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Phys. Rev. B **95**, 235130 — Published 16 June 2017

DOI: 10.1103/PhysRevB.95.235130

Modular Anomalies in $(2+1)$ and $(3+1)$-D Edge Theories

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(Dated: May 22, 2017)

The classification of topological phases of matter in the presence of interactions is an area of intense interest. One possible means of classification is via studying the partition function under modular transforms, as the presence of an anomalous phase arising in the edge theory of a D-dimensional system under modular transformation, or modular anomaly, signals the presence of a $(D+1)$-D non-trivial bulk. In this work, we discuss the modular transformations of conformal field theories along a $(2+1)$-D and a $(3+1)$-D edge. Using both analytical and numerical methods, we show that chiral complex free fermions in $(2+1)$-D and $(3+1)$-D are modular invariant. However, we show in $(3+1)$-D that when the edge theory is coupled to a background $U(1)$ gauge field this results in the presence of a modular anomaly that is the manifestation of a quantum Hall effect in a $(4+1)$-D bulk. Using the modular anomaly, we find that the edge theory of $(4+1)$-D insulator with spacetime inversion symmetry$(P*T)$ and fermion number parity symmetry for each spin becomes modular invariant when 8 copies of the edges exist.

INTRODUCTION

The quantum Hall effect[1] has been an intense area of research in condensed matter physics for several decades. The presence of a chiral metallic edge mode that is robust to disorder and interactions at the boundary of 2D bulk Fermi liquid in strong magnetic field is a key feature of the quantum Hall effect. The existence of such an edge and the corresponding nontrivial topology of the bulk can be detected by computing a bulk topological number[2–16]. Yet, in a more general sense, the robust gapless edge states within the quantum Hall effect are well-known to result in a U(1) chiral anomaly[17–21]. The presence of anomalies in an edge theory and the resultant charge pumping imply the edge lives on the boundary of a higher dimensional manifold. In principle, the concept of quantum anomalies may be extended to characterize topological phases in the presence of interactions as the coefficients of the anomalies, which are quantized, are known to be stable against interactions[22].

Recent studies[23–27] have proposed that an analysis of the anomalies in gapless $(1+1)$-D theories can also indicate the presence of a topological phase in $(2+1)$-D dimensions. This is based on the fact that if the edge theory has non-trivial response to certain transformations, which in $(1+1)$-D are chosen to be modular transformations, then the edge theory cannot be consistent on the $(1+1)$-D manifold and manifests itself as the edge of a $(2+1)$-D system. This method is known to give the correct results for chiral edge states in $(1+1)$-D, as well as for some more complex gapless edges involving spatial mirror symmetries[28]. A necessary step is to extend this method beyond $(1+1)$-D to higher space dimension. In this letter, we extend concept of modular transformations of gapless free fermion theories beyond $(1+1)$-D to examine higher dimensional edge theories. We show that the complex free fermions in both $(2+1)$-D Dirac and $(3+1)$-D chiral edge theories are modularly invariant. However, when an external magnetic field is coupled to the edge, the resultant Weyl modes show that a modular anomaly arises in the $(3+1)$-D edge theory indicating the presence of $(4+1)$-D quantum Hall effect. We further show using modular transformations that the edge theory of $(4+1)$-D insulators with the spacetime inversion symmetry$(P*T)$ and the fermion number parity symmetry for each spin becomes modular invariant when 8 copies of the edges exist.

MODULAR TRANSFORMATION IN $(1+1)$-D

To begin, consider a relativistic conformal field theory (CFT) defined in a $(1+1)$-D compact space manifold $T^1 \times T^1$ where T^1 is a torus (a circle in 1D). On such a space, the theory can exhibit invariance at a classical level under modular transformations[29]. However, interesting cases arise when theories are not invariant under modular transformations resulting in the accumulation of an additional anomalous phase. The resultant anomaly is referred to as a large gravitational anomaly in the sense that it cannot be generated via continuous deformation of the original action[23,30]. The modular group is defined as the group of linear fractional transformations of the upper half of the complex plane in which $\tau = L_0/L_1$ where L_0 and L_1 are the periods of the space and time coordinates respectively. τ transforms under the modular transformation:

$$\tau' = \frac{a\tau + b}{c\tau + d}, \tag{1}$$

where a, b, c, d are integers satisfying $ad - bc = 1$. The modular group is isomorphic to the projective special linear group $PSL(\mathbb{Z}, 2)$[29]. In $(1+1)$-D, the generators of the group are $S : \tau \to -1/\tau$ and $T : \tau \to \tau + 1$. S and T act on the periods of each coordinate by $S : (L_0, L_1) \to (-L_1, L_0)$ and $T : (L_0, L_1) \to (L_0 + L_1, L_1)$. To generalize modular transformation to higher dimensions, we consider the group generated by two generators, which they act on the periods of each coordinate as, $S : (L_0, L_1, L_2) \to (L_1, L_2, L_0)$, $T : (L_0, L_1, L_2) \to (L_0 + L_1, L_1, L_2)$ in $(2+1)$-D, and $S : (L_0, L_1, L_2, L_3) \to (-L_1, L_2, L_3, L_0)$ and $T : (L_0, L_1, L_2, L_3) \to (L_0 + L_1, L_1, L_2, L_3)$ in $(3+1)$-D. In this case, the generalized modular transformation is then isomorphic to $PSL(\mathbb{Z}, d)$ (See Appendix A in supplementary for the precise description of the modular transformation[31]). Under the S and T transformation, we can define the transformation matrices, A, for example, in $(3+1)$-D as

$$A_S = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, A_T = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \qquad (2)$$

