Topological gap labeling with third Chern numbers in three-dimensional quasicrystals

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Topological gap labeling with third Chern numbers in three-dimensional quasicrystals

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We study the topological gap labeling of general 3D quasicrystals and we find that every gap in the spectrum is characterized by a set of the third Chern numbers. We show that a quasi-periodic structure has multiple Brillouin zones defined by redundant wavevectors, and the number of states below a gap is quantized as an integer linear combination of volumes of these Brillouin zones. The associated quantum numbers to characterize energy gaps can be expressed as third Chern numbers by considering a formal relationship between an adiabatic charge pumping under cyclic deformation of the quasi-periodic potential and a topological nonlinear electromagnetic response in 6D band insulators.

I. INTRODUCTION

Quasicrystals are non-periodic but long-range ordered systems found in a wide variety of physical systems including metallic alloys[1–5], photonic quasicrystals[6–11], ultra cold-atom systems [12–14] and twisted two-dimensional (2D) materials. [15–19] Despite the increasing importance of quasicrystalline systems, the theoretical description of their physical properties is limited by the lack of the Bloch theorem. In periodic crystals, the energy spectrum is quantized into the Bloch bands with equal numbers of states, which corresponds to the area of the Brillouin zone (BZ). Therefore each energy gap is characterized by an integer, which is the number of the bands below the gap. In contrast, it is supposed that quasicrystals do not have such a quantum unit to count the number of states, but rather the spectrum splits to a set of infinitely many bands (the Cantor set) as the infinite-period limit of a periodic system.

In our previous works [16, 20], we studied spectral quantization of general 2D quasi-periodic systems and showed that the gap labeling is actually possible in the following sense. Specifically, the energy spectrum of a quasicrystal is characterized by multiple BZs defined with redundant wavevectors, and the number of states below the gap is always quantized as an integer linear combination of the areas of these BZs. The quantum numbers to characterize energy gaps were shown to be topological invariants expressed as the second Chern numbers, by considering a mapping between 2D quasicrystals and four-dimensional quantum Hall insulators. Topological characterization of energy gaps in quasicrystals was also studied in different contexts for in one-dimensional (1D)[21–32] and two-dimensional (2D) quasiperiodic systems [33–41], while the gap labeling of three dimensional (3D) quasicrystals is yet to be explored.

In this paper, we extend the argument for 2D [16, 20] to 3D, and show that the spectrum of a 3D quasicrystal is quantized by the third Chern numbers, which correspond to electromagnetic response in six-dimensional (6D) insulator. We consider a general 3D quasicrystalline system with the number of reciprocal lattice vectors greater than the number of the spatial dimensions. Specifically, it is described by the Hamiltonian in a 3D space,

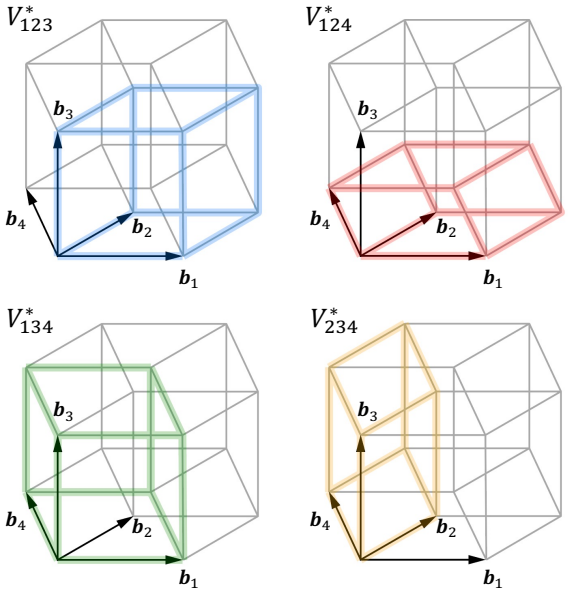

FIG. 1. Fundamental Brillouin zones in a 3D quasiperiodic system with four reciprocal lattice vectors, $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3, \boldsymbol{b}_4$

$$H = \frac{\boldsymbol{p}^2}{2m} + U(\boldsymbol{r}),$$
$$U(\boldsymbol{r}) = \sum_{m_1,\ldots,m_N} U_{m_1,\ldots,m_N} e^{i\sum_{i=1}^{N} m_i \boldsymbol{b}_i \cdot \boldsymbol{r}}, \tag{1}$$

where $m_1, ..., m_N$ are integers and $\boldsymbol{b}_i\,(i = 1, 2, ..., N)$ are a set of redundant reciprocal lattice vectors ($N > 3$). Then, we can define multiple Brillouin zones by taking three distinct vectors $\boldsymbol{b}_i, \boldsymbol{b}_j$ and $\boldsymbol{b}_k$ from N reciprocal lattice vectors, as illustrated in Fig. 1 for the case of $N = 4$. There are $N!/[(N-3)!3!]$ distinct Brillouin zones with generally different volumes of $V^*_{ijk} = \boldsymbol{b}_i \cdot (\boldsymbol{b}_j \times \boldsymbol{b}_k)$. We claim that, when the energy spectrum has a gap, the electron density below the gap is quantized as

$$n_e = \frac{1}{(2\pi)^3} \sum_{ijk} C^{(3)}_{ijk} V^*_{ijk}, \tag{2}$$

where $C^{(3)}_{ijk}$ is the third Chern number calculated from the occupied states. As we have $N!/[(N-3)!3!]$ choices of (i,j,k), every single gap is characterized by a set of $N!/[(N-3)!3!]$ third Chern numbers. The statement can be proved by considering a formal relationship between an adiabatic charge pumping under cyclic deformation of the potential and a topological electromagnetic response in a fictitious 6D band insulator.[42]

