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Z_2 antiferromagnetic topological insulators with broken C_4 symmetry

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A two-dimensional topological insulator may arise in a centrosymmetric commensurate Néel antiferromagnet (AF), where staggered magnetization breaks both the elementary translation and time reversal, but retains their product as a symmetry. Fang *et al.*, [Phys. Rev. B **88**, 085406 (2013)] proposed an expression for a Z_2 topological invariant to characterize such systems. Here, we show that this expression does not allow to detect all the existing phases if a certain lattice symmetry is lacking. We implement numerical techniques to diagnose topological phases of a toy Hamiltonian, and verify our results by computing the Chern numbers of degenerate bands, and also by explicitly constructing the edge states, thus illustrating the efficiency of the method.

Physical phenomena, whose description involves topology, have been invariably attracting attention regardless of whether the word “topology” was actually used at the time: early examples involve topologically non-trivial stable defects such as dislocations in crystals, as well as vortices in superconductors and superfluids. Quantum Hall Effect and its remarkably precise conductance quantization [1] marked the advent of an entirely new class of phenomena, related not so much to the appearance in the sample of finite-size topological objects, but rather to the electron state of the *entire* sample changing its topology in a way, that could no longer be undone by a local perturbation. More recently, it was understood that, in fact, non-trivial topology may appear even in zero magnetic field: the fact that a commonplace band insulator may find itself in distinct electron states that cannot be continuously transformed one into another without a phase transition, came as a major surprise [2, 3].

These phenomena invite the question of classifying topologically distinct states of matter: labeling each state by a set of discrete indices in such a way as to have different sets for any two phases that cannot be continuously transformed one into another without the system undergoing a phase transition. In the general setting, the problem remains unsolved.

In fact, open questions are present even in a non-interacting description of systems that are believed to admit a Z_2 (“even-odd”) classification, and thus have only one topologically trivial and one topologically non-trivial phase, commonly called topological. Here, we address one such question, that has recently attracted attention: diagnosing the topological phase of a Z_2 insulating Néel antiferromagnet.

To put the subsequent presentation in context, we recapitulate the key results for the prototypical Z_2 system: a paramagnetic topological insulator. Fu and Kane [4] have shown that the Z_2 invariant for such a system can be defined via the so-called sewing matrix $w(\mathbf{k})_{mn}$:

$$w(\mathbf{k})_{mn} = \langle \Psi_{m,-\mathbf{k}} | \Theta | \Psi_{n,\mathbf{k}} \rangle, \quad (1)$$

where the $|\Psi_{n,\mathbf{k}}\rangle$ is the Bloch eigenstate of the n -th band at momentum \mathbf{k} . The $w(\mathbf{k})_{mn}$ turns out to be

of particular interest at special momenta Γ_i such that $-\Gamma_i = \Gamma_i + \mathbf{G}$, with \mathbf{G} a reciprocal lattice vector. Such Γ_i are now commonly called the “time reversal-invariant momenta” (TRIM). In the Brillouin zone, a Γ_i is equivalent to its opposite, and thus the $w(\Gamma_i)_{mn}$ is antisymmetric. Since each band has its Kramers partner, the number of bands at hand is even, and the above two properties allow one to define the Pfaffian $Pf[w(\Gamma_i)_{mn}]$. As established by Fu and Kane [4], the Z_2 topological invariant Δ can be expressed in a continuous gauge via the $w(\Gamma_i)_{mn}$ as per

$$(-1)^\Delta = \prod_i \frac{\sqrt{\det[w(\Gamma_i)]}}{Pf[w(\Gamma_i)]}. \quad (2)$$

Moreover, in the presence of inversion symmetry, the Eq. (2) may be recast in terms of the parity eigenvalues $\xi(\Gamma_i)$ of Bloch eigenstates at the TRIM Γ_i :

$$(-1)^\Delta = \prod_i \prod_\alpha \xi_\alpha(\Gamma_i) \quad (3)$$

where the i labels the TRIM and the α counts one band per each pair of the $2N$ filled Kramers-partner bands.

Néel antiferromagnetism explicitly violates the symmetry with respect to time reversal Θ . However, both the Θ and the translation \mathbf{T}_a by half the Néel period invert the local magnetization, and thus the combination $\Theta_{AF} \equiv \Theta \mathbf{T}_a$ of the two remains a symmetry.

