle\!\rangle$. Let us consider a unitary operator U acting on $\mathcal{H}$. We introduce a state $|U\rangle\!\rangle$ corresponding to U as

$$|U\rangle\!\rangle = (U\otimes I)|\Omega\rangle\!\rangle. \tag{3}$$

It is customary to represent the state-operator map diagramatically as



(4)

Here, the reference state $|\Omega\rangle\!\rangle$ appears as a "cup."

Note that the overlap of two states corresponding to unitaries U and U' can be written as

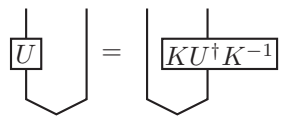
$$\langle\langle U|U'\rangle\rangle = (1/\mathcal{N})\mathrm{Tr}[U^\dagger U'] = \mathrm{Tr}[U'\rho_0 U^\dagger], \tag{5}$$

where the trace is taken over the original (single) Hilbert space $\mathcal{H}$, and $\rho_0 = I/\mathcal{N}$ is the infinite temperature state. This overlap can be interpreted (represented) as a Schwinger-Keldysh path-integral with the infinite temperature thermal state as the initial state.

c. The shift property. Using the invariance of the reference state under U, $|\Omega\rangle\rangle = (U^\dagger \otimes KU^\dagger K^{-1})|\Omega\rangle\rangle$, the state $|U\rangle\rangle$ can also be written as

$$\begin{aligned}|U\rangle\rangle &= (U\otimes I)(U^\dagger \otimes KU^\dagger K^{-1})|\Omega\rangle\rangle \\ &= (I\otimes KU^\dagger K^{-1})|\Omega\rangle\rangle,\end{aligned} \tag{6}$$

i.e., one can "shift" U from the left (out) to right (in), by conjugating with K. This reflects the fact that acting an arbitrary operator O on Ω from the right and left give the identical result, $O = O\cdot\Omega = \Omega\cdot O = \sqrt{\mathcal{N}}^{-1}\sum_i O|i\rangle\langle i| = \sqrt{\mathcal{N}}^{-1}\sum_i |i\rangle\langle i|O$. The shift property of $|\Omega\rangle\rangle$ can be represented pictorially as



(7)

In other words, by the reference state, one can establish a correspondence or an isomorphism between the spaces of operators acting on the output and input Hilbert spaces. Intuitively, the reference state acts as a perfect mirror ("reflector") that "reflects" all information from the output to input Hilbert space, and vice versa.

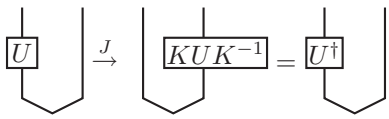
d. The modular conjugation. In the language of Tomita-Takesaki theory, the state operator map naturally comes with an antiunitary operator acting on the doubled Hilbert space, called the modular conjugation operator, which we denote by J. For the setting we are working with, it is simply an operation that exchanges the in and out Hilbert spaces; J can be introduced as

$$J\big(|i\rangle|j\rangle^*\big) = |j\rangle|i\rangle^*, \tag{8}$$

i.e., $J = K\cdot SWAP$, where K is complex conjugation acting on $\mathcal{H}_{\mathrm{out}}\otimes\mathcal{H}_{\mathrm{in}}$, and $SWAP$ exchanges the in and out Hilbert spaces. Note that the reference state $|\Omega\rangle\rangle$ is invariant under J. The modular conjugation J acts on $|U\rangle\rangle$ as

$$\begin{aligned}J|U\rangle\rangle &= J(U\otimes I)J\cdot J|\Omega\rangle\rangle = (I\otimes KUK^{-1})|\Omega\rangle\rangle \\ &= (U^\dagger\otimes I)|\Omega\rangle\rangle = |U^\dagger\rangle\rangle.\end{aligned} \tag{9}$$

Here, we used the shift property of $|\Omega\rangle\rangle$. Diagramatically,



(10)

Formally, Eq. (9) is nothing but the *KMS condition* for the infinite temperature state. In Appendix A, we review the KMS condition for finite temperature states, using the framework of the thermofield dynamics. There, the KMS condition can once again be stated by using J. Intuitively, J can be understood as an operation that exchanges the system of our interest and "heat bath.'

In the next section, we will see the KMS condition, in the presence of time-reversal symmetry, is used to form the KMS symmetry.

III. GAUGING SYMMETRIES

A. Review: gauging static (topological) phases

Gauging a global symmetry is a useful framework to detect nontrivial (symmetry-protected) topological phases of matter (see, for example, Refs. [22–26,31]). Here, by gauging, we mean introducing a nondynamical, background gauge field associated with the symmetry group. In the following, our goal is to extend this paradigm to unitary operators with symmetries; we will discuss the gauging procedure for topological/anomalous unitary operators.

Let us first recall a few essential points of the gauging procedure for the case of static topological phases. To be concrete, suppose we have a static gapped (topological) phase described by the Euclidean path integral which is given schematically by $Z[X] = \int \mathcal{D}\phi\, e^{-S[\phi,X]}$, where ϕ symbolically represents the "matter" degrees of freedom, and $S[\phi, X]$ is the Euclidean action on a closed $(d+1)$-dimensional space-time manifold X. In the presence of a background gauge field, we consider

$$Z[X,A] = \int \mathcal{D}\phi\, e^{-S[\phi,X,A]}. \tag{11}$$

(Here, for simplicity, we mainly focus on on-site unitary symmetry. It is also possible to gauge space-time symmetry, such as time-reversal, reflection, and other space group symmetry, by considering, e.g., unoriented space-time [24–26,51].) For gapped phases (with the unique ground state), the effective action $-\ln Z[X,A]$ is expected to be a local functional of A. It may also have a pure imaginary, topological part, signaling a nontrivial topological response of the ground state, $Z[X,A]\sim \exp iS_{\mathrm{top}}[X,A]$. The topological term $S_{\mathrm{top}}[X,A]$ can be thought of as a topological invariant characterizing the topological phase.

As an example, let us consider gapped phases in (1+1) space-time dimensions, protected by on-site unitary symmetry. We consider the Euclidean path integral on the space-time torus T^2. The nontrivial background gauge field configurations are then characterized by holonomies (Wilson loops) along the two noncontractible loops on T^2. The effect of the background can be thought of as twisting boundary conditions of the matter field ϕ along the two noncontractible loops, $\phi(\tau+T,x) = g\cdot\phi(\tau,x)$ and $\phi(\tau,x+L) = h\cdot\phi(\tau,x)$, where $\tau\in[0,T]$ and $x\in[0,L]$ coordinatize the temporal and spatial directions, respectively, and g and h are elements of the symmetry group. We thus consider

$$Z[T^2,(g,h)] = \int_{\substack{\phi(\tau+T,x)=g\cdot\phi(\tau,x),\\ \phi(\tau,x+L)=h\cdot\phi(\tau,x)}} \mathcal{D}\phi\, e^{-S[\phi,T^2]}. \tag{12}$$

The topological term, i.e., the phase of the partition function, is known to be classified by $H^2(G, \mathrm{U}(1))$ [23,52,53]. More generally, (especially in the case of orientation reversing symmetries), $S_{\mathrm{top}}[X, A]$ can be thought of as a topological quantum field theory which depends only on the cobordism class of $[X, A]$ [24] (including spin structures in the case of fermions [26]), and is denoted by $\Omega^{\mathrm{str}}_{d+1}(BG)$. Here, str refers to the corresponding spin (or pin) structure for fermions and BG is the classifying space of G. When there is no symmetry, we simply put a single point as BG, $BG = pt$. In this language, the topological term may be viewed as a homomorphism $e^{iS_{top}} : \Omega^{\mathrm{str}}_{d+1}(BG) \to U(1)$. Hence, the torsion part of the cobordism group Tor $\Omega^{\mathrm{str}}_{d+1}(BG)$ can be used to provide a classification of topological phases protected by a symmetry group G [24,26,54]. For instance, time-reversal symmetric fermionic systems in (1+1) space-time dimensions with $T^2 = 1$ have a $\Omega^{\mathrm{Pin}-}_2(BG) = \mathbb{Z}_8$ classification and the partition function on $\mathbb{R}P^2$ can be used as the corresponding $\mathbb{Z}_8$ topological invariant.

Quite often it is also possible to extract the topological term using the canonical (operator) formalism, in particular, solely from the ground state. The partition function (12) can be written in the operator formalism as $Z[T^2, (g, h)] = \mathrm{Tr}\,[V_g\, e^{-TH_h}]$. Here, H_h is the system's Hamiltonian with twisted spatial boundary condition by h, and the trace is taken in the Hilbert space with the twisted boundary condition; V_g implements the symmetry operation g in the (h-twisted) Hilbert space. In the zero-temperature limit $T \to \infty$, the ground state dominates the partition sum,

$$Z[T^2, (g, h)] = {}_h\langle GS|\, V_g\, |GS\rangle_h, \tag{13}$$

where $|GS\rangle_h$ is the ground state in the h-twisted sector. Observe that the twisting boundary condition in the temporal direction is implemented as the operator insertion V_g within the trace.

Our strategy to study the anomalous properties of unitary operators is to map them to corresponding states in the doubled Hilbert space (the operator-state map). In particular, when the mapped states are short-range entangled, which may be viewed as unique ground states of some gapped Hamiltonians, we can use tools from the physics of symmetry-protected topological phases to study the mapped states; we can follow the gauging procedure outlined above for static topological phases of matter.[1] For the rest of this section, we will develop the gauging procedure for unitary and antiunitary symmetries, by focusing first on the "temporal" component of background gauge fields. In particular, we will observe that, while time-reversal symmetry is antiunitary in the original (single) Hilbert space, it can be implemented as a unitary on-site symmetry (the KMS symmetry), and can be gauged following the standard procedure. We will also establish the connection between the temporal gauging procedure and the approach in Ref. [16] that deals with anomalous operator algebras appearing on boundaries of 1d topological Floquet systems. In Sec. III E, we will also discuss spatial gauging (turning on spatial components of background gauge fields) – the idea will be further developed in the following sections by taking examples of various kinds. (While we use the language of the operator-state map, and the doubled Hilbert space, this may not be entirely necessary to develop the gauging procedure, although we find it is quite convenient in many cases. We will mention the perspective without using the operator-state map when possible.)

[1]It is not entirely obvious for which Hamiltonian they are considered to be ground states. While not unique, such "parent" Hamiltonian can be constructed formally as $\mathbb{H} = (U_{\mathrm{out}} \otimes I_{\mathrm{in}})\mathbb{H}_0(U^\dagger_{\mathrm{out}} \otimes I_{\mathrm{in}})$ where $\mathbb{H}_0$ is the gapped parent Hamiltonian for $|\Omega\rangle\!\rangle$.

B. Gauging unitary symmetries

Let us consider a unitary time-evolution operator U with symmetries. We denote a symmetry group by $\mathscr{G}$. For a given element $g \in \mathscr{G}$, there is a unitary or an anti unitary operator V_g acting on the (physical) Hilbert space $\mathcal{H}$. We say a unitary U is symmetric under $\mathscr{G}$ when

$$V_g U V_g^{-1} = e^{i\phi_g(U)} U, \quad V_g : \text{unitary}, \tag{14}$$

$$V_g U V_g^{-1} = e^{i\phi_g(U)} U^\dagger, \quad V_g : \text{anti unitary}. \tag{15}$$

Here, note that we allow a projective phase in these operator algebras. Such projective phases may appear when unitary operators are realized on the boundary of topologically nontrivial bulk (Floquet) unitaries: While symmetry can be realized in the bulk without projective phases, boundary unitaries can be anomalous and may pick up projective phases when acted by symmetries [16]. As we will see momentarily, the projected phases can be detected by introducing a temporal component of the background gauge field.

