Topological Hamiltonian as an exact tool for topological invariants

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Abstract

We propose the concept of ‘topological Hamiltonian’ for topological insulators and superconductors in interacting systems. The eigenvalues of the topological Hamiltonian are significantly different from the physical energy spectra, but we show that the topological Hamiltonian contains the information of gapless surface states, therefore it is an exact tool for topological invariants.

(Some figures may appear in colour only in the online journal)

1. Introduction

Topological insulators are new states of matter with insulating bulk and topologically protected gapless surfaces, which are robust in the presence of disorder (Qi and Zhang 2010, Moore 2010, Hasan and Kane 2010, Qi and Zhang 2011). In the noninteracting limit, the existence of gapless surface states can be traced back to the bulk topological invariants (Thouless et al 1982, Kane and Mele 2005, Moore and Balents 2007, Roy 2009, Fu and Kane 2006, Fu et al 2007, Fu and Kane 2007, Qi et al 2008, Schnyder et al 2008, Ryu et al 2010, Wang et al 2010a), which are defined in terms of the noninteracting Bloch band states. Unfortunately, these topological invariants are inapplicable to systems with electron–electron interactions. For instance, both the definitions of Thouless–Kohmoto–Nightingale–den Nijs (TKNN) invariant (Thouless et al 1982) and the \(\mathbb{Z}_2\) invariants (Kane and Mele 2005, Fu and Kane 2006) crucially depend on the concept of ‘occupied band’, which is not readily generalizable to interacting insulators.

Recently, topological insulators with strong electron–electron interactions have attracted much interest (Raghu et al 2008, Shitade et al 2009, Zhang et al 2009, Seradjeh et al 2009, Pesin and Balents 2010, Fidkowski and Kitaev 2010, Li et al 2010, Dzero et al 2010, Rachel and Le Hur 2010, Wen et al 2010, Maciejko et al 2010, Levin and Stern 2009, Zhang et al 2012, Hohenadler et al 2011, Yu et al 2011, Neupert et al 2012, Yoshida et al 2012), therefore, it is highly desirable to find simple and powerful topological invariants for interacting insulators. For this purpose, the Green’s function has proved to be a useful tool. It has been applied to quantum Hall insulators (Ishikawa and Matsuyama 1986, Volovik 2003), and has also been proposed (Wang et al 2010b) for time reversal invariant topological insulators in three and two spatial dimensions (3D and 2D). These topological invariants, which are expressed in terms of integrals of the Green’s function, were identified as the quantized coefficients of topological field theory (Qi et al 2008). There are numerous recent works making wide use of Green’s functions (Wang et al 2011, 2012, Guralic 2011, Essin and Guralic 2011, Yazyev et al 2012). However, it was a long-standing difficulty that the Green’s function at the entire frequency domain was needed to obtain topological invariants (Ishikawa and Matsuyama 1986, Wang et al 2010b, Volovik 2003), which is very laborious in numerical and analytical calculations.

More recently, it has been explicitly shown (Wang and Zhang 2012a) that all the topological information of Green’s function is encoded in zero frequency, therefore, the Green’s function at nonzero frequency is always superfluous for the purpose of topological invariants. With this observation, a generalized Chern number expressed in terms of a zero frequency Green’s function was defined for quantum Hall insulators, which was also generalized to time reversal invariant topological insulators in 3D and 2D (Wang and Zhang 2012a), and to topological superconductors (Wang and Zhang 2012b). These topological invariants avoid the
difficulty of frequency integrals and have found interesting applications in recent works (Go et al 2012, Wang et al 2012, Budich et al 2012, Budich and Trauzettel 2012, Mannana et al 2012). In addition to these developments, we would like to mention that a 3D winding number of the zero frequency Green’s function has been defined in Volovik (2010, 2011) to study the topology of the 3D standard model of particle physics.

The applicability of the zero frequency Green’s function approach is beyond the ‘renormalized bands’ (or quasiparticle) picture. Generally speaking, the quasiparticle picture is not applicable in the calculation of topological invariants, because the concept of ‘quasiparticle’ itself can break down in strongly correlated systems. In the present paper, we will show that the quasiparticle approach to topological invariants can also fail for a different reason. Let us describe this failure in a little more detail. A quasiparticle with an approximate energy $\omega$ and momentum $k$ has a self-energy $\Sigma(\omega, k)$, therefore, we may expect that $\Sigma(\omega, k)$ should play an important role in defining topological invariants. To our surprise, we can see that only $\Sigma(0, k)$ appears in the exact topological invariants (Wang and Zhang 2012a). Because electrons are gapped in insulators, it is unexpected that only zero frequency quantities appear in topological invariants. It is the purpose of the present paper to understand this counterintuitive result.

