Disordered topological insulators via C*-algebras

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Abstract – The theory of almost commuting matrices can be used to quantify topological obstructions to the existence of localized Wannier functions with time-reversal symmetry in systems with time-reversal symmetry and strong spin-orbit coupling. We present a numerical procedure that calculates a Z² invariant using these techniques, and apply it to a model of HgTe. This numerical procedure allows us to access sizes significantly larger than procedures based on studying twisted boundary conditions. Our numerical results indicate the existence of a metallic phase in the presence of scattering between up and down spin components, while there is a sharp transition when the system decouples into two copies of the quantum Hall effect. In addition to the Z² invariant calculation in the case when up and down components are coupled, we also present a simple method of evaluating the integer invariant in the quantum Hall case where they are decoupled.

The study of topological insulators is one of the most active areas of physics today. Experimental and theoretical work has shown physical realizations of time-reversal invariant insulators with strong spin-orbit coupling in both two [1] and three dimensions [2] and a complete classification of different insulating phases has been recently obtained using methods of Anderson localization [3] and, more generally, K-theoretic techniques [4].

However, numerically it is difficult to determine the Z² invariants that are signatures of topological insulating phases. For systems with translational invariance, one can study the bundle over the momentum torus [5], while for systems without translation invariance, Essin and Moore [6] were able to study the phase diagram of a graphene model by studying the model over a flux torus corresponding to twisted boundary conditions. Unfortunately, the flux torus approach is very computationally intensive: for each disorder realization, the Hamiltonian must be diagonalized once for each point on a discrete grid on the flux torus, and then the connection on the torus must be computed. This limited the study to small systems, with at most 64 sites.

In this paper, we present a different approach to calculating a Z² invariant, based on ideas in C*-algebras, in particular the K-theory of almost commuting matrices. We present a fast numerical algorithm based on these ideas. Computing the invariant requires a single diagonalization of the Hamiltonian, matrix function calculations on matrices at most half the size of the Hamiltonian, and finally the calculation of the Pfaffian of a real antisymmetric matrix that is at most the size of the Hamiltonian. The most costly step is a single diagonalization, allowing us to study significantly larger samples, up to 1600 sites.

We apply this method to a model of HgTe [1], including the additional term H_BIA in [8] which breaks inversion symmetry. The Hamiltonian we use is H of [8], with an additional on-site disorder term. This can be written as

\[ H = \begin{pmatrix} h & 0 \\ 0 & h^* \end{pmatrix} + H_{BIA} + V, \]

where in the notation of [8]

\[ H_{BIA} = \begin{pmatrix} \Delta & \Delta & -\Delta \\ -\Delta & \Delta & -\Delta \\ \Delta & -\Delta & \Delta \end{pmatrix} \]
is a $k$-independent term that couples up and down spin components, and $V$ is a random disorder term, diagonal in spin and band indices, described below. We map out part of the phase diagram, focusing on the transition with and without coupling between up and down spins.

**Band projected position operators and Wannier functions in systems without time-reversal symmetry.** We describe first an integer invariant in the case of systems without time-reversal symmetry. We largely follow [9], which described an integer invariant for two-dimensional systems on the sphere or torus, and a $Z_2$ invariant in the case of a sphere. In the next section, we present a $Z_2$ invariant for systems on a torus.

Consider a lattice Hamiltonian $H$ for a single-particle, tight-binding model on the surface of a torus. We assume that the hopping is short-ranged, so that the matrix tight-binding model on the surface of a torus. We assume that the hopping is short-ranged, so that the matrix elements $H_{ij}$ is small if sites $i$ and $j$ are far separated on the torus. Let $P$ be the projector onto the states below the Fermi energy $E_F$. If the Fermi energy lies in a spectral gap, then one can show using the locality of $H$ that $P$ is also local: $P_{ij}$ is small if $i$ and $j$ are far separated. In fact, $P$ is still local even if the Fermi energy lies in a mobility gap. We parametrize the position of a given site $i$ on the surface of the torus by two angles, $\theta_i$ and $\phi_i$, between 0 and $2\pi$. Introduce two Hermitian matrices, $\Theta$ and $\Phi$. These are both diagonal matrices, with matrix elements $\Theta_{ii} = \theta_i$ and $\Phi_{ii} = \phi_i$.

