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Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances

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We present a manifestly gauge-invariant description of Chern numbers associated with the Berry connection defined on a discretized Brillouin zone. It provides an efficient method of computing (spin) Hall conductances without specifying gauge-fixing conditions. We demonstrate that it correctly reproduces quantized Hall conductances even on a coarsely discretized Brillouin zone. A gauge-dependent integer-valued field, which plays a key role in the formulation, is evaluated in several gauges. An extension to the non-Abelian Berry connection is also given.

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Topological phase transitions have been of considerable interest in recent condensed matter physics.[1–3] In lower dimensions, topological quantum numbers are known to play a crucial role in characterizing various phase transitions. A typical example is the integer quantum Hall transition, where quantized Hall conductances are given by Chern numbers associated with the Berry connection.[4–7] Its extension to the case of spin currents is also attracting much current interest.[8–11] These topological quantum numbers present a chance to characterize quantum liquids without using conventional symmetry breaking.[2,3]

Generically, the Chern numbers can be defined for quantum states with two periodic parameters. As shown below, they are given by an integral of fictitious magnetic fields (field strengths of the Berry connection) over two-dimensional compact surfaces such as the Brillouin zone. In practical numerical calculations, however, we can diagonalize Hamiltonians only on a set of discrete points chosen appropriately within the surfaces. It is thus crucial to develop an efficient method of calculating the Chern numbers using restricted data of wave functions given only on such discrete points. In these calculations, a phase ambiguity of the wave function causes a gauge ambiguity for the Berry connection. Therefore, one must be careful if gauge-dependent quantities are used.

In this letter, we propose an efficient method of calculating the Chern numbers on a discretized Brillouin zone. This is an application of a geometrical formulation of topological charges in lattice gauge theory.[12–16] We show that the Chern numbers thus obtained are *manifestly gauge-invariant* and *integer-valued* even for a discretized Brillouin zone. This implies that one can compute the Chern numbers using wave functions in *any gauge* or *without specifying gauge fixing-conditions*. For the purpose of demonstration, we apply our method to a simple model describing the integer Hall system. We find that even for coarsely discretized Brillouin zones, the method reproduces correct Chern numbers known so far. Our method can be useful in a practical computation for more complicated systems with a topological order for which a number of data points of the wave functions cannot easily be increased.

To be specific, we focus on the Chern numbers in the quantum Hall effect. An extension to different topological ordered states is straightforward. The spin Hall conductances, for example, can be treated in a similar way. We consider a two-dimensional system in which the Brillouin zone is defined by $0 \le k_\mu < 2\pi/q_\mu$ ($\mu = 1,\ 2$ with some integers q_μ). Since the Hamiltonian $H(k)$ is periodic in both directions, $H(k_1, k_2) = H(k_1 + 2\pi/q_1, k_2) = H(k_1, k_2 + 2\pi/q_2)$, the (magnetic) Brillouin zone can be regarded as a two-dimensional torus T^2. When the Fermi energy lies in a gap, the Hall conductance is given by $\sigma_{xy} = -(e^2/h)\sum_n c_n$, where c_n denotes the Chern number of the nth Bloch band, and the sum over n is restricted to the bands below the Fermi energy.[4,5] The Chern number assigned to the nth band is defined by

$$c_n = \frac{1}{2\pi \mathrm{i}} \int_{T^2} \mathrm{d}^2 k\, F_{12}(k), \tag{1}$$

where the Berry connection $A_\mu(k)$ ($\mu = 1, 2$) and the associated field strength $F_{12}(k)$ are given by[4,6,7]

$$\begin{aligned} A_\mu(k) &= \langle n(k)|\partial_\mu|n(k)\rangle, \\ F_{12}(k) &= \partial_1 A_2(k) - \partial_2 A_1(k), \end{aligned} \tag{2}$$

with $|n(k)\rangle$ being a normalized wave function of the nth Bloch band such that $H(k)|n(k)\rangle = E_n(k)|n(k)\rangle$. In the above expressions, the derivative ∂_μ stands for $\partial/\partial k_\mu$. We assume that there is no degeneracy for the nth state.[2,3] The phase of the wave function is not yet determined here; that is, $|n(k)\rangle$ is defined on T^2 only up to its phase.

If the gauge potential $A_\mu(k)$ is globally well defined over the continuum Brillouin zone T^2, the Chern number (1) vanishes because the torus has no boundary: It can be nonzero only when the gauge potential cannot be defined as a global function over T^2. In this case, one covers T^2 by several coordinate patches and then, within each patch, one can take a gauge (that is, a phase convention for the wave functions) such that the gauge potential is a smooth and well defined function. In an overlap between two patches, gauge potentials defined on each patch are related by a U(1) gauge transformation:

$$|n(k)\rangle \to \mathrm{e}^{-\mathrm{i}\lambda(k)}|n(k)\rangle, \quad A_\mu(k) \to A_\mu(k) - i\partial_\mu \lambda(k). \tag{3}$$

The Chern number (1) is then given by a sum of the winding number of the U(1) gauge transformation along a boundary of a patch. As a consequence, the Chern number is an *integer*.