This paper is organized as follows. In Sec. II, we present a general description of the electromagnetic response of the (6+1)D system using an effective action formalism. In Sec. III, we consider an adiabatic pumping in the 3D quasicrystal and a mapping to the 6D system. With the aid of the formula obtained in Sec. II and the dimensional reduction technique, we will finally obtain the result Eq. (2). A brief conclusion is given in Sec. IV. Throughout the paper, we use the natural unit $\hbar = c = e = 1$ and the Minkowski metric $\eta_{\mu\nu} = \mathrm{diag}(-1,+1,...,+1)$.

II. ELECTROMAGNETIC RESPONSE OF (6+1)D SYSTEMS

In this section, we describe a topological nonlinear response of a generic 6D band insulator in an electromagnetic field, and express the response coefficient with a third Chern number. The problem was also studied by the semiclassical approach. [42, 43] Here we use the Euclidean path integral formalism, by extending the argument for (4+1)D systems [44] to (6+1)D. The effective action $S_{\rm eff}$ in (6+1)D is defined as

$$e^{iS_{\rm eff}} = \int Dc^\dagger Dc\, e^{-S-S_{\rm int}} \tag{3}$$

where

$$S = \int d\tau \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}}(\tau)\Big(\frac{\partial}{\partial\tau} - h(\boldsymbol{k})\Big)c_{\boldsymbol{k}}(\tau) \tag{4}$$

$$= \sum_{\boldsymbol{k}n} c^\dagger_{\boldsymbol{k}n}\Big(i\omega_n - h(\boldsymbol{k})\Big)c_{\boldsymbol{k}n}, \tag{5}$$

$$S_{\rm int} = \sum_{\boldsymbol{q}\omega} A^\mu(\boldsymbol{q},\omega)J_\mu(-\boldsymbol{q},-\omega). \tag{6}$$

Here, $\tau = -it$ is imaginary time and $A^\mu(\boldsymbol{q},\omega) = (A^0,\boldsymbol{A})$ is an external electromagnetic four-potential with wavenumber $\boldsymbol{q}$ and frequency ω. The one-particle Hamiltonian is represented by $h(\boldsymbol{k})$, and $c^\dagger_{\boldsymbol{k}n}$ and $c_{\boldsymbol{k}n}$ are Grassmann numbers of an electron with Bloch wavenumber $\boldsymbol{k}$ and Matsubara frequency ω_n. The current $J^\mu = (J^0,\boldsymbol{J})$ is expressed as

$$J^0(\boldsymbol{q},\omega) = -\sum_{\boldsymbol{k}n} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\omega}c_{\boldsymbol{k},\omega_n} \tag{7}$$

$$\boldsymbol{J}(\boldsymbol{q},\omega) = -\sum_{\boldsymbol{k}n} \nabla_{\boldsymbol{k}}h(\boldsymbol{k})c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\omega}c_{\boldsymbol{k},\omega_n}. \tag{8}$$

For the (6+1)-dimensional insulator, the effective action contains a topological term called the third Chern-Simons term,

$$S_{\rm eff} = \frac{C^{(3)}}{192\pi^3}\int A\wedge dA\wedge dA\wedge dA, \tag{9}$$

with

$$C^{(3)} = \frac{\pi^3}{105}\int\frac{d^7l}{(2\pi)^7}\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\,\mathrm{tr}\,G(\partial_\mu G^{-1})G(\partial_\nu G^{-1}) \times G(\partial_\rho G^{-1})G(\partial_\sigma G^{-1})G(\partial_\tau G^{-1})G(\partial_\lambda G^{-1})G(\partial_\delta G^{-1}), \tag{10}$$

where $l^\mu = (i\omega,\boldsymbol{l})$ is the frequency-momentum vector and $G(l) = (i\omega - h(\boldsymbol{l}))^{-1}$ is the one-particle Green's function. The detailed derivation of Eqs.(9) and (10) is presented in Appendix A. We obtain the topological nonlinear response to an external electromagnetic field A^μ as

$$j^\mu = \frac{\delta S_{\rm eff}}{\delta A_\mu} = \frac{C^{(3)}}{48\pi^3}\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\partial_\nu A_\rho\partial_\sigma A_\tau\partial_\lambda A_\delta. \tag{11}$$

The coefficient $C^{(3)}$ in Eq. (10) is expressed as the third Chern number of the non-abelian Berry connection in the 6D Brillouin zone (BZ). Specifically, it is written as

$$C^{(3)} = \frac{1}{48\pi^3}\int_{BZ}\mathrm{tr}\,f\wedge f\wedge f, \tag{12}$$

where f is the Berry curvature defined by

$$f = \frac{1}{2}f_{ij}\,dk^i\wedge dk^j$$
$$f^{\alpha\beta}_{ij} = \partial_i a^{\alpha\beta}_j - \partial_j a^{\alpha\beta}_i - i[a_i,a_j]^{\alpha\beta},$$
$$a^{\alpha\beta}_i = i\,\langle\alpha\boldsymbol{k}|\,\partial_i\,|\beta\boldsymbol{k}\rangle\,, \tag{13}$$

and the indices α,β represent the occupied bands. The derivation of Eq. (12) is described in Appendix B. The $C^{(3)}$ is a topological number which is invariant under continuous deformations without closing an energy gap.