With these definitions, we consider the action of the modular group on the partition function in $(1+1)$-D[32], which is well-known to possess an anomaly. The most direct method to see the anomaly under the modular transformation is to calculate the partition function explicitly and apply the transformation. The partition function of $(1+1)$-D edge can be obtained in a well-regularized form as (For detailed calculation, see Appendix B in supplementary[31])

$$\begin{aligned} Z_{\lambda_0\lambda_1} &= [e^{2\pi i(1/2-\lambda_0)(1/2-\lambda_1)} q^{(\lambda_1^2-\lambda_1+1/6)/2}] \\ &\times [(1-\omega) \prod_{n_1=1}^{\infty} (1-\omega q^{n_1})(1-\omega^{-1} q^{n_1})] \qquad (3) \end{aligned}$$

where $\omega = q^{\lambda_1} e^{2\pi i \lambda_0}$, $q = e^{2\pi i \tau}$. $\lambda_0, \lambda_1 = 0(1/2)$ refers to the periodic (anti-periodic) boundary condition of the time and space coordinate directions respectively. By explicitly applying the modular transform, one derives the modular anomaly[24],

$$\begin{aligned} T[Z(\tau)_{\lambda_0\lambda_1}] &= e^{i\pi(\lambda_1^2-\lambda_1+1/6)} Z(\tau)_{\lambda_0'\lambda_1'} \qquad (4) \\ S[Z(\tau)_{\lambda_0\lambda_1}] &= e^{i2\pi(\lambda_1-1/2)(\lambda_0-1/2))} Z(\tau)_{\lambda_0'\lambda_1'} \end{aligned}$$

λ' is the transformed boundary conditions under the modular transformation where $\lambda'_\mu = A_{\mu\nu}\lambda_\nu$. The sign of anomalous phase flips if the chirality of the $(1+1)$-D mode is reversed. Therefore, the combination of two edges of opposite chirality achieves modular invariance[26]. This result is consistent with the fact that two opposite chiral edges can be gapped out by adding mass term. However, it is also possible to achieve modular invariance with finite copies of the same chirality[23].

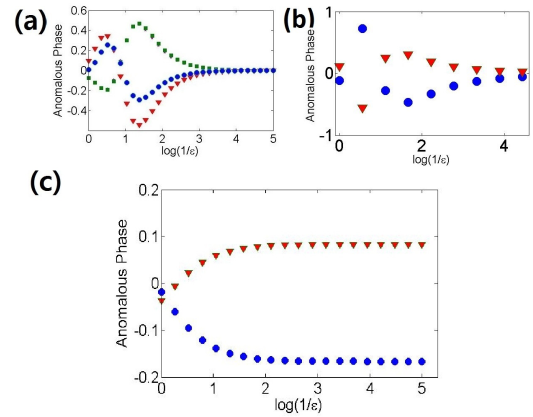

FIG. 1. Calculation of numerical regularization scheme for: (a) T transformation of (2+1)-D chiral edge. (b)(3+1)-D (c)(3+1)-D with magnetic field. Each lines represent different values of boundary condition. In (a), blue circles, red triangles and green squares represent $(\lambda_1, \lambda_2) = (0, 0), (0.5, 0), (0.5, 0.5)$ respectively. In (b), blue circles and red triangles represent $(\lambda_1, \lambda_2, \lambda_3) = (0, 0, 0), (0.5, 0, 0)$. In (c), blue circles and red triangles represent $(\lambda_1, \lambda_2, \lambda_3) = (0.5, 0, 0), (0, 0, 0)$. We include sufficient numbers of high energy states within each calculation of the energy cutoff until the anomalous phase value converges. In (a) and (b) all choices of boundary conditions converge to zero indicating modular invariance. When the magnetic field is inserted, the anomaly approaches to the value(1/6,-1/12) in accordance with Eq. (42) with $N_\phi = 1$. Details of the numerical calculation method are provided in Appendix D).

METHOD

Now we wish to elucidate higher dimensional gapless edges, thus we examine $(2+1)$-D and $(3+1)$-D edge theories where the action is given by

$$\mathcal{S} = \int d^d x \bar{\psi}(\partial_\tau + \sigma \cdot k)\psi \qquad (5)$$

In contrast to $(1+1)$-D, we cannot simply perform the transformation of the partition function since an expression of the well-regularized partition function is not available. We can understand the failure of the regularization more clearly by applying the zeta function regularization method[33,34] to higher dimensional edge theories. In given edge theory, the expression of the unregularized partition function contains a summation of the energy eigenvalues over all states. In $(2+1)$-D, we have $\sum_{k_x,k_y} \sqrt{k_x^2 + k_y^2}$ and in $(3+1)$-D, $\sum_{k_x,k_y,k_z} \sqrt{k_x^2 + k_y^2 + k_z^2}$. When the sum is divergent, a successful zeta function regularization should utilize analytic continuation to assign a finite value to the divergent sum. Unfortunately, this is difficult since the Epstein-Hurwitz zeta (EZ) functions in $(3+1)$-D, $\zeta(\epsilon) = \sum_{n_1,n_2,n_3} ({n_1}^2 + {n_2}^2 + {n_3}^2)^{-\epsilon}$, and $(2+1)$-D, $\sum_{n_1,n_2} ({n_1}^2 + {n_2}^2)^{-\epsilon}$, are meromorphic at $\epsilon = -1/2$[35], which forbids assigning a finite value to the summation of energy eigenvalues. To circumvent this issue, we instead focus on the change of path integral measure[36,37]. The calculation of the change of the measure only requires EZ function at $\epsilon = 0$ and $\epsilon = -1$, which have well defined finite values (See Appendix C in supplementary[31]).