The central observation of the present paper is that the zero frequency Green’s function contains the information of the gapless surface states (e.g. their existence or absence), while the more conventional ‘effective Hamiltonian’, though an accurate tool for bulk energy spectra, fails to do this. This physical observation confirms the zero frequency Green’s function as a crucial tool in calculating interacting topological invariants, which will be of great use in searching for new candidates for topological insulators in systems with strong interactions. As a convenient language, the concept of ‘topological Hamiltonian’ (see equation (3)) is coined for the inverse Green’s function at zero frequency, from which various topological invariants can be readily calculated.

The two main conclusions of this paper can be summarized as follows. First, the self-consistent quasiparticle approach is unsuitable for producing topological invariants; second, and more notably, the topological Hamiltonian determines the gapless surface states (see equation (14)). Therefore, it is a general tool for calculating topological invariants.

The rest of this paper is organized as follows. In section 2 we will review the zero frequency Green’s function approach, and define the ‘topological Hamiltonian’. In section 3, we will show that the quasiparticle effective Hamiltonian is unsuitable for calculating topological invariants, then in section 4 we present the main result of this paper, namely that the counterintuitive topological Hamiltonian can determine topological surface states (see equation (14)). Lastly, we will make several concluding remarks in section 5. In the appendix, we list formulas for topological invariants defined in terms of the topological Hamiltonian.

2. Topological Hamiltonian and effective Hamiltonian

In this section we will briefly review the zero frequency Green’s function approach, then we will define the ‘topological Hamiltonian’, which is a convenient language for this approach. We then highlight the difference between the topological Hamiltonian and the conventional ‘effective Hamiltonian’.

Let us fix the notation first. The many-body Hamiltonian is given as $H = H_0 + H_1$, where $H_0 = \sum_k c_k \bar{c}_k = \sum_{k, \alpha, \beta} \epsilon_{\alpha \beta}^k c_{\alpha(k)} \bar{c}_{\beta(k)}$ is the free quadratic Hamiltonian ($\alpha, \beta$ run through all degrees of freedom other than momenta, and the chemical potential has been absorbed into the definition of $H_0$), and $H_1$ term describes the electron–electron interactions. Various (Matsubara, retarded, etc) Green’s functions are defined in the frequency–momentum space in the standard forms (Mahan 2000). For instance, the free fermion system has the Matsubara Green’s function $G(\omega, k) = 1/\{i\omega - h_0(k)\}$. For interacting systems, Green’s functions are still fully determined by the many-body Hamiltonian, though their explicit forms can be very complicated. We note that the Matsubara Green’s functions and the retarded Green’s functions are equal at zero frequency, therefore either can be used in this paper.

As we have discussed in section 1, the early topological invariants (Ishikawa and Matsuyama 1986, Volovik 2003, Wang et al 2010b, Gurarie 2011) constructed from the Green’s function require integrals over the entire frequency domain, thus they are difficult to calculate. Recently it has been shown mathematically that the Green’s function at zero frequency contains all the topological information (Wang and Zhang 2012a). Here we would like to briefly review this approach without going into details. The zero frequency Green’s function $G(\omega = 0, k)$ is a Hermitian matrix, therefore, in the eigenvalue equation (at zero frequency)

$$G^{-1}(\omega = 0, k) \alpha(\omega = 0, k) = \mu_\alpha(\omega = 0, k) |\alpha(\omega = 0, k)\rangle$$

all $\mu_\alpha(0, k)$ are real numbers. An eigenvector $|\alpha(0, k)\rangle$ with $\mu_\alpha(0, k) > 0$ is called an ‘$R$-zero’ (Wang and Zhang 2012a, Wang et al 2012), and the space spanned by $R$-zeros is called ‘$R$-space’. We can define the Berry gauge field and Berry curvature in the $R$-space, as if the $R$-space is the ‘occupied band(s)’ of a noninteracting insulator. Therefore, we can define topological invariants just in the same way as the noninteracting cases. For example, for two-dimensional topological insulators with broken time reversal symmetry (namely the quantum Hall insulator), we have the ‘generalized Chern number’ (Wang and Zhang 2012a)

