

TKNN formula for general lattice Hamiltonian in odd dimensions

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Topological insulators in odd dimensions are characterized by topological numbers. We prove the well-known relation between the topological number given by the Chern character of the Berry curvature and the Chern-Simons level of the low energy effective action for a general class of Hamiltonians bilinear in the fermion with general U(1) gauge interactions including non-minimal couplings by an explicit calculation. A series of Ward-Takahashi identities are crucial to relate the Chern-Simons level to a winding number, which could then be directly reduced to Chern character of Berry curvature by carrying out the integral over the temporal momenta.

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1. Introduction

Topological insulators in $D = 2n + 1$ dimensions are characterized either by the Chern character of the Berry connection from the eigenfunctions of the Hamiltonian in the valence band [1, 2] or by the coefficient of the effective action as a function of an external U(1) gauge field, i.e., photon [3, 4, 5, 6]. These two characterizations are known to be equivalent because they both arise from the current correlation functions and there are explicit proofs for various cases [7, 8]. In Ref. [9] a proof is given for a large class of models for general odd dimensions, where they consider the most general lattice action for arbitrary free kinetic term on the lattice which is then coupled to U(1) gauge field in a minimal way, i.e. with the gauge interaction in the form of

$$H(A) = \sum_{m,n} \psi_m^\dagger h_{mn} e^{iA_{mn}} \psi_n + \sum_m \psi_m^\dagger \psi_m, \quad (1.1)$$

where m, n are the lattice sites h_{mn} are the hopping parameters and A_{mn} is the line integral of the gauge field along the straight line connecting the sites m and n . The advantage of this class of Hamiltonian is that the contact interactions such as fermion-fermion-multi-photon vertices do not contribute to the final expression so that only a set of Feynman diagram which appear also in the continuum theory gives non-vanishing contributions. Of course, this type of gauge interaction is physically motivated since it is based on the famous method of ‘Peierls substitution’ [10]. However, in more general situation, the gauge interaction may not always be described by such a single straight Wilson-line. In such cases, one has to include the contribution of contact interaction vertices. In this proceedings, we report our recent study on the equivalence for generalized lattice Hamiltonian so as to include arbitrary non-minimal gauge interactions [11].

2. Gapped fermion system on the lattice

We consider a gapped fermion system (with a gap Δ) on a lattice with the following action in Euclidean space in $D = 2n + 1$ dimensions.

$$S_E = \int dt \sum_{\vec{r}} \psi^\dagger(t, \vec{r}) \left[\frac{\partial}{\partial t} + iA_0 + H(\vec{A}) \right] \psi(t, \vec{r}), \quad (2.1)$$

where \vec{r} runs over the $2n$ dimensional spatial lattice points. We will set $x^0 = t$ in the followings. The Hamiltonian $H(\vec{A})$ is given by a summation over all the possible hoppings on the lattice which include gauge interactions with a smooth external U(1) gauge field $A_\mu = (A_0, \vec{A})$. The fermion fields $\psi^\dagger(t, \vec{r})$ and $\psi(t, \vec{r})$ give creation and annihilation operators of fermions after quantization. We assume that there are N_v bands and N_c bands below and above the fermi level, respectively. Therefore the fermion fields have $N_v + N_c$ components.

Since the fermion system is gapped with a gap size $\Delta > 0$, the effective gauge action obtained by integrating out fermions can be expanded in terms of gauge invariant local actions as $S_{\text{eff}} = \sum_k a_k S_k(A)$. Here, $S_{\text{eff}}(A)$ is defined as $e^{S_{\text{eff}}} = \int \mathcal{D}\psi \mathcal{D}\psi^\dagger e^{-S_E}$, and $S_k(A)$ are the gauge invariant actions given by the local Lagrangian $L_k(A)$ and a_k are the coefficients. By dimensional analysis, if the Lagrangian $L_k(A)$ has a mass dimension d_k the coefficient a_k is suppressed by the $d_k - (2n + 1)$ -powers in $\frac{1}{\Delta}$ or lattice spacing a . Many of the Lagrangians are given in terms of gauge invariant field

