Mixed Geometry-Charge Responses in Three-Dimensional Topological Crystalline Insulators

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Quantized responses are important tools for understanding and characterizing the universal features of topological phases of matter. In this work, we consider a class of topological crystalline insulators in $3+1$D with C_n lattice rotation symmetry along a fixed axis. We show that these insulators can realize a mixed geometry-charge response, where a quantized polarization is bound to line-like disclination defects. On the surface of the insulators, disclination carry a quantized charge, which is half the minimal amount that can occur in purely $2+1$D systems. If interactions are included, these insulators can host topologically ordered surface states with an anomalous lattice rotation symmetry. These effects, and others, are captured by a $3+1$D topological response therm that couples the lattice curvature to the electromagnetic field strength. We derive a topological invariant that determines the coefficient of this response term for certain classes of insulators with additional inversion symmetry.

I. INTRODUCTION

In modern condensed matter physics, it has been well established that for a given symmetry class, there can be multiple insulating phases of matter that are topologically distinct from one other[1, 2]. These topologically inequivalent insulators are denoted as symmetry protected topological phases (SPTs)[3–8], and have been a central area of condensed matter research for the last several decades. Concretely, SPTs are defined as symmetric insulators that cannot be smoothly deformed into a trivial insulator without either breaking the symmetry or closing the band gap. SPTs also display a bulk-boundary correspondence, where the topologically non-trivial bulk is accompanied by gapless degrees of freedom on symmetry preserving surfaces[9, 10].

One reason that topological phases of matter have attracted so much attention is that they can exhibit quantized responses. These responses arise from the underlying topology of the SPT and are robust to symmetry preserving disorder and perturbations. In experimental contexts, these quantized responses serve as smoking-gun characteristics of topological insulators[11–15]. The first observed, and most famous, topological response is the quantized Hall-conductance of $2+1$D insulators[16–19]. Similarly, $1+1$D insulators with particle hole symmetry (PHS) have a quantized polarization[20–23], and $3+1$D insulators with time-reversal symmetry (TRS) display quantized axion electrodynamics[24, 25]. All of these effects have a topological field theory description: Hall conductance corresponds to a Chern-Simons term[18], polarization corresponds to a Goldstone-Wilczek response term[26], and axion electrodynamics corresponds to a Θ-term[27].

More recently, the topological responses of topological crystalline insulators (TCIs)–SPTs that are protected by crystalline symmetries–have also gained attention[28–30]. Notably, it has been shown that certain TCIs can host mixed geometry-charge responses, where charge fluctuations are driven by lattice effects e.q. shears, strains, or defects[31–33]. A well known example of such a mixed geometry-charge response occurs in 2+1D, where charge is bound to disclination defects in TCIs with C_n lattice rotation symmetry[34, 35]. This effect is described by a Wen-Zee term in the effective field theory[36, 37].

In this work, we consider the mixed charge-geometry responses of $3+1$D systems with C_n lattice rotation symmetry around a fixed axis. We show that such a system can display a novel response, where line-like disclinations defects have an electromagnetic polarization. This response is described by a topological field theory term that directly couples the lattice curvature (R) to electromagnetism (F), which we denote as the RF-term. In general, the RF-term is unquantized, but, for systems with additional particle hole symmetry (PHS) or mirror symmetry along the z-direction, the RF-term is quantized, and defines a class of rotation invariant topological crystalline insulators (rTCIs).

We provide explicit lattice models of that realize these rTCIs for both spinless and spin-1/2 fermions. Using the RF-field theory description and the microscopic lattice models, we show that the rTCIs display a number of novel topological features. In particular, the surfaces of rTCIs host an even number of symmetry protected Dirac cones. These Dirac cones can be gapped out by breaking PHS breaking. The resulting massive surface hosts a Wen-Zee response term, indicating that surface disclinations of the rTCI bind charge. Interestingly, the coefficient of this Wen-Zee term is half the amount that is allowed in 2+1D. We also show that if interactions are included, the rTCI can host a symmetric gapped surface with symmetry-enriched topological order. This symmetry enriched surface topological order is anomalous and cannot be realized in a purely $2+1$D system with particle hole symmetry.

We generalize this analysis to certain classes of insulators that have a Dirac-like band structure at high-symmetry points. For spinless fermions with additional mirror symmetries, we show that the RF-term in response theory can be determined by the mirror eigenvalues and angular momentum of the occupied bands at the high-symmetry points. A similar relationship exists for spin-1/2 insulators that conserve spin.

The remainder of this paper is organized as follows. In Sec. II, we present the RF-response term, and discuss its physical properties, and show that it defines a new class of rTCIs. In Sec. III A we present a lattice model of the spinless rTCI. We show that the effective response theory of the rTCI contains a quantized RF-term, and that the surface of the rTCI is anomalous with respect to the spatial and onsite symmetries. In Sec. III B we present a lattice model for the spin-1/2 rTCI. We also analyze its bulk response theory and surfaces physics, as we did for the spinless model. In Sec. V we present a topological invariant for rTCIs with additional mirror symmetry, and show that the value of the invariant determines if the RF response is present. In Sec. VI we conclude this work and discuss possible extensions. We also have several appendixes that contain technical details.

II. RESPONSE THEORY

In this section, we will consider the effective field theory description of a 3 + 1D fermionic insulator with U(1) charge conservation, and C_n lattice rotation symmetry along a fixed axis–which we take to be the z-axis. Our main interest is in the following mixed geometry-charge response term,

$$\mathcal{L}_{RF} = \frac{\Phi}{4\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa, \tag{1}$$

where A_μ is the electromagnetic gauge field, and ω_μ is the C_n symmetry gauge field, both of which should be regarded as background probe fields. Physically, fluxes of ω_μ correspond to lattice disclinations, with Frank-vector parallel to the z-axis[38]. As we shall show in the following subsections, the response term in Eq. 1 describes a coupling between the lattice curvature (R) and the electromagnetic field strength (F), leading us to refer to it as the "RF-term". The RF-term is a total derivative, but nevertheless leads to a number of non-trivial responses. Furthermore, we shall show that the coefficient Φ is quantized for insulators with either particle hole symmetry (PHS) and/or mirror symmetry along the z-direction (which we will simply refer to as "mirror symmetry" unless otherwise noted).

A. Lattice Geometry in the Continuum Limit

The RF-term in Eq. 1 is defined in continuous spacetime. Because of this, it is worthwhile to discuss how lattice effects–an inherently discrete phenomena–can be described in the continuum limit. Here, for simplicity, we will consider the case of a cubic lattice, although this analysis applies to general lattices.

To begin, let us consider a cubic lattice embedded on a 3 + 1D manifold. In the continuum limit, the lattice constant is taken to zero, and the lattice points become continuum points on the manifold, which we label as x_μ ($\mu = 0, x, y, z$). The metric of the manifold, $g_{\mu\nu}$, should be consistent with the underlying lattice in the continuum limit. To this end, let us introduce the frame-fields (AKA vielbeins or tetrads)[39] e^A_μ ($A = 0, x, y, z$) such that $g_{\mu\nu} = e^A_\mu e^B_\nu \delta_{AB}$. In order for the metric of the manifold to be consistent with the lattice, the frame-fields e^A_μ with $A = x, y, z$, should be identified with the primitive lattice vectors (in units of lattice constant), and the $A = 0$ frame-field should be identified with the temporal direction. For a perfect lattice that is free of defects, we can take $e^0_\mu = i\delta^0_\mu$ and $e^A_\mu = \delta^A_\mu$ for $A = x, y, z$.

In this work, we are primarily interested in the continuum interpretation of lattice disclinations defects with Frank-vector parallel to the z-axis. These defects are fluxes of the C_n lattice rotation symmetry around the z-axis ($n = 4$ for the cubic lattice). In 3 + 1D, disclinations are line-like objects. With this in mind, let us consider a lattice where the only defects are disclinations with Frank-vector parallel to the z-axis (which we shall refer to simply as disclinations for brevity). Since the disclinations only rotate the lattice vectors that span the xy-plane, the frame-fields for a generic lattice with disclinations can be defined as

$$\begin{aligned} &e^0_\mu = i\delta^0_\mu, \quad e^z_\mu = \delta^z_\mu \\ &e^x_\mu = \cos(\varphi)\delta^x_\mu + \sin(\varphi)\delta^y_\mu, \\ &e^y_\mu = -\sin(\varphi)\delta^x_\mu + \cos(\varphi)\delta^y_\mu, \end{aligned} \tag{2}$$

for some spatially varying angle φ. For these frame-fields, the metric $g_{\mu\nu}$ is flat everywhere, which is a consequence of us only considering rotation symmetry fluxes. It should be noted that if non-trivial disclinations are present, a global definition of e^x and e^y is not possible, and it is necessary to work in coordinate patches where e^x and e^y can be consistently defined.

The spin connection is defined in terms of the frame-fields as $\omega^A_{B\mu} = E^\nu_B\partial_\mu e^A_\nu + \Gamma^\nu_{\rho\mu}e^A_\nu E^\rho_B$, where E^μ_A is the inverse frame-field ($e^A_\mu E^\nu_A = \delta^\nu_\mu$) and $\Gamma^\nu_{\rho\mu}$ is the Christoffel symbol[39]. For the frame-fields defined in Eq. 2 the only non-vanishing components of the spin connection are,

$$\omega_\mu \equiv \omega^x_{y\mu} = -\omega^y_{x\mu} = E^\nu_y\partial_\mu e^x_\nu. \tag{3}$$

For brevity, we will refer to ω_μ as the spin connection from here on out. Physically, ω_μ measures how much the lattice vectors that span the xy-plane rotate as we move along the μ-direction. The spin connection has a C_n gauge ambiguity, which correspond to a local redefinition of the lattice vectors that span the xy-plane. Under this C_n gauge symmetry, the frame-fields e^x and e^y transform as,

$$\begin{aligned} e^x_\mu &\to \cos(\theta)e^x_\mu + \sin(\theta)e^y_\mu, \\ e^y_\mu &\to -\sin(\theta)e^x_\mu + \cos(\theta)e^y_\mu, \end{aligned} \tag{4}$$

where θ is a function that takes on values in $\{0, \frac{2\pi}{n}, \frac{4\pi}{n}, ... \frac{(n-1)2\pi}{n}\}$. As we can see, the C_n gauge transformation does not change the metric. Using Eq. 3, the C_n gauge transformation act on the spin connection as

$$\omega_\mu \to \omega_\mu + \partial_\mu \theta. \tag{5}$$

For the theories we will consider in the following sections, this C_n gauge symmetry is actually part of an enlarger SO(2)=U(1) gauge symmetry that emerges within the continuum limit of the lattice model. The U(1) gauge symmetry transforms the frame-fields and spin connections as in Eq. 4 and 5 but with θ taking continuous values in $[0, 2\pi)$.

Based on the gauge transformation defined in Eq. 5, we define the gauge invariant lattice curvature tensor $R_{\mu\nu} = \partial_\mu \omega_\nu - \partial_\nu \omega_\mu$. This curvature, is related to the full curvature tensor of the 3+1D spacetime, $R^B_{\mu\nu A}$, as $R_{\mu\nu} \equiv R^x_{\mu\nu y}$[39]. The RF-term in Eq. 1 therefore describes a coupling between the effective lattice curvature $R_{\mu\nu}$ and the dual electromagnetic field strength $F^*_{\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\rho\kappa}F_{\rho\kappa}$. We note that, in principle, it is also possible to define torsion for the lattice system. However, for the frame-fields in Eq. 2 the torsion vanishes. At the level of the lattice, the absence of torsion is the result of the assumption that the lattice only has disclinations, and is free of dislocations[40].

As we shall now show, disclinations of the underlying lattice correspond to fluxes of ω_μ, and are singular points of the curvature R. Let us consider a disclination located at $x = y = 0$ with Frank-angle Θ_F. Away from the disclination core, the lattice vectors that span the xy-plane are rotated by Θ_F upon encircling the disclination. Using our previous identification of the frame-fields with the lattice vectors, we find that such a disclination corresponds to the frame-fields defined in Eq. 2, where φ winds by Θ_F on any loop that encircles $x = y = 0$, for example $\varphi(x, y) = \frac{\Theta_F}{2\pi}\tan^{-1}(x/y)$. Using Eq. 3, $\omega_\mu = \partial_\mu \varphi$, and $\oint \omega = \Theta_F$, where the loop integral is defined on a loop that encircles the disclination line. This confirms that fluxes of the spin connection correspond to lattice disclinations. Since we are considering a lattice system with C_n symmetry, the Frank angles are necessarily multiples of $2\pi/n$, and the physical fluxes of ω_μ are quantized in multiples of $2\pi/n$.

B. Physical Implications of the Response Theory

To set the stage for a discussion of the physical implications of the RF-term in Eq. 1 it will be useful to first discuss a related response term, the (axion) Θ-term[41–43],

$$\mathcal{L}_\Theta = \frac{\Theta}{8\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu A_\nu \partial_\rho A_\kappa. \tag{6}$$

which describes time-reversal invariant fermionic topological insulators when $\Theta = \pi$[27], and bosonic topological insulators when $\Theta = 2\pi$[44]. As we shall show, many features of the Θ-term have direct analogs in the RF-term. For a more detailed discussion of the Θ-term in the context of fermionic and bosonic topological phases of matter, see Ref. 27 and 44.

The first feature of note, is that for a non-vanishing value of Θ, Eq. 6 indicates that magnetic monopoles carry charge $-\Theta/2\pi$. This is known as the Witten effect[45]. Second, the Θ-term imparts magnetic flux tubes with non-trivial braiding statistics, where linking a pair of 2π $(\frac{hc}{e})$ electromagnetic vortices produces a phase of $e^{i\Theta}$ relative to the unlinked configuration. Third, at domain walls where the value of Θ changes by $\Delta\Theta$, there is a $2 + 1$D Chern-Simons term of the form

$$\mathcal{L}_{\text{CS-DW}} = \frac{\Delta\Theta}{8\pi^2}\epsilon^{\mu\nu\rho}A_\mu \partial_\nu A_\rho. \tag{7}$$

It is also important to note that in Eq. 6, Θ is periodic. For fermionic system, the period of Θ is 2π. This is easily demonstrated by considering a domain wall where Θ changes by $\Delta\Theta$. According to Eq. 7 this leads to a $2 + 1$D domain wall Chern-Simons term with coefficient $\Delta\Theta/8\pi^2$. For a purely $2 + 1$D fermionic system without topological order, the Chern-Simons coefficient must be an integer multiple of $1/4\pi$[46]. So, when $\Delta\Theta$ is an integer multiple of 2π, the domain wall physics can be trivialized by adding a purely $2 + 1$D system, indicating that the value of Θ in Eq. 6 is only meaningfully defined modulo 2π in fermionic systems. The periodicity of Θ in bosonic systems can be found using the same logic. For $2 + 1$D bosonic systems without topological order, the Chern-Simons coefficient must be an integer multiple of $1/2\pi$[47]. Because of this, Θ is defined modulo 4π in bosonic systems.

Having discussed the essential features of the Θ-term in Eq. 6, let us now consider the analogous features of the RF-term in Eq. 1. Since the RF-term couples the electromagnetic gauge field A_μ and the spin connection ω_μ, it gives rise to mixed charge-geometric effects. As is well known, the U(1) symmetry indicates that there is a conserved electromagnetic charge 4-current $j^\mu = \delta S/\delta A_\mu$, where S is the minimally coupled action. Similarly, the C_n symmetry leads to a conserved angular momentum 4-current $j^\mu_{AM} = \delta S/\delta \omega_\mu$. Since we are considering C_n symmetry, the angular momentum is only defined modulo n.

Using this, we first note that, for a non-vanishing value of Φ, there is a mixed Witten effect, where magnetic monopoles carry angular momentum $-\Phi/2\pi$. We can also define a $2\pi/n$ "disclination monopole" where a $2\pi/n$ disclination line terminates in the bulk of the insulator. Such a disclination monopole will likely have a large energy cost in an actual crystalline solid, but the disclination monopoles are still useful to consider as a theoretical tool. The mixed Witten effect indicates that a $2\pi/n$ disclination monopole carries electromagnetic charge $-\Phi/n$. Equivalently, the RF-term binds polarization $-\Phi/n$ to $2\pi/n$ disclination lines.

The RF-term also indicates that the electromagnetic flux lines and disclination lines have non-trivial braiding statistics. Linking a 2π electromagnetic flux line with a $2\pi/n$ disclination line produces a phase of $e^{i\Phi/n}$ compared to the unlinked configuration. The RF-term does not affect the self-statistics of the flux or disclination lines.

Finally, we can consider domain walls, where the value of Φ change by $\Delta\Phi$. For a domain wall that preserves C_n symmetry, i.e. a domain wall normal to the z-axis, there will be a $2+1$D Wen-Zee term of the form[36]

$$\mathcal{L}_{\text{WZ-DW}} = \frac{\Delta\Phi}{4\pi^2}\epsilon^{\mu\nu\rho}\omega_\mu\partial_\nu A_\rho. \tag{8}$$

At this domain wall, the electromagnetic 3-current is

$$j^\mu = -\frac{\Delta\Phi}{4\pi^2}\epsilon^{\mu\nu\rho}\partial_\nu\omega_\rho, \tag{9}$$

indicating that at the domain wall, a $2\pi/n$ disclination binds charge $-\Delta\Phi/2\pi n$. Similarly, the domain wall angular momentum 3-current is

$$j^\mu_{\text{AM}} = \frac{\Delta\Phi}{4\pi^2}\epsilon^{\mu\nu\rho}\partial_\nu A_\rho, \tag{10}$$

and a 2π magnetic flux on the surface has angular momentum $\Delta\Phi/2\pi$. These effects are shown schematically in Fig. 1.

The value of the Φ coefficient of the RF-term is also periodic, the period of which depends on if time-reversal symmetry is present, and on the spin of the fermions. Here, and throughout we will be primarily interested in systems with time-reversal symmetry, as it will simplify our discussions and make it more applicable to realistic materials. We provide a discussion of the periodicity of Φ in systems without time-reversal symmetry in Appendix A.

Similar to before, the period of Φ can be determined by finding the value of $\Delta\Phi$ where the domain wall Wen-Zee term in Eq. 8 can be realized in a purely $2+1$D system without topological order. For spinless fermions with time-reversals symmetry ($\hat{\mathcal{T}}^2 = +1$), the minimal disclination charge is $1/n$[35]. This indicates that Φ has period 2π. For spin-1/2 fermions where $\hat{\mathcal{T}}^2 = -1$, the minimal disclination charges is $2/n$ due to Kramer's degeneracy[35]. This response corresponds to a Wen-Zee term with coefficient π. Therefore, for spin-1/2 fermions with additional TRS, Φ has period 4π. We also note that for bosonic systems with integer spin, we expect that Φ will have period 2π, although here we are primarily interested in fermionic systems here.