$$C_1 = \frac{1}{2\pi} \int d^2 k \mathcal{F}_{xy}$$

where $\mathcal{F}_{ij} = \partial_i A_j - \partial_j A_i$, and $A_i = -i \sum_\alpha \langle k\alpha | \partial_i | k\alpha \rangle$. Here $|k\alpha\rangle$ runs through an orthonormal basis of the $R$-space. This is a topological invariant for 2D interacting insulators. Now we may ask a crucial question: Can we justify discarding Green’s function at nonzero frequencies? Fortunately, the answer is
yes. Taking advantage of general mathematical properties
of Green’s function, it has been established (Wang and
Zhang 2012a) that nonzero frequencies are always superfluous
for the purpose of defining topological invariants; in other
words, zero frequency is sufficient. It is also useful to mention
that the physical Hall response is determined (Wang and
Zhang 2012a) by this generalized Chern number if there is
no nontrivial ground state degeneracy. This approach has
been systematically generalized (Wang and Zhang 2012a, 2012b)
to topological insulators and superconductors in other
symmetry classes.
Since $G^{-1}(0, \mathbf{k})$ plays a crucial role in this approach, let
us define the ‘topological Hamiltonian’ as
$$h_{0}(\mathbf{k}) = -G^{-1}(0, \mathbf{k})$$
(3)
which can also be written as
$$h_{1}(\mathbf{k}) = h_{0}(\mathbf{k}) + \Sigma(0, \mathbf{k})$$
(4)
following the Dyson equation. In the absence of electron–
electron interactions, $h_{1}$ is reduced to the free Hamiltonian
$h_{0}$. With the definition in equation (3), the generalized Chern
number for interacting insulators, given in equation (2), is
equivalent to the Chern number of an ‘noninteracting system’
with free Hamiltonian $h_{0}(\mathbf{k})$. Therefore, $h_{1}$ is a convenient
language for the zero frequency Green’s function approach. It
can be applied (Wang and Zhang 2012a, 2012b) to topological
insulators and topological superconductors in all symmetry
classes in the periodic table (Kitaev 2009). In the appendix
we list explicit formulas for these $h_{1}$ topological invariants
to make this paper self-contained.

A naïve understanding of $h_{1}$ is to think of it as an
effective Hamiltonian for quasiparticles, namely that $h_{1}$
describes ‘renormalized energy bands’. As we will see,
this understanding is incorrect. In fact, the natural effective
Hamiltonian producing the ‘would-be’ quasiparticles\(^3\) and
accurate energy spectra can be described as follows. Let us
start from the self-consistent equations (Hybertsen and Louie
1985, 1986) for quasiparticle spectra, which can be written in
a simplified notation as
$$[h_{0}(\mathbf{k}) + \Sigma(\omega_{q}, \mathbf{k})]u_{\alpha}(\mathbf{k}) = \omega_{\alpha}(\mathbf{k})u_{\alpha}(\mathbf{k})$$
(5)
which can be more compactly written as
$$G^{-1}(\omega_{\alpha}, \mathbf{k})u_{\alpha}(\mathbf{k}) = 0.$$  
(6)
Equation (5) is a self-consistent equation with the self-energy
$\Sigma$ depending on the spectra $\omega_{\alpha}$. It is worth emphasizing that it is
$\Sigma(\omega_{\alpha}, \mathbf{k})$ instead of $\Sigma(0, \mathbf{k})$ that appears in equation (5). In
a general interacting system, $\Sigma(0, \mathbf{k})$ can be far away from
$\Sigma(\omega_{\alpha}, \mathbf{k})$, therefore the topological Hamiltonian approach
using $\Sigma(0, \mathbf{k})$ is a poor tool for energy spectra. Unlike $\omega_{\alpha}$
and $|u_{\alpha}(\mathbf{k})|$ given by equation (5), which can be interpreted
as energy spectra and ‘quasiparticles’, the eigenvalues and
eigenvectors of $h_{1}(\mathbf{k})$ lack clear physical meaning at this stage.
The powerful aspect of the topological Hamiltonian approach
\(^3\) It is called ‘would-be quasiparticle’ because the concept of quasiparticle
is precise only when the imaginary part of self-energy is negligible. This
condition is not generally satisfied at nonzero frequency for insulators.
is its ability to produce topological invariants rather than
energy spectra.