A number of authors [5–11] attempted to classify the topological phases that may appear in an antiferromagnet. However, contrary to the paramagnetic case, the relevant anti-unitary operator does not square to -1: instead, its action on a Bloch eigenstate $|\Psi_{n,\mathbf{k}}\rangle$ is given by

$$\Theta_{AF}^2 |\Psi_{n,\mathbf{k}}\rangle = -e^{i2\mathbf{k}\cdot\mathbf{a}} |\Psi_{n,\mathbf{k}}\rangle. \quad (4)$$

In the presence of inversion symmetry \mathbf{I} , the combined symmetry $\mathbf{I}\Theta_{AF}$ enforces double degeneracy at all momenta in the Brillouin zone. Moreover, the TRIM split into two kinds: the A-TRIM, where $\Theta_{AF}^2 = 1$ – and the B-TRIM, where $\Theta_{AF}^2 = -1$. In three dimensions, it has

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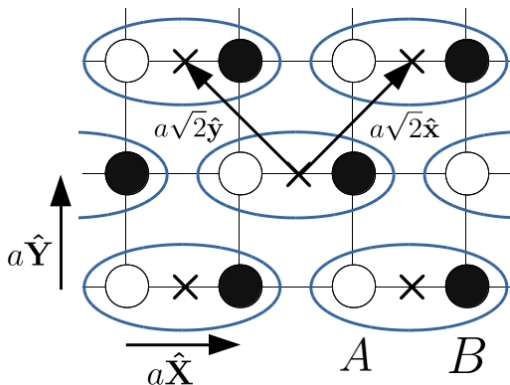


FIG. 1: Square lattice, on which the Hamiltonian is defined. In the absence of a staggered magnetic field, the primitive Bravais lattice vectors are $a\hat{\mathbf{X}}$ and $a\hat{\mathbf{Y}}$. In the presence of staggered magnetization, the dimerized lattice is defined by the primitive vectors $a\sqrt{2}\hat{\mathbf{x}}$ and $a\sqrt{2}\hat{\mathbf{y}}$. In this case, a unit cell (in blue) comprises two sites, A and B (white and black dots, respectively).

been argued that the B-TRIM suffice to define a topological invariant, as the Eq. (2) remains gauge-invariant as long as the product in the r.h.s. is taken over the B-TRIM only [7, 9, 11]. Similarly, Fang *et al.* argued that in two dimensions, the product of the parity eigenvalues ξ at the two B-TRIM would also be a Z_2 topological invariant.

The expression above, restricted to the B-TRIM only, appeared to work in the cases studied in the Refs. [7, 9, 11, 12]. Such an expression tacitly implies, that the parity eigenvalues at the two A-TRIM either change simultaneously or not at all, and thus do not affect the Z_2 invariant. However, if a band inversion were to occur only at a *single* A-TRIM, then the full Z_2 invariant of the Eq. (3) would change sign, and this would *not* be accounted for by the invariant, involving the parity eigenvalues at the B-TRIM only.

Below, we use a method developed in a previous work [12] to illustrate this possibility by a toy Hamiltonian.

i) The model – We consider a non-interacting electron system on a square lattice (of lattice vectors $a\hat{\mathbf{X}}$ and $a\hat{\mathbf{Y}}$), with an s- and a p-wave symmetry orbital on each site, as in the Bernevig-Hughes-Zhang (BHZ) model [13]. The lattice can be divided into two sub-lattices, A and B (see Fig.(1)), corresponding to the opposite orientation of magnetization in the z direction. In this case, the natural lattice vectors for the super-lattice will be $a\sqrt{2}\hat{\mathbf{x}} = a\hat{\mathbf{X}} + a\hat{\mathbf{Y}}$ and $a\sqrt{2}\hat{\mathbf{y}} = -a\hat{\mathbf{X}} + a\hat{\mathbf{Y}}$. In what follows, we choose $a = \frac{1}{\sqrt{2}}$. In this case, the TRIM will correspond to $(k_x, k_y) = (0, 0), (\pi, \pi), (0, \pi)$ and $(\pi, 0)$, the first two being the B-TRIM and the latter two being the A-TRIM. The Bloch Hamiltonian $H(\mathbf{k}) = e^{-i\mathbf{k}\mathbf{r}} H e^{i\mathbf{k}\mathbf{r}}$ can be written as:

$$\begin{aligned}
 H(\mathbf{k}) = & \mu + \Delta\mu\tau^z \\
 & - 2t(C_- + C_+)(C_- \sigma^x + S_- \sigma^y) \\
 & - 2(t'_x \cos(k_x) + t'_y \cos(k_y))\tau^z \\
 & + 2\alpha(S_+ C_+ s^y \tau^y \sigma^z - S_- C_- s^x \tau^x \sigma^z) \\
 & + ms^z \sigma^z
 \end{aligned} \tag{5}$$

where $C_{\pm} \equiv \cos[(k_x \pm k_y)/2]$ and $S_{\pm} \equiv \sin[(k_x \pm k_y)/2]$, while σ , s and τ are the Pauli matrices acting in the sublattice (A and B), spin and orbital spaces, respectively. The first term ($\mu_{\pm} = \mu \pm \Delta\mu$) originates from the energy difference of the s- and p-symmetric orbitals. The second term corresponds to the nearest-neighbor hopping between the same orbitals, the third – to second-neighbor hopping. We choose the latter to be anisotropic and orbital-dependent. This term breaks the C_4 symmetry, as explained later. The following term hybridizes the two orbitals via the amplitude α , and is of a spin-orbital nature, it is a third nearest neighbor hopping. This term is responsible for a gap at half-filling, and thus for bulk insulating behavior. Finally, the last term describes the staggered magnetization.

In the following, we choose $\mu = 0, \Delta\mu = 3, t = 1, t'_x = 1, t'_y = 0.5, \alpha = 2$ and $m > 0$. This choice is made to render the figures more legible, the same conclusions hold for more realistic parameters, such that $\alpha < t'_x, t'_y < t$.

Upon variation of m , the criterion due to Fang *et al.* would predict a single phase transition at $m = 6$. For $0 < m < 6$, the product of the parity eigenvalues over a half of the filled bands (for every pair of doubly degenerate bands, such a product counts only a single parity eigenvalue) at the B-TRIM equals -1 , and thus the system should be in a topological phase, while for $m > 6$ this product is equal to 1, and so the system should be in the trivial phase.

However, this criterion tacitly assumes that no topological phase transition may take place via closing the gap at an A-TRIM. Indeed, this is true if the system is C_4 -symmetric: this symmetry would guarantee that band inversion could occur only at both of the A-TRIM simultaneously, thus keeping the topological invariant intact. However, our Hamiltonian explicitly breaks the C_4 symmetry via the terms t'_x and t'_y , hence the argument above no longer applies.

ii) Phase diagram – We use a numerical method inspired by the Ref. [14] and adapted to the AF case in Ref. [12] to compute the topological invariant of the system for several sets of parameters. This method comprises two parts. First we obtain a smooth definition of the eigenstates over the BZ using a parallel transport method, and then compute the position of the Wannier charge centers (WCC) as a function of k_y . The sum of the WCC positions over the filled band may not have the same value for $k_y = -\pi$ and $k_y = \pi$, but the difference

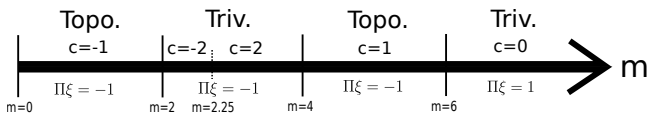


FIG. 2: The phase diagram, obtained by the WCC method for $\mu = 0, \Delta\mu = 3, t = 1, t'_x = 1, t'_y = 0.5, \alpha = 2$ and $m > 0$. “Topo.” corresponds to the topological phase (an odd jump of the WCC position), and “Triv.” to the trivial phase (an even jump). Below we show the total Chern number of the two lowest energy bands, restricted to the stable subspace spanned by the four states ($|\uparrow sA\rangle, |\uparrow sB\rangle, |\downarrow pA\rangle, |\downarrow pB\rangle$). The $\Pi\xi$ corresponds to the product of half the parity eigenvalues of the Bloch states at the B-TRIM. For $2 < m < 4$, the phase is trivial while $\Pi\xi = -1$, showing that $\Pi\xi$ alone cannot characterize the topology of the phase.

of these two values is an integer [14–16]. If this integer is odd, the system is in a topological phase; if it is even, the phase is topologically trivial. Keeping all the other parameters fixed, we vary the strength m of the staggered magnetization. In the Fig.(3), we see that for different values of m the gap closes at a different TRIM – and that each time the topology of the phase changes (see Fig.(4)). One may also note that for $m \simeq 2.25$ the gap closes at non-TRIM points, but this does not change the value of the Z_2 invariant.