To calculate the change of measure, we work on the Fourier transformed field basis:

$$\psi_{\boldsymbol{\lambda}}(\mathbf{x},\mathbf{s}) = \sum_{\mathbf{n},\mathbf{s}} a_{\mathbf{n},s}\Phi_{\mathbf{n}+\boldsymbol{\lambda}}(\mathbf{x})\chi_{\mathbf{s}} \tag{6}$$

$\mathbf{n} = (n_0, n_1, n_2, n_3)$ are integers, which n_i refers the frequency of i-th direction in the Fourier transformed basis. $\boldsymbol{\lambda} = (\lambda_0, \lambda_1, \lambda_2, \lambda_3)$ are the boundary conditions, which $\lambda_i = 0(1/2)$ refers to the periodic (anti-periodic) boundary condition. We simplify the notations by defining $\widetilde{\mathbf{n}} = \mathbf{n} + \boldsymbol{\lambda}$. In other words,

$$\Phi_{(\widetilde{n}_0,\widetilde{n}_1,\widetilde{n}_2,\widetilde{n}_3)}(x) = e^{2\pi i(\sum_{i=0}^{4}(n_i+\lambda_i)x_i)} \tag{7}$$

and $\chi_{\mathbf{s}}(\mathbf{s} = \pm)$ is a two component spinor such that $\chi_+ = (1,0)^T, \chi_- = (0,1)^T$. By following the transformation rule in appendix A, we represent the change of coefficient a' under modular transformation as,

$$a'_{\mathbf{n}',\mathbf{s}'} = \int d^d x \Phi^\dagger_{\mathbf{n}'+\boldsymbol{\lambda}'}\chi^\dagger_{\mathbf{s}}\psi_{\boldsymbol{\lambda}}(A^T x) \tag{8}$$
$$= \sum_{\mathbf{n},\mathbf{s}}[\int d^d x \Phi^\dagger_{\mathbf{n}'+\boldsymbol{\lambda}'}(\mathbf{x})\Phi_{\mathbf{n}+\boldsymbol{\lambda}}(A^T\mathbf{x})][\chi^\dagger_{\mathbf{s}'}\chi_{\mathbf{s}}]a_{\mathbf{n},\mathbf{s}},$$

where A is the matrix representations of the generators. The above equation leads us to define the transformation matrix C between $a_{\mathbf{n},\mathbf{s}}$ and $a'_{\mathbf{n},\mathbf{s}}$.

$$C_{\mathbf{n}',\mathbf{n},\mathbf{s}',\mathbf{s}} = \int d^d x \Phi^\dagger_{\mathbf{n}'+\boldsymbol{\lambda}'}(\mathbf{x})\Phi_{\mathbf{n}+\boldsymbol{\lambda}}(A^T\mathbf{x})[\chi^\dagger_{\mathbf{s}'}\chi_{\mathbf{s}}] \tag{9}$$

In terms of Fourier transformed field basis, the change of path integral measure is given by,

$$D\bar{\psi}'D\psi' = D\bar{a}'Da' = D\bar{a}Da\ det(C)^{-2} \tag{10}$$

We treat ψ and $\bar{\psi}$ independently, hence we obtain an additional contribution of -2 sign from the Grassman algebra. In $(3+1)$-D, each momentum mode Φ transforms under modular transformation by (Appendix A),

$$T[\Phi_{\widetilde{n}_0,\widetilde{n}_1,\widetilde{n}_2,\widetilde{n}_3}] = \Phi_{\widetilde{n}_0+\widetilde{n}_1,\widetilde{n}_1,\widetilde{n}_2,\widetilde{n}_3}, \tag{11}$$
$$S[\Phi_{\widetilde{n}_0,\widetilde{n}_1,\widetilde{n}_2,\widetilde{n}_3}] = \Phi_{-\widetilde{n}_1,\widetilde{n}_2,\widetilde{n}_3,\widetilde{n}_0}.$$

To calculate $Det(C)$, we select a basis that diagonalizes C. We define the basis as linear combinations of modes under successive applications of T and S as,

$$|\theta,\overrightarrow{n}\rangle_{\boldsymbol{\lambda}}\eta_{s,\overrightarrow{\widetilde{n}}} = \Phi_{\boldsymbol{\lambda}}\sum_{n_0=0}^{n_1-1}\sum_{j=-\infty}^{\infty} e^{2\pi i(\widetilde{n}_0+n_1 j)\theta}T^j[\Phi_{n_0,\overrightarrow{n}}]\eta_{s,\overrightarrow{\widetilde{n}}} \tag{12}$$
$$|\phi,\mathbf{n}\rangle_{\boldsymbol{\lambda}}\chi_s = \Phi_{\boldsymbol{\lambda}-1/2}\sum_{j=0}^{N-1} e^{2\pi i j\phi/N}S^j[\Phi_{\mathbf{n}+1/2}]\chi_s,$$

where $\overrightarrow{n}$ is the vector of the frequencies in spatial directions. N is the order of S such that Φ_{n_0,n_1,n_2,n_3} returns to the original mode under N application of S. In $(1+1),(2+1),(3+1)$-D, $N = 4,3,8$ respectively, except for modes Φ_{n_0,n_0,n_0} in $(2+1)$-D. $\theta \in [0,1)$ and $\phi \in \{-(\frac{N}{2}-1), -\frac{N-2}{2}, .., \frac{N}{2}\}$(In $(2+1)$-D,$\phi \in \{-1,0,1\}$). To avoid double counting of the basis for S, we restrict the momentum indices to $n_0, n_1 \geq 0$ in $(1+1)$-D, $n_0 \geq n_1 \geq n_2$ in $(2+1)$-D, and $n_0, n_1, n_2 \geq 0$ in $(3+1)$-D. η is the spinor which diagonalizes the Hamiltonian simultaneously. Then the basis satisfies

$$T|\theta,\overrightarrow{n}\rangle_{\boldsymbol{\lambda}} = e^{-2\pi i\widetilde{n}_1\theta}|\theta,\overrightarrow{n}\rangle_{T[\boldsymbol{\lambda}]} \tag{13}$$
$$S|\phi,\mathbf{n}\rangle_{\boldsymbol{\lambda}} = e^{-2\pi i\phi/N}|\phi,\mathbf{n}\rangle_{S[\boldsymbol{\lambda}]}$$

In $(2+1)$-D, the C matrix, using the new basis for T and S, is a diagonal matrix given by

$$C^{2D}_{T,\{\theta,n_1,n_2,\theta',n_1',n_2'\}} = (e^{-2\pi i\widetilde{n}_1\theta})\delta(\theta-\theta')\delta_{\overrightarrow{n},\overrightarrow{n}'} \tag{14}$$
$$C^{2D}_{S,\{\phi,n_0,n_1,n_2,\phi',n_0',n_1',n_2'\}} = (e^{-2\pi i\phi/N})\delta_{\phi,\phi'}\delta_{\mathbf{n},\mathbf{n}'}.$$

To regulate the determinant of C, we use the Epstein-Hurwitz type zeta function regulator that has the same form as energy dispersion, $|p|^{-\epsilon}$, where ϵ, in this instance, is a scale which cuts off the high energy states.