Can we define physically meaningful topological
invariants in terms of $|u_{\alpha}(\mathbf{k})|$ (or equivalently, in $\Sigma(\omega_{\alpha}, \mathbf{k})$)\(^2\)?
As we will see in the following, this effective Hamiltonian
approach turns out to be less fruitful than the topological
Hamiltonian approach. Let us proceed to see how far we can
go in the effective Hamiltonian approach. It is natural to define
a frequency-dependent ‘effective Hamiltonian’
$$h_{\text{eff}}(\omega, \mathbf{k}) = h_{0}(\mathbf{k}) + \Sigma(\omega, \mathbf{k}).$$
(7)
Furthermore, it seems also natural to define Berry connection
in terms of $|u_{\alpha}(\mathbf{k})|$ instead of $|\langle\mathbf{0}, \mathbf{k}\rangle|$ given in equation (1),
since $|u_{\alpha}(\mathbf{k})|$ represents the quasiparticle picture in the
interacting system. Now there is a difficulty in doing so,
namely that $\Sigma(\omega, \mathbf{k})$ is generally not a Hermitian matrix. Let
us partially circumvent this difficulty by writing $\Sigma(\omega, \mathbf{k}) =
\Sigma_{1}(\omega, \mathbf{k}) + i\Sigma_{2}(\omega, \mathbf{k})$, with both $\Sigma_{1}$ and $\Sigma_{2}$ Hermitian.
Assuming that the imaginary part $\Sigma_{2}$ can be safely ignored,
we replace $\Sigma(\omega, \mathbf{k})$ by $\Sigma_{1}(\omega, \mathbf{k})$ in equation (5), which now reads
$$h_{0}(\mathbf{k}) + \Sigma_{1}(\omega_{\alpha}, \mathbf{k})|u_{\alpha}(\mathbf{k})| = \omega_{\alpha}(\mathbf{k})|u_{\alpha}(\mathbf{k})|.$$  
(8)
Here we encounter another difficulty, namely that $|u_{\alpha}(\mathbf{k})|$ are
generally not orthogonal to each other. This is a relatively
minor problem since we can obtain an orthonormal basis by the
Gram–Schmidt process. For 2D quantum Hall systems, let us
define the ‘quasiparticle Chern number’ as
$$\tilde{C}_{1} = \frac{1}{2\pi} \int d^{2}\mathbf{k} \tilde{F}_{xy}$$
(9)
where $\tilde{F}_{ij} = \partial_{\mathbf{k}} \tilde{A}_{j} - \partial_{\mathbf{k}} \tilde{A}_{i}$, and $\tilde{A}_{i} = -i\sum_{\alpha} (u_{\alpha}(\mathbf{k})|\partial_{\mathbf{k}} |u_{\alpha}(\mathbf{k})|)$, in
which $|u_{\alpha}(\mathbf{k})|$ is an orthonormal basis in the space spanned by
those $|u_{\alpha}(\mathbf{k})|$ with negative $\omega_{\alpha}(\mathbf{k})$. The motivation to choose
equivalent $\omega_{\alpha}(\mathbf{k})$ is to generalize the ‘occupied band’, which is
a crucial concept for the definitions of topological invariants
in noninteracting system.

In the remaining parts of this paper, we will show by
an explicit example that equation (9) is unsuitable because
it can differ from the correct topological invariants given by
equation (2). We then explain the reason why equation (2)
instead of equation (9) is the suitable topological invariants
from the surface state picture.

3. Effective Hamiltonian is a poor tool for
topological invariant

In this section we study a toy model to show that the self-
consistent ‘quasiparticle’ approach starting from equation (5)
is unsuitable for calculating topological invariants. For
instance, equation (9) can fail for a quantum Hall system. Let
us begin with a two-dimensional (2D) model of the quantum
anomalous Hall effect (Haldane 1988, Qi et al 2006) with
electron–electron interactions. The free Hamiltonian part $H_{0}$
describes a two-band model (Qi et al 2006) with
$$h_{0}(\mathbf{k}) = \sin k_{x} \sigma_{x} + \sin k_{y} \sigma_{y}
+ [m_{0} + (2 - \cos k_{x} - \cos k_{y})] \sigma_{z}.$$  
(10)
Instead of giving an explicit form for the interaction term $H_i$, in the following we will choose an ansatz for self-energy $\Sigma(\omega, \mathbf{k})$, which is sufficient for our purpose.

Let us make a simple ansatz that $\Sigma(\omega, \mathbf{k}) \approx \Sigma_c(\omega, \mathbf{k})\sigma_z$ near $\mathbf{k} = 0$, in which case the main idea can be most readily appreciated. Near $\mathbf{k} = 0$ we have $h_{\text{eff}}(\omega, \mathbf{k}) \approx k_x\sigma_x + k_y\sigma_y + m(\omega)\sigma_z$, where $m(\omega) = m_0 + \Sigma(\omega, \mathbf{k} = 0)$. Additionally, we assume that the interaction preserves particle–hole symmetry, implying that $\Sigma_c(\omega, 0) = \Sigma_c(-\omega, 0)$. From equation (5) (taking $\mathbf{k} = 0$) we can obtain the self-consistent equation

$$m_{\text{eff}} = m_0 + \Sigma_c(m_{\text{eff}}, \mathbf{k} = 0). \quad (11)$$

This effective mass will be crucial in calculating $\tilde{C}_1$. On the other hand, the topological mass is defined as

$$m_t = m_0 + \Sigma_c(0, \mathbf{k} = 0). \quad (12)$$

Near $\mathbf{k} = 0$ we have $h_i(\mathbf{k}) \approx k_x\sigma_x + k_y\sigma_y + m_0\sigma_z$. Following equation (2), we can obtain the correct topological invariants as

$$C_1 = \frac{1}{4\pi} \int d^2\mathbf{k} \cdot (\partial_k \mathbf{n} \times \partial_\mathbf{k} \mathbf{n}) \quad (13)$$