Alternatively, the $C^{(3)}$ of Eq. (12) can be written as

$$C^{(3)} = \frac{i}{48\pi^3}\int_{BZ}\mathrm{tr}[dP\wedge PdP]^3 = \frac{i}{48\pi^3}\int_{BZ}d^6\boldsymbol{k}\,\epsilon^{ijklmn} \times\mathrm{tr}\big[(\partial_iP)P(\partial_jP)(\partial_kP)P(\partial_lP)(\partial_mP)P(\partial_nP)\big], \tag{14}$$

where $P = \sum_{\alpha\in\mathrm{occ}}|\alpha\boldsymbol{k}\rangle\langle\alpha\boldsymbol{k}|$ is the projection operator to the occupied states below the gap. This expression is convenient for practical calculations since the gauge fixing of the wavefunctions is not needed.

III. TOPOLOGICAL NUMBERS IN 3D QUASI-PERIODIC SYSTEMS

A. Adiabatic quantum pumping

Let us consider a 3D quasicrystalline system expressed by Eq. (1), and calculate the adiabatic charge pumping under a cyclic change of the potential $U(\boldsymbol{r})$. We introduce phase parameters $\phi_1, ..., \phi_N$ to the potential as

$$U(\boldsymbol{r};\, \phi_1, ..., \phi_N) = \sum_{m_1,...m_N} U_{m_1,...,m_N} e^{i\sum_{i=1}^{N} m_i(\boldsymbol{b}_i\cdot\boldsymbol{r}-\phi_i)}, \tag{15}$$

and consider a cyclic process where ϕ_i, with a certain i, is adiabatically increased from 0 to 2π. In a periodic case with $N = 3$, the process corresponds to just a parallel translation of the potential $U(\boldsymbol{r})$ by a real-space lattice period $\boldsymbol{a}_i$ where $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$. Eq. (15) is a generalization to quasiperiodic systems, while it is not generally expressed as a simple translation. If the potential $U(\boldsymbol{r})$ is a summation of independent periodic potentials $U_1(\boldsymbol{r}), U_2(\boldsymbol{r}), \cdots$ not sharing the same $\boldsymbol{b}_i$, in particular, a change of ϕ_i is equivalent to a relative sliding of a U_n with respect to the rest U_m's. In 2D, this corresponds to interlayer sliding in moiré multilayer systems. [16, 19, 40, 41]

We define $\Delta\boldsymbol{P_i}$ as the change of the electric polarization during a single cycle from $\phi_i = 0$ to 2π. When the spectrum has an energy gap, $\Delta\boldsymbol{P_i}$ is given by

$$\Delta\boldsymbol{P_i} = 2\pi\frac{\partial n_e}{\partial \boldsymbol{b}_i}, \tag{16}$$

where n_e is the electron density below the energy gap.[20] Eq. (16) can be proved by the following consideration. When a specific reciprocal lattice vector $\boldsymbol{b}_i$ is infinitesimally changed to $\boldsymbol{b}_i + \delta\boldsymbol{b}_i$, this leads to a change to the potential U at a point $\boldsymbol{r}$ which is equivalent to a phase change by $\delta\phi_i = -\delta\boldsymbol{b}_i \cdot \boldsymbol{r}$. This causes a polarization change by

$$\Delta\boldsymbol{P}_i\frac{\delta\phi_i}{2\pi} = \Delta\boldsymbol{P_i}\frac{(-\delta\boldsymbol{b}_i\cdot\boldsymbol{r})}{2\pi}. \tag{17}$$

Now, we consider a closed curved surface S, and let N_e be the number of electrons inside S. When $\boldsymbol{b}_i$ is changed to $\boldsymbol{b}_i + \delta\boldsymbol{b}_i$, the number of electrons passing through S is

$$\begin{aligned}\delta N_e &= \int_S \frac{\delta\boldsymbol{b}_i\cdot\boldsymbol{r}}{2\pi}\Delta\boldsymbol{P_i}\cdot d\boldsymbol{S} \\ &= \int_\Omega \mathrm{div}\left(\frac{\delta\boldsymbol{b}_i\cdot\boldsymbol{r}}{2\pi}\Delta\boldsymbol{P_i}\right)dV = \frac{\Omega}{2\pi}\Delta\boldsymbol{P_i}\cdot\delta\boldsymbol{b}_i,\end{aligned} \tag{18}$$

where Ω is the volume enclosed inside of S. Noting that the electron density is defined as $n_e = N_e/\Omega$, we obtain Eq. (16).

B. Mapping to a $(3+N)$-dimensional system

The adiabatic charge pumping in 3D quasicrystal discussed above can be described in an alternative approach considering an electromagnetic response in a $(3+N)$-dimensional system. By using the mapping, we will show that the transferred charge in the pumping is interpreted as integer-quantized response current in 6D[42], and it finally leads to the zone quantization rule, Eq. (2). The formulation is basically an extension of the argument for 2D quasicrystal [20] to 3D.