In a similar manner with $(2+1)$-D, the modular transformations, S and T, of the transformation matrix, C, in $(3+1)$-D are given by(See Appendix C in supplementary[31]),

$$C^{3D}_{T,\{\theta,n_1,n_2,n_3,\theta',n_1',n_2',n_3'\}} = (e^{-2\pi i\widetilde{n}_1\theta})\delta(\theta-\theta')\delta_{\overrightarrow{n},\overrightarrow{n}'}. \tag{15}$$
$$C^{3D}_{S,\{\phi,n_0,n_1,n_2,n_3,\phi',n_0',n_1',n_2',n_3'\}} = (e^{-2\pi i\phi/N})\delta_{\phi,\phi'}\delta_{\mathbf{n},\mathbf{n}'}.$$

By regulating the determinants above matrices with zeta function regularization method, we can derive the expression of the anomaly.

T TRANSFORMATION

In this section, we show that the anomalous phases under T transformation cancel out in both $(2+1)$-D and $(3+1)$-D. We begin by reproducing the modular anomaly of $(1+1)$-D chiral edge. The basis which diagonalizes the transformation matrix, C, under the T transformation is given according to Eq. (12).

$$|\theta,n_1\rangle_{\lambda_0,\lambda_1} = \Phi_{\lambda_0,\lambda_1}\sum_{n_0=0}^{n_1-1}\sum_{j=-\infty}^{\infty} e^{2\pi i(\widetilde{n}_0+n_1 j)\theta}T^j[\Phi_{n_0,n_1}], \tag{16}$$

where $\theta \in [0,1)$. Application of the T transformation to $|\theta, n_1\rangle_{\lambda_0,\lambda_1}$ is given as,

$$\begin{aligned} &T|\theta, n_1\rangle_{\lambda_0,\lambda_1} \qquad (17)\\ &= T[\Phi_{\lambda_0,\lambda_1}\sum_{n_0=0}^{n_1-1}\sum_{j=-\infty}^{\infty} e^{2\pi i(\widetilde{n}_0+n_1 j)\theta}T^j[\Phi_{n_0,n_1}]]\\ &= \sum_{n_0=0}^{n_1-1}\sum_{j=-\infty}^{\infty} e^{2\pi i(\widetilde{n}_0+n_1 j)\theta}\Phi_{(n_0+n_1)+jn_1+(\lambda_0+\lambda_1),n_1+\lambda_1}\\ &= e^{-2\pi i(n_1+\lambda_1)\theta}|\theta, n_1\rangle_{\lambda_0+\lambda_1,\lambda_1}. \end{aligned}$$

As a result, the newly selected basis diagonalizes C_T^{1D} matrix resulting in Eq. (12), namely

$$C^{1D}_{T,\{\theta,n_1,\theta',n_1'\}} = (e^{-2\pi i(n_1+\lambda)\theta})\delta(\theta-\theta')\delta_{n_1,n_1'}. \quad (18)$$

After the diagonalization of C_T^{1D} matrix, the determinant is given as the product of the diagonal entries. We divide the partition function of the path integral form into the anomalous divergent contribution, Z_A, and the regular contribution, Z_R, with the total partition function, $Z_{total} = Z_A Z_R$. In the calculation of the total partition function, we note that the anomalous contribution, Z_A, is the path integral of the negative dispersion modes only. The regular contribution to the total partition function, Z_R is invariant under the T transformation, $Z_{R,\lambda}(\tau+1) = \prod_{n_1=0}^{\infty}(1-e^{(2i\pi\tau(n_1+\lambda_1)+2i\pi(\lambda_0+\lambda_1))}) = Z_{R,\lambda'}$ indicating that the contribution to the modular anomaly under the T transformation comes entirely from Z_A. In other words, the regularized form of the total partition function transforms under the T transformation as

$$\begin{aligned} Z_{total,\lambda}(\tau+1) &= [Z_{A,\lambda}(\tau+1)][Z_{R,\lambda}(\tau+1)] \qquad (19)\\ &= [C_T^{1D^{-2}} Z_{A,\lambda'}(\tau)][Z_{R,\lambda'}(\tau)]. \end{aligned}$$

Therefore, we regularize the change of the measure of Z_A, which restricts the C matrix to the negative momentums. Then, the anomalous phase of C_T^{1D} is given by

$$\begin{aligned} arg(det(C_T^{1D})) &= -2\pi[\int_0^1 d\theta\theta][\sum_{n_1=-\infty}^{-1}(n_1+\lambda)] \qquad (20)\\ &= -\pi\frac{1}{2}(\lambda^2-\lambda+1/6). \end{aligned}$$

The above anomalous phase reproduces the known modular anomaly in $(1+1)$-D under the T transformation.