$F_{\mu\nu}$ Since we do not have the Lorentz-invariance on the lattice, the structure of the coefficients a_k in the effective action heavily depend the geometry of the lattice. However, there is a very special parity-violating term called Chern-Simons action $S_{\text{cs}}(A)$ given by

$$S_{\text{cs}}(A) = \int d^{2n+1}x \epsilon_{\alpha_0\beta_1\alpha_1\cdots\beta_n\alpha_n} A_{\alpha_0} \partial_{\beta_1} A_{\alpha_1} \cdots \partial_{\beta_n} A_{\alpha_n}. \quad (2.2)$$

This action is topological and always takes this form no matter what the geometry of the lattice is. Topological information of the fermion system is contained in the effective action through the coefficient c_{cs} as $S_{\text{eff}}(A) = ic_{\text{cs}}S_{\text{cs}} + \cdots$ where " \cdots " stands for other gauge invariant terms. Here the gauge invariance of the action requires that the coefficient is quantized as

$$c_{\text{cs}} = \frac{k}{(2\pi)^n(n+1)!}, \quad k \in \mathbb{Z}. \quad (2.3)$$

Since the Chern-Simons action is of the lowest dimension in the parity-violating sector, the coefficient c_{cs} can be obtained by the following quantity

$$c_{\text{cs}} = \frac{(-i)^{n+1} \epsilon_{\alpha_0\beta_1\alpha_1\cdots\beta_n\alpha_n}}{(n+1)!(2n+1)!} \left(\frac{\partial}{\partial(q_1)_{\beta_1}} \right) \cdots \left(\frac{\partial}{\partial(q_n)_{\beta_n}} \right) \prod_{i=1}^n \int d^D x_i e^{iq_{\alpha_i} x_i} \frac{\delta^{n+1} S_{\text{eff}}(A)}{\delta A_{\alpha_0}(x_0) \delta A_{\alpha_1}(x_1) \cdots \delta A_{\alpha_n}(x_n)} \Bigg|_{q_i=0} \quad (2.4)$$

The effective action can be given by the log of the fermion determinant as $S_{\text{eff}}(A) = \text{Tr}[\ln(D_0 + H(A))]$, where $D_0 = \frac{\partial}{\partial x_0} + iA_0$. Splitting the kinetic operator $D_0 + H(A)$ into free part and interaction part as $D_0 + H(A) = \frac{\partial}{\partial x_0} + H_0 - \Gamma(A)$, where H_0 is the free fermion part defined as $H_0 \equiv H(A)|_{A=0}$ and $\Gamma(A)$ is the interaction part defined as $\Gamma(A) \equiv -iA_0 - H(A) + H_0$. Expanding in $\Gamma(A)$, we obtain

$$S_{\text{eff}}(A) - \text{const.} = - \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} \left[\left(\frac{1}{\frac{\partial}{\partial x_0} + H_0} \Gamma(A) \right)^n \right] \quad (2.5)$$

From Eq.(2.4), we find that the Chern-Simons coupling for $D = 2 + 1$ dimension is given by

$$c_{\text{cs}} = - \frac{(-i)^2}{2!3!} \int \frac{d^3 p}{(2\pi)^3} \epsilon_{\alpha_0\beta_1\alpha_1} \left(\frac{\partial}{\partial q_1} \right)_{\beta_1} \left\{ \text{Tr} \left[S_F(p) \Gamma^{(2)}[-q_1, \alpha_0; q_1, \alpha_1; p] \right] + \text{Tr} \left[S_F(p - q_1) \Gamma^{(1)}[-q_1, \alpha_0; p] S_F(p) \Gamma^{(1)}[q_1, \alpha_1; p - q_1] \right] \right\} \Bigg|_{q_i=0} \quad (2.6)$$