Let us start with the case of unitary symmetry. To discuss the gauging procedure, we begin by noting that while symmetry g acts on U by conjugation, $U \to V_g U V_g^{-1}$, it acts on $|U\rangle\!\rangle$ as $|U\rangle\!\rangle \to [V_g \otimes K V_g K^{-1}]|U\rangle\!\rangle$. Now, if we view $|U\rangle\!\rangle$ as a ground state (of a gapped parent Hamiltonian), we consider, following the static case (13),

$$Z_g := \langle\!\langle U|\, V_g \otimes K V_g K^{-1}\, |U\rangle\!\rangle. \tag{16}$$

This quantity can be interpreted as a partition function in the space-time manifold $S^1 \times M$ (where M is the spatial part) in the presence of twisted boundary condition by g in the temporal direction. Here, "time" is a fictitious one, and the time-evolution is generated by the putative parent Hamiltonian; $V_g \otimes K V_g K^{-1}$ should be the symmetry of the parent Hamiltonian. The phase of this partition function may detect an anomaly (topological information) of $|U\rangle\!\rangle$. Using the shift property of $|U\rangle\!\rangle$,

$$\begin{aligned} V_g \otimes K V_g K^{-1} |U\rangle\!\rangle &= V_g U \otimes K V_g K^{-1} |\Omega\rangle\!\rangle \\ &= (V_g U V_g^{-1} \otimes I)|\Omega\rangle\!\rangle \\ &= \left|V_g U V_g^{-1}\right\rangle\!\rangle, \end{aligned} \tag{17}$$

so the "partition function" (16) is nothing but the overlap $\langle\!\langle U|V_g U V_g^{-1}\rangle\!\rangle$. It can be further rewritten as

$$Z_g = \mathcal{N}^{-1}\mathrm{Tr}\left[U^\dagger V_g U V_g^{-1}\right]. \tag{18}$$

When U is symmetric in the sense that $V_g U V_g^{-1} = e^{i\phi_g(U)} U$,

$$\left|V_g U V_g^{-1}\right\rangle\!\!\right\rangle = e^{i\phi_g(U)} |U\rangle\!\rangle, \tag{19}$$

and the partition function is a pure phase quantity, $Z_g = e^{i\phi_g(U)}$. The nonzero phase signals the anomalous nature of the unitary operator. Note also that by construction, $|I\rangle\!\rangle = |\Omega\rangle\!\rangle$ is invariant under $V_g \otimes K V_g K^{-1}$.

As mentioned around (5), we can also interpret Z_g in terms of the Schwinger-Keldysh path-integral (trace) with a temporal background gauge field.

C. Gauging the KMS symmetry

Let us now turn to the case of antiunitary symmetry. To be concrete, we will work with a time-reversal symmetric unitary,

$$TUT^{-1} = e^{i\phi_T(U)} U^\dagger. \tag{20}$$

We note that in general T can be written as $T = W \times$ (complex conjugation) where W is a unitary matrix. In the basis $\{|i\rangle\}$, T is defined by its action on $\{|i\rangle\}$ as

$$T|i\rangle = \sum_j W_{ij}|j\rangle, \quad TiT^{-1} = -i, \tag{21}$$

with $W_{ij} = \langle j|W|i\rangle$. We note that the fact that time reversal squares to the identity, $T^2 = I$, possibly up to the fermion number parity operator for fermionic systems, $T^2 = (-1)^F$, imposes a restriction on the projective phase (20). To see this, we first find the Hermitian conjugate of (20), $TU^\dagger T^{-1} = e^{-i\phi_T(U)} U$, and then apply T, which gives $T^2 U^\dagger T^{-2} = e^{i\phi_T(U)} TUT^{-1} = e^{2i\phi_T(U)} U^\dagger$. Assuming U is fermion number parity even (odd), the projective phase is quantized as $e^{2i\phi_T(U)} = \pm 1$.

To gauge time-reversal symmetry, we first need to discuss how time reversal acts in the doubled Hilbert space, as we did for the case of unitary symmetry. We should note that antiunitary symmetry does not allow tensor factorization in the doubled Hilbert space, in contrast with unitary symmetry g, which acts on the doubled Hilbert space as $V_g \otimes K V_g K^{-1}$. Nevertheless, the time reversal T can be naturally extended to the doubled Hilbert space as

$$T|i\rangle|j\rangle^* = \sum_{i'j'} W_{ii'} (W^\dagger)_{j'j} |i'\rangle|j'\rangle^* = \sum_{i'j'} W_{ii'} (W_{jj'})^* |i'\rangle|j'\rangle^*. \tag{22}$$

Here we recall that $\{|i\rangle^*\}$ is the conjugate representation of $\{|i\rangle\}$. T is an antiunitary operator on $\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}}$.

One can check easily $T|\Omega\rangle\!\rangle = |\Omega\rangle\!\rangle$. The symmetry condition $TUT^{-1} = e^{i\phi_T(U)} U^\dagger$ is translated into $T|U\rangle\!\rangle = |TUT^{-1}\rangle\!\rangle = e^{i\phi_T(U)} |U^\dagger\rangle\!\rangle$ [cf. Eq. (19)]. Then, analogously to (18), we can consider the overlap

$$\begin{aligned} \langle\!\langle U^\dagger | T | U\rangle\!\rangle &= \langle\!\langle U^\dagger | TUT^{-1}\rangle\!\rangle \\ &= \mathcal{N}^{-1} \mathrm{Tr}[UTUT^{-1}] = e^{i\phi_T(U)}. \end{aligned} \tag{23}$$

As in (16) this overlap can be interpreted as the partition function on $S^1 \times M$ with twisted temporal boundary condition by some symmetry. As explained below, the relevant symmetry is TJ – the composition of time-reversal and modular conjugation—which we will call the KMS symmetry. This symmetry is unitary, while both J and T are antiunitary.

To see this, we can first verify that the combined operation TJ is a symmetry of $|U\rangle\!\rangle$ by using the KMS condition (9),

$$\begin{aligned} TJ|U\rangle\!\rangle &= T(U^\dagger \otimes I)|\Omega\rangle\!\rangle = (TU^\dagger T^{-1} \otimes I) T|\Omega\rangle\!\rangle \\ &= e^{-i\phi_T(U)} (U \otimes I)|\Omega\rangle\!\rangle = e^{-i\phi_T(U)} |U\rangle\!\rangle, \end{aligned} \tag{24}$$

where we recall that $JA|\Omega\rangle\!\rangle = A^\dagger|\Omega\rangle\!\rangle$. Namely, neither J nor T are a symmetry in the doubled Hilbert space (they do not leave $|U\rangle\!\rangle$ invariant), but JT is (JT leaves $|U\rangle\!\rangle$ invariant up to possibly a phase factor $e^{-i\phi_T(U)}$). In other words, the KMS condition, once combined with time reversal, can be "promoted" to a unitary symmetry in the doubled Hilbert space. The KMS symmetry, here identified by using the operator-state map, also has its counterpart in the Schwinger-Keldysh path integral language. In the path-integral language, Ref. [39] (see also [55]) proposed a symmetry of the Schwinger-Keldysh path integral under $\psi_\sigma(t, \mathbf{r}) \to \psi_\sigma^*(-t + i\sigma\beta/2, \mathbf{r})$, $\psi_\sigma^*(t, \mathbf{r}) \to \psi_\sigma(-t + i\sigma\beta/2, \mathbf{r})$, as the KMS condition. Here, $\psi_\sigma(t, \mathbf{r})$ schematically represents quantum fields in the Schwinger-Keldysh path integral where $\sigma = \pm$ represents the forward and backward branches. Note that the KMS symmetry can be defined (and gauged) at finite temperature, although in this paper we set temperature to be infinite.

Now, the KMS symmetry, being unitary on-site symmetry in the doubled Hilbert space, can be gauged in a straight forward way. Following the static case (13), we consider the partition function with twisted temporal boundary condition by the KMS symmetry,

$$Z_{\text{KMS}} = \langle\!\langle U | (TJ) | U\rangle\!\rangle. \tag{25}$$

Using (24) Z_{KMS} is nothing but (the complex conjugate of) (23),

$$Z_{\text{KMS}} = \langle\!\langle U | TU^\dagger T^{-1}\rangle\!\rangle = e^{-i\phi_T(U)}. \tag{26}$$

D. Unitarity condition and chiral symmetry in the doubled Hilbert space

In the forthcoming sections, we will study the anomalous properties of unitary operators using the gauging procedure outlined above. It should be noted however that it is not entirely obvious if all anomalous (topological) properties of unitaries can be detected this way. For example, we should note that the state-operator map can be applied to any operator acting on the original Hilbert space, not just unitaries. Hence, we need to narrow our focus down to the set of states in the doubled Hilbert space that correspond to unitary operators in the original Hilbert space.[2]

[2]To illustrate this point, let us consider the Berry phase of mapped states in the doubled Hilbert space, when we have unitaries $|U(R)\rangle\!\rangle$ parameterized by adiabatic parameters $R = (R_1, R_2, \dots)$. Noting that the Berry connection is given explicitly by $A^i = i\langle\!\langle U | (\partial/\partial R_i) | U\rangle\!\rangle = i\mathrm{Tr}\,[U^\dagger (\partial U/\partial R_i)]$, the Berry phase associated to any closed loop in the parameter space is quantized to an integer multiple of 2π, $\oint A^i dR_i = 2\pi \times$ integer. Clearly, this is not the case for generic states in $\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}}$. This is one of the consequences of the unitarity condition.

For matrix product unitaries, the unitarity condition (requirement) can be taken into account by using the standard form of matrix product unitaries [32,33]. Moreover, the chiral unitary index (GNVW index), a rational number that characterizes asymmetric quantum information flow, can be introduced to classify unitaries. [14,15,32,33]. For the case of noninteracting fermionic systems (Gaussian unitaries), we can impose an additional symmetry, the so-called chiral symmetry, in the doubled Hilbert space, to limit our focus to states corresponding to unitary operators (and enforce the quantization of the Berry phase) [20,21,46]. (In the context of free fermion systems (Gaussian unitaries), the operator-state map is called the Hermitian map.)

In the following, we will deal with 1d examples with time-reversal symmetry, for which the chiral unitary index vanishes. Following the case of on-site unitary symmetries for (bosonic) 1d unitaries [32,35], we expect that the anomalies (group cohomology class) associated with the KMS symmetry (together with other symmetries) are enough to classify these unitaries.

E. Spatial gauging

The spatial component of the background gauge field can also implemented in the unitary operator. For example, the spatial component of the background KMS gauge field can be introduced by twisting the spatial boundary condition. To do this, we need to have a closer look at the local (spatial) structure of unitaries. As we will discuss in the next section, once a unitary is given as a matrix product unitary, the spatial component of the background gauge field can be introduced, following the gauging procedure of matrix product states [53]. [See below around (33)]. Another way to introduce spatial gauging is to make use of a parent Hamiltonian that has $|U\rangle\!\rangle$ as its ground state. If it exists, we can introduce the background gauge field by minimally coupling it to matter degrees of freedom in the parent Hamiltonian. We will discuss this in the forthcoming sections by using examples, see Secs. V and VI. Finally, we also note that it is known that torus partition functions with twisted boundary conditions (topological invariants) can be computed solely by using ground state wave functions (without using Hamiltonians) by using the partial swap operator [53,56].

In the presence of a spatial component of a gauge field, the operator algebra (14) can be generalized as

$$V_g U(A_h) V_g^{-1} = e^{i\phi_g(U(A_h))} U(A_h)^{s(g)}, \tag{27}$$

where $s(g) = 1$ or $s(g) = -1 = \dagger$ when V_g is a unitary or antiunitary symmetry, respectively, and A_h is the background h gauge field. (Here, we are assuming g is a nonspatial symmetry. When g is a spatial symmetry, e.g., parity, the gauge field A_h also has to be transformed—see (70).) Correspondingly, we can consider the overlap

$$\begin{aligned} Z_g(A_h) &:= \langle\!\langle U(A_h)^{s_g} |\, V_g \otimes K V_g K^{-1} \,| U(A_h) \rangle\!\rangle \\ &= \mathcal{N}^{-1} \mathrm{Tr}\left[(U^\dagger(A_h))^{s_g} V_g U(A_h) V_g^{-1} \right], \end{aligned} \tag{28}$$

which can be interpreted as a partition function on $S^1 \times M$ with twisted temporal boundary condition by g, and spatial background gauge field A_h on M.

IV. MATRIX PRODUCT UNITARIES

All locality-preserving 1d unitaries (in bosonic systems) can be represented in the form of a matrix product unitary [32,33]. In this section, we discuss how we can gauge the KMS symmetry in matrix product unitaries. A matrix product unitary U is expressed as

$$U = \sum_{\{i,j\}} \mathrm{Tr}(A^{i_1 j_1} \cdots A^{i_L j_L}) \, |i_1 \cdots i_L\rangle \, \langle j_1 \cdots j_L| \,, \tag{29}$$

where $\{|i_1 \cdots i_L\rangle\}$ is the basis of the total Hilbert space of the 1d chain consisting of L sites, given as a tensor product of basis states $\{|i\rangle\}$ of the local Hilbert space at each site; A is a $\chi \times \chi$ dimensional matrix where χ is the "bond dimension" of the auxiliary space. By the operator-state map, the corresponding state in the doubled Hilbert space is

$$|U\rangle\!\rangle = \sum_{\{i,j\}} \mathrm{Tr}(A^{i_1 j_1} \cdots A^{i_L j_L}) \, |i_1 \cdots i_L\rangle \, |j_1 \cdots j_L\rangle^* . \tag{30}$$

Once written in this form, we can apply results from matrix product states, in particular their classification. However, this does not fully capture the full classification of unitaries. The reason is that we have not included the unitarity requirement, and the chiral unitary index. (See Sec. III D.) References [32,33] introduced the standard form of matrix product unitaries that takes into account the unitarity requirement, and defined the chiral unitary index. Using the standard form, symmetry protected indices can also be introduced for on-site unitary symmetry [35]. The gauging procedure we introduced is agnostic about the unitarity condition.