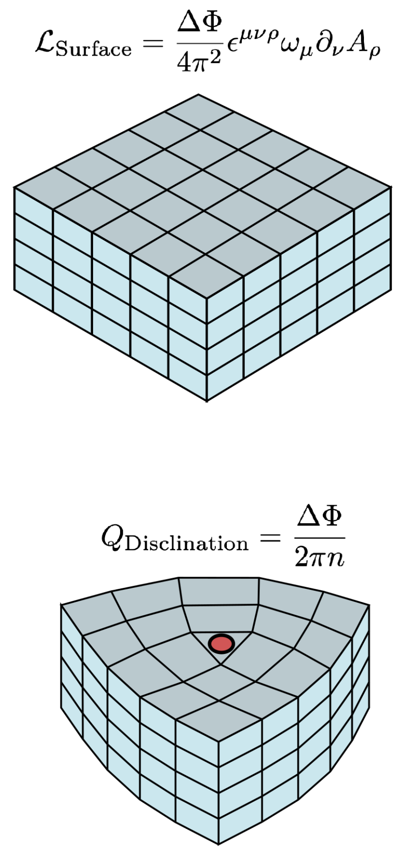

FIG. 1: Top) A schematic of a surface, where the coefficient of Eq. 1 changes by $\Delta\Phi$. This surface hosts Wen-Zee term with coefficient $\Delta\Phi/4\pi^2$. Bottom) The surface charge, $Q_{\text{Disclination}} = \Delta\Phi/2\pi n$, that is bound to a $2\pi/n$ disinclination, shown here for $n=4$. A domain wall where t

C. Quantized Responses in Insulators with Particle-Hole Symmetry

It is well known that the coefficient of the Θ-term in Eq. 6 is quantized by TRS[27]. This can be determined by noting that Eq. 6 is odd under TRS, such that $\Theta = -\Theta$ for a time-reversal invariant insulator. Recalling the periodicity of Θ, we find that $\Theta = -\Theta$ has solutions 0 and $\pi(2\pi)$, for fermions (bosons). In both cases, the former corresponds to a trivial insulator, while the latter corresponds to a time-reversal invariant topological insulator.

Similarly, the Φ coefficient of the RF-term is quantized by particle-hole-symmetry (PHS). Here, for simplicity, we will only consider systems with time-reversal symmetry (see Appendix A for a discussion of systems without TRS). The RF-term is odd under PHS, (PHS: $A_\mu \to -A_\mu$, and $\omega_\mu \to \omega_\mu$), so that the RF-term of a particle-hole symmetric insulator satisfies $\Phi = -\Phi$. As noted previously, for spinless insulators with TRS, Φ is 2π periodic, indicating that $\Phi = 0$, or π in spinless insulators with PHS and TRS. For spin-1/2 insulators with TRS, Φ is again 4π periodic, and so the RF-term has $\Phi = 0$, or 2π. Here, a non-zero value of Φ indicates that the system is a non-trivial rTCI.

One of the most important features of the RF-term is that domain walls of Φ can host Wen-Zee term. For the spinless rTCIs (with PHS and TRS), a domain wall where the value of Φ changes from $\Phi = \pi$ to $\Phi = 0$ correspond to a surface where PHS is explicitly broken. Based on Eq. 8, this PHS breaking surface hosts a Wen-Zee term with coefficient $1/4\pi + m/2\pi$ with $m \in \mathbb{Z}$, where the factor of $m/2\pi$ comes from purely surface effects. For such a surface, a $2\pi/n$ disclination binds charge $1/2n + m/n$. The surface disclination charge modulo $1/n$ is therefore a quantized signature of the bulk topology of the spinless rTCI. Similarly, for the spin-1/2 rTCIs, a domain wall where the value of Φ changes from $\Phi = 2\pi$ to $\Phi = 0$ corresponds to a PHS broken surface that hosts a Wen-Zee terms with coefficient $1/2\pi + m/\pi$. For this surface, a $2\pi/n$ surface disclination binds charge $1/n + 2m/n$. So, for spin-1/2 rTCIs, the surface disclination charge bound modulo $2/n$ is the quantized signature of the bulk topology.

D. Quantized Responses in Mirror Symmetric Insulators

In addition to PHS, the RF-term is also quantized by mirror symmetry along the z-direction. As before, this arises from the fact that the RF-term is odd under mirror symmetry ($\mathcal{M}_z : (A_0, A_x, A_y, A_z) \to (A_0, A_x, A_y, -A_z)$, and $(\omega_0, \omega_x, \omega_y, \omega_z) \to (\omega_0, \omega_x, \omega_y, -\omega_z)$). Hence, for spinless insulators with TRS and mirror symmetry, $\Phi = 0$ or π , and for spin-1/2 insulators with TRS and mirror symmetry, $\Phi = 0$ or 2π. Again, the non-trivial values of Φ correspond to a non-trivial rTCI with mirror symmetry.

The bulk physics is much the same for rTCIs with PHS and rTCIs with mirror symmetry. However, these two classes of rTCIs have different surface physics, since PHS is an onsite symmetry, while mirror symmetry is a spatial symmetry that exchanges surfaces. In particular, a non-trivial RF-term does not necessarily lead to symmetry protected surface modes for mirror symmetric insulators. To see this, we note that if Φ is a function of the z coordinate, mirror symmetry requires that $\Phi(z) = -\Phi(-z)$ (PHS requires that $\Phi(z) = -\Phi(z)$). With this in mind, let us consider an insulator with mirror symmetry, TRS, and a non-trivial RF-term that is separated from two trivial insulators by two domain walls. These domain walls can be gapped, while preserve mirror symmetry and TRS, if at one domain wall Φ winds by $\pi+2\pi q$ for spinless fermions ($2\pi+4\pi q$ for spin-1/2 fermions) and at the other domain wall, Φ winds by $-\pi - 2\pi q$ ($-2\pi - 4\pi q$ for spin-1/2 fermions), with $q \in \mathbb{Z}$. Other definitions of Φ lead to mirror symmetry breaking surfaces.

For the mirror symmetry preserving surfaces, each surface theory consists of a Wen-Zee term with the same coefficient, and a disclination binds the same amount of charge on both mirror related surfaces. On the other hand, for mirror symmetry breaking surfaces, each surface consists of a Wen-Zee term with opposite coefficients (modulo local surface terms). Disclinations of the two mirror symmetry breaking surfaces will bind opposite amounts of charge, up to local contributions.

As a final point, it is worth noting that a system with mirror symmetry and C_n rotation symmetry with $n = 2, 4, 6$ also has inversion symmetry, since inversion symmetry is the product of mirror symmetry and C_2 rotations.

E. Origin of Quantized RF-term

Here, we will consider the microscopic origin of the RF-term in the particle-hole symmetric or mirror symmetric rTCIs we discussed in the previous subsections. In principle, there are two distinct mechanisms that can give rise to the RF-term. First, the RF-term can be generated by the coupling between the microscopic fermions, the lattice curvature. As we shall show in the following sections, this contribution to the RF-term can be determined using linear response theory, where the coupling between the fermions and curvature is treated perturbatively.

Second, an RF-term can also arise if the disclination defects host lower dimensional SPTs. In 3 + 1D disclinations are line-like objects, and can in principle host 1 + 1D SPTs. This SPTs will be protected by either PHS or mirror symmetry, depending on the relevant symmetry protecting the rTCI. For both PHS and mirror symmetry, there exist 1 + 1D SPTs with quantized polarization, i.e. Su-Schrieffer-Heeger (SSH) chains. Adding such an SPT to a $2\pi/n$ disclination shift the polarization of the disclination by $\frac{1}{2}$ in spinless systems, since the spinless SSH chain has half-integer polarization[27]. For spin-1/2 systems, this effect can shift the polarization of a disclination by 1, since the spin-1/2 SSH chain has odd-integer polarization[35]. As noted previously, the polarization of a $2\pi/n$ disclination lines is equal to $\Phi/2\pi n$. So if the $2\pi/n$ disclinations host polarized SPTs, the coefficient of the RF-term will be shifted by πn for spinless fermions and $2\pi n$ for spin-1/2 fermions. This effect arises from the discrete properties of the disclinations and cannot be probed within the linear response framework discussed previously.

These two effects–the coupling of the fermions to the disclination curvature and the topology of the disclinations–are independent, and in principle both must be considered separately to determine the full RF-response term. For $n = 2, 4, 6$, the contribution to Φ from the topology of the disclinations comes in multiple of 2π for spinless fermions and a multiple of 4π for spin-1/2 fermions. Due to the periodicity of Φ, these contributions are trivial for both spinless and spin-1/2 fermions, and so the RF-term is determined solely by the coupling of the fermions to lattice curvature. The RF-term for such systems can therefore be uniquely determined within linear response theory. However, for $n = 3$, the contribution to Φ from the topology of the disclinations is non-trivial, and hence the full RF-term cannot be fully determined by linear response theory.

III. ROTATION INVARIANT TOPOLOGICAL CRYSTALLINE INSULATORS WITH PARTICLE-HOLE SYMMETRY

In this section, we shall consider time-reversal invariant rTCIs that have a RF-term that is quantized by PHS. We will consider both rTCIs composed of both spinless and spin-1/2 fermions, which are described by an RF-term with $\Phi = \pi$ and $\Phi = 2\pi$ receptively.

It is worth noting that PHS does not occur as an exact symmetry in realistic electronic insulators[48]. Nevertheless, it is useful to discuss rTCIs with PHS as theoretical constructions to better understand the physical consequences of the RF-term. The rTCIs with PHS will also serve as a primer for our forthcoming discussion of rTCIs with mirror symmetry in Sec. IV. Since mirror symmetry is common in electronic insulators, the mirror symmetric rTCIs are more likely to be realized in real materials. However, as we shall discuss, the mirror symmetric rTCIs have a more complex theoretical structure, since mirror symmetry is also a spatial symmetry. For this reason, it is useful to consider the rTCIs with PHS first, in order to gain intuition about the mixed charge-geometry responses that are described by the RF-term.

A. Spinless Lattice Model

In this subsection, we will present and analyze an 8-band minimal model for the spinless rTCI with PHS and C_4 rotation symmetry (generalizations to other C_n symmetries will be discussed in Sec. V). The Bloch Hamiltonian of the minimal model is,

$$\begin{aligned}\mathcal{H}(\boldsymbol{k}) =& \sin(k_x)\Gamma^x\sigma^0 + \sin(k_y)\Gamma^y\sigma^0 + \sin(k_z)\Gamma^z\sigma^0 \\ &+ (M + \cos(k_x) + \cos(k_y) + \cos(k_z))\Gamma^0\sigma^z.\end{aligned} \tag{11}$$

where $\sigma^{x,y,z,0}$ are the Pauli matrices, plus the 2×2 identity. The 4×4 Γ matrices are defined as $\Gamma^x = \sigma^x\sigma^0$, $\Gamma^y = \sigma^y\sigma^0$, $\Gamma^z = \sigma^z\sigma^z$, $\Gamma^0 = \sigma^z\sigma^x$, and $\Gamma^5 = \sigma^z\sigma^y$. The bulk spectrum of Eq. 11 is

$$\begin{aligned}E^2 =& \sin(k_x)^2 + \sin(k_y)^2 + \sin(k_z)^2 \\ &+ (M + \cos(k_x) + \cos(k_y) + \cos(k_z))^2.\end{aligned} \tag{12}$$

The bulk spectrum is gapped unless $|M| = 1, 3$. For $|M| > 3$, the lattice model is a trivial insulator, and is adiabatically connected to the atomic limit ($M \to \pm\infty$). As we shall show, for $1 < |M| < 3$ the lattice model is an rTCI with a $\Phi = \pi$ RF-term. For $|M| < 1$ the RF-term again vanishes.

The model in Eq. 11 has U(1) charge conservation, and is invariant under TRS, PHS, and C_4 rotation symmetry. The onsite TRS and PHS operators are

$$\begin{aligned}\hat{\mathcal{T}} &= \Gamma^y\sigma^y K = \sigma^y\sigma^0\sigma^y\mathcal{K}, \\ \hat{\mathcal{C}} &= \Gamma^{5y}\sigma^y K = \sigma^x\sigma^y\sigma^y\mathcal{K}.\end{aligned} \tag{13}$$

where $\Gamma^{ab} \equiv -i\Gamma^a\Gamma^b$ $(a, b = 0, x, y, z, 5)$ and $\mathcal{K}$ is complex conjugation. Since the fermions are spinless, $\hat{\mathcal{T}}^2 = \hat{\mathcal{C}}^2 = 1$. There is also the chiral symmetry, defined as $\hat{\Pi} = \hat{\mathcal{T}}\hat{\mathcal{C}}$. The C_4 symmetry operation is

$$\hat{U}_4 = \exp\Big(i\frac{\pi}{4}[\Gamma^{yx}\sigma^0 + \mathrm{I}\sigma^z]\Big), \tag{14}$$

such that $\hat{U}_4^{-1}\mathcal{H}(\boldsymbol{k})\hat{U}_4 = \mathcal{H}(R_4^z\boldsymbol{k})$, where R_4^z rotates the lattice momentum by $\pi/2$ around the z-axis. Since we are considering spinless fermions, $(\hat{U}_4)^4 = +1$. If the C_4 symmetry were absent, this system would be trivial. This can be seen from the fact that without C_4 symmetry, this model is in symmetry class BDI, which has no non-trivial system in $3 + 1$D[1, 2].

1. Response Theory

To derive the effective response theory of the lattice model in Eq. 11, we will consider the system close to the band crossing at $M = -3$. At this point, a pair of 4-component Dirac fermions form at $\boldsymbol{k} = (0, 0, 0)$. The low energy continuum Hamiltonian for the Dirac fermions is

$$\begin{aligned}\hat{\mathcal{H}} =& \Psi^\dagger\mathcal{H}\Psi \\ \mathcal{H} =& \Gamma^x\sigma^0 i\partial_x + \Gamma^y\sigma^0 i\partial_y + \Gamma^z\sigma^0 i\partial_z + m\Gamma^0\sigma^z\end{aligned} \tag{15}$$

where $m \sim M+3$, and Ψ is an 8 component Dirac fermion operator. Here, $m < 0$ corresponds to the lattice model with $M < -3$. As discussed, in this regime the lattice model is a trivial insulator. Similarly, $m > 0$ corresponds to the lattice model with $-3 < M < -1$, and as we shall show, in this regime the lattice model is an rTCI with a $\Phi = \pi$ RF-term.

To determine the response theory of Eq. 15, we will gauge the U(1) and C_4 symmetries, and introduce the gauge fields A_μ and spin connection ω_μ. As shown in Appendix B, in the continuum limit, the spin connection minimally couples to the Dirac fermions, via a term proportional to the angular momentum in the covariant derivative,

$$D_\mu = \partial_\mu - iA_\mu - i\frac{1}{2}\omega_\mu[\Gamma^{yx}\sigma^0 + \mathrm{I}\sigma^z]. \tag{16}$$

The Lagrangian for the minimally coupled Dirac fermions in curved space is given by[49]

$$\mathcal{L} = \bar{\Psi}[iE^\mu_A\bar{\Gamma}^A\sigma^z D_\mu - m\mathrm{I}\sigma^0]\Psi \tag{17}$$

where E^μ_A are the inverse frame-field introduced in Sec. II A, $\bar{\Psi} = \Psi^\dagger\bar{\Gamma}^0\sigma^z$ and $\bar{\Gamma}$ are 4×4 gamma-matrices. In relation to the matrices in the Hamiltonian in Eq. 11, $\bar{\Gamma}^A = \Gamma^0\Gamma^A$ for $A = x, y, z$ $\bar{\Gamma}^5 = \Gamma^0\Gamma^5$, and $\bar{\Gamma}^0 = \Gamma^0$. Under a C_4 gauge transformations, the frame-fields, spin connection, and continuum fermions transform as

$$\begin{aligned}
&E^\mu_x \to \cos(\theta)E^\mu_x + \sin(\theta)E^\mu_y,\\
&E^\mu_y \to -\sin(\theta)E^\mu_x + \cos(\theta)E^\mu_y,\\
&\omega_\mu \to \omega_\mu + \partial_\mu\theta,\\
&\Psi \to e^{i\theta\frac{1}{2}[\Gamma^{xy}\sigma^0 + \mathrm{I}\sigma^z]}\Psi,
\end{aligned} \tag{18}$$

where θ is a function of x_μ that takes values in $\{0, \pi/2, \pi, 3\pi/2\}$. Here, the C_4 gauge symmetry is actually part of a larger SO(2)=U(1) gauge symmetry that continuously rotates the Dirac fermions. This U(1) gauge symmetry is defined as in 18, but with θ taking continuous values in $[0, 2\pi)$. The original lattice model does not have this U(1) gauge symmetry. Rather, it is a new feature that emerges in the continuum limit.

In addition to the gauge fields, we will also add an additional PHS breaking perturbation to Eq. 17,

$$\hat{\mathcal{H}}' = \bar{\Psi}m'\bar{\Gamma}^5\sigma^0\Psi, \tag{19}$$

and set $m = -\bar{m}\cos(\phi)$ and $m' = -\bar{m}\sin(\phi)$, where ϕ is a background field. We will keep $\bar{m} > 0$ fixed, and treat ϕ as a new parameter for the theory, such $\phi = 0$ corresponds to the $m < 0$, trivial insulator, and $\phi = \pi$ corresponds to the $m > 0$ insulator[27]. Physically, non-constant values of ϕ encode either domain walls or adiabatic evolutions of the Hamiltonian. For examples, $\phi = \frac{\pi}{2}[1 - \tanh(z/\xi)]$ corresponds to a PHS breaking domain wall between the $m < 0$ and $m > 0$ insulators that is located near $z = 0$ and has width ξ. Similarly, $\phi = \pi t/T$ corresponds to an PHS breaking adiabatic evolution from the $m > 0$ insulator at $t = 0$ to the $m < 0$ insulator at $t = T$.

The effective response theory in terms of A_μ, ω_μ, and ϕ can be found by integrated out the massive fermions via a diagrammatic expansion[50]. Here, we are interested in the contributions from the triangle diagrams in Fig 2. These diagrams evaluate to

$$\mathcal{L}_{\text{eff}} = \frac{\phi}{4\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa. \tag{20}$$

For $m < 0$ ($\phi = 0$) the effective response vanishes, in agreement with the fact that the lattice model is trivial for $M < -3$. For $m > 0$ ($\phi = \pi$) the effective response is,

$$\mathcal{L}_{\text{eff}} = \frac{1}{4\pi}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa, \tag{21}$$

which is the RF-term from Eq. 1 with $\Phi = \pi$. As discussed in Sec. II C, the value of Φ is quantized to be 0 or π by PHS. Because of this, higher-order diagrams do not contribute to the value of the RF-term for the particle hole-symmetric rTCI. We therefore conclude that the lattice model is an rTCI with non-trivial RF-term when $-3 < M < -1$. Similar calculations show that the coefficient of the RF-term, Φ, vanishes for $|M| < 1$ and $|M| > 3$, and that $\Phi = \pi$ for $1 < |M| < 3$.