where $S_F(p)$ is the fermion propagator $\frac{1}{ip_0 + H_0(\vec{p})}$ and $\Gamma^{(1)}[q_1, \alpha_1; p]$ and $\Gamma^{(2)}[q_1, \alpha_1; q_2, \alpha_2; p]$ are fermion-fermion-photon and fermion-fermion-photon-photon vertices with in-coming fermion momentum p and in-coming photon momenta q_i ($i = 1, 2$) with Lorentz index α_i ($i = 1, 2$)

$$\Gamma^{(1)}[q_1, \alpha_1; p] = \int d^{2n+1}x_1 e^{iq_1 \cdot x_1} \int d^{2n+1}y e^{ip \cdot y} \frac{\delta \Gamma[A](x, y)}{\delta A_{\alpha_1}(x_1)} \Bigg|_{A=0}, \quad (2.7)$$

$$\Gamma^{(2)}[q_1, \alpha_1, q_2, \alpha_2; p] = \prod_{i=1}^2 \left(\int d^{2n+1}x_i e^{iq_i \cdot x_i} \right) \int d^{2n+1}y e^{ip \cdot y} \frac{\delta^2 \Gamma[A](x, y)}{\delta A_{\alpha_1}(x_1) \delta A_{\alpha_2}(x_2)} \Bigg|_{A=0}, \quad (2.8)$$

Note that the contributions with multi-photon vertices vanishes for the class of Hamiltonians with gauge interactions given by a single straight Wilson-line because the multi-photon vertices are

symmetric under the interchange of Lorentz indices of photons. When contracted with the anti-symmetric tensor, such contributions vanish. However, in general Hamiltonian we must consider these contributions.

In addition to the usual Ward-Takahashi identity $\Gamma^{(1)}[0, \alpha; p] = -\frac{\partial S_F^{-1}(p)}{\partial p_\alpha}$, we derive the Ward-Takahashi identities in Appendix A as

$$\left. \frac{\partial^2 \Gamma^{(1)}[k, \mu; p]}{\partial k_\nu \partial p_\lambda} \right|_{k=0} = \left. \frac{\partial \Gamma^{(2)}[k, \mu; 0, \lambda; p]}{\partial k_\nu} \right|_{k=0} = \left. \frac{\partial \Gamma^{(2)}[0, \lambda; l, \mu; p]}{\partial l_\nu} \right|_{l=0}. \quad (2.9)$$

Using these identities, the integrand of Eq. (2.6) can be rewritten as

$$\epsilon_{\alpha_0 \beta_1 \alpha_1} \text{Tr} \left[\frac{\partial}{\partial p_{\alpha_0}} \left(2S_F(p) \frac{\partial \Gamma^{(1)}[q, \alpha_1; p]}{\partial q_{\beta_1}} \right) + S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} \right] \Bigg|_{q=0} \quad (2.10)$$

The first term is a total divergence which vanishes when we integrate over the momentum. Therefore, one finds that the Chern-Simons coupling is given by the winding number as

$$c_{\text{cs}} = \frac{(-i)^2 \epsilon_{\alpha_0 \beta_1 \alpha_1}}{2!3!} \int \frac{dp_0}{2\pi} \int_{\text{BZ}} \frac{d^2 p}{(2\pi)^2} \text{Tr} \left[S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} \right] \quad (2.11)$$

For the case for $D = 4 + 1$ dimension ($n = 2$), we also have the following Ward-Takahashi identity given in Appendix A

$$\left. \frac{\partial^2 \Gamma^{(3)}[q, \mu; r, \nu; 0, \lambda; p]}{\partial q_\alpha \partial r_\beta} \right|_{q=r=0} = \left. \frac{\partial^3 \Gamma^{(2)}[q, \mu; r, \nu; p]}{\partial q_\alpha \partial r_\beta \partial p_\lambda} \right|_{q=r=0}. \quad (2.12)$$

with which one can show extra terms add up to total derivatives so we obtain

$$c_{\text{cs}} = -\frac{(-i)^3 \cdot 2}{3!5!} \int \frac{d^5 p}{(2\pi)^5} \epsilon_{\alpha_0 \beta_1 \alpha_1 \beta_2 \alpha_2} \text{Tr} \left[S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_2}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_2}} \right] \quad (2.13)$$

Therefore, Chern-Simons coupling is given by the winding number with fermion propagator also for $D = 4 + 1$ case.