We however note that the double Hilbert space structure allows us to define the operator entanglement, the correlation measure between (suitable sub regions of) the input and output spaces, that can capture the chiral unitary index [57]. We also note that for unitaries of our interest, namely, those that are invariant under time reversal, the chiral unitary index always vanishes.

While the gauging procedure may not capture all topological/anomalous aspects of unitary operators, topological invariants (quantum anomalies) derived from gauging provides a bona fide diagnostic of anomalous unitary operators.

Let us now assume the unitary U is time-reversal symmetric in the sense that $TUT^{-1} = U^\dagger$ (up to a projective phase), where T is time reversal, which, as in (21), can be written as $T = WK$ with some unitary W. The time reversal T can be naturally extended to the doubled Hilbert space as in (22). Together with the antiunitary modular conjugation operator, $J(|i\rangle|j\rangle^*) = |j\rangle|i\rangle^*$, $J|U\rangle\!\rangle = |U^\dagger\rangle\!\rangle$, we can construct the KMS symmetry JT, which is a unitary, on-site, $\mathbb{Z}_2$ symmetry. For the matrix product unitary, JT acts on $|U\rangle\!\rangle$ as

$$\begin{aligned} JT\,|U\rangle\!\rangle = \sum_{\{i,j,i',j'\}} & \mathrm{Tr}\,(A^{j_1 i_1} \cdots A^{j_L i_L}) \\ & \times W_{i_1 i'_1} \left(W_{j_1 j'_1}\right)^* \cdots W_{i_L i'_L} \left(W_{j_L j'_L}\right)^* |i'_1 \cdots i'_L\rangle \, |j'_1 \cdots j'_L\rangle^* . \end{aligned} \tag{31}$$

The invariance under JT implies that each matrix A transforms as [58–60]

$$\sum_{ij} A^{ji}_{ab} W_{ii'} (W_{jj'})^* = e^{i\theta} \sum_{a'b'} (M^\dagger)_{aa'} A^{i'j'}_{a'b'} M_{b'b} \tag{32}$$

with some matrix M and phase $e^{i\theta}$. In one spatial dimension, a unitary on-site $\mathbb{Z}_2$ symmetry alone does not lead to nontrivial SPT phases, as $H^2(\mathbb{Z}_2, U(1)) = 0$. (This is consistent with [32].)[3] However, in the presence of other symmetries, we can discuss the discrete torsion phase with KMS symmetry.

We can gauge the state $|U\rangle\!\rangle$ by the KMS symmetry; the state under the twisted boundary condition by the KMS symmetry is given by [61]

$$|U\rangle\!\rangle_{\rm KMS} = \sum_{\{i,j\}} {\rm Tr}(A^{i_1 j_1} \cdots A^{i_L j_L} M) \, |i_1 \cdots i_L\rangle \, |j_1 \cdots j_L\rangle^* . \tag{33}$$

Let us now imagine that U is symmetric under an additional unitary symmetry X, $XUX^{-1} = U$ (up to possibly a phase factor). The torus partition function (13) can be computed, in the presence of another symmetry generator X, ${}_{\rm KMS}\langle\!\langle U|X|U\rangle\!\rangle_{\rm KMS}$, which extract a topological invariant (cocycle). Note that once the matrix product operator form is given, it is not necessary to use the parent Hamiltonian to gauge symmetries.

Using the operator-state map, we can map $|U\rangle\!\rangle_{\rm KMS}$ back to an operator $U_{\rm KMS}$,

$$U_{\rm KMS} = \sum_{\{i,j\}} {\rm Tr}(A^{i_1 j_1} \cdots A^{i_L j_L} M) \, |i_1 \cdots i_L\rangle \, \langle j_1 \cdots j_L| . \tag{34}$$

This can be thought of as the gauged unitary operator, in the presence of background KMS gauge field. When U is symmetric under an additional unitary on-site symmetry X, X induces an action on the auxiliary space by a unitary matrix M_X, as in (32). Then, the operator algebra between X and $U_{\rm KMS}$ is given by

$$X \, U_{\rm KMS} \, X^{-1} = e^{i\phi_{X,{\rm KMS}}} \, U_{\rm KMS}, \tag{35}$$

where we note that

$$X \, U_{\rm KMS} \, X^{-1} = \sum_{\{i,j\}} {\rm Tr}(A^{i_1 j_1} \cdots A^{i_L j_L} M_X M M_X^\dagger) \times |i_1 \cdots i_L\rangle \, \langle j_1 \cdots j_L| \tag{36}$$

and $e^{i\phi_{X,{\rm KMS}}}$ is the group cohomology phase, $M_X M = e^{i\phi_{X,{\rm KMS}}} M M_X$. Thus (the phase of) the torus partition function and the anomalous phase that appears in the operator algebra between the *gauged* unitary operator and symmetry generator is equivalent.

[3]Note that in Ref. [32] unitaries satisfying $U = U^\dagger$ are called "time-reversal symmetric." Here, we stick with time reversal which is realized as a antiunitary operation in the physical Hilbert space, as Wigner's symmetry representation theorem. Reference [32] also studied unitaries satisfying $U = U^T$, which corresponds (up to possibly a unitary operation) to our definition of time-reversal symmetry. For the latter case, Ref. [32] showed that there is no nontrivial unitary, consistent with $H^2(\mathbb{Z}_2, {\rm U}(1)) = 0$.

a. Example: the CZX model. As a simple example, let us consider the CZX model [32,62]. It is defined on a one-dimensional lattice with two-dimensional local Hilbert space at each site, $\{|0\rangle, |1\rangle\}$. The explicit matrix product unitary form is given as

$$A^{01} = |0\rangle \langle +| , \quad A^{10} = |1\rangle \langle -| , \quad A^{00} = A^{11} = 0, \tag{37}$$

with two-dimensional internal (auxiliary) Hilbert space, and $|\pm\rangle = |0\rangle \pm |1\rangle$. The chiral unitary index is trivial for the CZX model. The CZX unitary U is invariant under time reversal $KUK^{-1} = U^\dagger$. Hence, under JT, A's are transformed as $A^{ji}_{ab} = e^{i\theta} (W^\dagger)_{aa'} A^{ij}_{a'b'} W_{b'b}$. It is easy to check that we can take $W = \sigma_y$, $A^{ij} = -\sigma_y A^{ji} \sigma_y^\dagger$.

Now, let us consider an additional $\mathbb{Z}_2$ symmetry. We can consider, for example, $X = \prod_i^{odd} s_i^x$, which commutes with time reversal. (Here, s_i^x is the x component of a physical spin 1/2 operator at site i.) It is convenient to "block," i.e., take two adjacent spins as a single degrees of freedom; at each site, we now have a four-dimensional local Hilbert space spanned by $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Under blocking, we consider the matrix product unitary with

$$\begin{aligned} A^{0101} &= A^{01} A^{01} = |0\rangle \langle +| , \quad A^{0110} = A^{01} A^{10} = |0\rangle \langle -| , \\ A^{1001} &= A^{10} A^{01} = |1\rangle \langle +| , \quad A^{1010} = A^{10} A^{10} = -|1\rangle \langle -| . \end{aligned} \tag{38}$$

Under symmetry X, $A^{ijkl} \to A^{\bar{i}\bar{j}kl}$ (where $\bar{0} = 1$ and $\bar{1} = 0$). One can check that the invariance under X can be implemented by $A^{ijkl} \to A^{\bar{i}\bar{j}kl} = \sigma_x A^{ijkl} \sigma_x^\dagger$. Now, while the JT and X commute when acting on the physical Hilbert space, in the two-dimensional auxiliary space, $\sigma_y \sigma_x = -\sigma_x \sigma_y$, implying that the CZX model is protected by time reversal and X.

V. MAJORANA FERMION MODELS

In this section, we consider unitary time-evolution operators in Majorana fermion systems in one spatial dimension without/with time-reversal symmetry. As a specific model, we consider the boundary unitaries which are realized at the boundary of topological Floquet drives without/with time-reversal symmetry. We first consider the model without time-reversal symmetry ("the single copy theory") on the boundary of the 2d topological chiral Floquet drive considered in Ref. [14]. The time-reversal symmetric model ("the two copy theory") can then be constructed from two copies of the above model with opposite chiralities. We will then discuss nontrivial 2d time-reversal symmetric unitaries that can be realized at the boundary of 3d topological Floquet systems.

A. The single copy theory

Let us first have a closer look at the single copy theory. At the boundary of 2d topological chiral Floquet drive [14], discrete time-evolution is given by a boundary unitary S, which is a lattice translation operator (or shift operator):

$$S \lambda_x S^\dagger = \lambda_{x+1}. \tag{39}$$

Here $\{\lambda_x\}$ is the set Majorana fermion operators defined on sites x located at the boundary of the 2d system, $\{\lambda_x, \lambda_{x'}\} =$

$2\delta_{xx'}$. Throughout this section, we impose the periodic boundary condition. The translation operator S can be written down explicitly as [63]

$$S := e^{i\delta}\lambda_1 \frac{1+\lambda_1\lambda_2}{\sqrt{2}} \cdots \frac{1+\lambda_{L-1}\lambda_L}{\sqrt{2}}. \tag{40}$$

The phase can be chosen such that the translation operator S satisfies $S^L = 1$ where L is the total number of sites. The phase factor satisfies $e^{i\delta} = 1$ when $L/2 = 4, 5, 8, 9$ while $e^{i\delta} = e^{i\pi L}$ when $L/2 = 2, 3, 6, 7$ (mod 8).

This shift operator is characterized by nonzero chiral unitary index (GNVW index) [14,15]. The chiral unitary index can be defined without referencing to any symmetry, and hence the topological Floquet drive does not require any symmetry for its stability/existence. As mentioned briefly in Sec. III D, for Gaussian unitaries, the unitarity condition can be implemented by imposing a chiral symmetry. Imposing both fermion number parity conservation and chiral symmetry leads to the $\mathbb{Z}$ topological classification of single-particle topological Floquet unitaries [20]. On the other hand, for many-body unitaries, there appears no such simple symmetry that can be used to implement the unitarity condition.

Beside the chiral unitary index, we can also discuss an anomaly associated with the fermion number parity $\mathbb{Z}_2^f$, $(-1)^F = \prod_{n=1}^{L/2}(i\lambda_{2n-1}\lambda_{2n})$. We can verify that the shift operator is odd under the fermion number parity [64],

$$(-1)^F S (-1)^F = -S, \tag{41}$$

and hence, the partition function twisted by the fermion number parity is

$$\mathcal{N}^{-1}\mathrm{Tr}\,[(-1)^F S(-1)^F S^\dagger] = (-1). \tag{42}$$

The $\mathbb{Z}_2$ phase (minus sign) on the RHS is indicative of a $\mathbb{Z}_2$ quantum anomaly, occurring at the boundary of the bulk 2d Floquet system. The $\mathbb{Z}_2$ anomaly is independent of the chiral unitary index, and provides an additional characterization.