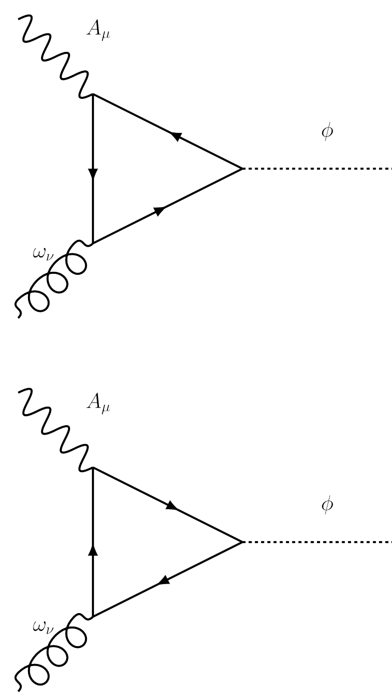

FIG. 2: The relevant Feynman diagrams for calculating the response theory in Eq. 20.

As a final point, we also note that increasing ϕ from 0 to 2π, in Eq. 17 is a periodic process that takes the trivial insulator back to itself. Based on the diagrammatic calculation in Eq. 20, an RF-term with $\Phi = 2\pi$ is generated during this process. This agrees with our earlier conclusion that Φ is 2π periodic for spinless fermions.

2. *Surface Theory*

In this subsection, we will analyze the surface theory of the rTCI. This will be done by considering a domain wall where $-3 < M < 1$ for $z < 0$, and $M < -3$ for

$z > 0$, i.e. a domain wall between the rTCI and a trivial insulator. This mass configuration generates a pair of gapless 2-component Dirac fermions that are localized at the $2+1$D domain wall[51]. The Hamiltonian for the surface Dirac fermions is

$$\begin{aligned} \hat{\mathcal{H}}_{\mathrm{surf}} &= \psi^\dagger \mathcal{H}_{\mathrm{surf}} \psi, \\ \mathcal{H}_{\mathrm{surf}} &= [\sigma^x\sigma^0] i\partial_x - [\sigma^y\sigma^0] i\partial_y, \end{aligned} \tag{22}$$

where ψ is a 4-component spinor. The TRS, PHS, and C_4 symmetry act on the surface Hamiltonian as

$$\begin{aligned} \hat{\mathcal{T}}_{\mathrm{surf}} &= \sigma^y\sigma^y K, \\ \hat{\mathcal{C}}_{\mathrm{surf}} &= \sigma^x\sigma^x K, \\ \hat{U}_{4-\mathrm{surf}} &= \exp\Big(i\frac{\pi}{4}[-\sigma^z\sigma^0 + \sigma^0\sigma^z]\Big). \end{aligned} \tag{23}$$

Consistent with the bulk theory, $\hat{\mathcal{T}}^2_{\mathrm{surf}} = \hat{\mathcal{C}}^2_{\mathrm{surf}} = (\hat{U}_{4-\mathrm{surf}})^4 = +1$. To show that the surface Dirac cones are symmetry protected, we note that a mass term for Eq. 22 must be proportional to $\sigma^z\sigma^{0,x,y,z}$. All of these terms break one of the symmetries in Eq. 23. Specifically, the $\sigma^z\sigma^0$ term breaks TRS and chiral symmetry, the $\sigma^z\sigma^z$ term breaks PHS and chiral symmetry, and the $\sigma^z\sigma^{x,y}$ terms breaks C_4 symmetry.

Based on our discussion of the effective field theory in Sec. II C, we now consider gapping the surface by adding a PHS breaking mass term $m_s\sigma^z\sigma^z$. The response theory for the massive symmetry broken surface is found by coupling the fermions to the gauge field A_μ and spin connection ω_μ via the covariant derivative

$$D_j = \partial_j - iA_j - i\frac{1}{2}\omega_j[\sigma^z\sigma^0 + \omega_j\sigma^0\sigma^z], \tag{24}$$

and integrating out the massive fermions via a diagrammatic expansion. The resulting response theory contains a Wen-Zee term,

$$\mathcal{L}_{\mathrm{surf}} = \frac{\mathrm{sgn}(m_s)}{4\pi}\epsilon^{\mu\nu\rho}\omega_\mu\partial_\nu A_\rho. \tag{25}$$

This is exactly the anomalous surface term from Eq. 8 with $\Delta\Phi = \pm\pi$. Addition local surface effects can shift the coefficient of the surface Wen-Zee term by $1/2\pi$, and, in general, a $\pi/2$ surface disclination bind charge $\frac{1}{8} + \frac{m}{4}$ with $m \in \mathbb{Z}$.

If there is both a top and bottom surface, a disclination of the top surface will be accompanied by a disclination on the bottom surface, provided that any disclination-lines do not terminate in the bulk. Based on our previous analysis, and charge conservation, the surface disclinations will bind charge $\pm(\frac{1}{8} + \frac{m}{4})$ respectively. The disclinated $3+1$D rTCI will therefore have a net z-direction polarization $P_z = \frac{1}{8} + \frac{m}{4}$. The disclinations of the rTCI therefore carry a quantized polarization, as predicted by the RF-term.

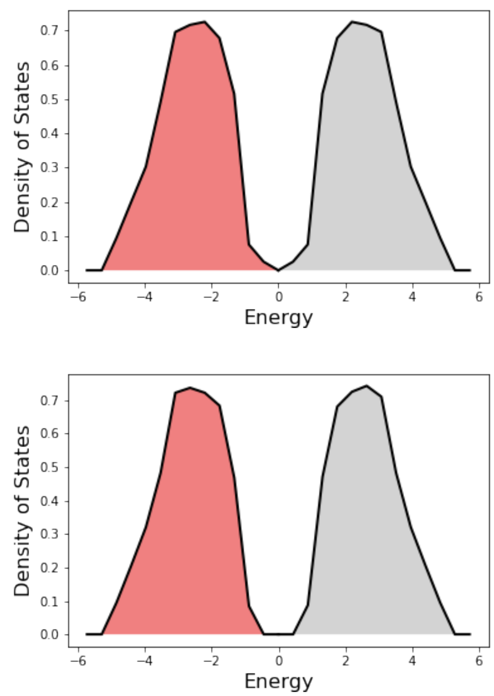

FIG. 3: Numerical calculations of the density of states of the lattice model in Eq. 11 with $M = -2$, defined on a $8 \times 8 \times 16$ lattice with open boundaries. Top) The spectrum for symmetry preserving surface, which have midgap surface states. Bottom) The energy spectrum when PHS is broken at the surfaces by Eq. 26 with $m_s = 0.5$, gapping the surface states.

3. *Numerics*

In this subsection, we will numerically verify our previous analysis. To do this, we consider the model in Eq. 11 defined on a lattice with open boundaries. For this geometry, we find midgap states in the rTCI density of states (see Fig. 3 top). The midgap states correspond to the gapless surface states of the rTCI, and can be gapped out by adding an oniste PHS breaking term of the form

$$\hat{\mathcal{H}}_s = m_s c^\dagger(r)\Gamma^5\sigma^0 c(r) \tag{26}$$

to all surfaces of the lattice model. Here, $c^\dagger(r)$ is the 8-component fermion creation operator at site r. The density of states with the additional surface perturbation shows no midgap states (see Fig. 3 bottom).

Let us now consider the charge distribution of the rTCI when PHS symmetry is broken at the surface by Eq. 26. Here, we will add negative background charges at each lattice site, such that the system is charge neutral at half-filling. Physically, these negative charges correspond to the ions that form a crystalline solid. When the lattice is free of disclinations, the charge distribution is uniform, as shown in Fig 5 top). To probe the mixed geometry-charge response of the rTCI with PHS breaking surfaces, we add a $\pi/2$ disclination-line to the lattice via the setup

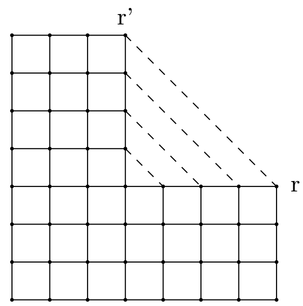

FIG. 4: An xy-cross section of the disclinated lattice.

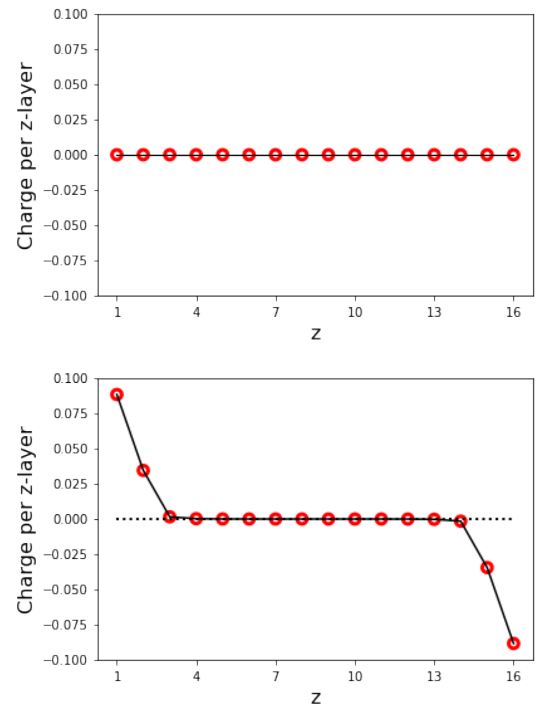

FIG. 5: The charge distribution along the z-direction for the Hamiltonian in Eq. 11 with $M = -2$ and PHS breaking surface term in Eq. 26 with $m_s = 0.5$. The system is defined on a $8 \times 8 \times 16$ lattice with open boundaries, and background charges are added such that the system is charge neutral at half-filling. (a) The charge distribution when the lattice is free of disclinations (b) The charge distribution when the lattice has a $\pi/2$ disclination, as shown in Fig 4.

shown in Fig 4. The dashed bonds correspond to hopping terms of the form $c^\dagger(r')T_{disc}c(r)$, where the matrix T_{disc} is defined as

$$T_{disc} = T_x^\dagger U_4^{-1} = U_4^{-1} T_y, \tag{27}$$

where T_x and T_y are the single particle hopping matrices for neighboring sites in the x and y directions, respectively. As shown in Fig. 5 bottom, when there is a disclination, excess charge is localized on the top and bottom surfaces of the rTCI. As noted previously, the charge that is bound to a surface disclination is only meaningfully defined modulo $\frac{1}{4}$, due to surface effects.

Fig 6 shows the net charge (mod($\frac{1}{4}$)) that is localized on the top surface of the disclinated lattice model for various values of M. When $1 < |M| < 3$ the disclinated surface has an extra $\frac{1}{8}$ surface charge, indicating that the lattice model is an rTCI with a non-trivial RF-term is these regimes. When $|M| > 3$ and $|M| < 1$ the surface charge is 0 mod($\frac{1}{4}$), indicating that the RF-term is trivial in these regimes. These results are in full agreement with our previous analysis.

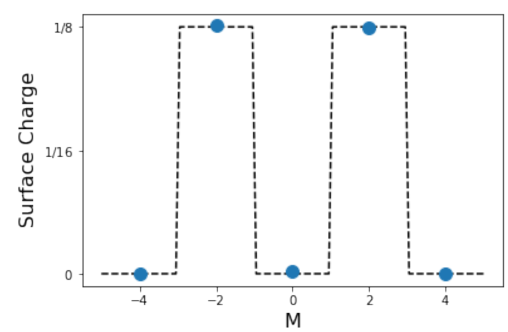

FIG. 6: The charge bound to a $\pi/2$ surface disclination for the Hamiltonian in Eq. 11 and 26, for $M = 0, \pm 2, \pm 4$ with $m_s = 0.5$. The calculations were done using a $8 \times 8 \times 16$ with open boundaries and a $\pi/2$ disclination, as shown in Fig 4. The dashes lines indicate the theoretical value of the surface charge.

4. Dimensional reduction to a 1+1D SPT

In Ref. 29, Song et al. showed that a TCI protected by a crystalline symmetry is adiabatically connected to a lower-dimensional SPT, and the crystalline symmetry of the higher-dimensional TCI becomes an onsite symmetry of the lower-dimensional SPT. In the subsection, we will use this logic to dimensionally reduce the $3+1$D rTCI to a $1+1$D SPT with an onsite U(1) symmetry, PHS, TRS, and $\mathbb{Z}_4$ symmetry, the latter of which is inherited from the C_4 rotation symmetry of the rTCI. As we shall show, this $1+1$D SPT is equivalent to the topological phase of the well known Su-Schrieffer-Heeger (SSH)[20] chain with an additional trivial $\mathbb{Z}_4$ symmetry.

This connection will be established as follows. Using the rTCI surface theory from Sec. III A 2, we will show that there exists a symmetry preserving deformation that trivialized the entire rTCI surface, except for the C_4 rotation center of the surface. The rotation center of the deformed surface hosts a zero-energy mode that is protected by PHS. The rotation center also binds an additional half integer of charge. These are exactly the same topological features that are found at the edge of an SSH chain. The equivalence of the deformed rTCI and the SSH chain therefore follows from the bulk-boundary correspondence.

To this end, we consider the surface theory for a single domain wall oriented normal to the z-direction in Eq. 22.

To the surface Hamiltonian, we add the following generic mass deformation term,

$$\mathcal{H}_{\text{surf-mass}} = m_x\sigma^z\sigma^x + m_y\sigma^z\sigma^y + m_z\sigma^z\sigma^z, \tag{28}$$

and set $m_z = 0$, $m_x + im_y = m_s(r)\exp(i\theta)$, where (r, θ) are polar coordinates on the surface, and $m_s(r) \geq 0$ is a function of the radial coordinate that vanishes at $r = 0$, and goes to a non-zero constant $\bar{m}_s$, as $r \to \infty$. Due to the dependence on the radial angle θ, this term is invariant under C_4 rotations, as well as PHS and TRS. The single particle spectrum of the surface theory can be explicitly solved. In Appendix C we show that the deformed surface has a single zero-energy mode ψ_0 that is localized at the rotation center, $r = 0$. This mode is protected by PHS, and transforms trivially under C_4 rotations.

Additionally, a net half-integer of charge is localized at $r = 0$. To show this, we take the zero-energy mode to be empty, and integrate out the remaining massive fermions. The effective theory for the massive fermions can be written in terms of the fluctuations of the mass terms $m_{x,y,z}$[52, 53],

$$\begin{aligned}\mathcal{L}_{\text{surf-mass}} &= \frac{\epsilon^{\mu\nu\rho}}{8\pi}\boldsymbol{n}\cdot(\partial_\mu\boldsymbol{n}\times\partial_\nu\boldsymbol{n})A_\rho,\\ \boldsymbol{n} &= \frac{\boldsymbol{m}}{|\boldsymbol{m}|}, \quad \boldsymbol{m} = (m_x, m_y, m_z).\end{aligned} \tag{29}$$

Using Eq. 29, we find that a charge $Q = -\frac{1}{2}$ is localized at $r = 0$ for the mass configuration defined above[54]. Due to the aforementioned zero-energy mode, this charge is only meaningfully defined modulo 1.

In total, we find that the surface of the rTCI can be symmetrically gapped expect for a single zero-energy mode that is localized at the rotation center and protected by PHS. The rotation center also binds charge $\frac{1}{2}$ mod (1). These are exactly the topological features that are found at the edge of a $1 + 1$D SSH chain. Using the bulk-boundary correspondence, we can conclude that since the surface physics of the deformed rTCI and SSH chain are equivalent, the bulks of the two systems are also equivalent, up to an adiabatic deformation.

It is also possible to apply this procedure to an rTCI with fully open boundary conditions on all surfaces. In this case, the surface mass term defined in Eq. 28 must be continued into a mass term that covers all surfaces. This mass term will fully gap the spectrum, except for at two point, one at the rotation center on the top surface and one at the rotation center on the bottom surface. These points host protected zero-modes, and bind a half-integer of charge. The rotation centers are therefore equivalent to the two edges of a finite SSH chain.

5. *Surface Topological Order*

If interactions are not present, the spinless rTCI does not support a fully gapped symmetric surface. However, as we shall show, if interactions are included, the rTCI can support a fully gapped symmetric surface with topologically order. This is similar to the topological orders that are found on the surfaces of the time-reversal invariant topological insulators[44, 55–57].

The rTCI surface topological ordered is Abelian, with anyon content $\{1, e, e^2, e^3, m, m^2, m^3, e^a m^b\} \times \{1, f\}$, for $a, b = 1, 2, 3$. The f particle is a fermion and the e and m anyons are self bosons with $\pi/2$ mutual statistics. The surface topological order is enriched by C_4 rotation symmetry[58], such that the anyons carry both charge and angular momentum. Specifically, the e anyon has charge $\frac{1}{2}$ and angular momentum 0, and the m anyon has charge 0 and angular momentum $\frac{1}{4}$. As we shall discuss, This topological order is anomalous for $2 + 1$D system with PHS, but can be realized on the surface of the $3 + 1$D rTCI with PHS.

To construct this topologically ordered surface state, we will use a vortex proliferation argument[55]. The first step of this argument is to gap out the surface fermions by adding superconducting terms that break U(1) charge conservation, C_4, rotation symmetry, TRS, PHS and chiral symmetry. To do this, it will be useful to rewrite the 4 component surface spinor ψ from Eq. 22 as $\psi = (\psi_1, \psi_2)$, where $\psi_{1,2}$ is a two-component Dirac spinors. In terms of these spinors, the superconducting terms are

$$\hat{\mathcal{H}}_{\text{SC}} = i\Delta_1\psi_1\sigma^y\psi_1 + i\Delta_2\psi_2\sigma^y\psi_2 + h.c.. \tag{30}$$

Under the U(1) and C_4 symmetries, $\Delta_{1,2}$ transforms as

$$\begin{aligned}&\text{U}(1) : (\Delta_1, \Delta_2) \to (\Delta_1^{i2\theta}, \Delta_2^{i2\theta})\\ &C_4 : (\Delta_1, \Delta_2) \to (\Delta_1^{i\pi/2}, \Delta_2^{-i\pi/2}).\end{aligned} \tag{31}$$

The surface superconductivity therefore consists of a condensate of Cooper pairs with charge 2 and angular momentum ± 1. The rest of the symmetries act as $T : \Delta_{1,2} \to \Delta_{2,1}^*$, and $C : \Delta_{1,2} \to -\Delta_{2,1}^*$.

To restore the surface symmetries, we can follow the well known procedure of vortex proliferation and disorder the superconducting terms, ($\langle\Delta_i\rangle = 0$). There are two types of vortices that we must consider here. First there are vortices where Δ_1 and Δ_2 both wind by $2\pi n$ ($n \in \mathbb{Z}$). Preempting our later identification of these vortices with the m anyons of the theory, we shall refer to them as $2\pi n$ m-vortices. Second, there are vortices where Δ_1 winds by $2\pi n$, and Δ_2 winds by $-2\pi n$, which we will refer to as $2\pi n$ e-vortices. To understand why we must consider both e and m-vortices, we note that if we just proliferate m-vortices, the composite operator $\Delta_1\Delta_2^*$ would not be disordered (see Eq. 31). This composite operator breaks C_4 symmetry, so the resulting surface would have U(1) symmetry, but not C_4 symmetry. A similar argument shows that only proliferating the e-vortices results in a surface state with unbroken C_4 symmetry, and broken U(1) charge conservation.