where the integral range is the Brillouin zone, $\mathbf{n} = n/|n|$, and $\mathbf{n} = (n_x(\mathbf{k}), n_y(\mathbf{k}), n_z(\mathbf{k}))$ is extracted from $h_i(\mathbf{k}) = h_0(\mathbf{k}) + \Sigma(0, \mathbf{k}) = \sigma \cdot \mathbf{n}$. As a concrete example, let us pick $m_0 = -0.2$, $\Sigma_c(0, \mathbf{k} = 0) = 0.1$, then $m_t = -0.1$, from which it follows that $C_1 = -1$. If we pick $\Sigma_c(0.1, \mathbf{k} = 0) = 0.3$ (as an example), then $m_{\text{eff}} = 0.1$ is self-consistently obtained from equation (11). It follows that $\tilde{C}_1$ determined by equation (9) is $\tilde{C}_1 = 0$. We knew that equation (2) produces the correct topological invariants $C_1$ (Wang and Zhang 2012a), therefore, equation (9) fails in this case because $\tilde{C}_1 \neq C_1$.

### 4. Topological Hamiltonian determines topological surface states

In the previous sections we have shown that the natural self-consistent $h_{\text{eff}}$ approach starting from equation (5) can produce the wrong topological invariants, while the ‘topological Hamiltonian’ $h_i(\mathbf{k}) = -G^{-1}(0, \mathbf{k})$ produces the correct topological invariants. This seems mysterious because the eigenvectors $|u_i(\mathbf{k})\rangle$ of $h_{\text{eff}}$ (see equation (5)) can be interpreted as the ‘would-be’ quasiparticles’, while the eigenvectors of $h_i$ have no clear physical meaning. Why should we expect $h_i$ instead of $h_{\text{eff}}$ to produce the correct topological invariants? The answer, as we will show, is that the gapless surface states are determined by $h_i$. The key idea is that the zero energy surface states, if they exist, will feel the self-energy $\Sigma(\omega = 0)$ because they have zero energy. Explicitly, the zero energy surface states $|\psi\rangle$ satisfy the formal equation

$$h_i|\psi\rangle = 0 \quad (14)$$

which is self-consistent because it follows from $G^{-1}(\omega)|\psi\rangle = 0$ (or $[\omega - h_0 - \Sigma(\omega)]|\psi\rangle = 0$) by taking $\omega = 0$. Equation (14) remains meaningful when the translational symmetry is broken, because $h_i = -G^{-1}(\omega = 0) = h_0 + \Sigma(\omega = 0)$ can also be defined in coordinate instead of momentum space. Now we can see that $h_i$ is a tailor-made ‘Hamiltonian’ for the gapless surface states. The existence of robustly gapless surface states is a holographic manifestation of the bulk topology, therefore, the direct connection between $h_i$ and surface states firmly establishes the $h_i$ approach to bulk topological invariants.

Now let us flesh out the above idea in the simple two-band model studied in section 3. Consider a 2D system with coordinate $(x, y)$ (see figure 1). What we shall show is that at the interface between two bulk states with different $C_1$ (calculated from topological Hamiltonian), there is gapless surface state. Let us suppose that the many-body Hamiltonian $H$ is a function of $x$, namely that certain parameters (e.g. interaction strength) of $H$ vary as functions of $x$, then the topological Hamiltonian $h_i$ is also a function of $x$. Assuming the form of $h_i$ given in section 3, we now have $h_i(x) \approx -\sigma_x\partial_x + \sigma_yk_y + \sigma_xm(x)$, since the translational symmetry along the $x$-direction is broken. Because it will not affect our conclusion, we take $|m_t(x)| \ll 1$ to simplify our analysis. Let us suppose that

$$m_t(x \to +\infty) \to M; \quad m_t(x \to -\infty) \to -M \quad (15)$$

and that $m_t$ smoothly interpolates between these two limits near $x = 0$ (see figure 1(b)).

Due to the translational symmetry in the $y$-direction, $k_y$ is a good quantum number, thus we can study the $k_y = 0$ branch first. Now $h_i$ reads

$$h_i \approx -i\sigma_x \partial_x + \sigma_xm_t(x). \quad (16)$$

We have omitted terms of higher order in $\mathbf{k}$ since we are concerned with low-energy modes. If $M > 0$ ($M$ is defined in equation (15)), the solution of the zero mode from equation (14) is readily obtained as

$$|\psi(x)\rangle_{\text{zero mode}} = \frac{1}{\sqrt{2}} |\frac{1}{i}\rangle \exp\left[-\int x' m_t(x')\right]. \quad (17)$$

The assumption of existence of this zero mode requires that $m_t(x) < 0$ when $x \to -\infty$ and $m_t(x) > 0$ when $x \to \infty$.
(otherwise the wavefunction diverges) (Jackiw and Rebbi 1976, Goldstone and Wilczek 1981), which is satisfied by this solution. If \( M < 0 \), then there is also a zero mode solution with \((1, -i)^T\) replacing the \((1, i)^T\) factor in equation (17). Note that the existence of a zero mode is fully determined by the asymptotic behaviors of \( h_0(x) \) as \(|x| \gg 0\), therefore it is determined by the bulk topology. From the above explicit calculation at the interface we have seen that when \( m_k(x) \) changes sign at the interface near \( x = 0 \), there are exact zero modes. The above calculation looks in parallel with the noninteracting cases in which we start from \( h_0 \) instead of \( h_t \), however, the crucial difference is that in interacting cases we have a frequency-dependent self-energy, and \( \Sigma(\omega = 0) \) appears in a self-consistent manner.