Let us now have a closer look at how the operator-state map works in this problem. We will be slightly generic and consider an arbitrary Gaussian unitary operator U. It transforms Majorana fermion operators $\{\lambda_a\}$ (satisfying $\{\lambda_a, \lambda_b\} = 2\delta_{ab}$) as

$$U\lambda_a U^\dagger = \mathcal{Q}_{ab}\lambda_b \tag{43}$$

where $\mathcal{Q}$ is a real orthogonal matrix. To deploy the state operator map, we introduce the doubled Hilbert space by considering the two sets of Majorana fermion operators $\{\lambda_{i,x}\}$ and $\{\lambda_{o,x}\}$ acting on the in and out Hilbert spaces, respectively. The construction of the reference state proceeds in a way slightly different than the bosonic case reviewed in Sec. II. As the reference state (1), we need to look for a maximally entangled state in the ($\mathbb{Z}_2$-graded) fermionic Hilbert space, which satisfies the shift property, and is invariant under a properly defined modular conjugation operator. We choose as the reference state the state consisting of maximal number of "Majorana dimers" connecting the in and out Hilbert spaces. Conveniently, the reference state can be taken as a ground state of the parent Hamiltonian

$$\mathbb{H}_0 = i\sum_x \lambda_{i,x}\lambda_{o,x}. \tag{44}$$

We identify the modular conjugation operator as[4]

$$J\lambda_{i,x}J^{-1} = \lambda_{o,x}, \quad J\lambda_{o,x}J^{-1} = \lambda_{i,x}. \tag{45}$$

One can check easily that $J\mathbb{H}_0 J^{-1} = \mathbb{H}_0$ and hence $J|\Omega\rangle\rangle \equiv |\Omega\rangle\rangle$. Furthermore, one can also check $\lambda_{ox}|\Omega\rangle\rangle = -i\lambda_{ix}|\Omega\rangle\rangle$. This means that by using $|\Omega\rangle\rangle$, we can map any bosonic operator O_{out} acting on the output Hilbert space to the corresponding operator O_{in} acting on the input Hilbert space; The reference state acts as a "perfect reflector" that reflects all operators from the output to input Hilbert space [recall Eqs. (4) and (7)]. For fermionic operators, applying two successive reflections is equivalent to a 2π rotation, under which they must pick up -1; this follows from the simplest case mentioned above, $\lambda_{ox}|\Omega\rangle\rangle = -i\lambda_{ix}|\Omega\rangle\rangle$.

We now consider the state $|U\rangle\rangle = (U_o \otimes I_i)|\Omega\rangle\rangle$, which can be thought of as a ground state of

$$\mathbb{H} = i\sum_{xy} \lambda_{i,x}\mathcal{Q}_{xy}\lambda_{o,y}. \tag{46}$$

The shift property of $|\Omega\rangle\rangle$ can be read off from $\mathbb{H}$ as

$$\mathbb{H} = i\sum_{xy} \lambda_{i,x}(\mathcal{Q}_{xy}\lambda_{o,y}) = i\sum_{xy} \left(\mathcal{Q}^{-1}_{yx}\lambda_{i,x}\right)\lambda_{o,y} \tag{47}$$

where we noted $\mathcal{Q}_{yx} = \mathcal{Q}^{-1}_{xy}$. Hence, $|U\rangle\rangle = (U_o \otimes I_i)|\Omega\rangle\rangle \propto (I_o \otimes U_i^\dagger)|\Omega\rangle\rangle$. We observe that $\mathbb{H}$ is not invariant under J, while $\mathbb{H}_0$ is, as expected.

Let us now consider the unitary in (39). Then, the parent Hamiltonian is

$$\mathbb{H} = i\sum_x \lambda_{i,x}\lambda_{o,x+1}. \tag{48}$$

This is essentially the Hamiltonian of the Kitaev chain in its topologically nontrivial phase. The ground state is characterized by the $\mathbb{Z}_2$ topological invariant associated with $\mathbb{Z}_2^f$ symmetry in one spatial dimension, consistent with the $\mathbb{Z}_2$ anomaly (41).

B. The two copy theory with time-reversal symmetry

The shift operator S is odd under time-reversal symmetry. In order to construct a time-reversal symmetric model of our interest, we introduce two copies of the 2d chiral topological Floquet model with opposite chiralities. We use $\uparrow$ / $\downarrow$ to label these two copies. At the boundary, this time-reversal symmetric model realizes the boundary unitary $U = S_\uparrow S_\downarrow^\dagger$, where $S_{\uparrow/\downarrow}$ is the shift operator that acts exclusively on the first/second copy. The boundary unitary U acts on the boundary Majorana fermion operators as

$$U\lambda_{\uparrow x}U^\dagger = \lambda_{\uparrow x+1}, \quad U\lambda_{\downarrow x}U^\dagger = \lambda_{\downarrow x-1}. \tag{49}$$

[4]Generically, the modular conjugation operator should satisfy $[J\mathcal{A}_{\text{in}}J, \mathcal{A}_{\text{in}}] = 0$, while for the J operator defined here, $J\lambda_i J$ and λ_i anticommute. The J operator here is actually the tilde conjugation in the thermofield dynamics [49]. While for bosonic systems the modular conjugation and the tilde conjugation are equivalent, for fermionic systems, they differ by a Klein factor (Jordan-Wigner string) [50].

The model is symmetric under the following time reversal,

$$T\lambda_{\uparrow x}T^{-1}=\lambda_{\downarrow x},\quad T\lambda_{\downarrow x}T^{-1}=\epsilon\lambda_{\uparrow x},\quad T^2=\epsilon^F. \tag{50}$$

where $(-1)^F=\prod_x(i\lambda_{\uparrow x}\lambda_{\downarrow x})$ is the total fermion number parity operator; $\epsilon=\pm1$ distinguishes two possible cases. The unitary is time-reversal symmetric in the sense that $TUT^{-1}=TS_\uparrow T^{-1}\cdot TS_\downarrow^\dagger T^{-1}=\epsilon S_\downarrow S_\uparrow^\dagger=\epsilon(S_\uparrow S_\downarrow^\dagger)^\dagger=\epsilon U^\dagger$. In particular, when $\epsilon=-1$, the operator algebra between U and T is nontrivial, while it is trivial when $\epsilon=+1$.

Below, we will try to detect the nontriviality (quantum anomaly) of the above time-reversal symmetric unitary when $\epsilon=-1$. At the noninteracting level, Floquet unitaries in symmetry class DIII (corresponding to $\epsilon=-1$) are classified by $\mathbb{Z}_2$ [20]. When we enforce time-reversal symmetry with $\epsilon=-1$, by the operator-state map, we consider a short-range entangled state in the doubled Hilbert space. The relevant symmetry group is $\mathcal{G}=\mathbb{Z}_2^f\times\mathbb{Z}_2$ where $\mathbb{Z}_2^f$ represents the fermion number parity conservation, and $\mathbb{Z}_2$ is the KMS symmetry (JT symmetry). Such short-range entangled states in (1+1)-dimensions are classified by $\Omega_2^{\rm Spin}(B\mathbb{Z}_2)=\mathbb{Z}_2^2$ [26]. In the following, we will show explicitly that the above unitary is a nontrivial element of this group. Additionally, we also study the operator entanglement spectrum of U. We then find two zero modes which form a doublet under the KMS symmetry.

Let us start by applying the operator-state map to the unitary (49). We denote the Majorana fermion operators acting on the in and out Hilbert spaces by $\{\lambda_{i/o,\uparrow/\downarrow,x}\}$. In the doubled Hilbert space, we introduce time reversal T acting on the fermion operators as

$$T\,\Lambda\,T^{-1}=[\mathbb{1}_2\otimes(i\sigma_2)\otimes\mathbb{1}_L]\,\Lambda, \tag{51}$$

where $\Lambda=(\lambda_{i\uparrow x},\lambda_{i\downarrow x},\lambda_{o\uparrow x},\lambda_{o\downarrow x})^T$ is a $4L$ component vector with x taking values from 1 to L. $\mathbb{1}_2, i\sigma_2, \mathbb{1}_L$ act on in/out, spin and position degree of freedoms, respectively.

We choose, as the reference state $|\Omega\rangle\!\rangle$, the ground state of the quadratic Hamiltonian:

$$\begin{aligned}\mathbb{H}_0&=i\sum_x(\lambda_{i\uparrow x}\lambda_{o\uparrow x}-\lambda_{i\downarrow x}\lambda_{o\downarrow x})\\&=\frac{i}{2}\Lambda^T\begin{pmatrix}0&(\sigma_3\otimes\mathbb{1}_L)\\-(\sigma_3\otimes\mathbb{1}_L)&0\end{pmatrix}\Lambda.\end{aligned} \tag{52}$$

One can check easily $T\mathbb{H}_0T^{-1}=\mathbb{H}_0$. We next construct the state $|U\rangle\!\rangle$. Let U be a generic Gaussian unitary operator that acts on the fermion operators as

$$U\begin{pmatrix}\lambda_\uparrow\\\lambda_\downarrow\end{pmatrix}U^\dagger=\mathcal{Q}\begin{pmatrix}\lambda_\uparrow\\\lambda_\downarrow\end{pmatrix}, \tag{53}$$

where $\mathcal{Q}$ is a $2L\times2L$ real orthogonal matrix, acting on "in" and "out" space in the same way. When U is time-reversal symmetric, $\mathcal{Q}$ satisfies $(-i\sigma_2)\mathcal{Q}(i\sigma_2)=\mathcal{Q}^T$. The state $|U\rangle\!\rangle$ can then be thought of as the ground state of the parent Hamiltonian

$$\mathbb{H}=\frac{i}{2}\Lambda^T\mathcal{K}\,\Lambda,\quad \mathcal{K}=\begin{pmatrix}0&(\sigma_3\otimes\mathbb{1}_L)\mathcal{Q}\\-\mathcal{Q}^T(\sigma_3\otimes\mathbb{1}_L)&0\end{pmatrix}. \tag{54}$$

For the case of our interest, this reduces to

$$\mathbb{H}=i\sum_x(\lambda_{i,\uparrow,x}\lambda_{o,\uparrow,x+1}-\lambda_{i,\downarrow,x}\lambda_{o,\downarrow,x-1}). \tag{55}$$

The parent Hamiltonian is invariant under the following unitary operation:

$$(JT)\,\Lambda\,(JT)^{-1}=\left[\begin{pmatrix}0&\sigma_1\\\sigma_1&0\end{pmatrix}\otimes\mathbb{1}_L\right]\Lambda \tag{56}$$

as one can check easily:

$$\left[\begin{pmatrix}0&\sigma_1\\\sigma_1&0\end{pmatrix}\otimes\mathbb{1}_L\right]\cdot\mathcal{K}\cdot\left[\begin{pmatrix}0&\sigma_1\\\sigma_1&0\end{pmatrix}\otimes\mathbb{1}_L\right]=\mathcal{K}, \tag{57}$$

by using the time-reversal symmetry of $\mathcal{Q}$. This operation can be understood as the composition of the modular conjugation

$$J\,\Lambda\,J^{-1}=\left[\begin{pmatrix}0&-\sigma_3\\-\sigma_3&0\end{pmatrix}\otimes\mathbb{1}_L\right]\Lambda, \tag{58}$$

and time reversal. We can check that J leaves $\mathbb{H}_0$ invariant, $J\mathbb{H}_0J^{-1}=\mathbb{H}_0$. (Also, while $\mathbb{H}$ is not invariant under T nor J, as we checked, JT is a symmetry of $\mathbb{H}$.) Finally, the single-particle Hamiltonian $\mathcal{K}$ is chiral symmetric,

$$\left[\begin{pmatrix}\mathbb{1}_2&0\\0&-\mathbb{1}_2\end{pmatrix}\otimes\mathbb{1}_L\right]\cdot\mathcal{K}\cdot\left[\begin{pmatrix}\mathbb{1}_2&0\\0&-\mathbb{1}_2\end{pmatrix}\otimes\mathbb{1}_L\right]=-\mathcal{K}. \tag{59}$$

a. Gauging the KMS symmetry. Let us now gauge the KMS (JT) symmetry. Specifically, we can introduce the background KMS gauge field, such that we twist the temporal and/or spatial boundary conditions. As for the temporal twisting, we note, $TUT^{-1}U=(-1)$ and hence

$$\langle\!\langle U|(JT)|U\rangle\!\rangle=(-1). \tag{60}$$

This quantity can be interpreted as a partition function on T^2 with the twisted temporal direction by the KMS symmetry, and periodic spatial boundary condition. This confirms that the unitary is a nontrivial element of the $\Omega_2^{\rm Spin}(B\mathbb{Z}_2)=\mathbb{Z}_2^2$ classification.