We consider a $(3+N)$D system in $(x, y, z, w_1, w_2, ..., w_N)$ space, which is continuous in x, y, and z directions and discrete in $w_i (i = 1, 2, ..., N)$ directions with lattice spacing a_i. For the w_i-direction, we assume nearest-neighbor tight-binding coupling t_i between adjacent layers. We apply a uniform magnetic field B_{xi}, B_{yi} and B_{zi} perpendicular to xw_i-plane, yw_i-plane and zw_i-plane, respectively. We take the vector potential as $\boldsymbol{A} = \sum_{i=1}^{N}(B_{xi}x + B_{yi}y + B_{zi}z)\boldsymbol{e}_i$, where $\boldsymbol{e}_i$ is the unit vector in the w_i-direction.

Since the Hamiltonian is periodic in any of the w_i-directions, the wavefunction can be written as $\Psi(x, y, z, w_1, w_2, ..., w_N) = \psi(x, y, z)e^{i\sum_i k_i w_i}$, where k_i is the Bloch wave number defined in $-\pi/a_i \le k_i \le \pi/a_i$. The $(3+N)$D Schrödinger equation is reduced to the 3D equation as

$$\Big[\frac{\boldsymbol{p}^2}{2m} - \sum_{i=1}^{N} 2t_i\cos(\boldsymbol{b}_i\cdot\boldsymbol{r} + \phi_i)\Big]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}), \tag{19}$$

where

$$\boldsymbol{b}_i = a_i\boldsymbol{B}_i = a_i(B_{xi}, B_{yi}, B_{zi}), \tag{20}$$

$$\phi_i = k_i a_i. \tag{21}$$

This is nothing but a 3D quasi-periodic system considered in the previous seciton. Higher harmonic terms in $\boldsymbol{b}_i$ can be incorporated by including further-range hoppings in w_i direction in the original $(3+N)$D model.

Now we consider an electronic response of the $(3+N)$D system to a weak external electric field E_i applied in the w_i direction. The E_i adiabatically changes the wavenumber k_i as $dk_i/dt = -E_i$, where the factor -1 is the charge of an electron in natural unit. In the corresponding 3D equation, Eq. (19), it is equivalent to an adiabatic potential change by shifting ϕ_i, which was considered in the previous section. A cyclic change from $\phi_i = 0$ to 2π corresponds to a translation of k_i by the Brillouin zone width, $2\pi/a_i$, which takes a time $T = (2\pi/a_i)/E_i$.

We assume that the Fermi energy is in an energy gap in the $(3+N)$D system. The response electric current induced by E_i is obtained by calculating those for 6D subspaces (x, y, z, w_i, w_j, w_k), and taking a sum over indeces $j, k(\neq i)$. According to Eq. (11), the response current in the 6D subspace is given by

$$\boldsymbol{j}^{(6D)} = \frac{C^{(3)}_{ijk}}{8\pi^3}E_i(\boldsymbol{B}_j\times\boldsymbol{B}_k). \tag{22}$$

The corresponding 3D current density per layer is given by $\boldsymbol{j}^{(3D)} = \boldsymbol{j}^{(6D)}a_i a_j a_k$, leading to

$$\boldsymbol{j}^{(3D)} = \frac{C^{(3)}_{ijk}}{(2\pi)^2 T}\boldsymbol{b}_j\times\boldsymbol{b}_k. \tag{23}$$

The total polarization change in a cyclic process is $\Delta \boldsymbol{P}_i = \boldsymbol{j}^{(3D)}T$. Taking summations over j and k, we obtain

$$\Delta \boldsymbol{P}_i = \frac{1}{(2\pi)^2}\sum_{jk} C^{(3)}_{ijk}\boldsymbol{b}_j \times \boldsymbol{b}_k. \tag{24}$$

By applying Eq. (24) to Eq. (16), we finially obtain the result

$$n_e = \frac{1}{(2\pi)^3}\sum_{ijk} C^{(3)}_{ijk}\boldsymbol{b}_i \cdot (\boldsymbol{b}_j \times \boldsymbol{b}_k), \tag{25}$$

which is Eq. (2). The result is analogous to 2D quasicrystal where n_e is quantized by the second Chern number [20], and also to 1D quasicrystal quantized by the first Chern number [9]. In a d dimensional quasicrystal with N reciprocal lattice vectors, there are $N!/[(N-d)!d!]$ independent d-th Chern numbers.

The calculation for the Chern numbers requires the Brillouin zone, and practically it can be achieved by considering a commensurate approximant,[16, 20] where the periodicities of $\boldsymbol{b}_i (i = 1, 2, ..., N)$ have a common super unit cell. If we take an approximant with a sufficiently large unit cell, the Brilloin zone volume becomes small, and the integrand of Eq. (14) becomes almost independent of $\boldsymbol{k}$. In this limit, the integration over the 6D Brillouin zone is reduced to just a multiplication by the Brillouin zone volume.

The gap characterization scheme presented here is applicable to general 3D quasiperiodic systems such as quasicrystalline alloys[1–5] and 3D photonic quasicrystals[7, 8, 10] as long as the spectrum has an energy gap. These systems can be described by a set of basis vectors more than three [45], and hence the potential $U(\boldsymbol{r})$ can be expressed in the form of Eq. (1).