From the bulk calculation given in section 3, we have \( C_1(m_0 > 0) = 0 \) and \( C_1(m_0 < 0) = -1 \) (remember that we take \(|m| \ll 1\)), thus the topological invariants at the two sides of the interface are different. To summarize the above calculations, we have shown that the gapless surface states are associated with the difference of topological invariants (calculated from \( h_0 \)) at the two sides of the interface. In experiment, one side of the interface is often the vacuum, which can be regarded as a topologically trivial insulator, therefore, having ‘different topological invariants’ at the two sides of the interface means that the insulator has a nontrivial topological invariant \( C_1 \neq 0 \) in this quantum Hall example.

The fact that \( h_t \) self-consistently determines the basic properties of gapless surface modes (e.g. the existence or absence of these gapless modes), as given by equation (14), is among the central results of this paper. It is equally notable that \( h_{\text{eff}} \) plays no role in the solution of the zero energy surface mode. This is the simple reason why \( h_t \) instead of \( h_{\text{eff}} \) should determine the bulk topological invariants.

We would like to add a remark for symmetry protected topological insulators, for which the topology is well defined provided that the bulk has the given symmetry. Let us take the time reversal invariant \( Z_2 \) topological insulators in three dimensions (Moore 2010, Hasan and Kane 2010, Qi and Zhang 2011) as an example. Suppose that the bulk time reversal symmetry is preserved. If the time reversal symmetry at the surface is also preserved, then the relation between \( h_0 \) and the gapless surface states discussed in this paper is applicable. On the other hand, if the surface states break the time reversal symmetry, either by external perturbation (e.g. surface magnetism) or spontaneous symmetry breaking, the surface become gapped, and \( h_t \) calculates the coefficient of topological field theory (Qi et al 2008). The same relation between \( h_0 \) and topological field theory (Wang et al 2011, Ryu et al 2012, Nomura et al 2012, Stone 2012) is true for symmetry protected topological superconductors. Therefore, \( h_t \) can tell us about physical topological responses such as the half-quantum Hall effect (Fu and Kane 2007, Qi et al 2008) and thermal Hall effect (Wang et al 2011, Ryu et al 2012) at the surface of topological states, if the surfaces are gapped.

We also note that we can have another understanding of \( h_t \), if we treat \( h_t(\lambda) \) as a function of a tuning parameter \( \lambda \) instead of the spatial coordinate \( x \). This is an understanding from the perspective of topological phase transition, in which the low-energy modes near the transition point play the role of ‘gapless surface/interface state’ discussed in this section.

5. Conclusions

In conclusion, we have shown that, for interacting systems, the self-consistent quasiparticle approach given by equation (5), which is a natural generalization of the noninteracting ‘occupied band’, is unsuitable for the purpose of topological invariants. We have also confirmed that the topological Hamiltonian \( h_t \) is the suitable tool, though its eigenvalues are generally very different from the true energy spectra. The simple reason, as we have shown, is that \( h_t \) directly tells us about the information of gapless surface states.

Early topological invariants (Ishikawa and Matsuyama 1986, Volovik 2003, Wang et al 2010) derived from Green’s function require integrals over the entire frequency domain, which are difficult to implement. Recently it has been shown (Wang and Zhang 2012a) mathematically that only zero frequency is relevant for topological invariants. This result justifies discarding Green’s function at nonzero frequencies, however, a more physical understanding of this approach was absent. We hope that the present paper has filled this gap by looking at the surface states. It is worth noting that the purpose of this paper is to understand the topological Hamiltonian approach as an exact tool, while more realistic models in which this approach may find wide applications remain to be studied.

The \( h_t \) approach can be applied (Wang and Zhang 2012b) to topological insulators and superconductors in all symmetry classes in the ‘periodic table’ (Kitaev 2009). After obtaining \( h_t(k) \) for an interacting system, the task of calculating topological invariants is equivalent to doing this for a ‘free fermion system’ with Hamiltonian \( h_0(k) \), thus all noninteracting topological invariants are generalized to interacting systems (see the appendix).

Let us conclude with the remark that in band structure calculations we are usually more concerned with energy spectra, namely that various versions of the ‘effective Hamiltonian’ approach are preferred, however, as we have shown in this paper, such calculations are unsuitable for the purpose of obtaining topological invariants. The topological Hamiltonian approach faithfully produces the correct topological invariants, therefore, it is a crucial tool for searching topological insulators/superconductors with strong electron–electron interactions.