Similarly, the spatial boundary condition can also be twisted by the KMS symmetry. To this end, it is convenient to go to the basis that diagonalizes JT; we introduce

$$\eta_\pm=\lambda_{i\uparrow}\pm\lambda_{o\downarrow},\quad \xi_\pm=\lambda_{i\downarrow}\pm\lambda_{o\uparrow} \tag{61}$$

The action of JT on these rotated Majorana operators are diagonal:

$$(JT)\eta_\pm(JT)^{-1}=\pm\eta_\pm,\quad (JT)\xi_\pm(JT)^{-1}=\pm\xi_\pm. \tag{62}$$

In terms of these operators, the parent Hamiltonian is written as

$$\mathbb{H}\propto i\sum_x(\eta_{+,x+1}\xi_{+,x}-\eta_{-,x+1}\xi_{-,x}). \tag{63}$$

Then, twisting spatial boundary condition by JT affects only the minus sector. In other words, combined with the fermion number parity $(-1)^F$, we can give different boundary conditions to each sector independently. The state $|U\rangle\!\rangle$ can be factorized as $|U\rangle\!\rangle_{pq}=|U_+\rangle\!\rangle_p|U_-\rangle\!\rangle_q$, where p,q denote the spatial boundary condition for each sector, and can be either periodic boundary condition ("Ramond" boundary condition,

r), or antiperiodic boundary condition ("Neveu-Schwarz" boundary condition, ns). The state in the sector twisted by the KMS symmetry is $|U\rangle\!\rangle_{JT} = |U_+\rangle\!\rangle_r |U_-\rangle\!\rangle_{ns}$. Then, we see, for example,

$$\begin{aligned}
&{}_{JT}\langle\!\langle U|(-1)^F|U\rangle\!\rangle_{JT} \\
&\quad = {}_r\langle\!\langle U_+|(-1)^{F_+}|U_+\rangle\!\rangle_r \cdot {}_{ns}\langle\!\langle U_-|(-1)^{F_-}|U_-\rangle\!\rangle_{ns} \\
&\quad = Z[T^2,(r,r)]\cdot Z[T^2,(r,ns)] = -1, \\
&{}_{JT(-1)^F}\langle\!\langle U|(-1)^F|U\rangle\!\rangle_{JT(-1)^F} \\
&\quad = {}_{ns}\langle\!\langle U_+|(-1)^{F_+}|U_+\rangle\!\rangle_{ns} \cdot {}_r\langle\!\langle U_-|(-1)^{F_-}|U_-\rangle\!\rangle_r \\
&\quad = Z[T^2,(r,ns)]\cdot Z[T^2,(r,r)] = -1,
\end{aligned} \tag{64}$$

where $Z[T^2,(a,b)]$ is the torus partition function of (1+1)d topological superconductors (the Kitaev chain in its nontrivial phase) in the presence of temporal and spatial boundary conditions (a,b); $Z[T^2,(a,b)] = -1$ for $(a,b) = (r,r)$, and $Z[T^2,(a,b)] = 1$ otherwise [65]. We once again confirm that the state $|U\rangle\!\rangle$ is nontrivial in the presence of time reversal. The above example represents the nontrivial element $(-1,-1) \in \Omega_d^{\text{Spin}}(B\mathbb{Z}_2) = \mathbb{Z}_2^2$ [26].

b. Boundary analysis. The anomalous properties of U can also be detected by studying the boundary excitations or entanglement spectrum of $|U\rangle\!\rangle$. Here, we follow Ref. [66] to analyze symmetry actions on the boundary excitations. When the system (parent Hamiltonian) is cut, excitations at the boundary are built out of unpaired Majorana fermion operators: $\lambda_{i,\downarrow}$, $\lambda_{o,\uparrow}$. We can then study the algebra of symmetry operators within the boundary Hilbert space. JT and the fermion number parity, can be constructed explicitly as (see Refs. [67,68] for similar analysis)

$$JT = \frac{e^{i\delta}}{\sqrt{2}}(\lambda_{i,\downarrow} + \lambda_{o,\uparrow}), \quad (-1)^F = (i\lambda_{i,\downarrow}\lambda_{o,\uparrow}), \tag{65}$$

where the phase $e^{i\delta}$ can be chosen such that $(JT)^2 = 1$, $e^{2i\delta} = 1$. Now, the commutator between JT and the fermion number parity is

$$(-1)^F(JT)(-1)^F = (-1)(JT). \tag{66}$$

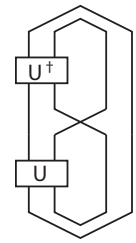
The projective phase factor (-1) indicates a $\mathbb{Z}_2$ anomaly.

C. Two spatial dimensions

One can analyze unitary operators of higher-dimensional Majorana fermion systems with time reversal. As an example, let us consider two spatial dimensions, and impose time-reversal symmetry which squares to $(-1)^F$. Let us once again assume the unitary condition does not play any role. Then, with the operator-state map, the relevant symmetry group is $\mathbb{Z}^f \times \mathbb{Z}_2$, where $\mathbb{Z}_2$ is the KMS symmetry (JT). Nontrivial fermionic SPT phases with this symmetry are classified by $\Omega_3^{\text{Spin}}(B\mathbb{Z}_2) = \mathbb{Z}_8$ [28,65,69]. The generating manifold is $\mathbb{R}P^3$. The corresponding topological invariant can be constructed by using partial symmetry transformation acting on a finite subregion of the space [65]. Specifically, we can consider the partial KMS symmetry, combined with π spatial rotation R_π, that acts only on a sub region of the total system, which we take as a disk D. Therefore the following expectation value

$$\langle\!\langle U|(JT\cdot R_\pi)_D|U\rangle\!\rangle \sim e^{\frac{2\pi\nu i}{8}}, \quad \nu \in \mathbb{Z}, \tag{67}$$

detects the $\mathbb{Z}_8$ classification. Diagramatically it can be represented as



(68)

In terms of the original unitary operator, this quantity may be obtained by taking the partial transpose of the unitary with respect to the disk D,

$$\text{Tr}\big[U^\dagger \cdot (R_\pi)_D U^{T_D}\big(R_\pi^{-1}\big)_D\big], \tag{69}$$

where A^{T_D} represents the partial transpose of an operator A with respect to D. (Here, we need to use partial transpose for fermionic systems, as explained in Refs. [30,70,71].)

We close this section with one remark. There is an isomorphism (Smith isomorphism) between $\Omega_{d+1}^{\text{Spin}}(B\mathbb{Z}_2)$ and $\Omega_d^{\text{Pin}^-}(pt)$. This means the classification of boundary unitary protected by time reversal with $\epsilon = -1$ in $d+1$ space-time dimension (= classification of topological Floquet unitary protected by time reversal with $\epsilon = -1$ in $d+2$) is equivalent to the classification of static SPT phases with $\epsilon = 1$ in d space-time dimension. This is consistent since the "Bott clock" differs by two (... AI, BDI, D, DIII ...).

VI. ANOMALOUS UNITARY OPERATORS WITH U(1) AND DISCRETE SYMMETRIES

A. Generalities

In this section, we consider topological/anomalous unitary time-evolution operators of charged fermion systems. This means that we have particle number conserving symmetry U(1) symmetry, $e^{i\theta Q}Ue^{-i\theta Q} = U$, where Q is the U(1) charge. In addition, we also discuss various discrete symmetries; they act on unitaries as in (14) and (15).

The U(1) symmetry can be gauged, and we can consider unitary operators in the presence of background U(1) gauge field, $U(A)$. In this paper, we focus on time-independent, spatial components of the U(1) gauge fields, $A_i(\mathbf{r})$ [46]. To detect topological/anomalous properties of the unitary operator, we will consider the operator algebra among the unitary symmetries in the presence of the background gauge field,

$$V_g U(A) V_g^{-1} = e^{i\phi_g(A)} U(g\cdot A)^{s(g)}, \tag{70}$$

analogous to (14) and (15). Here, $s(g) = 1$ or $s(g) = -1 = \dagger$ when V_g is a unitary or antiunitary symmetry, respectively, and again we allow a possible "projective" phase factor. $g\cdot A$ represents the background gauge field transformed by symmetry g. For example, $g\cdot A_i(\mathbf{r}) = -A_i(\mathbf{r})$ for particle-hole or time-reversal symmetry. As before (cf. Sec. III C), when an antiunitary symmetry squares to the identity (possibly up to the fermion number parity $(-1)^F$), the projective phase $e^{i\phi_g(A)}$

obeys a condition, $e^{i\phi_g(g\cdot A)} = e^{-i\phi_g(A)}e^{i\gamma}$, where $\gamma = \pi$ when $V_g^2 = (-1)^F$, and $U(A)$ is fermion number parity odd, and $\gamma = 0$ otherwise.

In addition to the algebraic relation (70), another closely related object of our interest is the Schwinger-Keldysh trace:

$$Z(A_1, A_2) = \mathcal{N}^{-1}\mathrm{Tr}\,[U(A_2)^\dagger U(A_1)] = \langle\langle U(A_2)|U(A_1)\rangle\rangle. \tag{71}$$

$Z(A_1, A_2)$ is the effective response theory (partition function) obtained by integrating over matter degrees of freedom. The Schwinger-Keldysh trace satisfies a couple of constants/conditions, such as (1) Schwinger-Keldysh symmetry:

$$Z(A, A) = 1; \tag{72}$$

(2) reality condition:

$$Z(A_1, A_2)^* = Z(A_2, A_1). \tag{73}$$

These conditions follow directly from (71). There are also other conditions, in particular, in the presence of symmetries [72]. From (70),

$$\mathrm{Tr}\big[V_g U(A_1)U(A_2)^\dagger V_g^{-1}\big] = e^{i[\phi_g(A_1)-\phi_g(A_2)]}\,\mathrm{Tr}[U(g\cdot A_1)^{s(g)}U(g\cdot A_2)^{-s(g)}], \tag{74}$$

we read off

$$Z(A_1, A_2) = e^{is(g)[\phi_g(A_1)-\phi_g(A_2)]}\,Z(g\cdot A_1, g\cdot A_2). \tag{75}$$

The phase factor $e^{is(g)[\phi_g(A_1)-\phi_g(A_2)]}$ is an anomaly in the sense that it represents the violation of the naive relation $Z(A_1, A_2) = Z(g\cdot A_1, g\cdot A_2)$ expected from the symmetry.

In what follows, we discuss some examples. We consider a series of unitaries in odd spatial dimensions, which, roughly speaking, realize chiral (Weyl) fermions in their single-particle quasienergy spectrum in momentum space. For example, their single-particle unitaries are given as $\mathcal{U}(k_x) = e^{ik_x}$ (1d), $\mathcal{U}(\mathbf{k}) \sim e^{i\mathbf{k}\cdot\boldsymbol{\sigma}}$ (3d), etc. These unitaries can be realized as boundary unitaries of bulk topological Floquet unitaries in one higher dimensions. The Schwinger-Keldysh trace for these unitaries is given in terms of topological terms, such as Chern-Simons terms (boundary) and theta terms (bulk). One of the key questions here is the interplay of these topological terms and discrete symmetries.

B. Example 1: (1+1)d with C

Let us start with the (1+1)d anomalous unitary, which is simply a lattice translation operator. We consider a one-dimensional lattice. At each site x on the lattice, we consider complex fermion creation/annihilation operators, which satisfy the canonical anticommutation relation, $\{\psi_x, \psi_y^\dagger\} = \delta_{xy}$. The unitary operator of our interest is the shift operator:

$$U\psi_x U^{-1} = \psi_{x+1}. \tag{76}$$

The unitary respects the particle number conserving U(1) symmetry, $e^{i\theta Q}Ue^{-i\theta Q} = U$ $(\theta \in [0, 2\pi])$, where $Q = \sum_x \psi_x^\dagger\psi_x$ is the total charge. This unitary arises as a boundary unitary of a topologically nontrivial 2d Floquet drive [12].[5]

As noted in Ref. [46], the unitary operator is invariant under particle-hole symmetry which is a unitary on-site symmetry defined by

$$C\psi_x C^{-1} = \psi_x^\dagger. \tag{77}$$

Also noted in Ref. [46], is that the (bulk and boundary) unitary operators are symmetric under particle-hole symmetry C, $CUC^{-1} \equiv U$, up to a projective phase for the boundary unitary. In the presence of the background U(1) gauge field, we expect that $CU(A)C^{-1}$ is equivalent to $U(-A)$, $CU(A)C^{-1} \equiv U(-A)$. While for the bulk without a boundary there is no projective phase $CU_{\mathrm{bulk}}(A)C^{-1} = U_{\mathrm{bulk}}(-A)$, one can verify by a direct calculation that a projective phase exists for the boundary unitary, and it is given by the one-dimensional Chern-Simons term (Wilson loop),

$$C\,U(A)\,C^{-1} = e^{iCS_1(A)}\,U(-A),$$
$$CS_1(A) = \oint dx\,A_x(x) = \oint A. \tag{78}$$

(Possibly up to a phase that is independent of A—see below.) We will provide the derivation of the projective phase shortly. By taking the trace and using the operator-state map, the anomalous relation (78) leads to

$$e^{iCS_1(A)} = \mathcal{N}^{-1}\mathrm{Tr}[CU(A)C^{-1}U^\dagger(-A)] = \langle\langle U(A)|\,C\,|U(-A)\rangle\rangle. \tag{79}$$

This can be interpreted as the path integral on two-dimensional space-time with twisted temporal boundary condition by C.