3. Equivalence of winding number and chern number

We now show the equivalence of the Chern-Simons coupling given by the winding number expression and the Chern character given by the Berry connection for the energy eigenstates in the valence bands. The proof of this part is already given in Ref. [9], but since the proof is simple, we give it here for completeness. We give the calculation for arbitrary odd ($D = 2n + 1$) dimensions, even though we have shown that the Chern-Simons coupling c_{cs} can be written by the winding number using S_F only for $D = 2 + 1$ and $D = 4 + 1$ dimensions.

In order to simplify the notation, hereafter we abbreviate the derivative with respect to the momentum p_μ as $\partial_\mu \equiv \frac{\partial}{\partial p_\mu}$. The result of the previous section for $D = 2 + 1$ and $D = 4 + 1$ can

be unified to the following results: In the expression using the fermion propagator $S(p) = \frac{1}{ip^0 + H}$ and inserting a complete set of energy eigenstates $\sum_{\alpha} |\alpha\rangle\langle\alpha|$, where α is the label of energy, the Chern-Simons coupling c_{cs} is given as

$$c_{cs} = \frac{n!(-i)^{n+2}}{(n+1)!(2n)!} \int \frac{d^{2n}p}{(2\pi)^{2n}} \sum_{\alpha_1, \dots, \alpha_{2n}} \varepsilon^{i_1 i_2 \dots i_{2n}} \int \frac{dp^0}{2\pi} \frac{\langle\alpha_1|\partial_{i_1}H|\alpha_2\rangle\langle\alpha_2|\partial_{i_2}H|\alpha_3\rangle\cdots\langle\alpha_{2n}|\partial_{i_{2n}}H|\alpha_1\rangle}{(ip^0 + E_{\alpha_1})^2(ip^0 + E_{\alpha_2})\cdots(ip^0 + E_{\alpha_{2n}})}, \quad (3.1)$$

where i_1, \dots, i_{2n} stand for the spatial indices.

All we have to do is to integrate over p^0 using Cauchy's theorem. Here, we use a trick to simplify the integration. It is easy to see that the expression Eqs. (2.10), (2.13) are invariant under continuous deformation of S_F (or H) provided that the integrand remains to have no singularities. Therefore, under a continuous change of the Hamiltonian, the winding number remains unchanged from its original value as long as the energy spectrum is kept gapped throughout the deformation. Now, the most general Hamiltonian with N_v valence bands and N_c conduction bands is expressed as

$$H(\vec{p}) \equiv \sum_{a=1}^{N_v} E_a(\vec{p}) |a(\vec{p})\rangle\langle a(\vec{p})| + \sum_{b=1}^{N_c} E_b(\vec{p}) |b(\vec{p})\rangle\langle b(\vec{p})|, \quad (3.2)$$

where $|a(\vec{p})\rangle$ labeled by a is the energy eigenstate in the valence band with spatial momentum \vec{p} and negative energy eigenvalue $E_a(\vec{p}) < 0$. The state $|b(\vec{p})\rangle$ labeled by b is the energy eigenstate in the conduction band with spatial momentum \vec{p} and positive energy eigenvalue $E_b(\vec{p}) > 0$. One can continuously deform the Hamiltonian without hitting the singularity of $S(p)$ (i.e. keeping the system gapped) so that all energy eigenvalues in the conduction bands and all energy eigenvalues in the valence bands are degenerate and momentum independent (i.e. flat band) respectively. Then the deformed Hamiltonian H_{new} which gives the same winding number becomes