The implementation of our gap labeling method for a given 3D quasicrystal is summarized as follows. First, we take a Fourier transform of the given quasiperiodic potential $U(\boldsymbol{r})$, and determine the fundamental reciprocal vectors $\boldsymbol{b}_1, \boldsymbol{b}_2, \cdots, \boldsymbol{b}_N$. Then we slightly deform these wave vectors to obtain a commensurate approximant which has a finite unit cell.[16, 20] For the approximant, the Hamiltonian is given as a function of parameters $(k_x, k_y, k_z, \phi_1, \cdots, \phi_N)$, where $\boldsymbol{k}^{(3D)} = (k_x, k_y, k_z)$ is the Bloch momentum in the BZ of the commensurate approximant, and ϕ_i's are the phases in Eq. (15) which move from 0 to 2π. We choose three non-overlapping labels i, j, k from $1, \cdots, N$ and consider the Bloch eigenstates in a 6D parameter space $\boldsymbol{k}^{(6D)} = (k_x, k_y, k_z, \phi_i, \phi_j, \phi_k)$ with the rest of ϕ_l's fixed. The third Chern number $C^{(3)}_{ijk}$ is calculated by applying Eq. (12) to the 6D Bloch states. We can obtain all of integers $C^{(3)}_{ijk}$ by performing the same procedure for all the combinations of i, j, k.

IV. CONCLUSION

We have provided a topological concept to characterize energy gaps in 3D quasicrystals. We found that the electron density below the gap is quantized as an integer linear combination of volumes of multiple Brillouin zones, which are defined by redundant reciprocal lattice vectors. Then we showed that these integers can be expressed as the third Chern numbers by considering a mapping between the 3D quasicrystal and a $(3+N)$D band insulator. Specifically, we showed that an adiabatic charge pumping in a potential phase change can be viewed as a projection of the nonlinear electromagnetic response in 6D subspaces in $(3+N)$D system, which is shown to be described by the third Chern numbers. The gap characterization scheme presented here is applicable to general 3D quasicrystalline systems having redundant periodicities more than the number of the spatial dimensions.

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Appendix A: Derivation of Eq. (9) and (10)

Here we show that the effective action S_{eff} of a 6D band insulator under an eletromagnetic field [Eq. (3)] includes the term of Eq. (9) with Eq. (10). We concentrate on the term proportional to A^4 in S_{eff}, and define the four-point function $\Pi^{\mu\rho\tau\delta}(x, y, z, w)$ as

$$S_{\text{eff}} = \frac{1}{4!}\int d^7x \int d^7y \int d^7z \int d^7w \Pi^{\mu\rho\tau\delta}(x, y, z, w)A_\mu(x)A_\rho(y)A_\tau(z)A_\delta(w).$$

Then $\Pi^{\mu\rho\tau\delta}(x, y, z, w)$ can be represented by

$$i\Pi_{\mu\rho\tau\delta}(x, y, z, w) = \frac{\int Dc^\dagger Dc\, J_\mu(x)J_\rho(y)J_\tau(z)J_\delta(w)\, e^{-S}}{\int Dc^\dagger Dc\, e^{-S}}.$$

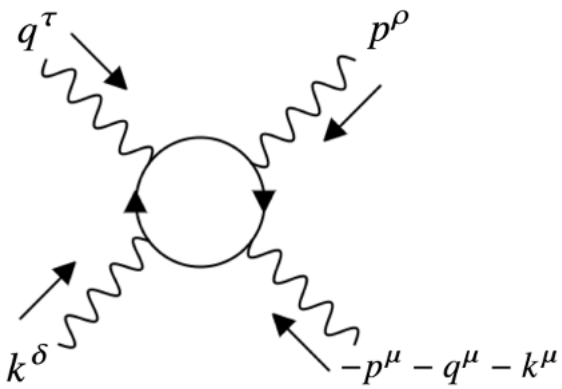

FIG. 2. One-loop Feynman diagram that contributes to $F_{\delta\tau\rho\mu}(k,q,p)$. The solid and wavy lines correspond to electron and the external electromagnetic field, respectively.

Since the current $J_\mu(x)$ satisfies the continuity equation $\partial_\mu J^\mu = 0$, $\Pi^{\mu\rho\tau\delta}(x,y,z,w)$ must satisfy

$$\frac{\partial}{\partial x^\mu}\Pi^{\mu\rho\tau\delta}(x,y,z,w) = \frac{\partial}{\partial y^\rho}\Pi^{\mu\rho\tau\delta}(x,y,z,w) = \frac{\partial}{\partial z^\tau}\Pi^{\mu\rho\tau\delta}(x,y,z,w) = \frac{\partial}{\partial w^\delta}\Pi^{\mu\rho\tau\delta}(x,y,z,w) = 0.$$