With this in mind, let us consider what vortices can be condensed to restore the surface symmetry. Following the usual logic, the condensable vortices must be commuting bosons with vanishing quantum numbers. Additionally, in order for the resulting surface to be gapped, the condensed vortices must not have any protected zero-modes. To determine the quantum numbers and statistics of the e and m-vortices, we first note that due to the symmetry transformations in Eq. 31, a 2π m-vortex is created by a π $(\frac{hc}{2e})$ U(1) flux, and a 2π e-vortex is generated by a 2π disclination. Let us now consider tunneling an electromagnetic monopole into the bulk of the rTCI. This process leaves behind a 2π U(1) flux on the surface, equiv. a 4π m-vortex. Based on our discussion of the RF term in Sec. II B a magnetic monopole in the bulk of the spinless rTCI carries angular momentum $\frac{1}{2}$. From conservation of angular momentum, the 4π m-vortex must have angular momentum $-\frac{1}{2}$, and the 2π m-vortex must have angular momentum $-\frac{1}{4}$. Similarly, a 2π disclination monopole in the bulk carries charge $\frac{1}{2}$, and so a 2π e-vortex has charge $-\frac{1}{2}$. Additionally, from the bulk braiding statistics of the flux and disclination lines, we can conclude that both types of vortices are self-bosons, and that a 2π e-vortex and a 2π m-vortex have $\pi/2$ mutual statistics.

Let us now consider the zero modes of the vortices. The 2π e and the 2π m-vortices both host a single complex fermion zero-mode. This comes from the fact that a 2π m-vortex is a combination of a 2π vortex of and a 2π vortex of Δ_2, each of which host a single Majorana zero mode[59]. This complex zero-mode is protected from acquiring a gap by PHS. The same logic indicates that a 2π e-vortex also has a complex zero-mode that is protected by PHS.

Based on these observations, the surface symmetry can be restored by simultaneously condensing the following two combinations of vortices 1) the combination of an 8π e-vortex, an 8π m-vortex, and a Cooper pair with charge 2 and angular momentum 1, and 2) the combination of an 8π e-vortex, a -8π m-vortex, and a Cooper pair with charge 2 and angular momentum -1. Both of these combinations have vanishing charge, vanishing angular momentum, and trivial mutual statistics. Additionally, both vortex combinations have a total of 8 complex fermions, and these fermions can be gapped out while preserving PHS. Under the first combination of vortices, Δ_1 winds by 16π, while Δ_2 winds by 0, and under the second combination Δ_1 winds by 0, while Δ_2 winds by 16π. Condensing both combinations of vortices therefore disorders Δ_1, Δ_2, and any composite operators descendants. The resulting surface state is therefore both gapped and symmetry preserving.

The resulting surface has several non-trivial deconfined excitations (anyons). First, there are the fermionic excitations that are the remnant of the gapped complex fermion zero modes. We will label these excitations as f. The rest of the anyons correspond to vortices that have trivial statistics with the condensed vortex combinations. Here, both $2\pi n$ e-vortices and $2\pi n$ m-vortices (as well as the fusions of the two) are deconfined. We will label the -2π e-vortex with an unoccupied complex zero-mode as the e anyon (the -2π e-vortex with an occupied complex zero-mode is $e \times f$). Similarly, we will label the -2π m-vortex with an unoccupied zero-mode as the m anyon. Based on our earlier observations, the e and m anyons are self bosons with $\pi/2$ mutual statistics. The e particle has charge $\frac{1}{2}$ and angular momentum 0, while the m particle has charge 0 and angular momentum $\frac{1}{4}$. Since the e^4 and m^4 anyons have trivial statistics with all other anyons and have non-fractionalized quantum numbers, they should be regarded as local particles and do not enter into the anyonic data of the theory. In addition to the non-trivial e and m particles, there are also

Having established the existence of the surface topological order, let us now show why this surface topological order is anomalous with respect to PHS. First, let us consider a purely 2+1D theory with the same anyon content as the surface topological order we have constructed. The bosonic part of the topological order can be represented in the K-matrix formalism as[36, 60]

$$\begin{aligned}\mathcal{L}_{\text{2D-top}} =& K_{IJ}\frac{\epsilon^{\mu\nu\rho}}{4\pi}a^I_\mu\partial_\nu a^J_\rho + \frac{\epsilon^{\mu\nu\rho}}{4\pi}q_I a^I_\mu \partial_\nu A_\rho \\ &+ \frac{\epsilon^{\mu\nu\rho}}{4\pi}s_I a^I_\mu\partial_\nu\omega_\rho\end{aligned} \tag{32}$$

where $K = 4\sigma^x$, $q_I = (2, 0)$, and $s_I = (0, 1)$. This $2+1$D theory is not consistent with PHS. This can clearly be seen from the fact that if we integrate out the dynamic gauge fields a^I_μ, the theory contains a Wen-Zee term

$$\mathcal{L}_{\text{2D-top}} = \frac{\epsilon^{\mu\nu\rho}}{4\pi}\omega_\mu\partial_\nu A_\rho, \tag{33}$$

which breaks PHS.

For an alternative perspective, let us consider a purely $2 + 1$D lattice system, with the same topological order as the gapped rTCI surface. We can consider an instanton process for this system, where a -2π U(1) flux is adiabatically inserted[57]. For a lattice system, this instanton even is a local process. However, the e anyons have charge $\frac{1}{2}$ and hence pick up an Aharonov-Bohm phase of -1 upon encircling the flux. The resolution to this seeming paradox is that the instanton event must bind an anyon that has π mutual statistics with the e anyon. This anyon must be the m^2 anyon. However, the m^2 anyons has angular momentum $\frac{1}{2}$. If angular momentum is conserved, the instanton even must therefore be accompanied by a flow of angular momentum current. The fact that inserting an electromagnetic flux drives an angular momentum current indicates that the $2 + 1$D lattice system must necessarily break PHS.

Let us now consider the same instanton event when the topological order is defined on the surface of the rTCI. Here, the flux insertion on the surface is accompanied by a monopole tunneling event in the bulk of the rTCI. As before, the flux insertion on the surface binds the m^2 anyon, which has angular momentum $\frac{1}{2}$. Additionally, due to the mixed Witten effect in the bulk of the rTCI, the monopole has angular momentum $-\frac{1}{2}$. So, the angular momentum of the full 3 + 1D system is conserved during the instanton event and there is no need for an accompanying angular momentum current on the surface. The topological order is therefore consistent with PHS when place on the surface of the rTCI.

B. Spin-1/2 Lattice Model

In this section, we will present a minimal model for the spin-1/2 rTCI with PHS and C_4 rotation symmetry. For spin-1/2 fermions, the minimal model consists of 16-band (8-bands per spin). The Bloch Hamiltonian for the minimal model is given by,

$$\begin{aligned}\mathcal{H}(\boldsymbol{k}) = &\sin(k_x)\Gamma^x\sigma^0\sigma^0 + \sin(k_y)\Gamma^y\sigma^0\sigma^0 + \sin(k_z)\Gamma^z\sigma^0\sigma^0 \\ &+ (M + \cos(k_x) + \cos(k_y) + \cos(k_z))\Gamma^0\sigma^z\sigma^0,\end{aligned} \tag{34}$$

where the spin of the fermions is given by $S^z = \frac{1}{2}\mathrm{I}\sigma^0\sigma^z$. The spectrum for the lattice model is

$$\begin{aligned}E^2 = &\sin(k_x)^2 + \sin(k_y)^2 + \sin(k_z)^2 \\ &+ (M + \cos(k_x) + \cos(k_y) + \cos(k_z))^2.\end{aligned} \tag{35}$$

The spectrum is gapped for $|M| \neq 1, 3$, and as we shall show, $1 < |M| < 3$ corresponds to the spin-1/2 rTCI with a $\Phi = 2\pi$ RF-term.

Eq. 34 conserves charge and is invariant under TRS, PHS, and C_4. The TRS and PHS operations are defined as

$$\begin{aligned}\hat{\mathcal{T}} &= i\Gamma^y\sigma^y\sigma^y K, \\ \hat{\mathcal{C}} &= i\Gamma^{5y}\sigma^y\sigma^y K.\end{aligned} \tag{36}$$

The C_4 rotations defined as

$$\hat{U}_4 = \exp\Big(i\frac{\pi}{4}[\Gamma^{yx}\sigma^0\sigma^0 + \mathrm{I}\sigma^z\sigma^0 + \mathrm{I}\sigma^0\sigma^z]\Big). \tag{37}$$

Here, $\hat{\mathcal{T}}^2 = (\hat{U}_4)^4 = -1$, since the fermions have spin-1/2.

C. Response Theory

To derive the response theory, we will follow the methodology used in Sec. III A 1 and consider the system close to the band crossing at $M = -3$ where the low energy degrees of freedom can be written in the Dirac-like form

$$\begin{aligned}\mathcal{H} = &[\Gamma^x\sigma^0\sigma^0]i\partial_x + [\Gamma^y\sigma^0\sigma^0]i\partial_y + [\Gamma^z\sigma^0\sigma^0]i\partial_z \\ &+ m\Gamma^0\sigma^z\sigma^0,\end{aligned} \tag{38}$$

with $m \sim M + 3$. To determine the effective response theory, we will gauge the U(1) charge and C_4 rotation symmetry and couple the fermions to the gauge field A_μ and spin connection ω_μ via the covariant derivative (see Appendix B),

$$D_\mu = \partial_\mu - iA_\mu - i\frac{1}{2}\omega_\mu[\Gamma^{xy}\sigma^0\sigma^0 + \mathrm{I}\sigma^z\sigma^0 + \mathrm{I}\sigma^0\sigma^z]. \tag{39}$$

Similar to before, the C_4 gauge symmetry of Eq. 38 is actually part of an enlarged U(1) gauge symmetry. In addition to the gauge fields, we will also include a PHS breaking perturbation

$$\mathcal{H}' = m'\Gamma^5\sigma^0\sigma^0, \tag{40}$$

and set $m = -\bar{m}\cos(\phi)$, and $m = -\bar{m}\sin(\phi)$, with $\bar{m} > 0$, such that $m < 0$ when $\phi = 0$, and $m > 0$ when $\phi = \pi$. The effective response theory can then be found by a diagrammatic expansion in terms of A_μ, ω_μ, and ϕ. As before, we are primarily interested in triangle diagrams shown in Fig. 2. Here, the contribution from the triangle diagrams is

$$\mathcal{L}_{\text{eff}} = \frac{\phi}{2\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa. \tag{41}$$

which differs by a factor of 2 from the effective response of the spinless lattice model, Eq. 20. For $\phi = \pi$, the effective response is,

$$\mathcal{L}_{\text{eff}} = \frac{1}{2\pi}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa, \tag{42}$$

which is exactly the RF-term in Eq. 1 with $\Phi = 2\pi$. We therefore find that the continuum model with $m > 0$ (equiv. the lattice model with $-3 < M < -1$) is a spin-1/2 rTCI with a $\Phi = 2\pi$ RF-term. Repeating this procedure for the band crossing at $M = \pm 1, 3$ we conclude that $\Phi = 2\pi$ for $1 < |M| < 3$ and vanishes otherwise.

We also note that for Eq. 38 and 40, increasing ϕ from 0 to 2π is a periodic process. During this process a $\Phi = 4\pi$ RF-term is generated, which agrees with our earlier conclusion that for spin-1/2 systems with TRS, Φ is 4π periodic.

1. *Surface Theory*

We shall now consider the surface theory of the spin-1/2 rTCI. For a C_4 invariant surface where $-3 < M < 1$ for $z < 0$, and $M < -3$ for $z > 0$, the surface theory consists of 4 2-component Dirac fermions,

$$\begin{aligned}\hat{\mathcal{H}}_{\text{surf}} &= \psi^\dagger\mathcal{H}_{\text{surf}}\psi, \\ \mathcal{H}_{\text{surf}} &= [\sigma^x\sigma^0\sigma^0]i\partial_x - [\sigma^y\sigma^0\sigma^0]i\partial_y,\end{aligned} \tag{43}$$

where ψ is an 8-component spinor. The spin of the surface fermions is given by $S^z_{\text{surf}} = \frac{1}{2}\sigma^0\sigma^0\sigma^z$. The surface symmetry operations are

$$\begin{aligned}\hat{\mathcal{T}}_{\text{surf}} &= \sigma^y\sigma^y\sigma^y K,\\ \hat{\mathcal{C}}_{\text{surf}} &= \sigma^x\sigma^x\sigma^y K,\\ \hat{U}_{4-\text{surf}} &= \exp\Big(i\frac{\pi}{4}[-\sigma^z\sigma^0\sigma^0+\sigma^0\sigma^z\sigma^0+\sigma^0\sigma^0\sigma^z]\Big).\end{aligned} \tag{44}$$

The symmetry operations satisfy $\hat{\mathcal{T}}^2_{\text{surf}} = \hat{\mathcal{C}}^2_{\text{surf}} = (\hat{U}_{4-\text{surf}})^4 = -1$, since the fermions have spin-1/2.

As expected, the surface theory can be gapped out via the PHS breaking surface mass term $m_s\sigma^z\sigma^z\sigma^0$. To find the response theory for the massive PHS breaking surface, we once again introduce the gauge field A_μ and spin connection ω_μ via the covariant derivative

$$D_\mu = \partial_\mu - iA_\mu - i\frac{1}{2}\omega_\mu[-\sigma^z\sigma^0\sigma^0+\sigma^0\sigma^z\sigma^0+\sigma^0\sigma^0\sigma^z]. \tag{45}$$

The response theory for the spin-1/2 surface is then given by the Wen-Zee term

$$\mathcal{L}_{\text{surf}} = \frac{\text{sgn}(m_s)}{2\pi}\epsilon^{\mu\nu\rho}\omega_\mu\partial_\nu A_\rho. \tag{46}$$

This is exactly the anomalous surface term associated with Eq. 1 with $\Delta\Theta = 2\pi$, and indicates that charge $\pm\frac{1}{4}$ is bound to $\pi/2$ disclinations of the surface. The coefficient of the surface Wen-Zee term can be shifted by $1/\pi$ by purely surface effects, and, in general, a surface $\pi/2$ disclination binds charge $\frac{1}{4}+\frac{m}{2}$ for $m\in\mathbb{Z}$.

2. Numerics

In this section, we numerically verify the mixed geometry-charge response of the spin-1/2 rTCI. To do this, we define Eq. 34 on a lattice with open boundaries, and a $\pi/2$ disclination a shown in Fig. 1. To gap out the surfaces of the lattice model, we add an onsite PHS breaking term of the form,

$$\hat{\mathcal{H}}_s = m_s c^\dagger(r)\Gamma^5\sigma^0\sigma^0 c(r) \tag{47}$$

to all surfaces of the disclinated the lattice. Here, $c^\dagger(r)$ is the 16-component fermion creation operator at site r.

Fig 7 shows the net charge ($\text{mod}(\frac{1}{2})$) that is localized on the top surface of the disclinated lattice model for various values of M. When $1<|M|<3$ the disclinated surface has an extra $\frac{1}{4}$ surface charge, indicating that the lattice model is a spin-1/2 rTCI with a non-trivial RF-term is these regimes. When $|M|>3$ and $|M|<1$ the surface charge is 0 $\text{mod}(\frac{1}{2})$, indicating that the RF-term is trivial in these regimes. These results are in full agreement with our previous analysis.

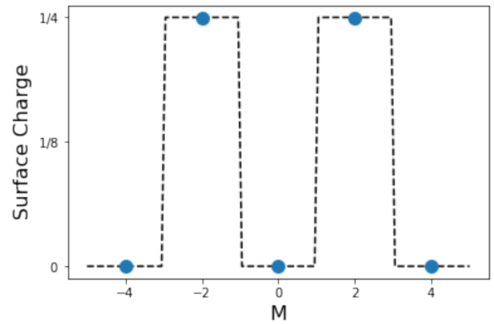

FIG. 7: The charge bound to a $\pi/2$ surface disclination for the Hamiltonian in Eq. 34 and 47, for $M=0,\pm2,\pm4$ with $m_s=0.5$. The calculations were done using a $8\times8\times16$ with open boundaries and a $\pi/2$ disclination, as shown in Fig 4. The dashes lines indicate the theoretical value of the surface charge.

3. Dimensional Reduction to a 1+1D SPT

In this subsection, we shall again use the logic of Ref. 29, and consider dimensionally reducing the $3+1$D spin-1/2 rTCI to a 1+1D SPT. As we shall show, the resulting $1+1$D SPT is equivalent to the spin-1/2 SSH chain, with an additional $\mathbb{Z}_4$ symmetry that is inherited from the C_4 symmetry of the rTCI. The spin-1/2 SSH chain can be though of as a doubled version of the spinless SSH, one copy per spin. The edge of this system hosts two zero-energy modes that form a Kramer's pair. The edge also has charge ±1 when TRS is preserved on the edge. The ±1 edge charge is protected for the spin-1/2 system, unlike the spinless version, since TRS requires that charges are added in Kramer's pairs, which carry charge 2. The $\mathbb{Z}_4$ symmetry of the SSH chain can be interpreted as a discrete internal spin rotation symmetry along the z-axis. In this interpretation, the two zero-energy modes of the spin-1/2 SSH chain have spin $S^z=\pm\frac{1}{2}$ respectively.

To show that the spin-1/2 rTCI can be dimensionally reduced to this system, we will add a mass term of the form,

$$\begin{aligned}\mathcal{H}_{\text{surf-mass}} =& m_x\sigma^z\sigma^x\sigma^0 + m_y\sigma^z\sigma^y\sigma^0\\ &+ m_z\sigma^z\sigma^z\sigma^0,\end{aligned} \tag{48}$$

to the surface theory in Eq. 43. Here, $m_z=0$, $m_x+im_y = m_s(r)\exp(i\theta)$, where (r,θ) are polar coordinates on the surface, $m_s(r)\geq0$ is a function of the radial coordinate that vanishes at $r=0$, and goes to a non-vanishing constant value $\bar{m}_s>0$ as $r\to\infty$. This mass term will trivialize the surface, except for at the C_4 rotation center. At the rotation center, there are two localized zero-energy modes, $\psi_{0\uparrow}$, and $\psi_{0\downarrow}$ (see Appendix C). These two zero-energy modes form a Kramer's pair under TRS, $\mathcal{T}:(\psi_{0\uparrow},\psi_{0\downarrow})\to(\psi_{0\downarrow},-\psi_{0\uparrow})$. Under a C_4 rotation the zero modes transform as $C_4:(\psi_{0\uparrow},\psi_{0\downarrow})\to(\psi_{0\uparrow}e^{i\frac{\pi}{4}},\psi_{0\downarrow}e^{-i\frac{\pi}{4}})$. Using the definition of the spin of the surface fermions from Sec. III C 1, $\psi_{0\uparrow}$ has spin $+1/2$ and

$\psi_{0\downarrow}$ has spin $-1/2$. Based on this the C_4 symmetry acts as a $\mathbb{Z}_4$ internal spin rotation symmetry, $\exp\left(i\frac{\pi}{2}S^z\right)$.

From this, we can conclude that there are two time-reversal symmetric surface configurations, one where both surface modes are empty, and one where both are filled. These two surface states differ by charge 2. Additionally, there are two time reversal breaking surface states, where only one of the two zero-energy modes are filled. These surface states have spin $S^z = \pm\frac{1}{2}$.