To extend the calculation beyond $(1+1)$-D, we use the matrices given by Eq. (14) and Eq. (15) to extend to $(2+1)$-D and $(3+1)$-D respectively. With the addition of the requisite extra dimensional momentum indices, we can write the phases of $det(C)$ in the same form as of Eq. (20) for both $(2+1)$-D and $(3+1)$-D cases as,

$$\begin{aligned} &arg(det(C_T^{2D})) = -2\pi\sum_{n_1,n_2\in\mathbb{Z}}\int_0^1 d\theta\theta(n_1+\lambda_1) \qquad (21)\\ &= -\pi\sum_{n_1,n_2\in\mathbb{Z}}(n_1+\lambda_1) = -\sum_{n_1,n_2=-\infty}^{\infty}\frac{L_x^2}{8\pi}\frac{\partial}{\partial\lambda_1}(F_2)^2. \end{aligned}$$

and

$$\begin{aligned} &arg(det(C_T^{3D})) = -2\pi\sum_{n_1,n_2,n_3\in\mathbb{Z}}\int_0^1 d\theta\theta(n_1+\lambda_1) \qquad (22)\\ &= -\pi\sum_{n_1,n_2,n_3\in\mathbb{Z}}(n_1+\lambda_1) = -\sum_{n_1,n_2,n_3=-\infty}^{\infty}\frac{L_x^2}{8\pi}\frac{\partial}{\partial\lambda_1}(F_3)^2, \end{aligned}$$

where $F_2 = 2\pi\sqrt{\widetilde{n_1}^2/L_x^2+\widetilde{n_2}^2/L_y^2}$ is the dispersion in $(2+1)$-D and $F_3 = 2\pi\sqrt{\widetilde{n_1}^2/L_x^2+\widetilde{n_2}^2/L_y^2+\widetilde{n_3}^2/L_z^2}$ is the dispersion in $(3+1)$-D. In order to evaluate the above summations, we must define the following Epstein-Zeta functions in which we use the variable ϵ to denote the scale that cuts off the high energy states:

$$\begin{aligned} &E_2(\epsilon, c_1, c_2, a_1, a_2) \qquad (23)\\ &\equiv \sum_{n_1,n_2=0}^{\infty}(a_1(n_1+c_1)^2+a_2(n_2+c_2)^2)^{-\epsilon}, \end{aligned}$$

$$\begin{aligned} &G_2(\epsilon, c_1, c_2, a_1, a_2) \qquad (24)\\ &\equiv \sum_{n_1,n_2=-\infty}^{\infty}(a_1(n_1+c_1)^2+a_2(n_2+c_2)^2)^{-\epsilon}, \end{aligned}$$

$$\begin{aligned} &E_3(\epsilon, c_1, c_2, c_3, a_1, a_2, a_3) \equiv \qquad (25)\\ &\sum_{n_1,n_2,n_3=0}^{\infty}(a_1(n_1+c_1)^2+a_2(n_2+c_2)^2+a_3(n_3+c_3)^2)^{-\epsilon}, \end{aligned}$$

$$\begin{aligned} &G_3(\epsilon, c_1, c_2, c_3, a_1, a_2, a_3) \equiv \qquad (26)\\ &\sum_{n_1,n_2,n_3=-\infty}^{\infty}(a_1(n_1+c_1)^2+a_2(n_2+c_2)^2+a_3(n_3+c_3)^2)^{-\epsilon}, \end{aligned}$$

$$\begin{aligned} &G_3(\epsilon, c_1, c_2, c_3, a_1, a_2, a_3) \equiv \qquad (27)\\ &\sum_{n_1,n_2=0,n_3=-\infty}^{\infty}(a_1(n_1+c_1)^2+a_2(n_2+c_2)^2+a_3(n_3+c_3)^2)^{-\epsilon}. \end{aligned}$$

We substitute previous summations over the dispersion relations, F, into the newly defined Zeta function expressions to obtain the anomalous phase resulting from the application of the T-transform in higher dimensions as

$$\begin{aligned} &arg(det(C_T^{2D})) \qquad (28)\\ &= -\frac{\pi}{2}L_x^2\frac{\partial}{\partial\lambda_1}G_2(-1,\lambda_1,\lambda_2,1/L_x^2,1/L_y^2) \end{aligned}$$

in $(2+1)$-D and

$$arg(det(C_T^{3D})) \quad (29)$$
$$= -\frac{\pi}{2} L_x^2 \frac{\partial}{\partial \lambda_1} G_3(-1, \lambda_1, \lambda_2, \lambda_3, 1/L_x^2, 1/L_y^2, 1/L_z^2)$$

in $(3+1)$-D. The expression of the above zeta function, G_3, is well-defined and vanishes at $\epsilon = -1$. We find that the resulting anomalous phases are zero which indicates the absence of the anomaly under the T transformation(For calculation of the value of the zeta function, see Appendix C in supplementary[31]).

S TRANSFORMATION

After establishing the the absence of the anomaly under the T transformation, we now prove the absence of the modular anomaly in $(2+1)$-D and $(3+1)$-D under the S transformation. We again start from the modular anomaly of a $(1+1)$-D edge. According to Eq. (12), the basis that diagonalizes the C matrix is given by

$$|\phi, n_0, n_1\rangle_{\lambda_0,\lambda_1} \quad (30)$$
$$= \Phi_{\lambda_0-1/2,\lambda_1-1/2}(\Phi_{n_0+1/2,n_1+1/2} + e^{2\pi i\phi/4}\Phi_{-n_1+1/2,n_0+1/2}$$
$$+e^{2\pi i2\phi/4}\Phi_{-n_0+1/2,-n_1+1/2} + e^{2\pi i3\phi/4}\Phi_{n_1+1/2,-n_0+1/2})$$

Where $\phi \in \{-1, 0, 1, 2\}$. The application of the S transformation to $|\phi, n_0, n_1\rangle$ is given as,

$$S|\phi, n_0, n_1\rangle_{\lambda_0,\lambda_1} \quad (31)$$
$$= \Phi_{-\lambda_1,\lambda_0}(\Phi_{-n_1,n_0} + e^{2\pi i\phi/4}\Phi_{-n_0,-n_1}$$
$$+e^{2\pi i2\phi/4}\Phi_{n_1,-n_0} + e^{2\pi i3\phi/4}\Phi_{n_0,n_1})$$
$$= e^{-2\pi i\phi/4}|\phi, n_0, n_1\rangle_{-\lambda_1,\lambda_0}$$

The C matrix is then a diagonal matrix given by the expression,

$$C^{1D}_{S,\{\phi,n_0,n_1,\phi',n_0',n_1'\}} = (e^{-2\pi i\phi/N})\delta_{\phi,\phi'}\delta_{n_0,n_0'}\delta_{n_1,n_1'} \quad (32)$$

As the determinant of diagonal matrix is the product of the diagonal entries, we have the unregulated phase of the C matrix under the S-transform

$$arg(det(C_S^{1D})) = \quad (33)$$
$$-2\pi[\sum_{\phi=-1,0,1,2} \phi/4][\sum_{n_0=0}^{\infty} 1][\sum_{n_1=0}^{\infty} 1]$$

We regularize the above sum by attaching the following regulator.

$$-2\pi \sum_{\phi=-1,0,1,2} \phi/4 \sum_{n_0=0}^{\infty} (n_0+\lambda_0)^0 \sum_{n_1=0}^{\infty} (n_1+\lambda_1)^0 \quad (34)$$
$$= -\pi\zeta(0,\lambda_0)\zeta(0,\lambda_1) = -\pi(1/2-\lambda_0)(1/2-\lambda_1)$$

The above expression of the anomalous phase again reproduces the modular anomaly of the S transformation.