The anomalous algebra (78) also leads to, for the ratio of the Schwinger-Keldysh partition functions,

$$\frac{Z(-A_1, -A_2)}{Z(A_1, A_2)} = e^{-i\oint(A_1-A_2)} \neq 1, \tag{80}$$

consistent with the result in Ref. [46]. Furthermore, in Ref. [46], it was found that the partition function of the corresponding bulk dynamics, defined on an open spatial manifold with a boundary, also picks up a phase under particle-hole symmetry but this has opposite sign: $Z_{\mathrm{bulk,open}}(-A_1, -A_2)/Z_{\mathrm{bulk,open}}(A_1, A_2) = e^{i\oint(A_1-A_2)}$. The total partition function is therefore invariant under C. This is an "anomaly inflow" for the mixed anomaly between the particle-hole and U(1) symmetries, in the sense that the anomalous phases in bulk and boundary cancel each other. This consideration extends to the p, q drives studied in Ref. [46], in which case (80) becomes $Z(-A_1, -A_2)/Z(A_1, A_2) = e^{-i\theta_{p,q}/2\pi\oint(A_1-A_2)}$, where $\theta_{\mathsf{p},\mathsf{q}}$ is an integer multiple of π and depends only on p/q. Note also that the anomalous relation

[5] It can also be viewed as an example of topologically nontrivial non-Hermitian Hamiltonian with a point gap.

(78) leads to $\mathrm{Tr}\, U(A)/\mathrm{Tr}\, U(-A) = e^{i\oint A}$, which was also verified in Ref. [46].[6]

The relation (78) can be verified by a direct calculation for the boundary unitary of the Floquet topological Anderson insulator, or by using the operator-state map and computing $\langle\langle U(A)|\, C\, |U(-A)\rangle\rangle$. Below, we will present both calculations. The following results depend on the total number of lattice sites (=L) being even or odd. We note that when we consider the 2d topological Floquet system defined on a cylinder, with two circular boundaries at its two ends, the number of boundary sites per boundary is always even. The number of boundary sites can be odd if we consider different geometries, e.g., a finite 2d square lattice with a single boundary around it. In the latter case, the boundary unitary is not a simple shift operator near the corners of the square lattice.

1. Direct calculation

Let us first have a look at the direct calculation. Following the case of Majorana fermions, we can construct U explicitly: $U = S_\lambda S_\gamma (-1)^F$, where $\psi_x = (\lambda_x + i\gamma_x)/2$ and S_λ and S_γ are the shift operators for λ_x and γ_x, respectively. Explicitly,

$$U = e^{i\delta}\lambda_1\gamma_1\Pi_{12}\Pi_{23}\cdots\Pi_{L-1,L}(-1)^F,$$
$$\Pi_{x,x'} = 1 + (\psi_x^\dagger\psi_{x'} - \psi_{x'}^\dagger\psi_x) - (n_x - n_{x'})^2. \quad (82)$$

(As before, the phase must be chosen such that $U^L = 1$.) We can then consider to gauge the U(1) symmetry. This amounts to $\psi_x^\dagger\psi_{x'} \to e^{iA_{x,x'}}\psi_x^\dagger\psi_{x'}$. In addition, we also consider

$$e^{i(A_{1,2}+A_{2,3}+\cdots+A_{L-1,L})\psi_1^\dagger\psi_1} \equiv e^{i\oint A\,\psi_1^\dagger\psi_1}, \quad (83)$$

to construct the operator

$$U(A) = e^{i\delta}e^{i\oint A\,\psi_1^\dagger\psi_1}\lambda_1\gamma_1\Pi_{12}(A)\cdots\Pi_{L-1,L}(A)(-1)^F, \quad (84)$$

as the gauged version of the translation operator. We can verify that the gauged version of (76) is given by

$$U(A)\,\psi_x\,U(A)^{-1} = e^{iA_{x,x+1}}\,\psi_{x+1}. \quad (85)$$

The unitary particle-hole transformation C, which acts on the Majorana operators as $C\lambda C^{-1} = \lambda$ and $C\gamma C^{-1} = -\gamma$, can also be constructed explicitly:

$$C = (i\gamma_1\gamma_2)(i\gamma_3\gamma_4)\cdots(i\gamma_{L-1}\gamma_L). \quad (86)$$

One can readily check that the following identities hold:

$$CUC^{-1} = (-1)^{L+1}U,$$
$$\mathcal{N}^{-1}\mathrm{Tr}\,[CUC^{-1}U^\dagger] = (-1)^{L+1}. \quad (87)$$

The minus sign is indicative of a $\mathbb{Z}_2$ anomaly. Now, in the presence of the background gauge field,

$$C\,U(A)\,C^{-1} = (-1)^{L+1}\,e^{i\oint A}U(-A). \quad (88)$$

2. Calculation via operator-state map

Next, let us use the operator-state map, and calculate $\langle\langle U(A)|\, C\, |U(-A)\rangle\rangle$. As in the case of Majorana fermion systems discussed in Sec. V, the construction of the reference state proceeds slightly differently from the bosonic case. Here, the reference state $|\Omega\rangle\rangle$ can be conveniently defined as the ground state of the parent Hamiltonian

$$\mathbb{H}_0 = -\sum_x(\psi_{i,x}^\dagger\psi_{o,x} + \psi_{o,x}^\dagger\psi_{i,x}), \quad (89)$$

where we denote the fermion creation/annihilation operators acting on the in and out Hilbert spaces as $\psi_{i,a}^\dagger/\psi_{i,a}$ and $\psi_{o,a}^\dagger/\psi_{o,a}$, respectively. Explicitly, the reference state is given by

$$|\Omega\rangle\rangle = \prod_x \frac{1}{\sqrt{2}}(\psi_{i,x}^\dagger + \psi_{o,x}^\dagger)|0\rangle\rangle. \quad (90)$$

Note that $|\Omega\rangle\rangle$ is given as a superposition of states of the form $|n_{\mathrm{in}}\rangle_i|L - n_{\mathrm{in}}\rangle_o = |n_{\mathrm{in}}\rangle_i(C|n_{\mathrm{in}}\rangle_o)$ with n_{in} being the occupation number for "in" fermions. Consequently, $|\Omega\rangle\rangle$ is invariant under "vectorial" U(1) rotations generated by $\exp[i\theta(Q_i + Q_o)]$, while it is not under "axial" U(1) rotations $\exp[i\theta(Q_i - Q_o)]$. Here, $Q_{i/o} = \sum_a \psi_{i/o,a}^\dagger\psi_{i/o,a}$ is the total U(1) charge for the in/out Hilbert space, and $\theta \in [0, 2\pi]$. Alternatively, we could work with a different reference state $|\Omega\rangle\rangle$, which is invariant under axial U(1) but not under vectorial U(1). These two choices are simply related by particle-hole transformation $\psi_{o,a} \leftrightarrow \psi_{o,a}^\dagger$. We can introduce a modular conjugation operator J as

$$J\psi_{i,a}J^{-1} = \psi_{o,a}^\dagger, \quad J\psi_{o,a}J^{-1} = -\psi_{i,a}^\dagger,$$
$$J|0\rangle\rangle = |full\rangle\rangle = \prod_x(\psi_{i,x}^\dagger\psi_{o,x}^\dagger)|0\rangle\rangle, \quad JiJ^{-1} = -i. \quad (91)$$

One can easily check $|\Omega\rangle\rangle$ is invariant under J.

To construct the mapped state $|U\rangle\rangle$ for the shift operator (76), we note that $|U\rangle\rangle$ is the ground state of the parent Hamiltonian

$$\mathbb{H} = -\sum_x(\psi_{i,x}^\dagger\psi_{o,x+1} + \psi_{o,x+1}^\dagger\psi_{i,x}). \quad (92)$$

Explicitly, $|U\rangle\rangle$ is given by

$$|U\rangle\rangle = \prod_x \frac{1}{\sqrt{2}}(\psi_{o,x+1}^\dagger + \psi_{i,x}^\dagger)|0\rangle\rangle. \quad (93)$$

Particle-hole transformation (77) can be properly extended to act on the doubled Hilbert space,

$$C\psi_{x,i}C^{-1} = \psi_{x,i}^\dagger, \quad C\psi_{x,o}C^{-1} = -\psi_{x,o}^\dagger, \quad C|0\rangle\rangle = |full\rangle\rangle. \quad (94)$$

Note that the parent Hamiltonians are invariant under C, $C\mathbb{H}_0C^{-1} = \mathbb{H}_0$, and $C\mathbb{H}C^{-1} = \mathbb{H}$, and so are their ground states. One can check explicitly $C|\Omega\rangle\rangle = |\Omega\rangle\rangle$ and $C|U\rangle\rangle = (-1)^{L+1}|U\rangle\rangle$, consistent with (87).

[6] We also note that the Schwinger-Keldysh trace itself (not the ratio) was computed in Ref. [46] both for (2+1)d bulk and (1+1)d boundary. In long-wave length limit, the bulk trace is given by

$$Z_{\mathrm{bulk}}(A_1, A_2) \sim \exp\left[\frac{i\theta}{2\pi}\int d^2x\,\varepsilon_{ij}\partial_i(A_{1j} - A_{2j})\right], \quad (81)$$

with $\theta = \pi$. There is no such limit for the boundary trace, being the dynamics on the boundary nonlocal. Clearly the above expression is consistent with the ratio presented in the main text. While (81) is valid for long wave lengths, the ratio presented in the main text for the bulk partition function [as well as (80)] is exact.

To study the mixed anomaly, we introduce the background U(1) gauge field via $U_o^\dagger \psi_{o,x} U_o \to \psi_{o,x+1} e^{iA_{x,x+1}}$, and consider the parent Hamiltonian

$$\mathbb{H}(A) = -\sum_x (\psi_{i,x}^\dagger \psi_{o,x+1} e^{iA_{x,x+1}} + \psi_{o,x+1}^\dagger \psi_{i,x} e^{-iA_{x,x+1}}). \quad (95)$$

The ground state is given by

$$|U(A)\rangle\!\rangle = \prod_x \frac{1}{\sqrt{2}} (\psi_{o,x+1}^\dagger e^{-iA_{x,x+1}} + \psi_{i,x}^\dagger)|0\rangle\!\rangle. \quad (96)$$

One can then verify explicitly (88), $C|U(A)\rangle\!\rangle = (-1)^{L+1} e^{-i\oint A} |U(-A)\rangle\!\rangle$.

C. Example 2: (3+1)d with *CP*

Let us now discuss the (4+1)d bulk topological Floquet unitary [61,73] and its (3+1)d boundary. The boundary unitary has a single Weyl point (or multiple Weyl points with nonvanishing total chiralities) in its single-particle quasienergy spectrum. We can discuss *CP* symmetry, which leaves the boundary unitary invariant, as seen from $CP : \mathbf{k}\cdot\boldsymbol{\sigma} \to \sigma_2(\mathbf{k}\cdot\boldsymbol{\sigma})^T\sigma_2 = -\mathbf{k}\cdot\boldsymbol{\sigma}$, where P sends $\mathbf{r} \to -\mathbf{r}$ (inversion). The following discussion using *CP* applies also to *CR* symmetry, where R sends $x \to -x$ (reflection).

Guided by the 1d case (78), we postulate the anomalous operator algebra relation with the three-dimensional Chern-Simons term $CS_3(A)$,

$$(CP)\,U(A)\,(CP)^{-1} = e^{iCS_3(A)}\,U(\tilde{A}),$$
$$CS_3(A) = \frac{1}{4\pi}\int d^3x\,\varepsilon_{ijk}A_i\partial_j A_k = \frac{1}{4\pi}\int AdA, \quad (97)$$

where $\tilde{A} = CP\cdot A$ is given by $\tilde{A}_i(\mathbf{r}) = A_i(-\mathbf{r})$. As before, by taking the trace and using the operator-state map,

$$e^{iCS_3(A)} = \mathcal{N}^{-1}\mathrm{Tr}[(CP)U(A)(CP)^{-1}U(\tilde{A})^\dagger]$$
$$= \langle\!\langle U(A)|(CP)|U(\tilde{A})\rangle\!\rangle, \quad (98)$$

where *CP* is properly extended so that it acts on the doubled Hilbert space. In addition, analogously to (80), (97) leads to

$$\frac{Z(A_1,A_2)}{Z(\tilde{A}_1,\tilde{A}_2)} = e^{i[CS_3(A_1)-CS_3(A_2)]} \neq 1. \quad (99)$$

Here, we note the Chern-Simons term $CS_3(A)$ flips its sign under *CP*, $\int d^3x\,\varepsilon_{ijk}A_i(-\mathbf{r})\partial_j A_k(-\mathbf{r}) = -\int d^3x\,\varepsilon_{ijk}A_i(\mathbf{r})\partial_j A_k(\mathbf{r})$. (This is also the case for *CR*.) We note that (97) is consistent with the Schwinger-Keldysh trace for (4+1)d bulk topological Floquet unitaries (put on a closed spatial manifold) and their (3+1) boundary unitaries, which are given, in the long-wave length limit, as [46]

$$Z_{\mathrm{bulk}}(A_1,A_2) \sim \exp\left[\frac{i\theta}{8\pi^2}\int (dA_1dA_1 - dA_2dA_2)\right],$$
$$Z_{bdry}(A_1,A_2) \sim \exp\left[\frac{i}{8\pi}\int (A_1dA_1 - A_2dA_2)\right]. \quad (100)$$

While $Z_{\mathrm{bulk}}(A_1,A_2)/Z_{\mathrm{bulk}}(\tilde{A}_1,\tilde{A}_2) = 1$ for the (4+1) bulk systems, as inferred from the effective action (100), this naive relation is violated at the boundary, (99).