Using a basis of eigenstates of $H$, we can conjugate the band-projected position matrices $P \exp(i\Theta)P$ and $P \exp(i\Phi)P$ by a single unitary matrix to produce block matrices

$$P \exp(i\Theta)P \approx \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}, \quad P \exp(i\Phi)P \approx \begin{pmatrix} 0 & 0 \\ 0 & V \end{pmatrix},$$

(3)

where the first block corresponds to the empty states (those projected onto by $1-P$) and the second block corresponds to the filled states (those projected onto by $P$).

The matrices $U$ and $V$ are approximately unitary ($UU \approx I$ and $VV \approx I$) whenever $E_F$ lies in a mobility gap and the system is large. To see this, note that if $P$ is local, then $P$ almost commutes with $\exp(i\Theta)$. More precise results for a system on a sphere are in [9]. Further, $U$ and $V$ almost commute if $E_F$ is in a mobility gap.

Now we ask: given two matrices, $U$ and $V$, which almost commute and which are almost unitary, does there exist a pair of matrices $U'$, $V'$ which exactly commute, are exactly unitary, and which are close to $U$ and $V$? This question of approximating almost commuting matrices by exactly commuting matrices is an old problem in $C^*$-algebras [10].

Consider the quantity

$$\text{tr}(\log (VUV^\dagger U^\dagger)) \equiv 2\pi m + r,$$

(4)

where $m$ and $r$ are real. We have $\exp(2\pi im + r)$ equal to $\det(VUV^\dagger U^\dagger)$. This determinant is real and positive (since $\det(U) = \det(U^\dagger)$) so $m$ is an integer. This integer $m$ is precisely the topological invariant called the **Bott index**. The approximation by exactly commuting matrices is possible if and only if $m = 0$ [11].

If $U$ and $V$ almost commute and are close to unitary, $VUV^\dagger U^\dagger$ is close to the identity. All of its eigenvalues stay away from the branch cut of the logarithm (chosen on the negative real axis), which is why the integer $m$ is a topological invariant. If $U$ and $V$ exactly commute then $m = 0$.

The physical importance of the Bott index is that when it is nonzero, it is not possible to find a complete, orthonormal basis of localized functions (so-called Wannier functions) spanning the occupied states [9].

This invariant can be computed very quickly. We perform a full diagonalization of the Hamiltonian to form the projector $P$ onto states below $E_F$. We then construct $U$ and $V$ and calculate the trace of the logarithm in eq. (4) from the eigenvalues of $VUV^\dagger U^\dagger$. The matrices $U$ and $V$ are of dimension equal to the number of occupied states. This is at most half the size of the dimension of $H$.

Figure 1, shows the results of this invariant on a model of HgTe studied in [8], with the up and down spin decoupled ($\Delta = 0$). We chose constants $A = 1, B = -1, D = 0, M = -2$, which sets the irrelevant terms of order $k^2$ to zero. The system had linear size $w$ giving $w^2$ sites and $2w^2$ states per spin component, and we added a diagonal disorder term on each site chosen uniformly from the interval $[-4, 4]$. The transition sharpens as $w$ increases. In the inset, we plot a scaling collapse with the exponent $\nu = 7/3$ from [12]. This collapse suggests that the transition is sharp in the thermodynamic limit.

One can also use the commutator of $U$ and $V$ as a signature of localization. In fig. 2, we plot this commutator as a function of $E_F$ for various system sizes. One may see that as $w$ increases, the commutator gets smaller away from the transition. In the inset, we show the same plot for a system with $\Delta = 0.64, M = -1$, to show the existence of a metallic phase in this case.