To extend the calculation into higher dimensions, we use the matrices given by Eq. (14) and (15). Using these, we write the phase of $det(C_S)$ in $(2+1)$-D and $(3+1)$-D as,

$$arg(det(C_S^{2D})) = -4\pi[\sum_{\phi=-1,0,1} \phi/3][\sum_{n_0\geq n_1\geq n_2} 1] \quad (35)$$

$$arg(det(C_S^{3D})) \quad (36)$$
$$= -4\pi[\sum_{\phi=-3,-2,..,4} \phi/8][\sum_{n_0,n_1,n_2=0,n_3=-\infty}^{\infty} 1]$$

Without requiring the complete summation of the modes, we immediately see that $arg(det(C_S^{2D})) = 0$ from the summation of ϕ. To calculate C_S^{3D}, we again connect the EZ zeta function to expression of the C matrix,

$$arg(det(C_S^{3D})) \quad (37)$$
$$= -2\pi \sum_{n_0=0}^{\infty} \sum_{n_1,n_2=0,n_3=-\infty}^{\infty} (n_0+\lambda_0)^0(F_3)^0,$$

The connection between the determinant of the transformation matrix, $det(C_S^{3D})$, and the EZ zeta function is given by

$$arg(det(C_S^{3D})) \quad (38)$$
$$= -2\pi(1/2-\lambda_0)g_3(0, \lambda_1, \lambda_2, \lambda_3, a_1, a_2, a_3),$$

Again, the zeta function g_3 vanishes at $\epsilon = 0$. Therefore, we find that the modular anomaly under the S transformation is absent. By showing that the free fermions in both $(2+1)$-D and $(3+1)$-D have no anomaly under S and T transformation, we conclude that the free fermions are modular anomaly free.

Beyond analytical calculations to confirm our result numerically, we calculate the Casmir energy of the (2+1)-D and $(3+1)$-D edge theory. In the numerical calculation, we explicitly calculate the partition function by summing up the Boltzmann weights of all the possible states with a given high energy cutoff. By comparing the numerical values of the partition functions before and after the modular transformation, we calculate the anomalous phase(For detailed implementation of the algorithm, see Appendix D in supplementary[31]). Fig. 1 (a) and (b) show the numerically calculated anomalous phase as a function of the high energy cut off scale. As we include more high energy states, we find the anomalous phases in Fig. 1 (a) and (b) converges to zero which indicates the absence of the modular anomaly in (2+1)-D and (3+1)-D edge theories. Unlike the zeta function regularization of the entire partition function, the explicit numerical summation of Boltzmann weights does not distinguish higher dimensional partition functions from slices of $(1+1)$-D partition functions where each $(1+1)$-D partition function has a specific transverse momentum. While each slice of the partition function is regularizable using the zeta function, our numerical calculation regularizes the slices one by one individually.

The cancellation of the modular anomaly is not surprising as one may represent a gapless theory in $(2+1)$-D on a lattice indicating that a higher dimensional bulk is not required to regularize a $(2+1)$-D theory. Further, this indicates that $(2+1)$-D gapless theory can be generically gapped out by breaking time-reversal symmetry. Nonetheless, by adding symmetry constraints, a modular anomaly can be found[27] in $(2+1)$-D. In contrast to $(2+1)$-D, the Nielsen-Ninomiya (NN) theorem in $(3+1)$-D suggests that the chiral edge of even dimension cannot be written without the aid of bulk theory[38]. Therefore, it is natural to expect an anomalous contribution in even dimensions even without symmetry projection. Thus, in the next section, we show that the chiral fermion in $(3+1)$-D shows a modular anomaly(mixed modular anomaly) when $U(1)$ gauge field is coupled to it.

MIXED MODULAR ANOMALY

While chiral free fermions in $(3+1)$-D are modular anomaly free, attaching a background $U(1)$ gauge field changes the situation. Consider the chiral edge under a uniform magnetic field pointing out-of-plane in the z-direction thereby breaking the periodicity of the in-plane x and y coordinates. Therefore, the full modular transformation that is isomorphic to $PSL(\mathbb{Z},4)$ is no longer a good symmetry of the action, Eq. (5). However, we can still safely consider $PSL(\mathbb{Z},2)$ acting on both z and the time component as a subgroup of the original $PSL(\mathbb{Z},4)$. We write the Hamiltonian for this situation as,

$$H = (\overrightarrow{k} - \overrightarrow{A}) \cdot \overrightarrow{\sigma}, \tag{39}$$

with magnetic vector potential A written in the Landau gauge, $A = (0, -Bx, 0)$. This Hamiltonian has two types of solutions. $E_{W(D)}$ is gapless(gapped) Landau level(LL).