We present the obtained phase diagram in the Fig.(2), and compare it to the one expected from the criterion due to Fang *et al.*. The discrepancies appear when a band inversion occurs at an A-TRIM, excluded from the Fang criterion, such as for $m = 2$ and $m = 4$. We verified the above result using the “reconnection phase” method, described in the Ref. [12]. These results are not presented here for brevity, but are in complete agreement with the WCC computation.

The Hamiltonian we discuss is block-diagonal, and can be separated into two blocks that are related by Θ_{AF} -symmetry. Hence it is possible to work with a single block, and compute the Chern number of the different bands. We restrict ourselves to a stable subspace spanned by the four states ($|\uparrow sA\rangle, |\uparrow sB\rangle, |\downarrow pA\rangle, |\downarrow pB\rangle$). We compute analytically the eigenstates as a function of k . Then, using the Eqs.(9) and (10) of the Ref [17], we integrate the Berry curvature numerically to obtain the first Chern number. We finally sum over all the filled bands. The resulting phase diagram is again in perfect agreement with the WCC and the reconnection phase computation. Concerning the validity and coherence of our results, we note that the computation of the Berry curvature is analytical, and thus, the only error could come from numerical integration to obtain the Chern number. The accuracy of our numerical integration is well controlled and rules out an inconsistency.

Finally, we realized an explicit construction of the edge states, following the methods discussed in [18] and [12]. In order to simplify the problem, we chose to work with

a unit cell containing four sites (forming a square) rather than two. Despite the fact that, with this choice, we have to work with a 16-band model, we now have hopping only between nearest-neighbor unit cells, which simplified finding the edge states. For the same set of parameters as before, we looked for edge states on an antiferromagnetic edge (alternating up and down magnetization), at the energy $E = 0$. For $m = 1$ and $m = 5$, we found a single pair of edge states, while we found two pairs for $m = 3$ and none at all for $m = 7$. The parity of the number of pairs of edge states is thus once again in perfect agreement with the phase diagram we found (see Fig.2).

To conclude, in this work we shed new light on topological phase transitions in centrosymmetric two-dimensional antiferromagnets. For such systems, one would like to find an easily computable form of the topological invariant such as in the Eq. (3). Fang and co-authors proposed such a form, but it holds only in the presence of a symmetry that assures identical behavior at both of the A-TRIM, as does the C_4 symmetry. Without the latter, we do not yet have a simple expression for the topological invariant in an antiferromagnetic insulating phase. However, we put forward a set of numerical methods that allow one to capture the topological behavior of the system. We verified these results by direct computation of the Chern number and by the explicit construction of edge states. Notice that such numerical methods (WCC and “reconnection phase”) are applicable even when direct computation of the Chern number is not easily accessible, for example when the Hamiltonian cannot be block-diagonalized by a fixed change of basis, as above. Finally, notice that for a three-dimensional antiferromagnetic insulator, the Refs. [5, 7] proposed a topological index involving the B-TRIM only. It would be interesting to verify whether in three dimensions the absence of symmetry between the A-TRIM could affect this result as it does in two dimensions.