$$H_{\text{new}}(\vec{p}) = E_v \sum_{a=1}^{N_v} |a(\vec{p})\rangle\langle a(\vec{p})| + E_c \sum_{b=1}^{N_c} |b(\vec{p})\rangle\langle b(\vec{p})|, \quad (3.3)$$

where $E_v < 0$, $E_c > 0$ are the momentum independent constant. Here the eigenstates are identical to those with the original Hamiltonian. Since there are only two poles, we can easily carry our p^0 integral to obtain

$$J = - \sum_{a_1, \dots, a_n=1}^{N_v} \sum_{\dot{a}_1, \dots, \dot{a}_n=1}^{N_c} \varepsilon^{i_1 j_1 \dots i_{2n} j_{2n}} \frac{(2n)!}{(n!)^2} \langle a_1 | \partial_{i_1} \dot{a}_1 \rangle \langle \dot{a}_1 | \partial_{j_1} a_2 \rangle \times \cdots \times \langle a_n | \partial_{i_n} \dot{a}_n \rangle \langle \dot{a}_n | \partial_{j_n} a_1 \rangle.$$

Let us define the Berry connection using the negative energy eigenstates as

$$\mathcal{A}^{ab} \equiv \mathcal{A}_{\mu}^{ab} dx^{\mu} = -i \langle a | \partial_{\mu} b \rangle dx^{\mu} \equiv -i \langle a | db \rangle. \quad (3.4)$$

Then it is straightforward to show that the Berry curvature \mathcal{F}^{ab} is

$$\mathcal{F}^{ab} \equiv (d\mathcal{A} + i\mathcal{A}\mathcal{A})^{ab} = i \sum_{c=1}^{N_c} \langle a | dc \rangle \langle c | db \rangle \quad (3.5)$$

Using Eq. (3.5), the Chern-Simons coupling can be expressed as

$$c_{\text{cs}} = \frac{(-1)^n}{(n+1)!(2\pi)^n} \int_{\text{BZ}} \text{ch}_n(\mathcal{A}), \quad (3.6)$$

where $\text{ch}_n(\mathcal{A})$ is the 2nd Chern character defined by $\text{ch}_n(\mathcal{A}) = \frac{1}{n!} \frac{1}{(2\pi)^n} \text{tr}(\mathcal{F}^n)$. Comparing this expression with Eq. (2.3) $c_{\text{cs}} = \frac{k}{(n+1)!(2\pi)^n}$,

$$k = (-1)^n \int_{\text{BZ}} \text{ch}_n(\mathcal{A}). \quad (3.7)$$

We have shown the Chern-Simons level and the topological number in terms of the Berry connection is identical. On the other hand, while the Berry connection approach is limited to the free theory case, the effective theory approach can be applied also to interacting theories.

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A. Ward-Takahashi identities

In this appendix, we derive various identities among vertex functions and the inverse fermion propagator obtained from gauge invariance, i.e. Ward-Takahashi identities. Finite difference operator which appears in the hopping term of the lattice fermion system can be expressed in terms of infinite series of derivatives. Therefore, we assume that the Hamiltonian can be expressed in terms of all sorts of fermion hopping terms connected by the Wilson-lines of arbitrary contours or superpositions of them. Then, the action can be formally expanded as

$$S = \int dt \sum_{\vec{x}} \sum_{n=0}^{\infty} \psi^\dagger(t, \vec{x}) M_{\mu_1 \dots \mu_n} (D_{\mu_1} \dots D_{\mu_n} \psi)(t, \vec{x}) \quad (A.1)$$

where summation over μ_1, \dots, μ_n are implicit. $M_{\mu_1 \dots \mu_n}$ are some $N \times N$ matrix where $N = N_c + N_v$ is the number of fermion degrees of freedom per site.