This requirement suggests that the term,

$$\Pi^{\mu\rho\tau\delta}(x,y,z,w) = s\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\frac{\partial}{\partial y^\nu}\delta(y-x)\frac{\partial}{\partial z^\sigma}\delta(z-x)\frac{\partial}{\partial w^\lambda}\delta(w-x) + \cdots$$

should be included in $\Pi^{\mu\rho\tau\delta}(x,y,z,w)$, where s is a certain constant. This term is specific to the $(6+1)$D system as it has 7 indices. Taking the Fourier transform of $\Pi^{\mu\rho\tau\delta}(x,y,z,w)$, we obtain

$$\begin{aligned}\Pi^{\mu\rho\tau\delta}(r,p,q,k) &= \int d^7x e^{-irx}\int d^7y e^{-ipy}\int d^7z e^{-iqz}\int e^{-ikw}\Pi^{\mu\rho\tau\delta}(x,y,z,w)\\ &= (2\pi)^7\delta(r+p+q+k)\tilde{\Pi}^{\mu\rho\tau\delta}(p,q,k),\end{aligned} \tag{A1}$$

where

$$\tilde{\Pi}^{\mu\rho\tau\delta}(p,q,k) = -is\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}p_\nu q_\sigma k_\lambda + \cdots. \tag{A2}$$

The constant s is given by

$$s = \frac{1}{7!}\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\frac{\partial}{\partial p^\nu}\frac{\partial}{\partial q^\sigma}\frac{\partial}{\partial k^\lambda}i\tilde{\Pi}_{\mu\rho\tau\delta}(p,q,k)\Big|_{p=q=k=0}. \tag{A3}$$

The four point function $i\tilde{\Pi}^{\mu\rho\tau\delta}(p,q,k)$ has contributions from 3! Feynman diagrams. One of them is illustrated in Fig. 2, and others are obtained by permutation. We can explicitly perform path integrals, giving

$$\begin{aligned}&i\tilde{\Pi}_{\mu\rho\tau\delta}(p,q,k)\\ =&\frac{\int Dc^\dagger Dc\, J_\mu(-p-q-k)J_\rho(p)J_\tau(q)J_\delta(k)\,e^{-S}}{\int Dc^\dagger Dc\, e^{-S}}\\ =&F_{\delta\tau\rho\mu}(k,q,p) + F_{\delta\rho\tau\mu}(k,p,q) + F_{\tau\delta\rho\mu}(q,k,p) + F_{\tau\rho\delta\mu}(q,p,k) + F_{\rho\tau\delta\mu}(p,q,k) + F_{\rho\delta\tau\mu}(p,k,q),\end{aligned} \tag{A4}$$

where we define

$$F_{\delta\tau\rho\mu}(k,q,p) = -\int\frac{d^7l}{(2\pi)^7}\,\mathrm{tr}\,G(l)\frac{\partial G^{-1}(l)}{\partial l^\delta}G(l+k)\frac{\partial G^{-1}(l+k)}{\partial l^\tau}G(l+k+q)\frac{\partial G^{-1}(l+k+q)}{\partial l^\rho}G(l+k+q+p)\frac{\partial G^{-1}(l)}{\partial l^\mu},$$

and the minus sign originates from the fermion loop. In the calculation, we used the expression

$$J^\mu(\boldsymbol{q},\omega) = \sum_{k,n} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\omega_n+\omega}\frac{\partial G^{-1}}{\partial k_\mu}c_{\boldsymbol{k},\omega_n}.$$

By applying Eq. (A4) to Eq. (A3), we finally obtain

$$s = -\frac{3!}{7!}\int \frac{d^7l}{(2\pi)^7}\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\,\mathrm{tr}\,G(\partial_\mu G^{-1})G(\partial_\nu G^{-1})G(\partial_\rho G^{-1})G(\partial_\sigma G^{-1})G(\partial_\tau G^{-1})G(\partial_\lambda G^{-1})G(\partial_\delta G^{-1}).$$

Appendix B: Derivation of Eq. (12)

Let us show that the coefficient $C^{(3)}$ in Eq. (10) is expressed as the third Chern number as in Eq. (12). The derivation is closely analogous to Ref. [44], which investigated the classification of (4+1)D time reversal invariant topological insulators in terms of the 2nd Chern number and (4+1)D Chern-Simons theory. Here we extend the argument to (6+1)D.

First, we show that any continuous deformation of $h(\boldsymbol{k})$ does not change Eq. (10). When $h(\boldsymbol{k})$ is infinitesimally changed to $h(\boldsymbol{k}) + \delta h$, the Green's function G is changed to $G + \delta G$. The change in each factor $G(\partial_\mu G^{-1})$ in Eq. (10) makes the same contribution to the change in Eq. (10), giving

$$\delta C^{(3)} = 7 \times \frac{\pi^3}{105}\int \frac{d^7l}{(2\pi)^7}\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\,\mathrm{tr}\,\delta\Big(G(\partial_\mu G^{-1})\Big)G(\partial_\nu G^{-1})G(\partial_\rho G^{-1})G(\partial_\sigma G^{-1})G(\partial_\tau G^{-1})G(\partial_\lambda G^{-1})G(\partial_\delta G^{-1}),$$

where the change of the factor $G(\partial_\mu G^{-1})$ is given by

$$\delta\Big(G(\partial_\mu G^{-1})\Big) = -G\partial_\mu(G^{-1}\delta G)G^{-1}.$$

Integrating by parts, we obtain $\delta C^{(3)} = 0$.