$$E_W(k_3) = k_z, E_D(n, k_3) = \pm\sqrt{Bn + k_3^2}, \tag{40}$$

where $k_3 = 2\pi(n_3 + \lambda_3)/L_z$ and n is an positive integer. We can write the unregularized partition function to be

$$Z_{\lambda_0,\lambda_3} = [\prod_{k_3}(1 - e^{2\pi i\lambda_0 - \beta E_W(k_z)}) \tag{41}$$
$$\times \prod_{n,k_z}(1 - e^{2\pi i\lambda_0 + \beta E_D(n,k_z)})(1 - e^{2\pi i\lambda_0 - \beta E_D(n,k_z)})]^{N_\phi},$$

where N_ϕ is the level degeneracy and $\omega = q^{\lambda_3} e^{2\pi i\lambda_0}$. After regularization, we find that the chiral modes contribute to the anomaly while gapped landau levels do not contribute as they are massive (For explicit calculations of massive mode, see Appendix E in supplementary[31]). This reflects the fact that the regularized Casimir energy has no contribution from gapped states. Therefore, the modular transforms of the partition function of a $(3+1)$-D edge theory coupled to a $U(1)$ gauge field are

$$T[Z_{\boldsymbol{\lambda}}] = e^{iN_\phi \pi(\lambda_3^2 - \lambda_3 + 1/6)} Z_{\boldsymbol{\lambda}'} \tag{42}$$
$$S[Z_{\boldsymbol{\lambda}}] = e^{iN_\phi 2\pi(\lambda_3 - 1/2)(\lambda_0 - 1/2))} Z_{\boldsymbol{\lambda}'}$$

and clearly contain a modular anomaly that is proportional to N_ϕ, which counts the number of $(1+1)$-D chiral modes. To confirm, we again look at the numerical calculation of the Casmir energy in Fig. 1(c) where we find that the anomalous phase value under T transformation reproduces the transformation rules given in Eq. (42). Thus, the $(3+1)$-D chiral edge, when coupled to a background gauge field, contains a modular anomaly. In contrast to $(1+1)$-D, $(3+1)$-D chiral edge has charge pumping but only in conjunction with the magnetic field, in analogy to the chiral anomaly[39]. Therefore, we conclude the presence of modular anomaly when $N_\phi \neq 0$, is a direct manifestation of quantum Hall effect of $(4+1)$-D.

PT SYMMETRIC EDGE STATE

After establishing the presence of the mixed modular anomaly, we apply our result to an edge theory of $(4+1)$-D insulator. Using the $(3+1)$-D chiral edge result enables us to extend our analysis to $(4+1)$-D insulators with the following two symmetries: the fermion parity of each spin component is preserved and the system is invariant under $(x, y, z, w, t) \to (-x, -y, -z, w, -t)$. Consider an open $(3+1)$-D surface with $w = const$, the second symmetry is equivalent to $P * T$, where P is parity in 3D. The first symmetry, in the non-interacting case, ensures the decoupling between spin-up and spin-down sectors, so each sector is itself a $(4+1)$-D quantum Hall state with $N_\uparrow$ ($N_\downarrow$) Weyl nodes on the surface. $P * T$ on the surface ensures that $N_\uparrow = N_\downarrow \equiv N_{edge}$, as it maps (i) spin-up to spin-down and (ii) a positive monopole to a negative monopole. The topological classification without interaction is hence $\mathbb{Z}$.

To calculate the modular anomaly of the edge theory, we consider N_{edge} copies of the Weyl fermions with positive monopole and negative monopole with the magnetic field. When the Weyl fermions with each monopole conserve the fermion number parity. We can consider the partition function of a sector labeled with a definite fermion number parity. This is accomplished by projecting the Hilbert space with the symmetry projection operator, P. the symmetry projection operator is given as

$$P = \frac{(1 + (-1)^{N_\uparrow})(1 + (-1)^{N_\downarrow})}{4} \tag{43}$$

where $N_{\uparrow(\downarrow)}$ refers the fermion number operator of positive(negative) monopole. P returns 1 only if $N_\uparrow$ and $N_\downarrow$ are even integers, thus P projects the Hilbert space into one of the sectors with a definite fermion number parity. Now the partition function with a definite fermion number parity can be expressed as

$$Z_{total,\lambda_3} = Tr(Pe^{i\tau H_\uparrow}e^{i\tau H_\downarrow}) \tag{44}$$
$$= \frac{1}{4}Tr[(1+e^{\pi i N_\uparrow})e^{i\tau H_\uparrow}]Tr[(1+e^{\pi i N_\downarrow})e^{i\tau H_\downarrow}] = \frac{Z_{\uparrow\lambda_3}Z_{\downarrow\lambda_3}}{4}.$$

where $Z_{\uparrow\lambda_3}$ is given as

$$Z_{\uparrow,\lambda_3} = [Z_{\lambda_0=0,\lambda_3}]^{N_{edge}} + [Z_{\lambda_0=1/2,\lambda_3}]^{N_{edge}}, \tag{45}$$

where $H_\uparrow$ refers the Hamiltonian of the edge with spin-up and we have used the fact that $Z_{\lambda_0,\lambda_3} = Tr(e^{-2\pi i N\lambda_0}e^{i\tau H_{\lambda_3}})$[23]. We consider the general case of the partition function, which is a linear combination of the periodic, $Z_{\lambda_3=0}$, and anti-periodic, $Z_{\lambda_3=1/2}$, boundary conditions, namely

$$Z_\uparrow = \sum_{\lambda_0=0,1/2,\lambda_3=0} Z^{N_{edge}}_{\lambda_0,\lambda_3} + s\sum_{\lambda_0=0,1/2,\lambda_3=1/2} Z^{N_{edge}}_{\lambda_0,\lambda_3}, \tag{46}$$

where s is the relative phase between the periodic and antiperiodic sector. From Eq. (42), we find that the partition function under the application of the T-transformation to be,

$$T[Z_\uparrow] = e^{iN_\phi N_{edge}\pi/6}[\sum_{\lambda_0=0,1/2,\lambda_3=0}[Z_{T[\lambda]}]]^{N_{edge}} \tag{47}$$
$$+se^{-i\pi N_\phi N_{edge}/4}\sum_{\lambda_0=0,1/2,\lambda_3=1/2}[Z_{T[\lambda]}]^{N_{edge}}].$$