Fig. 1: (Colour on-line) Average index as a function of the Fermi level $E_F$, for $w = 20$ (1200 samples), $w = 30$ (520 samples), $w = 40$ (800 samples), $w = 60$ (470 samples). Inset: scaling collapse with $\nu = 7/3$ [12].
which we call into the band of occupied states to form three matrices
triples (\[ \sigma \] sphere constructed in \[ 9 \]). This theory applies to all
begin with the invariant formatricesthat almost represent
with time-reversal symmetry. –
boundary modes and hence
number of positive and negative eigenvalues of
Bott index, is half the difference between the
matrices, there are two almost commuting band projected position
with open boundary conditions, such as a disk \([13]\), where
in this case, there is not an obstruction to finding exponentially localized Wannier
functions with time-reversal symmetry.

An obstruction to localized Wannier functions with time-reversal symmetry. – We now consider invariants in systems with time-reversal symmetry. We begin with the invariant for matrices that almost represent a sphere constructed in \([9]\). This theory applies to all triples \((H_1, H_2, H_3)\) of self-dual Hermitian matrices for which
\[
\| [H_r, H_s] \| \leq \delta, \quad \left\| I - \sum H_i \right\| \leq \delta \tag{6}
\]
with a small \(\delta\). We need not convert a lattice over the torus to a lattice over the sphere; we compute the band-
compressed periodic position operators and apply matrix functions to create matrices that satisfy eq. \(6\).

Consider the matrix \(B(H_1, H_2, H_3)\), which we define as
\[
\frac{1}{4} (1 + i \sigma_y \otimes \sigma_y) B(H_1, H_2, H_3) (1 - i \sigma_y \otimes \sigma_y), \tag{7}
\]
where \(\sigma_y \otimes \sigma_y\) is a product of the \(\sigma_y\) matrices on the physical spin of the particle and on the pseudospin introduced to define \(B\). The resulting matrix is real and antisymmetric. The sign of its Pfaffian represents a potential \(Z_2\) obstruction in the group \(Z_2 = \{-1, 1\}\).

We call this index the Pfaffian-Bott index. This index being \(-1\) is first of all an obstruction to our being able to approximate the \(H_r\) simultaneously by exactly commuting self-dual matrices. The analysis in paragraph V.B of \([9]\) is valid in the self-dual case, and it shows that this is also an obstruction to finding exponentially localized Wannier functions with time-reversal symmetry.

The spectrum of \(B(H_1, H_2, H_3)\) is pure imaginary and has a gap at zero. The smaller the commutators between the \(H_r\), the larger the gap and the larger the distance must be to exactly commuting self-dual matrices.

We prefer to study a physical system on a torus in order to have a regular lattice without defects. The \(Z_2\) invariant for the torus is not as simple as eq. \((4)\). We compute the matrices \(U\) and \(V\) as above; these matrices \(U, V\) will be self-dual if we are careful how we diagonalize the Hamiltonian. We need to diagonalize it via a symplectic matrix, found using a variation of an old algorithm \([16]\) designed for Hamiltonians with time-reversal symmetry.

We select a degree-one, continuous mapping from the torus to the sphere, a map \((\theta, \phi) \mapsto (x_1, x_2, x_3)\) with
\[
\begin{align*}
x_1 &= f(\phi), \\
x_2 &= g(\phi) + h(\phi) \cos 2\pi i \theta, \\
x_3 &= h(\phi) \sin 2\pi i \theta.
\end{align*}
\]

We then apply this map to \(U\) and \(V\) by defining
\[
\begin{align*}
H_1 &= f(V), \\
H_2 &= g(V) + \frac{1}{4} \{ h(V), U^\dagger \} + \frac{1}{4} \{ h(V), U \}, \\
H_3 &= \frac{1}{4} \{ h(V), U^\dagger \} - \frac{1}{4} \{ h(V), U \},
\end{align*}
\]
and then compute the \(Z_2\) invariant of \(H_1, H_2, H_3\). The anticommutators ensure that the \(H_r\) are self-dual.

Expressing the torus invariant in terms of the sphere invariant requires computing with the matrix \(B(H_1, H_2, H_3)\), which has dimension twice as large as the number of occupied states, and so is at most the size of the Hamiltonian. We need only tridiagonalize the matrix \(B\), which is real, further improving the speed.