Expanding this action in terms of gauge fields and making Fourier transformations, one can obtain the formal expressions of the inverse propagator and the vertex functions in the momentum space. In the following, let us denote the inverse fermion propagator with momentum p as $S_F^{-1}(p)$ and the vertex functions with incoming fermion momentum p and n photons with incoming momentum k_i and μ_i components ($i = 1, \dots, n$) and outgoing fermion with momentum $p + \sum_{i=1}^n k_i$ as $\Gamma^{(n)}[k_1, \mu_1; \dots; k_n, \mu_n; p]$. Then the formal expression gives

$$S_F^{-1}(p) = \sum_{n=0}^{\infty} M_{\mu_1 \dots \mu_n} \prod_{i=1}^n (ip_{\mu_i}), \quad (A.2)$$

$$\Gamma^{(1)}[k, \mu; p] = -i \sum_{n=1}^{\infty} \sum_{a=1}^n M_{\mu_1 \dots \mu_{a-1} \mu_{a+1} \dots \mu_n} \prod_{i=1}^{a-1} (i(p+k)_{\mu_i}) \prod_{i=a+1}^n (ip_{\mu_i}), \quad (A.3)$$

Substituting Eqs. (A.2) (A.3), it is easy to show the usual Ward-Takahashi identity in QED holds.

Now, it is interesting to note that we could also obtain Ward-Takahashi identities for quantities involving higher order terms in photon momenta and multi-photon vertex functions. For example the two-photon vertex is given as

$$\begin{aligned} & \Gamma^{(2)}[k, \mu; l, \nu; p] \\ &= -i^2 \sum_{n=1}^{\infty} \sum_{\substack{a, b=1 \\ a < b}}^n M_{\mu_1 \cdots \mu_{a-1} \nu \mu_{a+1} \cdots \mu_{b-1} \nu \mu_{b+1} \cdots \mu_n} \prod_{i=1}^{a-1} (i(p+k+l)_{\mu_i}) \prod_{i=a+1}^{b-1} (i(p+l)_{\mu_i}) \prod_{i=b+1}^n (ip_{\mu_i}) \\ &- i^2 \sum_{n=1}^{\infty} \sum_{\substack{a, b=1 \\ a < b}}^n M_{\mu_1 \cdots \mu_{a-1} \nu \mu_{a+1} \cdots \mu_{b-1} \mu \mu_{b+1} \cdots \mu_n} \prod_{i=1}^{a-1} (i(p+k+l)_{\mu_i}) \prod_{i=a+1}^{b-1} (i(p+k)_{\mu_i}) \prod_{i=b+1}^n (ip_{\mu_i}), \end{aligned} \quad (\text{A.4})$$

Using Eqs.(A.3) (A.4) , we obtain the following identities:

$$\left. \frac{\partial^2 \Gamma^{(1)}[k, \mu; p]}{\partial k_\nu \partial p_\lambda} \right|_{k=0} = \left. \frac{\partial \Gamma^{(2)}[k, \mu; l, \lambda; p]}{\partial k_\nu} \right|_{k, l=0} = \left. \frac{\partial \Gamma^{(2)}[k, \lambda; l, \mu; p]}{\partial l_\nu} \right|_{k, l=0} \quad (\text{A.5})$$

Carrying out similar calculations by simply differentiating $\Gamma^{(2)}$ and $\Gamma^{(3)}$, we can see that the following identity holds:

$$\left. \frac{\partial^2 \Gamma^{(3)}[q, \mu; r, \nu; s, \lambda; p]}{\partial q_\alpha \partial r_\beta} \right|_{q, r, s=0} = \left. \frac{\partial^3 \Gamma^{(2)}[q, \mu; r, \nu; p]}{\partial q_\alpha \partial r_\beta \partial p_\lambda} \right|_{q, r=0} \quad (\text{A.6})$$

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