Directly confirming (97) along the line of Sec. VI B 1 is rather difficult, unfortunately. Alternatively, similar to what we did in Sec. VI B 2, we can use the operator-state map and compute the overlap $\langle\!\langle U(A)|(CP)|U(\tilde{A})\rangle\!\rangle$ in (98). In particular, we numerically check that

$$\langle\!\langle U(\Phi_{xy} = 2\pi, \gamma_z)|CP|U(\Phi_{xy} = 2\pi, \tilde{\gamma}_z)\rangle\!\rangle \sim e^{i\gamma_z} \quad (101)$$

holds for a lattice implementation of $|U\rangle\!\rangle$ (see Appendix B for more details). Here, $|U(\Phi_{xy} = 2\pi, \gamma_z)\rangle\!\rangle$ is the mapped state in the presence of the unit background magnetic flux piercing the xy plane $\Phi_{xy} = \oint F_{xy} = 2\pi$ and the Wilson loop $\gamma_z = \oint A_z$ along z direction. Note that $\tilde{\gamma}_z = -\gamma_z$ as a result of *CP* transformation. This background gauge field configuration gives rise to $CS_3(A) = \gamma_z$. In the limit $\gamma_z = \pi$, the quantity (101) is essentially the same as the $\mathbb{Z}_2$ many-body topological invariant for fermionic short-range entangled states protected by *CP* (or *CR*) symmetry in (3+1) dimensions [topological insulators with symmetry $\mathrm{U}(1) + CR$ with $(CR)^2 = 1$], introduced in Ref. [71].

D. Comments

Let us close this section with some comments.

First of all, while we focused here on the anomalous unitaries preserving U(1) in one and three spatial dimensions (with *C* and *CP* symmetries, respectively), we expect that the pattern continues to all higher odd spatial dimensions. The anomalous operator algebras in higher dimensions signifying a mixed anomaly between U(1) and a discrete symmetry involve higher-dimensional Chern-Simons terms, $\int AdA\cdots dA$. This is analogous to the "primary series" of topological insulators/superconductors in even (odd) spatial dimensions that are classified/characterized by an integral topological invariant and the response Chern-Simons terms (θ terms) [22,47]. For a given spatial dimension, they belong to one of the ten Altland-Zirnbauer symmetry classes.

There are also topological states that are outside of the primary series, and are classified by $\mathbb{Z}_2$ topological invariants—they are obtained from the topological states in the primary series by dimensional reduction (called "(first/second) descendants" in Ref. [47]). For anomalous unitaries, we also expect that there are similar "descendants." For example, let us consider unitaries in two spatial dimensions respecting U(1) and *CR* symmetries. Following Ref. [71], we can construct the $\mathbb{Z}_2$ topological invariant as

$$\frac{\langle\!\langle U(\Phi_{xy} = 2\pi)|CR|U(\Phi_{xy} = 2\pi)\rangle\!\rangle}{\langle\!\langle U(\Phi_{xy} = 0)|CR|U(\Phi_{xy} = 0)\rangle\!\rangle} = \pm 1. \quad (102)$$

Here, the background gauge field configuration is invariant under *CR*. An anomalous unitary for which this topological invariant is nontrivial should have an even number of Weyl points in its quasienergy spectrum.

There is a close connection between the effective Schwinger-Keldysh functional $Z(A_1,A_2) = \langle\!\langle U(A_1)|U(A_2)\rangle\!\rangle$ and the Berry phase $\oint\langle\!\langle U(A)|U(A+dA)\rangle\!\rangle$. The relations like (100) can be guessed from (or at least consistent with) the Berry phase of the short-range entangled state $|U(A)\rangle\!\rangle$. For a short-range entangled state $|U(A)\rangle\!\rangle$ in the presence of a spatial background gauge field A, it is known that that the Berry phase is related to the response effective action [71]. For example,

for $\mathcal{U}(\mathbf{k}) \sim e^{i\mathbf{k}\cdot\sigma}$, the Berry phase is related to the θ term in the effective response action,

$$\oint dA\, i\langle\langle U(A)|\frac{d}{dA}|U(A)\rangle\rangle = \frac{i\theta}{8\pi^2}\int dt d^3x\, \varepsilon^{\mu\nu\kappa\lambda}\partial_\mu A_\nu \partial_\kappa A_\lambda \tag{103}$$

with $\theta = \pi$. specializing to the configuration for which $\varepsilon_{ij}\partial_i A_j$ $(i, j = x, y)$ is time-independent, but changing A_z adiabatically in time, and further discretizing the (adiabatic) time, $\partial_t A_\mu \to A_{1\mu} - A_{2\mu}$, (103) suggests

$$\langle\langle U(A_1)|U(A_2)\rangle\rangle \sim 1 + \frac{i\theta}{4\pi^2}\int d^3x\,(A_{1z} - A_{2z})\varepsilon_{ij}\partial_i A_j \tag{104}$$

where $A_y = A_{1y} = A_{2y} = (A_{1y} + A_{2y})/2$. This is consistent with (100). To summarize, we can use the operator-state map and the Berry phase to "guess" the Schwinger-Keldysh response effective action $Z(A_1, A_2)$ when A_1 and A_2 are close enough.

VII. CONCLUSION

In this paper, we discuss the characterizations of anomalous unitary time-evolution operators, that may be realized on the boundary of bulk topological Floquet systems. Much the same way as the boundaries of static topological phases that can be characterized, detected, and classified by quantum anomalies, we identified quantum anomalies for boundary unitaries.

We close by listing a few open questions and interesting directions to explore. First, while we focused on quantum anomalies on boundary unitaries, it is interesting to ask if there is a corresponding bulk topological field theory. This problem was explored already in Ref. [46] for the case of background U(1) gauge field. For the case of time-reversal symmetric boundary unitaries, it is interesting to ask if one can write down a topological field theory for the KMS gauge field.

As mentioned in Sec. III B, anomalous boundary unitaries are characterized by their algebraic relations with symmetry generators. In the presence of U(1) symmetry, we considered gauged versions of the anomalous operator algebra in Sec. VI. Instead of gauging U(1) symmetry, it would be interesting to consider the Lieb-Schultz-Mattis type twist operator, which has been useful in various Lieb-Schultz-Mattis type theorems and can be understood in terms of quantum anomalies.

It is interesting to apply/extend the framework developed in this paper to other symmetries. For example, in Sec. VI, we discussed the mixed anomaly between U(1) and discrete symmetric, C and CP. It would be interesting to discuss mixed anomalies between U(1) and other discrete symmetries.

It is also interesting to study "exotic" symmetries, such as $OUO^{-1} = U^\dagger$ where O is a unitary operator. The symmetry is called "many-body spectral reflection symmetry" or "unitary time-reflection symmetry" [32,74,75]. By combining with time reversal, we can also consider $O'UO'^{-1} = U$, where O' is an antiunitary operator. In the doubled Hilbert space, when $U = OU^\dagger O^{-1}$, the composition of the modular conjugation J with O is an antiunitary symmetry, $OJ|U\rangle\rangle = O|U^\dagger\rangle\rangle \equiv |U\rangle\rangle$. JO can be gauged, by putting the system on an unoriented space-time, $\mathbb{R}P^2$. It would be interesting to see if the associated topological invariant (the partition function on $\mathbb{R}P^2$) is related to the corresponding matrix-product-operator index discussed in Ref. [32].

Finally, while our focus in this paper is on unitaries with symmetries, it is interesting to see if one can understand the chiral unitary index of 1d unitaries, in terms of quantum anomalies. A natural candidate is a gravitational anomaly.

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APPENDIX A: THE KMS CONDITION AT FINITE TEMPERATURE

1. Thermofield double states

To introduce the KMS condition at finite temperature, we first introduce the thermofield double (TFD) states used in the thermofield dynamics, where a thermal density operator is mapped to a state (thermofield double state) in the doubled Hilbert space. For our purpose of studying (boundary) unitary operators, there is generically no (local) Hamiltonian, and hence there is no simple finite temperature thermofield double state. Nevertheless, thermofield double states still serve as a useful example to introduce and discuss the KMS condition. In TFD states, states from the first and second Hilbert spaces are paired up by using energy eigenvalues:

$$|\rho_\epsilon\rangle\rangle = (1/\sqrt{Z})\sum_i e^{-\epsilon E_i}|E_i\rangle|E_i\rangle^*, \tag{A1}$$

where $|E_i\rangle$ is the eigen state of the Hamiltonian H with energy E_i, and $|E_i\rangle^*$ is the time-reversal partner of $|E_i\rangle$, satisfying $(KHK^{-1})|E_i\rangle^* = E_i|E_i\rangle^*$. They evolve in time according to $+i\frac{d}{dt}|E_i(t)\rangle = H|E_i(t)\rangle$ and $-i\frac{d}{dt}|E_i(t)\rangle^* = KHK^{-1}|E(t)\rangle^*$, respectively.

The TFD state $|\rho_\epsilon\rangle\rangle$ is a purification of the thermal density matrix $\rho_\epsilon = (1/Z)e^{-2\epsilon H}$ at inverse temperature 2ϵ. While $|\rho_\epsilon\rangle\rangle$ is not maximally entangled between the in and out Hilbert spaces for $\epsilon > 0$, it can be used as a reference state to invoke the operator-state map. In the context of quantum many-body physics and quantum field theory, the TFD state is a convenient reference state, which provides a finite (but small) regularization (cutoff) $\epsilon > 0$. For example, the state corresponding to the unitary evolution operator $U(t) = \exp(-itH)$ is given by $|U_\epsilon(t)\rangle\rangle = (U(t)\otimes I)|\rho_\epsilon\rangle\rangle$. Note that the state $|U_\epsilon(t)\rangle\rangle$ enjoys the shift property, $|U_\epsilon(t)\rangle\rangle = (U(t)\otimes I)|\rho_\epsilon\rangle\rangle = (I\otimes KU(t)^\dagger K^{-1})|\rho_\epsilon\rangle\rangle$.

In the context of TFD, the modular conjugation operator is conventionally called the tilde conjugation [50]. The

antiunitary modular conjugation operator J satisfies

$$J^2 = 1, \quad J|\rho_\epsilon\rangle\rangle = |\rho_\epsilon\rangle\rangle, \quad J\mathcal{A}_{\text{in}}J = \mathcal{A}_{\text{out}}, \tag{A2}$$

where $\mathcal{A}_{\text{in}}/\mathcal{A}_{\text{out}}$ is the operator algebra acting on $\mathcal{H}_{\text{in}}/\mathcal{H}_{\text{out}}$. Observing that $|U_\epsilon\rangle\rangle$ is stationary (invariant) under $U(t)\otimes KU(t)K^{-1}$, we can introduce the modular Hamiltonian by $\exp(-it\bar{H}) = U(t)\otimes KU(t)K^{-1}$,

$$\bar{H} = H\otimes I - I\otimes KHK^{-1} = H\otimes I - J(H\otimes I)J, \tag{A3}$$

which generates a time-translation in the doubled Hilbert space. The modular Hamiltonian satisfies

$$\bar{H}|\rho_\epsilon\rangle\rangle = 0, \quad J\bar{H}J = -\bar{H}, \quad \Delta^{-it}\mathcal{A}_{\text{in/out}}\Delta^{+it} = \mathcal{A}_{\text{in/out}}. \tag{A4}$$

where $\Delta = \exp(-\beta\bar{H})$ is the modular operator.