There are issues with applying the formulas in eq. \((9)\). The matrix functions of \(V\) must be analytic functions, Laurent polynomials or polynomials in \(V\) and \(V^\dagger\) since we do not expect \(V\) to be normal. That limitation is not compatible with defining a degree-one map from the torus to the sphere. This we overcome by choosing \(f, g\) and \(h\) that define a map to three-space that is close to the sphere.
Our choice of $f$ is similar to that used in [9,17], only with three derivatives vanishing at the extrema. See fig. 3. We define $f_1$, $g_1$ and $h_1$, truncating the Fourier series for $g_1$ and $h_1$ to produce order-5 trigonometric polynomials:

$$f_1(\phi) = \frac{150}{128} \sin(2\pi \phi) + \frac{25}{128} \sin(6\pi \phi) + \frac{3}{128} \sin(10\pi \phi),$$

$$g_1(\phi) \approx \begin{cases} 0, & \frac{1}{4} \leq \theta < \frac{1}{2}, \\ \sqrt{1 - (f(\phi))^2}, & -\frac{1}{4} \leq \theta < \frac{1}{4}, \\ 0, & -\frac{1}{2} \leq \theta < -\frac{1}{4}. \end{cases}$$

$$h_1(\phi) \approx \begin{cases} 0, & \frac{1}{4} \leq \theta < \frac{1}{2}, \\ \sqrt{1 - (f(\phi))^2}, & -\frac{1}{4} \leq \theta < \frac{1}{4}, \\ 0, & -\frac{1}{2} \leq \theta < -\frac{1}{4}. \end{cases}$$

Our invariant is most meaningful when $\|V^1 - V^{-1}\|$ is small, so we replace $g_1(V)$ by a star-polynomial $g(V)$ so $g_1(V) = \sum_{n=-5}^{5} b_n V^n \approx g(V) = \sum_{n=-5}^{5} b_n V^n$, where $V^n$ equals $V^n$ for positive $n$ and $(V^{-1})^{-n}$ for negative $n$. This is much faster. Applied to scalars of unit modulus, there is no difference between $g_1(z)$ and $g(z)$. We do a similar replacement of inverse by adjoint to define $f(V)$ and $h(V)$. The underlying map from the two sphere is illustrated by fig. 4.

Based on earlier experience [17], we used also an alternative method. We computed the polar decomposition $V = V_0 [V]$ of $V$ and a symplectic diagonalization $WDW^\dagger$ of $V_0$. This allowed discontinuous functions

$$f(\phi) = 1 - 2\phi,$$

$$g(\phi) = 0,$$

$$h(\phi) = \sqrt{1 - f(\phi)^2},$$

as we can apply them to the diagonal of $D$.

Both methods work well, with the star-polynomial method, eq. (10), being faster. The log-based method, eq. (11), gave smaller values for the important numbers $\|H_{r}, H_{s}\|$ and $\|I - \sum H_{r}\|$. The data in the plots were generated using the log-based method. These matrix functions, and $O(n^3)$ algorithms for Pfaffians and symplectic diagonalization, will be discussed in [7].

The inability to approximate the $H_{r}$ by self-dual, exactly commuting matrices implies the inability to approximate the $U$ and $V$ by self-dual, exactly commuting matrices. We have an obstruction to the existence of exponentially localized Wannier functions with time-reversal symmetry in our original lattice model on the torus.

Results for a system with time-reversal symmetry. – In fig. 5 we plot the average value of this Pfaffian as a function of $E_F$ for a system using the model of HgTe studied in [8]. We include spin-orbit coupling, which in the terms of [8] means $\Delta = 0.64$, $M = -1$. Unlike in fig. 1, here the plots do not continue to sharpen as $\omega$ increases, suggesting the presence of a metallic phase. When the $U$ and $V$ are far from commuting, the spectral gap of $\tilde{B}(H_1, H_2, H_3)$ is small and the value of the Pfaffian-Bott index is less meaningful. The wide plateau in fig. 2 inset is perhaps a stronger indication of a metallic phase. The fluctuating index implies that the phase is metallic. We are not certain of the interpretation of the index in the metallic regime, but we note that the index is a well-defined topological invariant so long as the Green’s function has a sufficiently fast power-law decay.