When the two zero-energy modes are empty, the effective response theory for the massive surface is

$$\mathcal{L}_{\text{eff-surf}} = \frac{\epsilon^{\mu\nu\rho}}{4\pi}\boldsymbol{n}\cdot(\partial_\mu\boldsymbol{n}\times\partial_\nu\boldsymbol{n})A_\rho, \tag{49}$$

where $\boldsymbol{n}$ is defined as in Eq. 29. Due to Kramer's degeneracy, the charge response for the spin-1/2 rTCI is twice that of the spinless rTCI in Eq. 29. Using the definition of the mass terms from above, we find there is a charge $Q = -1$ localized at $r = 0$. Due to the aforementioned gapless modes at $r = 0$, this charge is only meaningfully defined modulo 2 for a time-reversal invariant surface.

Based on this, we can conclude that the surface physics of the mass deformed spin-1/2 rTCI matches the surface physics of a spin-1/2 SSH chain with additional $\mathbb{Z}_4$ spin rotation symmetry. Namely, both surfaces have two zero modes, which form a Kramer's pair and have spin $\pm 1/2$. Additionally, when TRS is preserved, the charge at the surfaces is 1 mod (2). Using the bulk boundary correspondence, we conclude that the spin-1/2 rTCI and spin-1/2 SSH chain with additional $\mathbb{Z}_4$ spin-rotation symmetry are equivalent.

4. Surface Topological Order

Similar to the spinless model, the spin-1/2 rTCI admits a symmetric gapped topologically ordered surface state. This surface state has anyon content $\{1, v, v^2, v^3, w, w^2, w^3, v^a w^b\} \times \{1, f\}$, for $a, b = 1, 2, 3$. Similar to before, the f particle is a fermion and the v and w anyons are self bosons with $\pi/2$ mutual statistics. The v particle has charge $\frac{1}{2}$ and angular momentum 0, and the w particle has charge 0 and angular momentum $\frac{1}{2}$. This topological order can be viewed as the spinless topological order described in Sec. III A 5, except that the m particle has angular momentum $\frac{1}{2}$ instead of $\frac{1}{4}$. Nevertheless, we shall label the anyons of the spin-1/2 surface topological order as v and w instead of e and m to avoid confusion.

The spin-1/2 topological order can be constructed using a vortex proliferation argument similar to that in Sec. III A 5. As before, the starting point is to add a superconducting term to the surface theory. If we divide the 8 component spinor in Eq. 43 into 4 2-component Dirac fermions, $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)$, the superconducting surface can be written as

$$\begin{aligned}\hat{\mathcal{H}}_{\text{SC}} =& i\Delta_1\psi_1\sigma^y\psi_1 + i\Delta_2\psi_2\sigma^y\psi_2\\ &+ i\Delta_3\psi_3\sigma^y\psi_3 + i\Delta_4\psi_4\sigma^y\psi_4 + h.c..\end{aligned} \tag{50}$$

Under $U(1)$ and C_4 rotations, the Δ_is transform as,

$$\begin{aligned}&\text{U}(1) : (\Delta_1, \Delta_2, \Delta_3, \Delta_4) \to (\Delta_1^{i2\theta}, \Delta_2^{i2\theta}, \Delta_3^{i2\theta}, \Delta_4^{i2\theta})\\ &C_4 : (\Delta_1, \Delta_2, \Delta_3, \Delta_4) \to (\Delta_1^{i\pi}, \Delta_2, \Delta_3, \Delta_4^{-i\pi}).\end{aligned} \tag{51}$$

Based on this Δ_1 describes a Cooper pair with charge 2 and angular momentum 2, Δ_2 and Δ_3 describe Cooper pairs with charge 2 and angular momentum 0, and Δ_4 describes a Cooper pair with charge 2 and angular momentum -2. By extension, there also exists composite Cooper pairs with charge 0 and angular momentum ± 2. The TRS, and PHS act via

$$\begin{aligned}&T : (\Delta_1, \Delta_2, \Delta_3, \Delta_4) \to -(\Delta_4^*, \Delta_3^*, \Delta_2^*, \Delta_1^*)\\ &C : (\Delta_1, \Delta_2, \Delta_3, \Delta_4) \to (\Delta_4^*, \Delta_3^*, \Delta_2^*, \Delta_1^*).\end{aligned} \tag{52}$$

Similar to before, we can identify 2-types of vortices that must be proliferated in order to restore the all symmetries. First, there are $2\pi n$ w-vortices, where all Δ_i wind by $2\pi n$. Second, there are $2\pi n$ v-vortices where Δ_1 winds by $2\pi n$, Δ_4 winds by $-2\pi n$ and Δ_2 and Δ_3 are left invariant. Based on Eq. 51, a 2π w-vortex is generated by a π electromagnetic flux, while a 2π v-vortex is generated by a π disclination.

Using the effective response theory, we find that a -2π w-vortex has charge 0 and angular momentum $\frac{1}{2}$, and a -2π v-vortex has charge $\frac{1}{2}$ and angular momentum 0. Both the w and v-vortices are self-bosons, and the 2π w and v-vortices have $\pi/2$ mutual statistics. Additionally, a 2π w-vortex binds 4 Majorana fermions (2-complex fermions) and a 2π v-vortex binds 2 Majorana fermions (1-complex fermion). Following the same logic used in Sec. III A 5, the following two types of vortices can be simultaneously condensed, 1) an 8π w-vortex and a charge 0 angular momentum -2 composite Cooper pair, and 2) an 8π v-vortex along and a charge 2 angular momentum 0 Cooper pair. The Majorana zero modes of these vortices can all be gapped while preserving symmetry. Based on Eq. 51 and 52 proliferating these two types of vortices restores the symmetry of the surface.

The anyon content of the gapped surface theory corresponds to the vortices that have trivial braiding statistics with the condensate. These are the $2\pi n$ w-vortices, $2\pi n$ v-vortices, and their combinations. There is also a fermion f, which is the remnant of the gapped fermionic zero modes. The -2π w-vortex is a self-boson with charge 0 and angular momentum $\frac{1}{2}$, and constitutes the w anyon. The -2π v-vortex is a self-boson with charge $\frac{1}{2}$ and angular momentum 0 and constitutes the v anyon. The v and w anyons have $\pi/2$ mutual statistics. The w^4 and v^4 anyons have trivial braiding statistics and unfractionalized quantum numbers, so they can be regarded as local particles that do not enter into the anyonic data.

We can therefore conclude that the topological order described at the beginning of the section can be realized on the surface of the spin-1/2 rTCI. Due to the same logic used in Sec. III A 5 this topological order cannot be realized in a purely $2+1$D system with PHS, but can be realized on the surface of the particle-hole symmetric spin-1/2 rTCI.

IV. ROTATION INVARIANT TOPOLOGICAL CRYSTALLINE INSULATORS WITH MIRROR SYMMETRY

In this section, we will discuss time-reversal invariant rTCIs with C_4 symmetry and mirror symmetry. Much of the bulk physics of the rTCIs with mirror symmetry is the same as that of the rTCIs with particle-hole symmetry, which we discussed in detail in Sec. III. However, as noted in Sec. II D, unlike the rTCI with PHS, the surfaces of the rTCI with mirror symmetry can be gapped while preserving mirror symmetry and without introducing surface topological order. These symmetric gapped surfaces still carry an anomaly, as a $\pi/2$ surface disclination bind charge 1/8 in spinless systems, and charge 1/4 in spin-1/2 systems (half the amount that is allowed in purely $2+1$D systems).

A. Spinless Lattice Model

The spinless rTCI with TRS and mirror symmetry is again realized by 8-band lattice model in Eq. 11. Here, the mirror symmetry acts as

$$\hat{U}_{m-z} = \Gamma^{5z}\sigma^z, \tag{53}$$

where $\hat{U}_{m-z}^{-1}\mathcal{H}(k_x,k_y,k_z)\hat{U}_{m-z} = \mathcal{H}(k_x,k_y,-k_z)$. Since mirror reflection is equivalent to the combination of a $\pi/2$ rotation and inversion, $(\hat{U}_{m-z})^2 = +1$ for spinless fermions. As noted before, Eq. 11 also has PHS, however it is possible to add additional perturbations to Eq. 11 that preserve mirror symmetry and break PHS. For example, the term

$$\begin{aligned}\mathcal{H}_{\text{mirror}}(\boldsymbol{k}) =& \sin(k_x)\sin(k_z)\sigma^z\sigma^0\sigma^x \\ &+ \sin(k_y)\sin(k_z)\sigma^z\sigma^0\sigma^y,\end{aligned} \tag{54}$$

preserves TRS, C_4 symmetry, and mirror symmetry, and breaks PHS. As we shall show, the inclusion of this term does not affect the bulk response. The spectrum of the lattice model with Eq. 54 is doubly degenerate with

$$\begin{aligned}E^2 =& (1+\sin(k_z)^2)\sin(k_x)^2 + (1+\sin(k_z)^2)\sin(k_y)^2 \\ &+ (1 \pm \sqrt{\sin(k_x)^2+\sin(k_y)^2})\sin(k_z)^2 \\ &+ (M+\cos(k_x)+\cos(k_y)+\cos(k_z))^2.\end{aligned} \tag{55}$$

Here, as before, the spectrum is gapped except when $|M| = 1, 3$.

1. Response Theory

The response theory for the rTCI with mirror symmetry is found in the same way as was outlined in Sec. III A 1. If we consider the band crossing near $M=-3$, the continuum theory is again given by Eq. 15. At this point, the PHS breaking perturbation in Eq. 54 corresponds to a term that is second order in momentum and hence can be ignored.

In the continuum limit, the effective response theory is once again found by coupling the Dirac fermions to the spin connection ω and U(1) gauge field A (see Eq. 16). We will also include the perturbation in Eq. 19 and set $m = -\bar{m}\cos(\phi)$ and $m' = -\bar{m}\sin(\phi)$. Here, if ϕ is a function of z, mirror symmetry is preserved only when $\phi(z) = -\phi(-z) \bmod (2\pi)$. After integrating out the massive fermions, the response theory as a function of ω, A, and ϕ is again given by Eq. 20.

When ϕ is constant, mirror symmetry requires that $\phi = 0$ or π. The former correspond to the $m<0$ insulator ($M<-3$ in the lattice model), which is a trivial with a trivial RF-term. The latter corresponds to the $m>0$ insulator ($-3<M<-1$ in the lattice model), which is a mirror symmetric rTCI with a $\Phi=\pi$ RF-term. This analysis is much the same as that of the rTCI with PHS. However, as noted before, the coefficient of the RF-term can fluctuate while preserving mirror symmetry, provided that $\Phi(z) = -\Phi(-z) \bmod (2\pi)$. Because of this, it is possible to have mirror symmetry preserving domain walls between the rTCI and a trivial insulator (see Sec. II D). We will show this explicitly in the following section

2. Surface Theory

In order to analyze the surface theory of the rTCI with mirror symmetry, we will consider a pair of domain walls that are related to one another by mirror symmetry. Specifically, we will consider a geometry, where $-3 < M < 1$ when $|z| < z_{\text{dw}}$, and where $M<-3$ when $|z| > z_{\text{dw}}$, which corresponds to a pair of symmetry related domain walls at $z = \pm z_{\text{dw}}$ (z_{dw} is taken to be large compared to the correlation length of the insulators).

The Hamiltonian for the two surfaces is,

$$\begin{aligned}\mathcal{H}_{\text{t}} &= [\sigma^x\sigma^0]i\partial_x - [\sigma^y\sigma^0]i\partial_y, \\ \mathcal{H}_{\text{b}} &= [\sigma^x\sigma^0]i\partial_x - [\sigma^y\sigma^0]i\partial_y,\end{aligned} \tag{56}$$

where the b and t subscript indicate the top and bottom surfaces, respectively. The two surface theories can be combined as,

$$\mathcal{H}_{\text{t-b}} = [\sigma^x\sigma^0\sigma^0]i\partial_x - [\sigma^y\sigma^0\sigma^0]i\partial_y, \tag{57}$$

where the two domain walls are indexed by $\sigma^0\sigma^0\sigma^z$. The mirror symmetry acts on Eq. 57 as

$$\hat{M}_{z-\mathrm{surf}} = \sigma^0\sigma^z\sigma^x. \tag{58}$$

The possible inclusion of the bulk perturbation in Eq. 54 does not change the surface theory.

Using the 8-band description of the surfaces in Eq. 57, there are two possible surface mass terms of note. First, the mass term promotional to $\sigma^z\sigma^z\sigma^z$, which preserves TRS, and breaks mirror symmetry. Second, there is the mass term proportional to $\sigma^z\sigma^z\sigma^0$, which preserves both TRS and mirror symmetry. Hence, in agreement with our discussion from Sec. II D, we find that the surface Dirac fermions are not protected by mirror symmetry.

For the mirror symmetry breaking surface masses, the surface response theory consists of two Wen-Zee terms, one per surface. The coefficients of these two Wen-Zee terms will be opposite, up to local contributions. Following the same logic used before, a $\pi/2$ disclination of the rTCI with mirror symmetry breaking surfaces with bind charge $\pm\frac{1}{8}$ mod($\frac{1}{4}$) on one surface, and charge $\mp\frac{1}{8}$ mod($\frac{1}{4}$) on the other surface, lead to a net polarization of $P_z = \frac{1}{8}$ mod($\frac{1}{4}$).

For the mirror symmetry preserving surface masses, after integrating out the fermions, the surface response theory consists of a Wen-Zee term of the form Eq. 46 on each of the two surfaces. Due to mirror symmetry, these Wen-Zee terms have the same coefficient. A $\pi/2$ disclination to the rTCI with mirror symmetry preserving surfaces will therefore bind charge $\pm\frac{1}{8}$ mod($\frac{1}{4}$) on *both* surfaces.

In conclusion, fractional charges are bound to disclination of the massive surfaces of the rTCI regardless of whether the surfaces break or preserve mirror symmetry, and that charge bound to the surface disclination is half the amount that is allowed in purely $2+1$D systems. Hence, the fractional charge bound to surface disclinations is a robust indicator of the topology of the rTCI with TRS and mirror symmetry, even the absence of symmetry protected surface states.

It should be noted that since the rTCI hosts symmetric, non-interacting gapped surfaces, it is not necessary to include additional interactions to generated gapped topologically ordered surfaces, as we did in Sec. III A 5.

3. *Dimensional Reduction to $1+1D$ SPT*

We can also consider dimensionally reducing the rTCI with mirror symmetry to a $1+1$D SPT, as in Sec. III A 4. Here, the resulting SPTs is the SSH chain protected by mirror symmetry and a trivial onsite $\mathbb{Z}_4$ symmetry. Much like the SSH chain with PHS, the SSH chain with mirror symmetry has half-integer quantized charges at its boundaries. However, the SSH chain with mirror symmetry does not have protected zero edge modes. This is because mirror symmetry only requires that the energies of the two edge modes are equal to each other, (under PHS, the energies of any edge modes must be exactly zero). Mirror symmetry also guarantees that the two edges of the SSH chain will have the same charge.

With this in mind, let us now consider the two surface Hamiltonians in Eq. 56, and add mass perturbations of the form

$$\begin{aligned}\mathcal{H}_{\text{t-mass}} &= m_{x,\mathrm{t}}\sigma^z\sigma^x + m_{y,\mathrm{t}}\sigma^z\sigma^y + m_{z,\mathrm{t}}\sigma^z\sigma^z,\\ \mathcal{H}_{\text{b-mass}} &= m_{x,\mathrm{b}}\sigma^z\sigma^x + m_{y,\mathrm{b}}\sigma^z\sigma^y + m_{z,\mathrm{b}}\sigma^z\sigma^z.\end{aligned} \tag{59}$$

Under mirror symmetry, $m_{x,\mathrm{t}} \to -m_{x,\mathrm{b}}$, $m_{y,\mathrm{t}} \to -m_{y,\mathrm{b}}$, and $m_{z,\mathrm{t}} \to m_{z,\mathrm{b}}$. As discussed in Sec. III A 4, the rTCI can be dimensionally reduced to an SSH chain with gapless edge modes is realized by setting $m_{z,\mathrm{t}} = m_{z,\mathrm{b}} = 0$, $m_{x,\mathrm{t}} + im_{y,\mathrm{t}} = m_s(r)\exp(i\theta)$, and $m_{x,\mathrm{b}} + im_{y,\mathrm{b}} = -m_s(r)\exp(i\theta)$ where (r,θ) are polar coordinates on the surface, and $m_s(r) \geq 0$ is a function of the radial coordinate that vanishes at $r=0$, and goes to a non-zero constant $\bar{m}_s$, as $r\to\infty$. For this configuration, there is a zero energy mode on each surface located near $r=0$, which transforms trivially under C_4 symmetry.

It is possible to gap out the edge modes of the SSH chain by instead setting $m_{z,\mathrm{t}} = m_{z,\mathrm{b}} = \sqrt{\bar{m}_s^2 - m_s(r)^2}$, such that $m_{z,\mathrm{t}}$ and $m_{z,\mathrm{b}}$ take on the same non-quantized value near $r=0$. This perturbation gaps out the zero modes located at $r=0$ on each surface (see Appendix C).

To determine the charge that is bound at $r=0$, we will integrate out the massive fermions, leading to the effective response theory

$$\begin{aligned}\mathcal{L}_{\text{eff-t}} &= \frac{\epsilon^{\mu\nu\rho}}{8\pi}\boldsymbol{n}_\mathrm{t}\cdot(\partial_\mu\boldsymbol{n}_\mathrm{t}\times\partial_\nu\boldsymbol{n}_\mathrm{t})A_\rho,\\ \mathcal{L}_{\text{eff-b}} &= \frac{\epsilon^{\mu\nu\rho}}{8\pi}\boldsymbol{n}_\mathrm{b}\cdot(\partial_\mu\boldsymbol{n}_\mathrm{b}\times\partial_\nu\boldsymbol{n}_\mathrm{b})A_\rho,\\ \boldsymbol{n}_{\mathrm{t/b}} &= \frac{\boldsymbol{m}_{\mathrm{t/b}}}{|\boldsymbol{m}_{\mathrm{t/b}}|},\quad \boldsymbol{m}_{\mathrm{t/b}} = (m_{x,\mathrm{t/b}}, m_{y,\mathrm{t/b}}, m_{z,\mathrm{t/b}}).\end{aligned} \tag{60}$$

For the mass configurations discussed above, the response theory indicates that charge 1/2 is localized near $r=0$ on both the top and bottom surfaces (this charge is only defined modulo 1 due to surface effects). We can therefore conclude the rTCI with mirror symmetry can be dimensionally reduced to a $1+1$D system with unprotected edge modes, and half-integer edge charges. These are exactly the characteristic features of the SSH chain with mirror symmetry, and we can conclude that the rTCI and SSH chain with mirror symmetry are adiabatically connected.

It is worth noting that the SSH chain with mirror symmetry can be further dimensionally reduced to a non-trivial $0+1$D system with onsite $\mathbb{Z}_2$ symmetry, which is inherited from the mirror symmetry (see Ref. 61 for further discussion). By extension, the rTCI can also be dimensionally reduced to the same $0+1$D system, with an additional trivial $\mathbb{Z}_4$ symmetry.