Without loss of generality, the chemical potential can be defined to be zero. Since any gapped Hamiltonian $h(\boldsymbol{k})$ can be continuously deformed into the simple Hamiltonian $h_0(\boldsymbol{k})$, that is the form

$$\begin{aligned} h_0(\boldsymbol{k}) &= \epsilon_G \sum_{1\le\alpha\le M} |\alpha\boldsymbol{k}\rangle\langle\alpha\boldsymbol{k}| + \epsilon_E \sum_{M+1\le\alpha'} |\alpha'\boldsymbol{k}\rangle\langle\alpha'\boldsymbol{k}| \\ &= \epsilon_G P_G(\boldsymbol{k}) + \epsilon_E P_E(\boldsymbol{k}), \end{aligned}$$

where $P_G(P_E)$ is the projection operator of ground states (excited states), $\alpha = 1, 2, ...M$ are occupied bands, and $\alpha' = M+1, ...$ are unoccupied bands. Here, $\epsilon_G(\epsilon_E)$ is the energy of the ground states (excited states) and satisfies $\epsilon_G < 0 < \epsilon_E$. Therefore, it is sufficient to prove Eq. (12) for the simple Hamiltonian $h_0(\boldsymbol{k})$. In this case, the one-particle Green's function is written as

$$G(\boldsymbol{k},\omega) = \frac{1}{i\omega - \epsilon_G P_G(\boldsymbol{k}) - \epsilon_E P_E(\boldsymbol{k})} = \frac{P_G(\boldsymbol{k})}{i\omega - \epsilon_G} + \frac{P_E(\boldsymbol{k})}{i\omega - \epsilon_E}. \tag{B1}$$

The derivatives of $G^{-1}(\boldsymbol{k},\omega)$ are calculated as

$$\begin{aligned} &\frac{\partial G^{-1}}{\partial k^0}(\boldsymbol{k},\omega) = 1, \\ &\frac{\partial G^{-1}}{\partial k^i}(\boldsymbol{k},\omega) = -\epsilon_G\frac{\partial P_G}{\partial k^i}(\boldsymbol{k}) - \epsilon_E\frac{\partial P_E}{\partial k^i}(\boldsymbol{k}) = (\epsilon_E - \epsilon_G)\frac{\partial P_G}{\partial k^i}(\boldsymbol{k}), \quad (i = 1,2,3,4,5,6). \end{aligned}$$

By using this, Eq. (10) can be written as

$$\begin{aligned} C^{(3)} &= \frac{\pi^3}{105}\int \frac{d^7k}{(2\pi)^7}\epsilon^{\mu\nu\rho\sigma\tau\lambda\delta}\,\mathrm{tr}\,G(\partial_\mu G^{-1})G(\partial_\nu G^{-1})G(\partial_\rho G^{-1})G(\partial_\sigma G^{-1})G(\partial_\tau G^{-1})G(\partial_\lambda G^{-1})G(\partial_\delta G^{-1}) \\ &= 7\times\frac{\pi^3}{105}\int \frac{d^7k}{(2\pi)^7}\epsilon^{ijklmn}\,\mathrm{tr}\,G(\partial_0 G^{-1})G(\partial_i G^{-1})G(\partial_j G^{-1})G(\partial_k G^{-1})G(\partial_l G^{-1})G(\partial_m G^{-1})G(\partial_n G^{-1}) \\ &= \frac{\pi^3}{15}\sum_{abcdef=G,E}\int \frac{d^7k}{(2\pi)^7}\epsilon^{ijklmn}\,\mathrm{tr}\,\frac{P_a(\partial_i P_G)P_b(\partial_j P_G)P_c(\partial_k P_G)P_d(\partial_l P_G)P_e(\partial_m P_G)P_f(\partial_n P_G)}{(i\omega-\epsilon_a)^2(i\omega-\epsilon_b)(i\omega-\epsilon_c)(i\omega-\epsilon_d)(i\omega-\epsilon_e)(i\omega-\epsilon_f)}(\epsilon_E-\epsilon_G)^6. \end{aligned} \tag{B2}$$

From the identities $P_G + P_E = 1$ and $P_G P_E = P_E P_G = 0$, we have

$$P_E\frac{\partial P_G}{\partial k^i} = \frac{\partial P_G}{\partial k^i}P_G, \quad P_G\frac{\partial P_G}{\partial k^i} = \frac{\partial P_G}{\partial k^i}P_E.$$

Hence the trace in Eq. (B2) can be nonzero only when $(a,b,c,d,e,f) = (G,E,G,E,G,E)$ or (E,G,E,G,E,G), giving