In fig. 5 inset, we compute for the case $\Delta = 0$ the average value of the $Z_2$ invariant to the $Z$ invariant for the same system, showing that the average value of the Pfaffian-Bott index is close to 1-2 $\ast m$. Recall that nonzero Bott index and Pfaffian-Bott index not equal to one both indicate topological insulators.

In fig. 6, we show the phase diagram as a function of $\Delta$ with $M = -1$; in fact, $\Delta$ cannot be varied in experiment, but the ratio $\Delta/M$ can be as $M$ depends on sample geometry [8]. For $\omega = 20$, we computed which values of $E_F$ gave average index equal to $\pm 1/3$ or $\pm 2/3$. Due to the finite $\omega$, even at $\Delta = 0$ there is a nonzero distance between the curves. In the thermodynamic limit, the insulator has average Pfaffian $\pm 1$,
and the metal has absolute value of average Pfaffian less than 1. Finite-size simulations cannot identify the insulating regime with certainty, but these simulations suggest that the topological insulator, where the index is always $-1$, is located a short distance inside the $-2/3$ curve and the ordinary insulator is located a short distance outside the $+2/3$ curve. The curves with $E_F > 0$ were obtained by mirroring the curves with $E_F < 0$; while our index is not obviously particle-hole symmetric, numeric tests indicate that the average Pfaffian is in fact close to invariant under this reflection.

Interestingly, for $\Delta \approx 2$, the system has a delocalized phase near zero energy, but there is no topological insulating phase at this value of $\Delta$ and the phase instead separates two ordinary insulating phases. Rather, the delocalized phase results from the proximity to the topological insulating phase at smaller values of $\Delta$.

**Relation of Bott index to Hall conductance.**

Finally, we relate the Bott index, in the case without time-reversal symmetry, to the Hall conductance. We do this by relating the Bott index to an invariant [18] which describes the response of charge to a magnetic field. Suppose $H$ has a spectral gap. Then, we can “spectrally flatten” $H$, to define a new matrix $H'$ whose eigenvalues are all equal to $\pm 1$, which is still local in the sense that the matrix elements of $H'$ are exponentially small between far-separated sites, and such that the space spanned by negative energy states of $H'$ is the same as that spanned by occupied states of $H$. From now on in this section, when we write $H$ we in fact mean the spectrally flattened Hamiltonian $H'$.

We add a pseudospin degree of freedom with a Zeeman coupling to a magnetic monopole in the center of the sphere, giving the Hamiltonian

$$
\tilde{H} = H \otimes I + h \sum_a X_a \otimes \sigma_a,
$$

with the radius of the sphere equal to one so $\sum_a X_a^2 = I$. Then, if the system is large, the lattice spacing $a$ is small, and we can choose $h$ such that $a \ll h \ll 1$. Let $H$ have $M$ negative eigenvalues. Then $\tilde{H}$ has $2M$ negative eigenvalues since $h \ll 1$. Since $a \ll h$, if the pseudospin is aligned with the magnetic field, and hops to a nearby site within distance $a$, the angle between the pseudospin and the magnetic field on the new site is small. So for $a \ll h$, we can describe the dynamics semiclassically: the particle hops on the lattice, with its pseudospin following the magnetic field. In this semiclassical limit, the negative eigenvalues are all close to $-1 \pm h$.

The invariant we will consider is the difference between the number of negative eigenvalues close to $-1 + h$, which we denote $M_+$, and the number of negative eigenvalues close to $-1 - h$, which we denote $M_-$, where $M_+ + M_- = 2M$. We compute $M_+ - M_-$ in two different ways.

First, we compute it semiclassically. Consider the eigenvalues close to $-1 + h$. If the pseudospin is aligned with the field, the Berry phase for transport of the pseudospin leads to an effective orbital magnetic field, as if there were a magnetic monopole inside the sphere. We will write $P = (1 - H)/2$ for the projector onto the negative energy states of $H$. We write $P(+) + P(-)$ for the projector onto the negative energy state of a modified Hamiltonian, $H(+)$, where $H(+)$ is the Hamiltonian $H$ modified by an orbital coupling to a magnetic monopole. We write $P(-)$ for the projector onto the negative energy states of a Hamiltonian $H(-)$, which has the opposite sign monopole. So, $M_+ - M_- = \text{tr}(P(+) - P(-))$. This quantity $\text{tr}(P(+) - P(-))$ has been suggested by [18].