B. Spin-1/2 Lattice Model

The spin-1/2 rTCI with mirror symmetry is again realized by 16-band lattice model in Eq. 34. Here, the mirror symmetry acts as

$$\hat{U}_{m-z} = i\Gamma^{5z}\sigma^z\sigma^0, \tag{61}$$

where $\hat{U}_{m-z}^{-1}\mathcal{H}(k_x, k_y, k_z)\hat{U}_{m-z} = \mathcal{H}(k_x, k_y, -k_z)$. Here, since we are considering spin-1/2 fermions, $(\hat{U}_{m-z})^2 = -1$. As noted before, Eq. 34 also has PHS. PHS can be broken, while preserve mirror symmetry by, for example, adding the term of the form

$$\begin{aligned}\mathcal{H}_{\text{mirror}}(\boldsymbol{k}) = &\sin(k_x)\sin(k_z)\sigma^z\sigma^0\sigma^x\sigma^0 \\ &+ \sin(k_y)\sin(k_z)\sigma^z\sigma^0\sigma^y\sigma^0.\end{aligned} \tag{62}$$

This term preserves TRS, C_4 symmetry, and mirror symmetry, and breaks PHS. The inclusion of this term does not affect the bulk response. With this term, the spectrum of the lattice model is 4-fold degenerate, with the same energy eigenvalues as given in Eq. 55.

1. *Response Theory*

The response theory for the rTCI with mirror symmetry is found in the same way as was outlined in Sec. III C. Specifically, we once again couple the Dirac fermions to the spin connection ω and U(1) gauge field A (see Eq. 39). We will also include the perturbation in Eq. 40 and set $m = -\bar{m}\cos(\phi)$ and $m' = -\bar{m}\sin(\phi)$. Here, mirror symmetry is preserved only when $\phi(z) = -\phi(-z) \bmod(2\pi)$. After integrating out the massive fermions, the response theory as a function of ω, A, and ϕ is again given by Eq. 41. The inclusion of the perturbation in Eq. 62 does not change this result.

When ϕ is constant, mirror symmetry requires that $\phi = 0$ or π. The former correspond to the $m < 0$ insulator ($M < -3$), which is a trivial with a trivial RF-term. The ladder corresponds to the $m > 0$ insulator $-3 < M < -1$, which is a mirror symmetric rTCI with a $\Phi = 2\pi$ RF-term. As noted before, the coefficient of the RF-term can fluctuate while preserving mirror symmetry, provided that $\Phi(z) = -\Phi(-z) \bmod(4\pi)$. Because of this, it is possible to have mirror symmetry preserving domain walls between the rTCI and a trivial insulator, as we shall show in the following subsection.

2. *Surface Theory*

In order to analyze the surface theory of the rTCI with mirror symmetry, we will consider a pair of domain walls, where $-3 < M < 1$ when $|z| < z_{\text{dw}}$, and where $M < -3$ when $|z| > z_{\text{dw}}$. The Hamiltonian for the two surfaces is

$$\begin{aligned}\mathcal{H}_{\text{t}} &= [\sigma^x\sigma^0\sigma^0]i\partial_x - [\sigma^y\sigma^0\sigma^0]i\partial_y, \\ \mathcal{H}_{\text{b}} &= [\sigma^x\sigma^0\sigma^0]i\partial_x - [\sigma^y\sigma^0\sigma^0]i\partial_y,\end{aligned} \tag{63}$$

or, equivalently,

$$\mathcal{H}_{\text{t-b}} = [\sigma^x\sigma^0\sigma^0\sigma^0]i\partial_x - [\sigma^y\sigma^0\sigma^0\sigma^0]i\partial_y, \tag{64}$$

where the two domain walls are indexed by $\sigma^0\sigma^0\sigma^0\sigma^z$. The mirror symmetry acts on Eq. 57 as

$$\hat{M}_{z-\text{surf}} = \sigma^0\sigma^z\sigma^0\sigma^x. \tag{65}$$

The possible inclusion of the bulk perturbation in Eq. 62 does not change the surface theory.

Eq. 64, has two surface mass terms of note. First, the mass term promotional to $\sigma^z\sigma^z\sigma^z\sigma^0$, which preserves TRS, and breaks mirror symmetry. Second, there is the mass term proportional to $\sigma^z\sigma^z\sigma^0\sigma^0$, which preserves TRS and mirror symmetry. Hence, in agreement with our discussion from Sec. II D, we find that the surface Dirac fermions are not protected by mirror symmetry.

For the mirror symmetry breaking surface masses, one surfaces hosts a Wen-Zee term with coefficient $1/2\pi$ and the other hosts a Wen-Zee term with coefficient $-1/2\pi$. A $\pi/2$ disclination of the rTCI with mirror symmetry therefore binds charge $\frac{1}{4}$ on one surface, and charge $-\frac{1}{4}$ on the other surface. In general, the value coefficient of the Wen-Zee term of each surface can be shifted by $1/\pi$ by additional surface perturbations.

For the mirror symmetry preserving surface masses, both surfaces host a Wen-Zee term with coefficient $\pm 1/2\pi$, and a $\pi/2$ disclination binds charge $\pm\frac{1}{4}$ on *both* surfaces. Surface effects can shift the coefficient of the Wen-Zee term by $1/\pi$ on both surfaces. In order to preserve mirror symmetry, such surface effects must shift the Wen-Zee terms on both surfaces by the same amount.

As before, the charge bound to surface disclinations is a robust signature of the topology of the rTCI with mirror symmetry, regardless of if the mirror symmetry is broken or preserved at the surfaces. The amount of charge that is bound to a surface disclinations is half the amount which can be bound to a disclination of purely $2+1$D spin-1/2 insulators with time-reversal symmetry, and is twice the amount which is bound to surface disclinations of the spinless rTCI with mirror symmetry.

Again, since the surfaces of the spin-1/2 rTCI with mirror symmetry hosts symmetric, non-interacting gapped surfaces, it is not necessary to include additional interactions to generated gapped topologically ordered surfaces, as we did in Sec. III C 4.

3. *Dimensional Reduction to $1+1D$ SPT*

The spin-1/2 rTCI with mirror symmetry can be dimensionally a $1+1$D spin-1/2 SSH chain protected by mirror symmetry and an onsite $\mathbb{Z}_4$ spin rotation symmetry. The spin-1/2 SSH chain with mirror symmetry has an odd integer of charge localized time-reversal symmetric boundaries, and has mirror symmetry preserving gapped boundaries. Mirror symmetry requires that the same amount of charge is bound to each boundary.

To show this, we will consider the two surface Hamiltonians in Eq. 63, and add mass perturbations of the form

$$\begin{aligned}\mathcal{H}_{\text{t-mass}} &= m_{x,\mathrm{t}}\sigma^z\sigma^x\sigma^0 + m_{y,\mathrm{t}}\sigma^z\sigma^y\sigma^0 + m_{z,\mathrm{t}}\sigma^z\sigma^z\sigma^0,\\ \mathcal{H}_{\text{b-mass}} &= m_{x,\mathrm{b}}\sigma^z\sigma^x\sigma^0 + m_{y,\mathrm{b}}\sigma^z\sigma^y\sigma^0 + m_{z,\mathrm{b}}\sigma^z\sigma^z\sigma^0.\end{aligned} \tag{66}$$

Under mirror symmetry, $m_{x,\mathrm{t}} \to -m_{x,\mathrm{b}}$, $m_{y,\mathrm{t}} \to -m_{y,\mathrm{b}}$, and $m_{z,\mathrm{t}} \to m_{z,\mathrm{b}}$. As discussed in Sec. III C 3, the rTCI can be dimensionally reduced to an SSH chain with gapless edge modes is realized by setting $m_{z,\mathrm{t}} = m_{z,\mathrm{b}} = 0$, $m_{x,\mathrm{t}} + im_{y,\mathrm{t}} = m_s(r)\exp(i\theta)$, and $m_{x,\mathrm{b}} + im_{y,\mathrm{b}} = -m_s(r)\exp(i\theta)$ where (r,θ) are polar coordinates on the surface, and $m_s(r) \geq 0$ is a function of the radial coordinate that vanishes at $r = 0$, and goes to a non-zero constant $\bar{m}_s$, as $r \to \infty$. For this configuration, there are two zero energy mode on each surface located near $r = 0$, that form a Kramer's pair and have C_4 symmetry eigenvalues $\pm 1/2$.

It is possible to gap out the edge modes of the SSH chain by instead setting $m_{z,\mathrm{t}} = m_{z,\mathrm{b}} = \sqrt{\bar{m}_s^2 - m_s(r)^2}$, such that $m_{z,\mathrm{t}}$ and $m_{z,\mathrm{b}}$ take on the same non-quantized value near $r = 0$. This perturbation gaps out the zero modes located at $r = 0$ on each surface, while preserving time-reversal symmetry. For this configuration, both of the zero modes are unoccupied on both surfaces in the ground state. If we were to instead set $m_{z,\mathrm{t}} = m_{z,\mathrm{b}} = -\sqrt{\bar{m}_s^2 - m_s(r)^2}$, then both zero modes are instead occupied on each surface in the ground state.

To determine the charge that is bound at $r = 0$, we will integrate out the massive fermions, leading to the effective response theory

$$\begin{aligned}\mathcal{L}_{\text{eff-t}} &= \frac{\epsilon^{\mu\nu\rho}}{4\pi}\boldsymbol{n}_{\mathrm{t}} \cdot (\partial_\mu \boldsymbol{n}_{\mathrm{t}} \times \partial_\nu \boldsymbol{n}_{\mathrm{t}})A_\rho,\\ \mathcal{L}_{\text{eff-b}} &= \frac{\epsilon^{\mu\nu\rho}}{4\pi}\boldsymbol{n}_{\mathrm{b}} \cdot (\partial_\mu \boldsymbol{n}_{\mathrm{b}} \times \partial_\nu \boldsymbol{n}_{\mathrm{b}})A_\rho,\end{aligned} \tag{67}$$

where $\boldsymbol{n}_{\mathrm{t/b}}$ is defined as in Eq. 60 For the mass configurations discussed above, the response theory indicates that charge 1 is localized near $r = 0$ on both the top and bottom surfaces (this charge is only defined modulo 2 due to surface effects). We can therefore conclude the rTCI with mirror symmetry can be dimensionally reduced to a $1 + 1$D system with unprotected edge modes, and odd integer edge charges. These are exactly the characteristic features of the spin-1/2 SSH chain with mirror symmetry, and we can conclude that the spin-1/2 rTCI and SSH chain with mirror symmetry are adiabatically connected.

Similar to the spinless case, the spin-1/2 SSH chain with mirror symmetry can be further dimensionally reduced to a non-trivial $0 + 1$D spin-1/2 system with onsite $\mathbb{Z}_2$ symmetry, which is inherited from the mirror symmetry[61]. By extension, the spin-1/2 rTCI can also be further dimensionally reduced to the same $0 + 1$D system, with an onsite $\mathbb{Z}_4$ spin rotation symmetry.

V. RESPONSES FOR INSULATORS WITH ADDITIONAL INVERSION SYMMETRY RENAME

In Sec. III A and III B we determined the coefficient of the RF-term, Φ, for lattice models with C_4 symmetry. This was done by treating the coupling of the fermions to the lattice curvature perturbatively, and using linear response theory. This linear response analysis can be directly extended to other C_n symmetric insulators with $n = 2, 4, 6$ that have a Dirac-like description at low energies. As we noted in Sec. II E, the perturbative approach used here is not sufficient to derive the RF-term in C_3 symmetric insulators.

In this section, we will show that for certain classes of insulators with additional inversion symmetry, the linear response analysis can be greatly simplified. Specifically, for these systems, the value of Φ can be determined by the symmetry eigenvalues of the occupied bands at the time-reversal invariant momentum (TRIM) of the Brillouin zone, i.e. lattice momentum $\boldsymbol{k}$ such that $\boldsymbol{k} = -\boldsymbol{k}$ modulo a reciprocal lattice vector.

The classes of insulators we will consider are as follows. 1) spinless insulators with TRS, C_n symmetry ($n = 2, 4, 6$), inversion symmetry, and PHS and/or mirror symmetry that have a Dirac-like the band-structure at the TRIM. 2) spin-1/2 insulators with TRS, C_n symmetry ($n = 2, 4, 6$), inversion symmetry, and PHS and/or mirror symmetry that have a Dirac-like the band-structure at the TRIM and conserve spin.

To simplify the discussion in the following sections, we note that for particle-hole, and C_n symmetric systems with $n = 2, 4, 6$, the coefficient of the RF-term, Φ, is determined by the electromagnetic response of the system to π disclinations *only*. This arises from the fact that the polarization of a $2\pi/n$ disclination is equal to $\Phi/2\pi n$ (see Sec. II B). For C_4 symmetric systems, a π disclination is a fusion of two $\pi/2$ disclination and for C_6 symmetric systems, a π disclination is a fusion of three $\pi/3$ disclination. Since the polarization must add under fusion, the polarization of a π disclination determine the value of Φ for C_4 and C_6 symmetric systems, (as well as C_2 symmetric systems, trivially). In terms of the response theory, only considering π disclinations in a C_4 or C_6 symmetric system is equivalent to only gauging the C_2 subgroup of the full rotation symmetry. Based on our previous argument, the coefficient of the RF-term that is derived from gauging only the C_2 subgroup must be the same as the coefficient of the RF-term that is derived from gauging the full rotation symmetry. We will use this in the following sections, where we will determine the value of Φ for a C_n invariant systems, by gauging only the C_2 subgroup. This will simplify our analysis, since the TRIM are invariant under C_2 rotations.

A. Spinless fermions

Here, we shall consider the RF-term for a lattice model of spinless fermions, where the band-structure is Dirac-like near the TRIM. We will take this model to have PHS, TRS (with $\mathcal{T}^2 = 1$), U(1) charge conservation, C_n symmetry, and M_x, M_y, and M_z mirror symmetries. As noted before, such a system necessarily has a C_2 rotation symmetry, and to determine the coefficient of the RF-term we only need to gauge this C_2 symmetry. Because of this, we will only consider the C_2 rotations here, but with the implicit understanding that it may be part of a larger rotation symmetry.

Before discussing the full lattice model, it will be useful to first determine the *change* in the RF-term during a generic Dirac-like band crossing. For $\mathcal{T}^2 = 1$, the most generic Dirac Hamiltonian consists of $8N$ bands, and in an appropriate basis can be written as

$$\begin{aligned}\mathcal{H}_{\text{Dirac}} =&\Gamma^x \mathrm{I}_{2N} i\partial_x + \Gamma^y \mathrm{I}_{2N} i\partial_y + \Gamma^z \mathrm{I}_{2N} i\partial_z \\ &+ m\Gamma^0 \mathrm{I}_{2N},\end{aligned} \tag{68}$$

where I_{2N} is the $2N \times 2N$ identity matrix. The TRS, PHS, C_2, inversion, and mirror symmetry act on Eq. 68 via

$$\begin{aligned}&\hat{\mathcal{T}} = \sigma^y \sigma^0 W \mathcal{K}, \\ &\hat{\mathcal{C}} = \sigma^x \sigma^y V \mathcal{K}, \\ &\hat{U}_2 = (\hat{U}_n)^{\frac{n}{2}} = \exp(i\pi[\Gamma^{xy} \mathrm{I}_{2N} + \mathrm{I}_4 S]) \\ &\hat{P} = \Gamma^0 R \\ &\hat{U}_{m-z} = \hat{U}_2 \hat{P}\end{aligned} \tag{69}$$

Here, W, V, S, and R are $2N \times 2N$ matrices that satisfy $\{S, W\} = \{S, V\} = 0$. Since spinless fermions have integer angular momentum, S must have half-integer eigenvalues. Additionally, since C_2 angular momentum is only defined mod(2), we can take S to have eigenvalues $\pm 1/2$. Based on this, and the compatibility conditions between the different symmetries, there exists a basis where

$$S = \frac{1}{2}\sigma^z \mathrm{I}_N. \tag{70}$$

In this basis inversion symmetry can be written as

$$\hat{P} = \Gamma^0 \sigma^0 R', \tag{71}$$

where R' is a $N \times N$ matrix.

Let us now consider how the RF-term changes in Eq. 68 during the band crossing, where m changes from a negative to a positive value. As before, we shall do this by gauging the U(1) and C_2 symmetries, and coupling the Dirac fermions to the electromagnetic gauge field A_μ and spin connection ω_μ, via the covariant derivative

$$D_\mu = \partial_\mu - iA_\mu - i\omega_\mu \frac{1}{2}[\sigma^z \sigma^0 \mathrm{I}_{2N} + \mathrm{I}_4 \sigma^z \mathrm{I}_N]. \tag{72}$$

We will also add an additional mass perturbation,

$$\mathcal{H}' = m' \Gamma^5 \sigma^z \mathrm{I}_N. \tag{73}$$

This term preserves TRS, but breaks PHS and mirror symmetry. Upon setting $m = -\bar{m}\cos(\phi)$, and $m' = -\bar{m}\sin(\phi)$ and integrating out the massive fermions, the RF-term in the effective Lagrangian is given by

$$\mathcal{L}_{\text{eff}}[A_\mu, \omega_\mu, \phi] = N\frac{\phi}{2\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu \omega_\nu \partial_\rho A_\kappa, \tag{74}$$

As we can see, when m changes sign, an RF-term with coefficient $\Phi = N\pi$ is generated. For spinless fermions, this term is trivial when N is even, and non-trivial when N is odd.

We would now like to relate the coefficient of the RF-term to the inversion and C_2 eigenvalues of the occupied bands. From our previous discussion of the symmetries of Eq. 68, the $4N$ occupied bands come in pairs with the same C_2 angular momentum, and the same inversion eigenvalue. This is true for any Dirac Hamiltonian with C_2 symmetry, inversion symmetry, and $\mathcal{T}^2 = 1$ TRS. To this end, let us arrange the $4N$ occupied bands such that the $2m^{\text{th}}$ and $2m-1^{\text{th}}$ occupied bands have the same inversion eigenvalue and C_2 angular momentum. We then define the following quantity

$$\beta = \prod_{m=1}^{2N} (\xi_{2m})^{\chi_{2m}}, \tag{75}$$

where ξ_{2m} and χ_{2m} are the inversion eigenvalue and C_2 angular momentum of the $2m^{\text{th}}$ occupied band respectively. Since the C_2 angular momentum is integer, $\beta = \pm 1$. During a phase transition where m changes sign, β will also change sign if a non-trivial RF-term is generated during the transition. To show this, we explicitly calculate β for the Hamiltonian in Eq. 68,

$$\beta = (-\text{sgn}(m))^N \det |R'|, \tag{76}$$

where the matrix R' is defined as in Eq. 71. Clearly, when m changes sign, β also changes sign when N is odd, and does not change sign when N is even. Since the RF-term generated when m changes sign is only non-trivial for N odd, we can conclude that a change in the RF-term is accompanied by a change in the sign of β.