$$\begin{aligned}
C^{(3)} &= \frac{\pi^3}{15}\int \frac{d^7k}{(2\pi)^7}\epsilon^{ijklmn}\,\mathrm{tr}\,\frac{P_G(\partial_i P_G)P_E(\partial_j P_G)P_G(\partial_k P_G)P_E(\partial_l P_G)P_G(\partial_m P_G)P_E(\partial_n P_G)}{(i\omega-\epsilon_G)^4(i\omega-\epsilon_E)^3}(\epsilon_E-\epsilon_G)^6 \\
&\quad + \mathrm{tr}\,\frac{P_E(\partial_i P_G)P_G(\partial_j P_G)P_E(\partial_k P_G)P_G(\partial_l P_G)P_E(\partial_m P_G)P_G(\partial_n P_G)}{(i\omega-\epsilon_G)^3(i\omega-\epsilon_E)^4}(\epsilon_E-\epsilon_G)^6 \\
&= -\frac{\pi^3}{15}\int \frac{d^7k}{(2\pi)^7}\epsilon^{ijklmn}\frac{(\epsilon_E-\epsilon_G)^7}{(i\omega-\epsilon_G)^4(i\omega-\epsilon_E)^4}\,\mathrm{tr}(\partial_i P_G)P_E(\partial_j P_G)(\partial_k P_G)P_E(\partial_l P_G)(\partial_m P_G)P_E(\partial_n P_G) \\
&= -\frac{\pi^3}{15}\int_{-\infty}^{+\infty}\frac{id\omega}{2\pi}\int\frac{d\boldsymbol{k}}{(2\pi)^6}\epsilon^{ijklmn}\frac{(\epsilon_E-\epsilon_G)^7}{(i\omega-\epsilon_G)^4(i\omega-\epsilon_E)^4}\,\mathrm{tr}(\partial_i P_G)P_E(\partial_j P_G)(\partial_k P_G)P_E(\partial_l P_G)(\partial_m P_G)P_E(\partial_n P_G) \\
&= \frac{-i}{48\pi^3}\int d^6\boldsymbol{k}\epsilon^{ijklmn}\,\mathrm{tr}(\partial_i P_G)P_E(\partial_j P_G)(\partial_k P_G)P_E(\partial_l P_G)(\partial_m P_G)P_E(\partial_n P_G). \qquad \text{(B3)}
\end{aligned}$$

Finally, we write this equation in terms of the Berry curvature. Using the Berry connection,

$$a_i^{\alpha\beta} = i\,\langle\alpha\boldsymbol{k}|\,\frac{\partial}{\partial k^i}\,|\beta\boldsymbol{k}\rangle,$$

the Berry curvature is expressed by

$$\begin{aligned}
f_{ij}^{\alpha\beta} &= \partial_i a_j^{\alpha\beta} - \partial_j a_i^{\alpha\beta} - i[a_i,a_j]^{\alpha\beta} \\
&= i\Big(\langle\partial_i\alpha\boldsymbol{k}|\partial_j\beta\boldsymbol{k}\rangle - \langle\partial_j\alpha\boldsymbol{k}|\partial_i\beta\boldsymbol{k}\rangle\Big) + i\Big(\langle\alpha\boldsymbol{k}|\partial_i\gamma\boldsymbol{k}\rangle\langle\gamma\boldsymbol{k}|\partial_j\beta\boldsymbol{k}\rangle - \langle\alpha\boldsymbol{k}|\partial_j\gamma\boldsymbol{k}\rangle\langle\gamma\boldsymbol{k}|\partial_i\beta\boldsymbol{k}\rangle\Big) \\
&= i\Big(\langle\partial_i\alpha\boldsymbol{k}|\partial_j\beta\boldsymbol{k}\rangle - \langle\partial_j\alpha\boldsymbol{k}|\partial_i\beta\boldsymbol{k}\rangle\Big) - i\Big(\langle\partial_i\alpha\boldsymbol{k}|\gamma\boldsymbol{k}\rangle\langle\gamma\boldsymbol{k}|\partial_j\beta\boldsymbol{k}\rangle - \langle\partial_j\alpha\boldsymbol{k}|\gamma\boldsymbol{k}\rangle\langle\gamma\boldsymbol{k}|\partial_i\beta\boldsymbol{k}\rangle\Big) \\
&= i\Big(\langle\partial_i\alpha\boldsymbol{k}|\partial_j\beta\boldsymbol{k}\rangle - \langle\partial_j\alpha\boldsymbol{k}|\partial_i\beta\boldsymbol{k}\rangle\Big) - i\Big(\langle\partial_i\alpha\boldsymbol{k}|\,P_G\,|\partial_j\beta\boldsymbol{k}\rangle - \langle\partial_j\alpha\boldsymbol{k}|\,P_G\,|\partial_i\beta\boldsymbol{k}\rangle\Big) \\
&= i\Big(\langle\partial_i\alpha\boldsymbol{k}|\,P_E\,|\partial_j\beta\boldsymbol{k}\rangle - \langle\partial_j\alpha\boldsymbol{k}|\,P_E\,|\partial_i\beta\boldsymbol{k}\rangle\Big).
\end{aligned}$$

Thus we have

$$\begin{aligned}
f_{ij} &= \sum_{\alpha\beta}|\alpha\boldsymbol{k}\rangle\, f_{ij}^{\alpha\beta}\,\langle\beta\boldsymbol{k}| \\
&= i\Big((\partial_i P_G)P_E(\partial_j P_G) - (\partial_j P_G)P_E(\partial_i P_G)\Big).
\end{aligned}$$

By using this, Eq. (B3) is transformed to

$$\begin{aligned}
C^{(3)} &= \frac{1}{2^3}\times\frac{-i}{48\pi^3}\int d^6\boldsymbol{k}\epsilon^{ijklmn}\,\mathrm{tr}\big(-if_{ij}\big)(-if_{kl})(-if_{mn}) \\
&= \frac{1}{2^3}\times\frac{1}{48\pi^3}\int d^6\boldsymbol{k}\epsilon^{ijklmn}\,\mathrm{tr}\,f_{ij}f_{kl}f_{mn} \\
&= \frac{1}{48\pi^3}\int_{BZ}\mathrm{tr}\,f\wedge f\wedge f.
\end{aligned}$$

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