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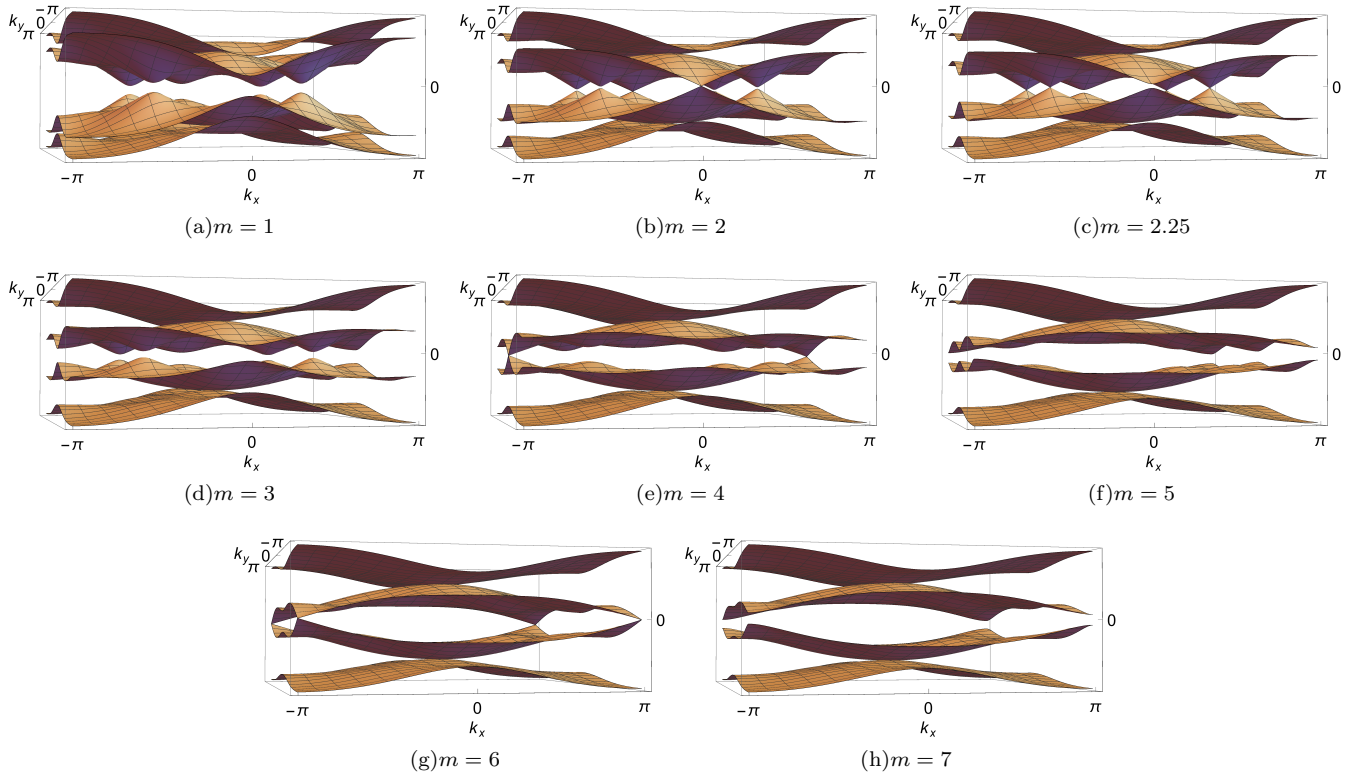


FIG. 3: Dispersion relation for $\mu = 0, \Delta\mu = 3, t = 1, t'_x = 1, t'_y = 0.5, \alpha = 2$ and different values of m . The gap closes at a B-TRIM for $m = 6$ and at the A-TRIM for two different values of m (2 and 4). For other values of m , a gap is present all over the BZ, insuring an insulating phase, except at $m \simeq 2.25$ where the gap closes at non TRIM points.

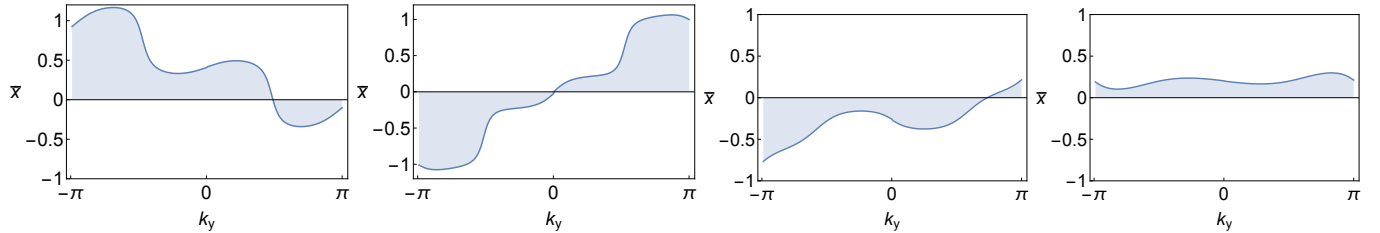


FIG. 4: Position of the WCC for $\mu = 0, \Delta\mu = 3, t = 1, t'_x = 1, t'_y = 0.5, \alpha = 2$ and $m = 1, 3, 5, 7$. The jump in the WCC positions between $-\pi$ and π is equal to (in absolute values) 1, 2, 1 and 0 respectively. We thus get a topological phase for $m = 1$ and 5 and the trivial phase for $m = 3$ and 7.

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