However, we can also compute $M_+ - M_-$ using degenerate perturbation theory. Since $h \ll 1$, we can ignore matrix elements of $h \sum_a X_a \otimes \sigma_a$ which couple negative and positive energy states of $H \otimes I$ and and just consider the operator $h \sum_a X_a \otimes \sigma_a$ projected onto the negative energy space of $H \otimes I$. This operator equals $h \sum_a P X_a P \otimes \sigma_a = h \cdot B(PX_1, PX_2, PX_3 P)$. Thus, in this semiclassical limit the Bott index equals the difference $\text{tr}(P(+)) - \text{tr}(P(-))/2$.

While the invariant of [18] may be unfamiliar, in fact physically it simply describes the response of charge to
flux. In a quantum Hall system, the adiabatic addition of
flux increases the charge by an amount proportional to the
Hall conductance [19]. It is possible in this way to equate
the Bott index we consider with the Hall conductance of
a system on a sphere in the limit of large system size.

We now turn to the torus. The relation between Hall
conductance and the Bott invariant as in eq. (4) will be
investigated in [7]. The calculation in this section suggests
that we want a map from the torus to the sphere such that
the pullback of the connection on $CP^1$ onto $T^2$ gives
a connection with constant curvature to give a constant
effective orbital magnetic field on the torus with a single
monopole. No such map exists but the map we used in
the log-method, eq. (11), gives constant curvature except
at the singularity $\phi = 0$.

Discussion. — We have presented an approach to cal-
culating $Z_2$ invariants in time-reversal invariant systems,
allowing us to study larger system sizes than previously.

In a numerical study of a model for HgTe, we observed
a metallic phase around the transition when the spin
components are not decoupled, as expected from the
existence of metallic phases in disordered systems with
spin-orbit scattering due to antilocalization [20].

We use methods of noncommutative topology, not
noncommutative geometry [21], to define our indices.
While no precise boundary exists between these fields in
the mathematics literature, our general approach is to
discard most of the information in the original Hamiltonian,
only retaining the band-projected position operators. This keeps topological properties while discarding
“metric information” [22,23] used in the noncommutative
geometry approach. By retaining the minimum of informa-
tion, we obtain an efficient, practical computational pro-
dure for these indices. The topological invariance of these
indices follows from standard linear algebra, although the
tighter estimates in [9] require recent results in matrix
theory.

Two distinct approaches to investigating topological
phases are common. One is via index and the other is
via transport. In this paper we have taken the approach
of studying an index. In contrast to flux-torus approaches
to $Z_2$ index, such as Essin-Moore, our approach allows
the numerical study of much larger systems. For systems
with coupling between spin components, studying the Hall conductance as in [24] does not work, so the transport
method requires boundaries. In contrast, on such systems
our method works without the introduction of boundaries. Although the transport approach allows larger system size,
introducing boundaries may increase finite-size effects.
Further, the conductance in a transport measurement is
not exactly quantized in finite-size systems, while the
index approach returns an integer topological invariant
even for finite sizes. Another interesting ability of the
index approach is in studying effects such as we have
seen near $\Delta = 2$. There, the delocalized phase has a
slightly negative average index (roughly $-0.3$) at $E_F = 0$,
implying that the index detects the nearby presence of
topological insulator. Ideally, we want access to all
properties of a topological insulator: bulk conductance,
conductance of boundary modes, and index. We expect
that a combination of transport and index techniques will
be needed to obtain a full understanding of these systems
in the presence of strong disorder.

Since our approach does not use twisted boundary
conditions, we maintain the time-reversal symmetry of
the problem throughout the calculation. This leads to a phi-
sophical advantage of our approach: rather than study-
ing the response of the system to a perturbation that
breaks the symmetry (the twisted boundary conditions),
we directly study an intrinsic property of the given Hamiltonian, in particular allowing us to show obstruc-
tions to localized Wannier functions for that Hamiltonian.

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