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Appendix. Topological invariants for interacting (integer) topological phases in general spatial dimensions

In this appendix we list topological invariants for interacting integer topological insulators and superconductors in the periodic table (Kitaev 2009). These formulas take the same mathematical forms as their noninteracting counterparts, except that they are expressed in term of the zero frequency Green’s function \( h_0(k) = -G^{-1}(0,k) \) for interacting systems instead of the free Hamiltonian \( h_0(k) \) for noninteracting systems. We list these formulas to make this paper self-contained. The noninteracting counterparts of the listed formulas can be found in previous literature, e.g. in Ryu et al (2010).

First we list topological invariants for the two complex classes, class A and AIII, which are characterized by integer topological invariants.

For topological insulators in class A in 2n dimensions (\( n \) is an arbitrary positive integer), we can define the Berry gauge field \( A \) and the Berry curvature \( F \) in the R-space (see section 2), which can be intuitively understood as the ‘occupied band’ of \( h_0(k) \), then we can define the \( n \)th generalized Chern number as

\[
A: C_n = \frac{1}{n!} \int \text{Tr} \left( \frac{F}{2\pi} \right)^n
= \frac{1}{2\pi^n n!(2\pi)^n} \times \int d^{2n} k e^{\alpha_1 \cdots \alpha_{2n}} \text{Tr} F_{\alpha_1 \alpha_2} \cdots F_{\alpha_{2n-1} \alpha_{2n}}
\]

(A.1)

which is a straightforward generalization of equation (2). Taking \( n = 1 \) in equation (A.1), we have equation (2) with a slightly different notation, namely that the trace in equation (A.1) has been absorbed into the definition of \( A \) in equation (2). The mathematical form in equation (A.1) is the same as that of the noninteracting Chern number (Thouless et al 1982, Nakahara 1990, Ryu et al 2010), but it is defined in terms of \( h_0(k) \); thus, it is applicable to interacting insulators and superconductors.

For topological insulators in class AIII in \( 2n + 1 \) dimensions, we have the chiral symmetry

\[
\{ h(k), \Gamma \} = 0
\]

(A.2)

where \( \Gamma \) satisfy \( \Gamma^2 = 1 \). It follows that \( h_1 \) can be written as

\[
h_1(k) = \begin{pmatrix} Q(k) \\ Q^\dagger(k) \end{pmatrix}
\]

(A.3)

in the basis in which \( \Gamma \) is diagonal. The topological invariant is given as a winding number

\[
\text{AIII: } W_{2n+1} = \frac{(-1)^n n!}{(2n+1)!} \left( \frac{i}{2\pi} \right)^{n+1} \int \text{Tr} (Q^{-1} dQ)^{2n+1}
= \frac{(-1)^n n!}{(2n+1)!} \left( \frac{i}{2\pi} \right)^{n+1} \int d^{2n+1} k e^{\alpha_1 \cdots \alpha_{2n+1}} \times \text{Tr} \left[ (Q^{-1} d\alpha_1 Q) \cdots (Q^{-1} d\alpha_{2n+1} Q) \right]
\]

(A.4)

which takes the same form as the noninteracting winding number (Schnyder et al 2008, Ryu et al 2010).

We have listed formulas for the two complex classes, A and AIII. The eight real classes are similar. For topological insulators/superconductors in AI and AII classes in \( 4n \) (\( n \) is an arbitrary positive integer) dimensions, and those in C and D classes in \( 4n - 2 \) dimensions, the topological invariants are Chern numbers with the same forms as given by equation (A.1). For topological insulators/superconductors in CI and DIII classes in \( 4n - 1 \) (\( n \) is an arbitrary positive integer) dimensions, and those in BDI and CII classes in \( 4n - 3 \) dimensions, the topological invariants are the winding numbers, whose forms are the same as equation (A.4).

This list has exhausted integer topological invariants (Chern numbers and winding numbers).