Similarly, under the S transformation, we find

$$S[Z_\uparrow] = \sum_{(\lambda_0,\lambda_3)=(0,1/2),(1/2,1/2)}[sZ_{S[\lambda]}]^{N_{edge}} \tag{48}$$
$$+e^{i\pi N_\phi N_{edge}/2}[Z_{S[\lambda=(0,0)]}]^{N_{edge}} + [Z_{S[\lambda=(1/2,0)]}]^{N_{edge}}.$$

This allows us to conclude that to achieve modular covariance($T[Z_\uparrow] = e^{iN_\phi N_{edge}\pi/6}Z_\uparrow$ and $S[Z_\uparrow] = Z_\uparrow$) $N_\phi N_{edge}$ must be multiples of 8. Therefore, the modular covariance is achieved when $N_{edge} = 8/gcd(N_\phi, 8)$. When $Z_\uparrow$ has modular covariance, $Z_{total} = Z_\uparrow Z_\downarrow$ has modular invariance. As N_ϕ can be any integer, the complete cancellation of the modular anomaly occurs when $N_{edge} = 8$.

CONCLUSION

In conclusion, we have generalized modular transformation in (1+1)-D CFT to higher dimensional edge theory with use of $PSL(\mathbb{Z}, d)$ group supported by numerical calculations of the Casmir energies. We have shown the gapless free fermion theories in (2+1)-D and (3+1)-D are modular invariant. We find a modular anomaly in (3+1)-D when the edge theory is coupled to a $U(1)$ gauge field resulting in a (4+1)-D quantum Hall effect. Moreover, we find that the edge theory of (4+1)-D insulator with spacetime inversion symmetry($P * T$) and fermion number parity symmetry for each spin achieves modular invariant when $N_{edge} = 8$. The cancellation of the modular anomaly when $N_{edge} = 8$ implies that the surface partition function does not have adiabatic pumping of stress-energy tensor. In other words, this implies that the corresponding surface theory has a trivial gravitational response when 8 copies of the edge theory are present.

MJG would like to thank Shinsei Ryu for enlightening conversations. MJP would like to thank Thomas Faulkner for helpful discussions. MJP, CF, and MJG were supported by ONR - N0014-11-1-0123. MJG and MJP were supported by NSF-CAREER EECS-1351871. BAB was supported by NSF CAREER DMR-095242, ONR - N00014-11-1-0635, MURI-130-6082, NSF-MRSEC DMR-0819860, DARPA under SPAWAR Grant No.: N66001-11-1-4110, Packard Foundation and Keck grant. CF was supported by Project 11674370 by NSFC and the National Key Research and Development Program under grant number 2016YFA0302400 and 2016YFA0300600.

[1] K. v. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett **45**, 494 (1980).
[2] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
[3] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
[4] B. A. Bernevig and S.-C. Zhang, Phys. Rev. Lett. **96**, 106802 (2006).
[5] T. H. B. A. Bernevig and S.-C. Zhang, Science **314**, 1757 (2006).
[6] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007).
[7] L. Fu and C. L. Kane, Phys. Rev. B **76**, 045302 (2007).
[8] T. L. Hughes and B. A. Bernevig, *Topological Insulators and Topological Superconductors* (Princeton University Press, 2013).
[9] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B **78**, 195125 (2008).
[10] S. Ryu, A. F. A. Schnyder, and A. W. W. Ludwig, New J. Phys. **12**, 065010 (2010).
[11] J. E. Moore and L. Balents, Phys. Rev. B **75**, 121306(R) (2007).
[12] A. Alexandradinata, C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. Lett. **113**, 116403 (2014).
[13] C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. B **86**, 115112 (2012).
[14] C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. Lett. **112**, 106401 (2014).

[15] N. H. Lindner, G. Refael, and V. Galitski, Nature Physics **7**, 490 (2011).
[16] M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. **104**, 106408 (2010).
[17] S. Adler, Phys. Rev. **5**, 177 (1969).
[18] J. Bell and R. Jackiw, Il Nuovo Cimento **60**, 47 (1969).
[19] G. 't Hooft, Phys. Rev. Lett. **8**, 37 (1976).
[20] K. Ishikawa, Phys. Rev. Lett **53**, 1615 (1984).
[21] R. B. Laughlin, Phys. Rev. B **23**, 5632 (1981).
[22] X.-L. Qi, E. Witten, and S.-C. Zhang, Phys. Rev. B **87**, 134519 (2013).
[23] S. Ryu and S. C. Zhang, Phys. Rev. B **85**, 245132 (2012).
[24] O. M. Sule, X. Chen, and S. Ryu, Phys. Rev. B **88**, 075125 (2013).
[25] C.-T. Hsieh, O. M. Sule, G. Y. Cho, S. Ryu, and R. G. Leigh, Phys. Rev. B **90**, 165134 (2014).
[26] A. Cappelli and E. Randellini, Journal of High Energy Physics **2013**, 101 (2013), 10.1007/JHEP12(2013)101.
[27] C.-T. Hsieh, G. Y. Cho, and S. Ryu, Phys. Rev. B **93**, 075135 (2016).
[28] H. Yao and S. Ryu, Phys. Rev. B **88**, 064507 (2013).
[29] J. Polchinski, *String Theory* (Cambridge University Press, 1998).
[30] E. Witten, Commum. Math. Phys. **100**, 197 (1985).
[31] See supplemental material at [URL will be inserted by publisher].
[32] A. Cappelli and G. R. Zemba, Nucl. Phys. B **490**, 595 (1997).
[33] S. Hawking, Commun. Math. Phys. **55**, 133 (1977).
[34] A. Actor, J. Phys. A **24**, 3741 (1991).
[35] E. Elizalde, *Ten Physical Applications of Spectral Zeta Functions* (Springer, 2012).
[36] K. Fujikawa, Phys. Rev. Lett. **42**, 1195 (1979).
[37] K. Fujikawa, Phys. Rev. D **21**, 2848 (1980).
[38] H. Nielsen and M. Ninomiya, Phys. Lett. B **105**, 219 (1981).
[39] H. Nielsen and M. Ninomiya, Phys. Lett. B **130**, 389 (1983).