2. The KMS condition

Let us now review the KMS condition at finite temperature. It is the statement characterizing states (density matrices), and it reads

$$\langle AB(t)\rangle_\beta = \langle B(t-i\beta)A\rangle_\beta \tag{A5}$$

for any two operators A and B, where $B(t) := e^{itH}Be^{-itH}$, and $\langle\cdots\rangle_\beta := \text{Tr}\,(\cdots e^{-\beta H})/\text{Tr}\,(e^{-\beta H})$.[7] The KMS condition can be rephrased in the language of thermofield dynamics [50]; the KMS condition is nothing but the statement

$$J\Delta^{1/2}O|\rho_{\beta/2}\rangle\rangle = O^\dagger|\rho_{\beta/2}\rangle\rangle, \quad O\in\mathcal{A}_{\text{out}}. \tag{A6}$$

To see the connection, we start from the TFD representation of the correlator, $\langle AB(t)\rangle_\beta = \langle\langle\rho_{\beta/2}|AB(t)|\rho_{\beta/2}\rangle\rangle$ (where on the RHS we write $A\equiv A\otimes I$, $B(t)\equiv B(t)\otimes I$ by abusing notation). Using (A6),

$$\begin{aligned}\langle AB(t)\rangle_\beta &= (J\Delta^{1/2}A|\rho_{\beta/2}\rangle\rangle, J\Delta^{1/2}B^\dagger(t)|\rho_{\beta/2}\rangle\rangle)\\ &= (\Delta^{1/2}A|\rho_{\beta/2}\rangle\rangle, \Delta^{1/2}B^\dagger(t)|\rho_{\beta/2}\rangle\rangle)^*\\ &= \langle\langle\rho_{\beta/2}|B(t)\Delta^{1/2}\cdot\Delta^{1/2}A|\rho_{\beta/2}\rangle\rangle,\end{aligned} \tag{A7}$$

where we use $(*,*)$ to represent the inner product in the doubled Hilbert space, and noted that J is antiunitary. Since $|\rho_{\beta/2}\rangle\rangle = \Delta^{-1/2}|\rho_{\beta/2}\rangle\rangle$, we conclude the KMS condition:

$$\begin{aligned}\langle AB(t)\rangle_\beta &= \langle\langle\rho_{\beta/2}|\Delta^{-1/2}\Delta^{-1/2}B(t)\Delta A|\rho_{\beta/2}\rangle\rangle\\ &= \langle\langle\rho_{\beta/2}|\Delta^{-1}B(t)\Delta A|\rho_{\beta/2}\rangle\rangle\\ &= \langle B(t-i\beta)A\rangle_\beta.\end{aligned} \tag{A8}$$

The point is that the modular conjugation operator J effectively implements the cyclic property of the trace, without relying on the finite dimensionality of the Hilbert space. In the main text, what corresponds to (A6) is (9), $J|U\rangle\rangle = |U^\dagger\rangle\rangle$, where the temperature is infinity. At infinite temperature, the Schwinger-Keldysh trace satisfies $\text{Tr}\,[U^\dagger V] = \text{Tr}\,[VU^\dagger]$ for two unitary operators U and V, which is just the cyclicity of the trace. In the state language, this follows from the existence of modular conjugation operator. Following (A7) with $\beta = 0$,

$$\begin{aligned}\frac{1}{\mathcal{N}}\text{Tr}[U^\dagger V] &= (JU^\dagger|\Omega\rangle\rangle, JV^\dagger|\Omega\rangle\rangle)\\ &= (U^\dagger|\Omega\rangle\rangle, V^\dagger|\Omega\rangle\rangle)^*\\ &= (V^\dagger|\Omega\rangle\rangle, U^\dagger|\Omega\rangle\rangle) = \frac{1}{\mathcal{N}}\text{Tr}[VU^\dagger].\end{aligned} \tag{A9}$$

The KMS condition also follows from the shift property: we note that the inner product $\langle\langle U|V\rangle\rangle = \mathcal{N}^{-1}\sum_{i,j}(U|i\rangle\otimes K|i\rangle, V|j\rangle\otimes K|j\rangle) = \mathcal{N}^{-1}\text{Tr}\,[U^\dagger V]$ can be computed by first using the shift property of $|\Omega\rangle\rangle$:

$$\begin{aligned}\langle\langle U|V\rangle\rangle &= \frac{1}{\mathcal{N}}\sum_{i,j}(\langle i|)\otimes(\langle i|UK)(|j\rangle\otimes KV^\dagger|j\rangle)\\ &= \frac{1}{\mathcal{N}}\sum_i(KU^\dagger|i\rangle, KV^\dagger|i\rangle)\\ &= \frac{1}{\mathcal{N}}\sum_i(V^\dagger|i\rangle, U^\dagger|i\rangle) = \frac{1}{\mathcal{N}}\text{Tr}[VU^\dagger].\end{aligned} \tag{A10}$$

Thus the shift property implies/is consistent with the cyclicity of the trace: $\text{Tr}\,[U^\dagger V] = \text{Tr}\,[VU^\dagger]$.

APPENDIX B: NUMERICAL VERIFICATION OF MANY-BODY TOPOLOGICAL INVARIANT IN EQ. (101)

In this Appendix, we consider a lattice Hamiltonian in the doubled Hilbert space and numerically show that the relation (101) holds.

Recall that the shift operator as a boundary unitary of (2 + 1)d Floquet topological is given by Eq. (76). The corresponding transformation in momentum space is then $U\psi_k U^{-1} = e^{ik}\psi_k$, where $\psi_k = \sum_x \psi_x e^{-ikx}$. Thus the (3 + 1)d generalization of this boundary unitary becomes

$$U\psi_{\mathbf{k}}U^{-1} = e^{i\mathbf{k}\cdot\boldsymbol{\sigma}}\psi_{\mathbf{k}}, \tag{B1}$$

where $\psi_{\mathbf{k}}$ is a two-component fermionic field. Our system is furnished with a CR symmetry which acts as

$$(CR)\psi(\mathbf{r})(CR)^{-1} = \psi^\dagger(R\mathbf{r}), \tag{B2}$$

where $R\mathbf{r} = (x, -y, z)$ involves a reflection with respect to xz plane. The corresponding transformation in momentum space reads as

$$(CR)\psi_{\mathbf{k}}(CR)^{-1} = \psi^\dagger_{-R\mathbf{k}}. \tag{B3}$$

where $-R\mathbf{k} = (-k_x, k_y, -k_z)$. It is easy to check that the unitary (B1) is invariant under CR.

To construct the mapped state $|U\rangle\rangle$ we use the reference state (90) which is the ground state of the Hamiltonian (89). Hence, the state $|U\rangle\rangle$ can be obtained as the ground state of the following Hamiltonian:

$$\mathbb{H} = -\sum_{\mathbf{k}}\Psi^\dagger_{\mathbf{k}}\begin{pmatrix}0 & e^{-i\mathbf{k}\cdot\boldsymbol{\sigma}}\\ e^{i\mathbf{k}\cdot\boldsymbol{\sigma}} & 0\end{pmatrix}\Psi_{\mathbf{k}}, \tag{B4}$$

[7] For a finite-dimensional Hilbert space, the KMS condition follows simply from the cyclic property of the trace, $\text{Tr}(e^{-\beta H}Ae^{itH}Be^{-itH}) = \text{Tr}(e^{-\beta H}e^{i(t-i\beta)H}Be^{-i(t-i\beta)H}A)$. However, the KMS condition holds beyond the finite Hilbert space setting. Note that the expression using the trace is meaningful only when operators such as the density matrix $e^{-\beta H}$ belong to the trace class.

where $\Psi^\dagger_{\mathbf{k}} = (\psi^\dagger_{o,\mathbf{k}}, \psi^\dagger_{i,\mathbf{k}})$. The proper CR transformations in the doubled Hilbert space are given by

$$\begin{aligned}(CR)\psi_{i,\mathbf{k}}(CR)^{-1} &= \psi^\dagger_{i,-R\mathbf{k}},\\ (CR)\psi_{o,\mathbf{k}}(CR)^{-1} &= -\psi^\dagger_{o,-R\mathbf{k}},\\ (CR)|0\rangle\rangle &= |full\rangle\rangle. \end{aligned} \tag{B5}$$

In order to calculate the quantity (101), we need to find the ground state in the presence of magnetic field in xy plane and twisted boundary condition in z direction. This requires a real-space implementation of the Hamiltonian. It is more convenient to consider the following Hamiltonian on a cubic lattice

$$\begin{aligned}\mathbb{H}_{\text{latt}} = \frac{1}{2}\sum_{\substack{\mathbf{r}\\ s=1,2,3}} [\Psi^\dagger(\mathbf{r}+\hat{x}_s)(it\alpha_s - r\beta)\Psi(\mathbf{r}) + \text{H.c.}]\\ + m\sum_{\mathbf{r}} \Psi^\dagger(\mathbf{r})\beta\Psi(\mathbf{r}),\end{aligned} \tag{B6}$$

which shares the same low-energy Hamiltonian as that of Eq. (B4). Here, the Dirac matrices are given by

$$\alpha_s = \tau_y \otimes \sigma_s = \begin{pmatrix} 0 & -i\sigma_s \\ i\sigma_s & 0 \end{pmatrix}, \tag{B7}$$

$$\beta = \tau_x \otimes I = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \tag{B8}$$

where τ acts on in/out degrees of freedom and σ acts on the inner degrees of freedom.

For simplicity, we set $t = r = 1$. Furthermore, the lattice Hamiltonian is also invariant under CR symmetry defined in Eq. (B5). We should note that the ground state of the lattice Hamiltonian with a mass term in the range $1 < |m| < 3$ is topologically equivalent to the mapped unitary $|U\rangle\rangle$.

To compute the ground state $|GS(\Phi_{xy} = 2\pi, \gamma_z)\rangle\rangle$, we modify the hopping terms in the lattice Hamiltonian (B6), which we call $\mathbb{H}_{\text{latt}}(\Phi_{xy} = 2\pi, \gamma_z)$, as follows. A simple way to prepare a 2π magnetic flux with uniform magnetic field is to set

$$\begin{aligned}A_x(x,y) &= -\frac{2\pi y}{L_x L_y},\\ A_y(x,y) &= \begin{cases} 0 & (y = 1,\ldots,L_y - 1)\\ \frac{2\pi x}{L_x} & (y = L_y)\end{cases},\end{aligned} \tag{B9}$$

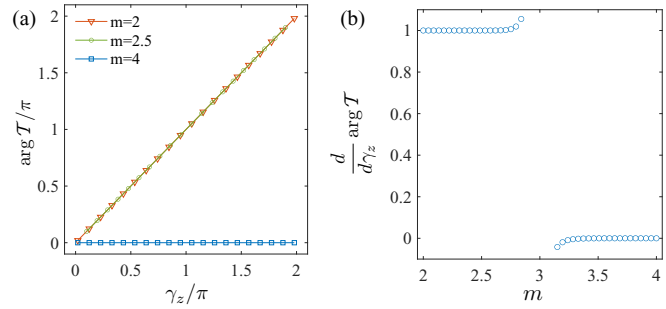

FIG. 1. Manybody topological invariant for CR-symmetric $(3+1)$d boundary unitary (Sec. VI C). The invariant was computed via (B11) for the ground state of the lattice Hamiltonian (B6) in the doubled Hilbert space. The topological phase of the lattice Hamiltonian (i.e., when $2 < m < 3$) is topologically equivalent to $|U\rangle\rangle$.

where L_x, L_y are the number of sites. This gauge configuration leads to a uniform magnetic flux $F(x,y) = A_x(x,y) + A_y(x+1,y) - A_x(x,y+1) - A_y(x,y) = 2\pi/(L_x L_y)$ inserted per unit cell. The twisted boundary condition in z direction is implemented as usual via multiplying the hopping amplitudes by a phase factor. It is important to note that the quantity (101) is well-defined since under CR symmetry we have

$$(CR)\,\mathbb{H}_{\text{latt}}(\Phi_{xy}, \gamma_z)(CR)^{-1} = \mathbb{H}_{\text{latt}}(\Phi_{xy}, -\gamma_z). \tag{B10}$$

Figure 1(a) shows how the argument of the following quantity

$$\mathcal{T}(\gamma_z) = \langle GS(\Phi_{xy} = 2\pi, \gamma_z)|CR|GS(\Phi_{xy} = 2\pi, -\gamma_z)\rangle, \tag{B11}$$

varies as a function of γ_z. We plotted two values for the mass term in the topological phase and one in the trivial phase. It is evident that in the former case $\arg\mathcal{T} = \gamma_z$ while in the latter $\arg\mathcal{T} = 0$. We further check that the linear behavior $\arg\mathcal{T} = \gamma_z$ is valid within the topological phase (away from the transition point $m = 3$ where finite-size effects dominate) in Fig. 1(b). Given the topological equivalence between the topological phase of $\mathbb{H}_{\text{latt}}$ and the ground state of $\mathbb{H}$, we deduce Eq. (101).

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