Let us now consider the RF-term for an N_{band} lattice model where the band-structure is Dirac-like at the TRIM. For $\hat{\mathcal{T}}^2 = 1$, $N_{\text{band}} \in 8\mathbb{Z}$. Let us consider the bands at a given TRIM, Λ_i. As discussed before, the

$N_{\text{band}}/2$ occupied bands Λ_i must come in pairs with the same angular momentum and inversion eigenvalues. These occupied bands at Λ_i can be organized such that $\xi_{2m}[\Lambda_i] = \xi_{2m-1}[\Lambda_i]$ and $\chi_{2m}[\Lambda_i] = \chi_{2m-1}[\Lambda_i]$ are the inversion eigenvalues and C_2 angular momentum of the $2m^{\text{th}}$ and $2m-1^{\text{th}}$ occupied bands, respectively. Using this, we define,

$$\beta[\Lambda_i] = \prod_{m=1}^{N_{\text{band}}/4} (\xi_{2m}[\Lambda_i])^{\chi_{2m}[\Lambda_i]} \tag{77}$$

As we shall discuss, the coefficient RF-term, Φ, is related to $\beta[\Lambda_i]$ via

$$e^{i\Phi} = \prod_i \beta[\Lambda_i], \tag{78}$$

where the product is taken over the 8 TRIM of the 3D Brillouin zone. To show this, we first note that any two insulators with the same symmetries (and representations) can be symmetrically evolved into one another via a sequence of band crossings. Since the RF-term is quantized in particle-hole symmetric insulators, the difference in the RF-term between two particle-hole symmetric insulators, is equal to the total change in the RF-term that occurs during the aforementioned band crossings. Based on this, we can conclude that Eq. 78 correctly determines the RF-response of a given insulator provided that the right-hand side (RHS) of Eq. 78 evaluates to 1 for a trivial symmetric insulator, and that any band crossing that generates a non-trivial RF-term also changes the sign of the RHS Eq. 78.

To this end, let us consider a trivial (atomic) insulator, where the lattice Hamiltonian only contains a constant onsite potential $\mathcal{H}_{\text{Triv}} = \Gamma^0 \mathrm{I}_{N_{\text{band}}/4}$. Importantly, the band structure is constant throughout the Brillouin zone, and $\beta[\Lambda_i]$ must take the same value at all 8 TRIM. Because of this, the RHS of Eq. 78 necessarily evaluates to 1 for such an insulator.

We will now consider a generic symmetric band crossing. This band crossing can either occur at a TRIM, or at an arbitrary point in the Brillouin zone. Let us first consider the former case, where the band crossing occurs at a TRIM, Λ_i. Since we are assuming that the band-structure is Dirac-like at the TRIM, our previous analysis indicates that when a non-trivial RF-term is generated by a band crossing at Λ_i, $\beta[\Lambda_i] \to -\beta[\Lambda_i]$. Therefore, when the coefficient of the RF-term changes due to a band-crossing at a TRIM, the RHS of Eq. 78 will change as well.

We can also consider a band crossing that occurs at an arbitrary point in the Brillouin zone. Due to the symmetries of the lattice Hamiltonian, such a band crossing must be accompanied by other symmetry related band crossings. In general, it is possible to adiabatically and symmetrically evolve the lattice Hamiltonian such that the momentum space distance between the multiple band crossings is taken to zero (modulo a reciprocal lattice vector). After this evolution, all band crossings occur at single TRIM, Λ_i. So, any two insulators that are connected by multiple band crossings that occurs at arbitrary points in the Brillouin zone, can also be connected by a single band crossings that occurs at a TRIM. The difference in the RF-term and the difference in the values of $\beta[\Lambda_i]$ between the two insulators must be independent of the location of the band crossing. We now note that if the band crossings occur away from Λ_i, then the inversion eigenvalues and angular momentum of the bands at Λ_i will not be affected, and $\beta[\Lambda_i]$ will be unchanged. Additionally, if the band crossing occurs at the TRIM Λ_i, a non-trivial change in the RF-term must be accompanied by a change in the sign of $\beta[\Lambda_i]$. Since the relative values of the RF-term and $\beta[\Lambda_i]$ must be independent of where the band crossing occurs, the only consistent possibility is that any band-crossings that occur away from the TRIM do not change RF-term. Only band-crossings at a TRIM can change the RF-term. Based on this, we can conclude that Eq. 78 correctly determines the value of the RF-term coefficient, Φ, for the lattice models we have considered here.

B. Spin-1/2 Fermions with Additional Spin Conservation

Having discussed spinless fermions, we now turn our attention and derive an analogous expression for the RF-term coefficient for spin-1/2 fermions, where the band-structure is Dirac-like near the TRIM. As before, we shall consider lattice models with TRS (with $\mathcal{T}^2 = -1$), U(1) charge conservation, C_n rotation symmetry, inversion symmetry, mirror symmetry, and PHS and/or mirror symmetry. As before, we shall only consider the C_2 rotation symmetry subgroup here. In addition to these symmetries, we shall also assume that the S^z component of spin is conserved (i.e. no spin-orbit coupling). The assumption provide several useful constraints on the possible band structures, and on C_2 transformation properties of the lattice fermions.

As before, our starting point will be a single Dirac Hamiltonian with the symmetries discussed above. In general, such a Dirac Hamiltonian must consist of $16N$ bands, ($8N$ per spin). In a suitable basis, the Hamiltonian can be written

$$\begin{aligned}\mathcal{H}_{\text{Dirac}} =& \Gamma^x \sigma^0 \mathrm{I}_{2N} i\partial_x + \Gamma^y \sigma^0 \mathrm{I}_{2N} i\partial_y + \Gamma^z \sigma^0 \mathrm{I}_{2N} i\partial_z \\ &+ m\Gamma^0 \sigma^0 \mathrm{I}_{2N},\end{aligned} \tag{79}$$

where I_{2N} is the $2N \times 2N$ identity matrix. In general, the TRS, PHS, C_2 rotation symmetry, and mirror symmetries act on Eq. 68 via

$$\begin{aligned}
&\hat{\mathcal{T}} = \sigma^y\sigma^0\sigma^y W\mathcal{K},\\
&\hat{\mathcal{C}} = \sigma^x\sigma^y\sigma^y V\mathcal{K},\\
&\hat{U}_2 = \exp\Big(i\pi[\frac{1}{2}\Gamma^{xy}\sigma^0\mathrm{I}_{2N} + \frac{1}{2}\mathrm{I}_4\sigma^z\mathrm{I}_{2N} + \mathrm{I}_4\sigma^0 S]\Big),\\
&\hat{P} = \Gamma^0\sigma^0 R\\
&\hat{U}_{m-z} = \hat{U}_2\hat{P}
\end{aligned} \tag{80}$$

where W, V, S and R are $2N\times 2N$ matrices that satisfy $\{S,W\} = \{S,V\} = 0$. Here, the S^z component of spin is labelled by,

$$S^z = \frac{1}{2}\mathrm{I}_4\sigma^z\mathrm{I}_{2N} \tag{81}$$

which is reflected in the definition of $\hat{U}_2$. Additionally, since $(\hat{U}_2)^2 = -1$, S must have half-integer eigenvalues, and, as before, we can choose a basis where $S = \sigma^z\mathrm{I}_N$. In this basis, the inversion symmetry operator can be written as

$$\hat{P} = \Gamma^0\sigma^0\sigma^0 R', \tag{82}$$

where R' is an $N\times N$ with eigenvalues ± 1.

To determine the change in the RF-term as m changes sign in Eq. 79, we will again minimally the spin-1/2 fermions via

$$\begin{aligned}
D_\mu =&\partial_\mu - iA_\mu\\
&- i\omega_\mu\frac{1}{2}[\Gamma^{xy}\sigma^0\mathrm{I}_{2N} + \mathrm{I}_4\sigma^z\mathrm{I}_{2N} + \mathrm{I}_4\sigma^0\sigma^z\mathrm{I}_N],
\end{aligned} \tag{83}$$

and add an additional mass perturbation of the form

$$\mathcal{H}'[\Lambda_i] = m'\Gamma^5\sigma^0\sigma^z\mathrm{I}_N. \tag{84}$$

This term preserves TRS, but breaks PHS and mirror symmetry. Upon setting $m = -\bar{m}\cos(\theta)$, and $m' = -\bar{m}\sin(\theta)$ and integrating out the massive fermions, the effective Lagrangian for is given by

$$\mathcal{L}_{\text{eff}}[\phi] = N\frac{\phi}{\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa, \tag{85}$$

As we can see, when the sign of m changes, an RF-term with coefficient $\Phi = 2\pi N$ is generated. Hence, we find that for spin-1/2 fermions with additional S^z spin conservation, this term is trivial when N is even, and non-trivial when N is odd.

We would now like to relate the change in the RF-term to the inversion eigenvalues and angular momentum of the occupied bands. To do this, we will consider the occupied bands $S^z = +\frac{1}{2}$. These bands come in pairs with the same total-angular momentum, and inversion eigenvalue. This is a general feature of Dirac Hamiltonians with C_2 symmetry, inversion symmetry, $\mathcal{T}^2 = -1$ TRS, and S^z spin conservation. Let us arrange the $4N$ occupied bands with $S^z = +\frac{1}{2}$ such that the $2m^{\text{th}}$ and $2m-1^{\text{th}}$ occupied bands have the same inversion eigenvalue and C_2 angular momentum. We then define the following quantity,

$$\beta_\uparrow = \prod_{m=1}^{2N}(\xi^\uparrow_{2m})^{\chi^\uparrow_{2m}-\frac{1}{2}}, \tag{86}$$

where $\xi^\uparrow_{2m}$ and $\chi^\uparrow_{2m}$ are the inversion eigenvalue and C_2 angular momentum of the $2m^{\text{th}}$ occupied band with $S^z = +\frac{1}{2}$. Since $\chi^\uparrow_{2m}$ is a half-integer for spin-1/2 fermions, $\beta_\uparrow = \pm 1$. As in the spinless case, $\beta\to-\beta$ for a band crossing where a non-trivial RF-term is generated. To show this, we will explicitly evaluate Eq. 86 for the Hamiltonian in Eq. 79. Upon doing so, we find that

$$\beta_\uparrow = (-\text{sgn}(m))^N\det|R'|. \tag{87}$$

where R' is defined as in Eq. 82. We therefor conclude that when N is odd, $\beta_\uparrow$ changes sign when m changes sign, and remains the same otherwise. Since a non-trivial value of Φ is only generated when N is odd, we can conclude that when a non-trivial RF term is generated during a band crossing, $\beta_\uparrow$ changes sign as well.

We now consider the RF-term for an N_{band} spin-1/2 lattice model, where the band-structure is Dirac-like at the TRIM. For an insulator with $\hat{\mathcal{T}}^2 = -1$ and S^z spin conservation, $N_{\text{band}}\in 16\mathbb{Z}$. As discussed, at a TRIM, Λ_i there are $N_{\text{band}}/4$ occupied bands with $S^z = +\frac{1}{2}$. These occupied bands come in pairs with the same angular momentum and inversion eigenvalues, and we can organize them such that $\xi^\uparrow_{2m}[\Lambda_i] = \xi^\uparrow_{2m-1}[\Lambda_i]$ and $\chi^\uparrow_{2m}[\Lambda_i] = \chi^\uparrow_{2m-1}[\Lambda_i]$, where $\xi^\uparrow_{2m}[\Lambda_i]$ and $\chi^\uparrow_{2m}[\Lambda_i]$ are the inversion eigenvalues and C_2 angular momentum of the $2m^{\text{th}}$ occupied band with $S^z = \frac{1}{2}$ respectively. Using this, we define

$$\beta_\uparrow[\Lambda_i] = \prod_{m=1}^{N_{\text{band}}/4}(\xi^\uparrow_{2m}[\Lambda_i])^{\chi^\uparrow_{2m}[\Lambda_i]-\frac{1}{2}}, \tag{88}$$

and the invariant

$$e^{i\Phi/2} = \prod_i\beta_\uparrow[\Lambda_i], \tag{89}$$

where the product is taken over the 8 TRIM of the 3D Brillouin zone. The validity of this expression can be confirmed using the logic that we used in Sec. V A. Namely, that for a trivial insulator the RHS of Eq. 89 evaluate to 1, and for band crossings where the coefficient of the RF-term changes by 2π, the RHS of Eq. 89 also change sign.

To conclude this section, it is worth reiterating that the expressions we have derived here, were based on the assumptions the lattice Hamiltonian is Dirac-like at the TRIM, and for the case of spin-1/2 fermions, the S^z component of spin was conserved. These assumption leave out many systems that may be relevant, and worth considering. In particular, our results do not apply to spin-1/2 systems with spin-orbit coupling. Determining a more general formula for the RF-term coefficient remains an open question for further research.

VI. CONCLUSION AND OUTLOOK

In this work, we analyzed how electromagnetic and geometric features can be intertwined in $3+1$D rotation invariant insulators. Our main point of focus was a mixed geometry-charge term, denoted the RF-term, that can occur in the effective response theories of such systems. The RF-term gives rise to a mixed Witten effect, and imparts fractional statistics to magnetic fluxes lines and disclination lines. Additionally, Wen-Zee terms are bound to domain walls where the coefficient of the RF-term changes. Using symmetry analysis, and lattice models, we showed that a quantized RF-term occurs for a class of rotation invariant topological crystalline insulators with TRS, PHS, and C_n symmetry. The coefficient of the RF-term depends on if the rTCI is composed of spinless fermions or spin-1/2 fermions. The surfaces of the rTCIs host an even number of symmetry protected Dirac fermions. These Dirac fermions can be gapped out by breaking PHS, leading to a surface state with a Wen-Zee response that has half the coefficient that is allowed in purely $2+1$D systems. Additionally, the rTCI can support symmetric gapped surface states with anomalous symmetry enriched topological order.

Based on our results, there are several open questions for future work. First, there is the question of what mixed geometry-charge response are exhibited by other $3+1$D topological crystalline insulators, and how to relate a given continuum response theory to a lattice model. Linear response theory was used to accomplish the latter in this work, however, this approach cannot be used on systems where the geometric effects are non-perturbative. Second, there is the question of what other anomalous symmetry enriched topological orders can only be realized on the surface of a topological crystalline insulator. A partial answer to this question would come from a set of anomaly indicator[62] for topological orders that are enriched by crystalline symmetries. Finally, there is the question of whether any physical systems can realize the RF-term we have discussed here. In this work we found that for certain C_n, and mirror symmetric insulators without spin-orbit coupling, the RF-term is determined by the angular momentum and inversion eigenvalues of the occupied bands at TRIM. To consider more realistic materials, it will likely be necessary to generalize this result to more generic band-structures and systems with possible spin-orbit coupling. In experiments, the RF-term could be observed by using scanning probes to detect the charge that is bound to disclinations on PHS breaking surfaces.

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Appendix A: The RF-term is Systems Without Time-Reversal symmetry

In this appendix, we will discuss the RF-term in systems that do not have time-reversal symmetry (TRS). As we shall discuss, without TRS the mixed-geometry charge responses arising from the RF-term can be intertwined with the charge responses of the Θ-term (Eq. 6 in the main text).

1. Disclination Charges in $2+1$D systems with broken TRS

To demonstrate this intertwining of responses in 3+1D, we will first have to consider the interplay between geometry-charge responses, and purely charge responses in $2+1$D systems with broken TRS. As in the case with unbroken TRS, the charge bound to disclinations in $2+1$D systems with broken TRS also depends on if the fermions are spinless or have spin-1/2. As we shall show, without TRS, the charge bound to disclinations of a spinless insulator comes in multiples of $1/2n$, and, importantly, if the disclination charge is an odd multiple of $1/2n$, the insulator must have an odd (non-zero) Chern number. For spin-1/2 insulators with broken TRS, the disclination charge comes in multiples of $1/n$, and the disclination charge is independent of the Chern number of the insulator[35].

To establish this, we first note that spinless fermions satisfy $(\hat{U}_n)^n+1$, and spinless fermions satisfy $(\hat{U}_n)^n-1$, where $\hat{U}_n$ is the $2\pi/n$ rotation operator. In systems without TRS, a system of spinless fermions can be mapped onto a system of spin-1/2 fermions, and vice versa, by redefining the rotation operator

$$\hat{U}_n \to \hat{U}'_n = \hat{U}_n e^{\pm i\pi/n}, \tag{A1}$$

This phase shift of the rotation operator also changes the structure of the lattice disclinations. In particular, to change from a spinless (spin-1/2) insulator with rotation operator $\hat{U}_n$ to a spin-1/2 (spinless) insulator with rotation operator $\hat{U}'_n$, one must add an additional $\pm\pi/n$ U(1) symmetry flux to $2\pi/n$ disclinations. This extra U(1) flux binds an additional charge $\pm C/2n$, where C is the Chern number of the insulator (note that redefinition of the rotation operator does not change the Chern number of the insulator).

Based on this, if there is a spin-1/2 insulator with $C=+1$, with disclination charge $Q^n_{disc}=0$, then there exist spinless insulators with $C=+1$, and disclination charge $Q^n_{disc}=\pm1/2n$. If this is true, then, by continuing this logic, it must be true that $Q^n_{disc}=N/n$ ($N\in\mathbb{Z}$) for spin-1/2 insulator, regardless of their Chern number, and $Q^n_{disc}=N/2n$ for spinless insulators, where an odd value of N indicates that the insulator also has an odd Chern number. Conversely, if there exists a spinless insulator with $C = +1$, and $Q^n_{disc} = 0$, then there exist spin-1/2 insulators with $C = +1$, and disclination charge $Q^n_{disc} = \pm 1/2n$. If this is true, then $Q^n_{disc} = N/n$ ($N \in \mathbb{Z}$) for spinless insulator, regardless of their Chern number, and $Q^n_{disc} = N/2n$ for spin-1/2 insulators, where an odd value of N indicates that the insulator also has an odd Chern number. Importantly, it is not possible to have *both* spinless and spin-1/2 insulators with $C = +1$ and $Q^n_{disc} = 0$, as that would imply that there exist insulators with zero Chern number, and $Q^n_{disc} = 1/2n$, violating the results of Ref. 35.

Based on the numerical calculations from in Ref. 34 and 35, there are spin-1/2 insulators with $C = +1$, and $Q^n_{disc} = 0$, and spinless insulators with $C = +1$, and $Q^n_{disc} = \pm 1/2n$. We therefore conjecture that $Q^n_{disc} = N/n$ ($N \in \mathbb{Z}$) for spin-1/2 insulator with broken TRS, regardless of Chern number, and $Q^n_{disc} = N/2n$ for spinless insulators with broken TRS, and an odd value of N indicates that the insulator also has an odd Chern number. In terms of the response theories, this means that a system of spinless fermions can have a Wen-Zee term with coefficient $1/4\pi \bmod (1/2\pi)$ if and only if it also has a Chern-Simons term with coefficient $1/4\pi \bmod (1/2\pi)$. Similarly, a spinless system can have a Wen-Zee term with coefficient $0 \bmod (1/2\pi)$ if and only if it also has a Chern-Simons term with coefficient $0 \bmod (1/2\pi)$.

2. Periodicity of the RF-term in system with broken TRS

To see how the intertwining of mixed geometry-charge and purely charge responses in $2+1$D insulators affects the $3+1$D RF-term, we will consider the periodicity of the coefficient of the RF-term Φ when TRS is broken. For spin-1/2 insulators with broken TRS, the disclination charge comes in multiples of $1/n$, regardless of Chern number, and the same logic used in the main text indicates that Φ has period 2π for these systems.