The \( Z_2 \) topological invariants can be obtained from the dimensional reductions of integers invariants. This has been done for noninteracting insulators (Qi et al 2008, Ryu et al 2010), and can also be generalized to interacting insulators using \( h_1 \). For instance, the time reversal invariant topological insulators in AI class in 3D and 2D can be obtained from dimensional reduction of a 4D topological insulator in the same class (Qi et al 2008), in other words, the \( Z_2 \) topological invariant in 3D and 2D (the quantum spin Hall insulator) can be obtained from the 4D Chern number. The details of this dimensional reduction in the zero frequency Green’s function approach can be found in Wang and Zhang (2012a). For the first descendants (i.e. time reversal invariant topological insulators in 3D), we can extend \( h_1(k) \) to \( h_1(k, u) \) by adding a Wess–Zumino–Witten parameter \( u \) (similar to the procedure in Wang et al 2010b). Now we have four variables \( (k_1, k_2, k_3, u) \), thus we can define the second Chern number \( C_2 \), and identify the 3D \( Z_2 \) topological invariant as \( C_2 \) (mod 2). For the second descendants (i.e. time reversal invariant topological insulators in 2D), we can extend \( h_1(k) \) to \( h_1(k, u, v) \), and the remaining procedure is the same. More generally, for interacting \( Z_2 \) topological insulators/superconductors in any spatial dimensions in which they do exist, we can implement a Wess–Zumino–Witten extension of \( h_1 \), so that the topological invariant of a topological insulator in lower dimensions can be compactly defined in terms of quantities in higher dimensions, though the final result is independent (mod even integer) of this dimensional extension. For the first descendants of Chern insulators, the result of dimensional reduction is exactly the Chern–Simons terms (Qi et al 2008, Ryu et al 2010, Nakahara 1990), therefore, there is no need to take the Wess–Zumino–Witten extension in the calculation. For the descendants of ‘winding number insulators’, we can take the Wess–Zumino–Witten terms as the definition of \( Z_2 \) topological invariants, though no simple form analogous to the Chern–Simons term can be found.

Since all these \( Z_2 \) topological invariants take the same forms as integer topological invariants, we do not need to list all of them. Let us just take the DIII class as an example to illustrate how the integer topological invariants in \( D \) dimensions can be regarded as \( Z_2 \) invariants in \( D - 1 \) and \( D - 2 \) dimensions. For topological insulators/superconductors
in the DIII class in $4n - 1$ dimensions, we have stated that the topological invarian is given by the winding number, namely that we just replace the dimension `$2n+1$' in equation $\left(A.4\right)$ by `$4n - 1$'. Now we can write down the $Z_2$ topological invariant in $4n - 2$ dimensions as

$$DIII: Z_2 = \frac{(2n - 1)!(-1)^{n+1}}{(4n - 1)!} \left(\frac{1}{2\pi}\right)^{2n} \times \int \text{Tr}\left(Q^{-1}dQ\right)^{n-1} = \frac{(2n - 1)!(-1)^{n+1}}{(4n - 1)!} \left(\frac{1}{2\pi}\right)^{2n} \times \int \text{d}a \text{d}^{4n-2}k e^{i\alpha_{1}...\alpha_{2n-1}} \text{Tr}\left[(Q^{-1}\partial_{\alpha_{1}}Q)\cdots(Q^{-1}\partial_{\alpha_{2n-1}}Q)\right]$$

(A.5)

where the variables are $k_1,\ldots,k_{4n-2},u$. Here $u$ is a Wess–Zumino–Witten-extension parameter. More precisely, we have extended $Q$ from the Brillouin zone $(k_1,\ldots,k_{4n-2})$ to $(k_1,\ldots,k_{4n-2},u)$ $(u \in [-1,1])$, with $(k_1,\ldots,k_{4n-2},0)$ identified as the original Brillouin zone $(k_1,\ldots,k_{4n-2})$ (see Wang et al 2010b for analogous treatment). We can see that equation (A.5) is exactly the winding number in $4n - 1$ dimensions if we regard $u$ as an additional momentum $k_{4n-1}$. The only subtlety is that equation (A.5) is defined mod 2, in other words, it is a $Z_2$ topological invariant. This (mod 2) ambiguity is a well-known fact of the Wess–Zumino–Witten terms (Witten 1983). For $4n - 3$ dimensional topological insulators/superconductors in class DIII, the $Z_2$ topological invariant can be written down just like equation (A.5), except that we have two parameters $u$ and $v$ in the Wess–Zumino–Witten extension.

All other $Z_2$ topological invariants can also be obtained from equations (A.1) and (A.4), with some momentum variables replaced by Wess–Zumino–Witten parameters. The resultant formulas are analogous to equation (A.5). Because the translation from equations (A.1) and (A.4) to these $Z_2$ topological invariants is straightforward, we do not list all the formulas here.

Equations (A.1) and (A.4), and their $Z_2$ descendants (through Wess–Zumino–Witten extensions) are topological invariants expressed in terms of $h_i$ for interacting systems. These topological invariants do not involve a frequency integral and are much easier to calculate than those with a frequency integral.

Although the Green’s function has rich behaviors of frequency dependence, it turns out that all the information about the topology is fully contained in its zero frequency, which has been proved using the Lehmann spectral representation of the Green’s function and a smooth deformation (Wang and Zhang 2012a). This mathematical fact established the zero frequency Green’s function as a precise tool for topological invariants, since it implies that we cannot obtain more topological invariants even if we study Green’s function in the entire frequency domain. In the present paper, we confirm the zero frequency Green’s function approach from the perspective of surface states, which is complementary to the calculations in the bulk (Wang and Zhang 2012a).

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