The situation for spinless insulators with broken TRS is more complex. As discussed previously, a spinless insulator with broken TRS must either have disclination charge $Q^n_{disc} = 2N + 1/n$ and an odd Chern number, or disclination charge $Q^n_{disc} = 2N/n$ and an even Chern number. Based on this, we find that the coefficient of the RF-term (Φ) and the coefficient of the Θ-term have a combined periodicity, where

$$\begin{aligned}(\Phi,\Theta) &\equiv (\Phi+\pi,\Theta+2\pi) \equiv (\Phi+\pi,\Theta-2\pi)\\ &\equiv (\Phi+2\pi,\Theta) \equiv (\Phi,\Theta+4\pi)\end{aligned} \tag{A2}$$

. It is important to note, this argument only applies to systems with gauged C_n symmetry.

To show this explicitly, let us consider a domain walls where the value of Φ changes by $\Delta\Phi$. If the domain wall response can be cancelled by a purely $2+1$D insulator without topological order, then Φ and $\Phi + \Delta\Phi$ are equivalent. As noted in the main, a domain wall where the value of Φ changes by $\Delta\Phi$ hosts a Wen-Zee term with coefficient $\Delta\Phi/4\pi^2$. Based on our previous discussion, when $\Delta\Phi = \pi$ the domain wall Wen-Zee term can be cancelled adding the spinless TRS breaking $2+1$ insulator we discussed above. However, as we noted, such an insulator also has a Chern-Simons term. Therefore, if we add such a $2+1$D insulator to the RF-term domain with $\Delta\Phi = \pi$, the domain wall will not host a Wen-Zee term, but will instead host a Chern Simons term with coefficient $1/4\pi \bmod (1/2\pi)$. Hence, a domain wall where Φ changes by π cannot be *completely* trivialized by adding a purely $2+1$D system.

However, we can instead consider a domain wall of both the RF-term and the Θ-term, where Φ changes by $\Delta\Phi$ and Θ changes by $\Delta\Theta$. At this domain wall, there will be a Wen-Zee term with coefficient $\Delta\Phi/4\pi^2$, and a Chern-Simons term with coefficient $\Delta\Theta/8\pi^2$. Based on our previous discussion, when $\Delta\Phi = \pi$ and $\Delta\Theta = 2\pi$, the domain wall can be completely trivialized by a $2+1$D insulator. The RF-term and the Θ term therefore have a combined periodicity where Φ is shifted by π and Θ is shifted by 2π. The other equivalence relationships in Eq. A2 can be established using similar logic.

3. Intertwining of Pure Charge, and Geometry-Charge Responses, in rTCIs without TRS

Based on Eq. A2, there exists a spinless mirror symmetric rTCI that can only exist in TRS breaking systems. To show this, we note that both the RF and Θ-terms are odd under mirror symmetry, and so for a mirror symmetric insulator $(\Phi,\Theta) = (-\Phi,-\Theta)$. This equation admits the non-trivial solution $(\Phi,\Theta) = (\pi/2,\pi)$, which describes a non-trivial rTCI with mirror symmetry. Hence, this insulator necessarily has a both a non-trivial RF-term and a non-trivial Θ-term. The Θ-term has the same quantized coefficient as the Θ-term that describes topological insulators with TRS. The coefficient of the RF-term is half that which is allowed for mirror symmetric insulators with TRS (see Sec. II D). Since both the Θ-term and the RF-term must be non-vanishing in this insulator, we see that there is a natural intertwining of pure charge responses and geometry-charge responses in this mirror symmetric rTCI with broken mirror symmetry.

One might also expect that there is also a particle-hole symmetric rTCI that can only exist in TRS breaking systems. However, we do not find any evidence for such a system. This is because the RF-term is odd under PHS, while the Θ term is even under PHS, so an insulator with PHS, $(\Phi,\Theta) = (-\Phi,\Theta)$. Using Eq. A2 the solutions to this equation have $\Phi = 0$ or $\Phi = 2\pi$, and the value of Θ is unconstrained. These are the same values of Φ that are allowed in systems with unbroken TRS.

4. Lattice Model for the Mirror Symmetric rTCI with broken TRS

In this subsection we will present a lattice model for the spinless rTCI with C_4 symmetry, mirror symmetry and broken TRS, which we discussed in the previous section. This rTCI is realized by the 4-band model,

$$\begin{aligned}\mathcal{H}(\boldsymbol{k}) =& \sin(k_x)\Gamma^x + \sin(k_y)\Gamma^y + \sin(k_z)\Gamma^z \\ &+ (M + \cos(k_x) + \cos(k_y) + \cos(k_z))\Gamma^0,\end{aligned} \tag{A3}$$

where the Γ matrices are defined as in the main body of the text. The C_4 rotation symmetry, and mirror symmetry act on Eq. A3 as

$$\begin{aligned}\hat{U}_4 &= \exp\Big(i\frac{\pi}{4}(\Gamma^{xy} + \mathrm{I}_4)\Big), \\ \hat{U}_{m-z} &= \Gamma^{z5},\end{aligned} \tag{A4}$$

where I_4 is the 4×4 identity matrix. This model is gapped expect when $|M| = 1, 3$, and as we shall show, when $1 < |M| < 3$, this model realizes the mirror symmetric rTCI with $\Theta = \pi$ and $\Phi = \pi/2$.

We can determine the response theory for this insulator using the same methods used in the main text. Specifically, we consider the band crossing near $M = -3$, and write the continuum Hamiltonian as

$$\mathcal{H} = \Gamma^x i\partial_x + \Gamma^y i\partial_y + \Gamma^z i\partial_z + m\Gamma^0. \tag{A5}$$

We will couple this system to the spin connection ω and U(1) gauge field A via the covariant derivative

$$D_\mu = \partial_\mu - iA_\mu - i\frac{1}{2}\omega_\mu(\Gamma^{xy} + \mathrm{I}_4), \tag{A6}$$

and add the mirror symmetry breaking perturbation

$$\mathcal{H}' = m'\Gamma^5. \tag{A7}$$

If we set $m = -\bar{m}\cos(\phi)$, and $m = -\bar{m}\sin(\phi)$, we find that the effective response theory in terms of ϕ, A and ω is given by

$$\begin{aligned}\mathcal{L}_{\text{eff}} =& \frac{\phi}{8\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa + \frac{\phi}{8\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu A_\nu\partial_\rho A_\kappa \\ &+ \frac{\phi}{32\pi^2}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho\omega_\kappa.\end{aligned} \tag{A8}$$

When $\phi = 0$ ($M < -3$ in the lattice model) the response theory vanishes. When $\phi = \pi$ ($-3 < M < -1$ in the lattice model), the response theory is

$$\begin{aligned}\mathcal{L}_{\text{eff}} =& \frac{1}{8\pi}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho A_\kappa + \frac{1}{8\pi}\epsilon^{\mu\nu\rho\kappa}\partial_\mu A_\nu\partial_\rho A_\kappa \\ &+ \frac{1}{32\pi}\epsilon^{\mu\nu\rho\kappa}\partial_\mu\omega_\nu\partial_\rho\omega_\kappa.\end{aligned} \tag{A9}$$

The first two terms are the RF-term with $\Phi = \pi/2$ and the Θ-term with $\Theta = \pi$, and so we can confirm that this model realized the mirror symmetric rTCI with broken TRS that we predicted in the previous subsection. Additionally, we find that there is an addition term that is quadratic in momentum. This term was not predicted by our earlier heuristic argument, but is not unexpected, and similar terms have been previously studied[63].

Since this model has a non-vanishing RF-term and a non-vanishing Θ term, this model exhibits topological charge responses, as well as topological geometry-charge responses. Individually, the charge responses should resemble those that have been previously studied in the contexts of $3+1$D topological insulators with $\Theta = \pi$[27]. Similarly, the geometry charge responses, should be similar to those that we discuss in the main body of the text, albeit with a different quantization. It is also possible that the combination of the RF-term and the Θ term may lead to fundamentally new phenomena, but determining such phenomena is beyond the scope of this work.

Appendix B: Coupling lattice Dirac Fermions to the Spin Connection

In this appendix, we will discuss how to couple Dirac fermions to the spin connection that encodes lattice disclinations. For our purposes, it will suffice to consider Dirac fermions that are located near n-fold high symmetry points (HSPs) of the Brillouin zone of a C_n symmetric lattice.

Let us consider a single Dirac fermion located at an n-fold HSP. The Hamiltonian for this fermion can be written as,

$$\begin{aligned}\hat{H} &= \psi^\dagger\mathcal{H}\psi \\ \mathcal{H} &= \Gamma^x i\partial_x + \Gamma^y i\partial_y + \Gamma^z i\partial_z + m\Gamma^0\end{aligned} \tag{B1}$$

where the Γ matrices are 4×4 anti-commuting matrices. Here, it will be useful to write the C_n rotation operator as

$$U_n \equiv \exp\left(i\frac{2\pi}{n}L\right), \tag{B2}$$

where L is the C_n angular momentum operator, and U_n satisfies

$$U_n^\dagger\mathcal{H}(\boldsymbol{k})U_n = \mathcal{H}(R_n\boldsymbol{k}), \tag{B3}$$

where $\mathcal{H}(\boldsymbol{k})$ is the Bloch Hamiltonian of Eq. B1. To proceed, we note that the continuum Dirac Hamiltonian in Eq. B1 has a continuous U(1) rotation symmetry. In order for the continuum theory to be consistent, the C_n lattice rotation symmetry should be embedded in this enlarged U(1), i.e.

$$\begin{aligned}U^\dagger(\theta)\mathcal{H}(\boldsymbol{k})U(\theta) &= \mathcal{H}(R(\theta)\boldsymbol{k}) \\ U(\theta) &\equiv \exp(i\theta L)\end{aligned} \tag{B4}$$

where $R(\theta)$ is a rotation of the momentum by θ. Based on this, the most general consistent definition of the C_n angular momentum is

$$L \equiv \frac{1}{2}\Gamma^{xy} + p\mathrm{I}_4, \tag{B5}$$

where I_4 is the 4×4 identity matrix, and $\Gamma^{xy} = i\Gamma^x\Gamma^y$. For spinless fermions $(U_n)^n = +1$ and for spin-1/2 fermions $(U_n)^n = -1$. So, for spinless fermions p must be a half-integer, while for spin-1/2 fermions, p must be an integer. Here, the value of p is only defined modulo n, and any physical quantity should only depend on the value of p modulo n.

Let us now consider gauging the C_n lattice rotation symmetry. To do this, we will need to introduce the frame-fields, e^A_μ (and inverses E^μ_A), and the spin connection ω. Under a local C_n transformation $\theta(x_\mu)$, the frame-fields, and Dirac fermions transform as

$$\begin{aligned} e^x_\mu &\to \cos(\theta)e^x_\mu + \sin(\theta)e^y_\mu, \\ e^y_\mu &\to -\sin(\theta)e^x_\mu + \cos(\theta)e^y_\mu, \\ \omega_\mu &\to \omega_\mu + \partial_\mu\theta \\ \psi &\to e^{i\theta L}\psi = e^{i\theta(\frac{1}{2}\Gamma^{xy}+p\mathrm{I}_4)}\psi \end{aligned} \tag{B6}$$

In terms of these fields, the minimally coupled Lagrangian is

$$\mathcal{L} = \bar{\psi}[iE^\mu_A\bar{\Gamma}^A D_\mu - m]\psi \tag{B7}$$

where

$$D_\mu = \partial_\mu - i\omega_\mu[\frac{1}{2}\Gamma^x\Gamma^y + p\mathrm{I}_4]. \tag{B8}$$

It can be directly confirmed that the Lagrangian in Eq. B7 is invariant under the C_n gauge transformation given in Eq. B6, as desired.

Appendix C: zero-energy Surface Mode

In this appendix, we demonstrate the existence of a zero energy mode on the surface of the spinless rTCI when a mass vortex is added. The continuum surface Hamiltonian is

$$H = \sigma^x\sigma^0(i\partial_x) - \sigma^y\sigma^0(i\partial_y) \tag{C1}$$

the mass vortex term takes the form

$$H_M = \sigma^z\sigma^x m_s(r)\cos\theta + \sigma^z\sigma^y m_s(r)\sin\theta \tag{C2}$$

Here $m_s(r)$ is a function which vanishes at $r=0$. Now we look for zero energy eigenstate of the Hamiltonian. It is convenient to go to polar coordinate, where the Hamiltonian is

$$\begin{aligned} H =& i\begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix} \otimes \sigma^0 \frac{\partial}{\partial r} - \begin{pmatrix} 0 & e^{i\theta} \\ -e^{-i\theta} & 0 \end{pmatrix} \otimes \sigma^0 \frac{1}{r}\frac{\partial}{\partial\theta} \\ &+ m_s(r)\sigma^z \otimes \begin{pmatrix} 0 & e^{-i\theta} \\ e^{i\theta} & 0 \end{pmatrix} \end{aligned} \tag{C3}$$

From this form of the Hamiltonian we can expect a solution of the following form

$$\Psi = \begin{pmatrix} u_1(r)e^{in\theta} \\ u_2(r)e^{i(n+1)\theta} \\ u_3(r)e^{i(n-1)\theta} \\ u_4(r)e^{in\theta} \end{pmatrix} \tag{C4}$$

We will take m_s to be zero for $r \le R$ and a non-zero constant $\bar{m}_s$ for $r > R$, $m_s = \bar{m}_s\Theta(r-R)$, where Θ is a step function. The zero energy solution satisfies the following equations

$$(\partial_r^2 - \frac{n(n+1)}{r^2} - m_s^2)u_1 = 0 \tag{C5}$$

$$(\partial_r^2 + \frac{2}{r}\partial_r - \frac{n(n+1)}{r^2} - m_s^2)u_2 = 0 \tag{C6}$$

$$(\partial_r^2 + \frac{2}{r}\partial_r - \frac{n(n-1)}{r^2} - m_s^2)u_3 = 0 \tag{C7}$$

$$(\partial_r^2 - \frac{n(n-1)}{r^2} - m_s^2)u_4 = 0 \tag{C8}$$

For the first and the last equation. We can make the substitution $u = r^{\frac{1}{2}}f$, and therefore obtain the equation

$$r^2\frac{d^2f}{dr^2} + r\frac{df}{dr} - [m_s^2r^2 + n(n\pm 1) + \frac{1}{4}]f = 0 \tag{C9}$$

while for the other two we take $u = r^{-\frac{1}{2}}f$ and obtain

$$r^2\frac{d^2f}{dr^2} + r\frac{df}{dr} - [m_s^2r^2 + n(n\pm 1) + \frac{1}{4}]f = 0 \tag{C10}$$

First look at $r < R$, in this region $m_s = 0$ and the four equations are decoupled, and we find that

$$u_1 = c_1r^{-n},\ u_2 = c_2r^{-n-1},\ u_3 = c_3r^{n-1},\ u_4 = c_4r^n \tag{C11}$$

For $r > R$ these equations are solved by modified Bessel functions. Now we impose boundary conditions, the solution must be regular at both $r = 0$ and $r \to \infty$, and it also needs to be continuous at $r = R$. It is easy to see that if $u_2 = 0$ for $r > R$ then u_3 must be so, thus by continuity at $r = R$ c_2 and c_3 have to be non-zero. However, this leads to singularity at $r = 0$ for arbitrary n. Therefore, $u_2 = u_3 \equiv 0$. Similar arguments hold for u_1 and u_4, and we find the only possible solution is the following one, with $n = 0$

$$u = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -i \end{pmatrix} \sqrt{\frac{\pi}{2\bar{m}_s}} \begin{cases} e^{-\bar{m}_s r} & (r > R) \\ e^{-\bar{m}_s R} & (r < R) \end{cases} \tag{C12}$$

Under the symmetry of the model: $\hat{T} = \sigma^y \otimes \sigma^y K$, $\hat{C} = \sigma^x \otimes \sigma^x K$ and $\hat{C}_4 = \exp\big[i\frac{\pi}{4}(-\sigma^z \otimes \sigma^0 + \sigma^0 \otimes \sigma^z)\big]$, the zero mode transforms as $\hat{T}u = -iu$, $\hat{C}u = iu$, and $\hat{C}_4 u = u$.

The existence of such zero modes had been demonstrated numerically. We took a $10 \times 10 \times 10$

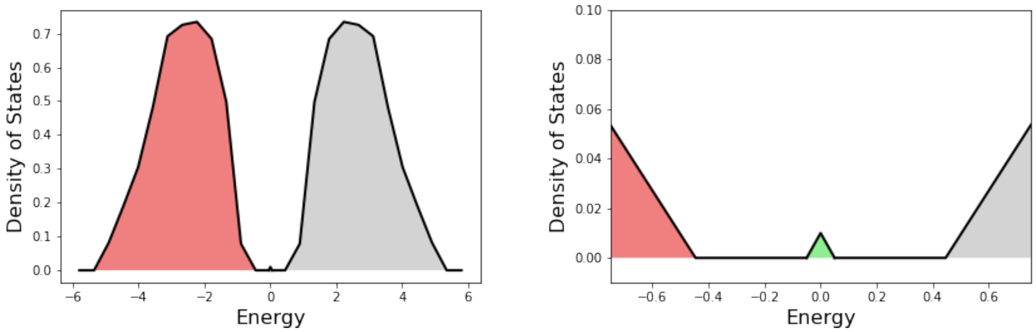

FIG. 8: Right) The density of states with $M = -2$ in the bulk, and a pair of mass vortices with $\bar{m}_s = 0.5$. There is a pair of zero-energy modes at $E = 0$. Left) The density of states around $E = 0$

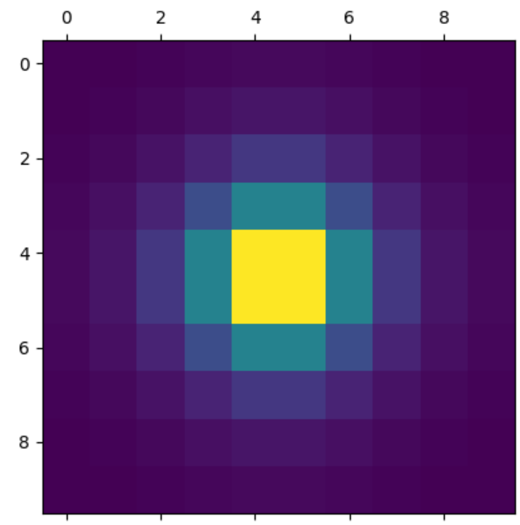

FIG. 9: The density distribution of a zero-energy mode at $z = 0$, which is localized around the core of the mass vortex.

lattice, with a pair of mass vortices of opposite vorticity created at the centers of the two z-surfaces. In the bulk, $M = -2$ and on the surface $\bar{m}_s = 0.5$. A small chemical potential is introduced on the surface to break hybridization between the two zero modes on the surface. Fig. 8 show the energy spectrum in the presence of the mass vortex. It can be seen that now we have two zero energy modes (the small difference in their energies is caused by the chemical potential). Fig. 9 shows the density distribution of the zero mode at $z = 0$, it can be seen that the density is localized around the core of the mass vortex and symmetric under C_4 rotations, as predicted theoretically above.