The above discussion is for the continuum Brillouin zone. Now suppose that we have data of wave functions only on discrete points within the Brillouin zone, as in actual numerical computations. A straightforward approach for computing the Chern number (1) would be to replace all the derivatives by discrete differences and the integral by a summation. Namely, one approximates the connection $A_\mu(k)dk_\mu$ by

$$A_\mu(k)\delta k_\mu = \langle n(k)|\delta_\mu|n(k)\rangle, \tag{4}$$

where δ_μ is an infinitesimal difference operator defined by $\delta_\mu f(k) = f(k+\delta\hat{k}_\mu) - f(k)$ with $\delta\hat{k}_\mu$ being an infinitesimal displacement vector in the direction μ (its magnitude is $|\delta k_\mu|$). Note that, to evaluate the difference, one must fix a local gauge with which the state $|n(k)\rangle$ is smoothly differentiable near k. Under this local gauge, the field strength in the continuum is also approximated by

$$F_{12}(k)\delta k_1\delta k_2 = [\delta_1 A_2(k) - \delta_2 A_1(k)]\delta k_1 \delta k_2. \tag{5}$$

Summing this $F_{12}(k)\delta k_1\delta k_2$ then gives the Chern number c_n in the limit $|\delta k_\mu| \to 0$. However, this direct procedure can be costly in taking the limit if the Hamiltonian concerned is complicated.

Here, we propose an alternative approach. Let us denote lattice points k_ℓ ($\ell = 1, \ldots, N_1 N_2$) on the discrete Brillouin zone as

$$k_\ell = (k_{j_1}, k_{j_2}), \quad k_{j_\mu} = \frac{2\pi j_\mu}{q_\mu N_\mu}, \quad (j_\mu = 0, \ldots, N_\mu - 1). \tag{6}$$

We assume that the state $|n(k_\ell)\rangle$ is periodic on the lattice, $|n(k_\ell + N_\mu\hat{\mu})\rangle = |n(k_\ell)\rangle$, where $\hat{\mu}$ is a vector in the direction μ with the magnitude $2\pi/(q_\mu N_\mu)$. Below, we set $N_\mu = q_\nu N_{\mathrm{B}}$ ($\mu \neq \nu$) so that the unit plaquette is a square of the size $2\pi/(q_1 q_2 N_{\mathrm{B}})$.

We first define a U(1) link variable from the wave functions of the nth band as

$$U_\mu(k_\ell) \equiv \langle n(k_\ell)|n(k_\ell + \hat{\mu})\rangle / \mathcal{N}_\mu(k_\ell), \tag{7}$$

where $\mathcal{N}_\mu(k_\ell) \equiv |\langle n(k_\ell)|n(k_\ell + \hat{\mu})\rangle|$. The link variables are well defined as long as $\mathcal{N}_\mu(k_\ell) \neq 0$, which can always be assumed to be the case (one can avoid a singularity $\mathcal{N}_\mu(k_\ell) = 0$ by an infinitesimal shift of the lattice). From the link variable (7), we next define a lattice field strength by

$$\tilde{F}_{12}(k_\ell) \equiv \ln U_1(k_\ell) U_2(k_\ell + \hat{1}) U_1(k_\ell + \hat{2})^{-1} U_2(k_\ell)^{-1},$$
$$-\pi < \frac{1}{\mathrm{i}}\tilde{F}_{12}(k_\ell) \leq \pi. \tag{8}$$

Note that the field strength is defined within the principal branch of the logarithm specified in eq. (8). It is obvious that this field strength is invariant under the gauge transformation (3). Finally, we define the Chern number on the lattice which is associated to the nth band as

$$\tilde{c}_n \equiv \frac{1}{2\pi\mathrm{i}} \sum_\ell \tilde{F}_{12}(k_\ell). \tag{9}$$

First of all, we note that $\tilde{c}_n$ is manifestly *gauge-invariant* under eq. (3). This implies that we do not need to determine which gauge is adopted; any choice of gauge gives an identical number $\tilde{c}_n$. Moreover, $\tilde{c}_n$ is *strictly an integer* for arbitrary lattice spacings. To show this, we introduce a gauge potential

$$\tilde{A}_\mu(k_\ell) = \ln U_\mu(k_\ell), \quad -\pi < \frac{1}{\mathrm{i}}\tilde{A}_\mu(k_\ell) \leq \pi, \tag{10}$$

which is periodic on the lattice: $\tilde{A}_\mu(k_\ell + N_\mu\hat{\mu}) = \tilde{A}_\mu(k_\ell)$. Recalling definition (8), one finds

$$\tilde{F}_{12}(k_\ell) = \Delta_1\tilde{A}_2(k_\ell) - \Delta_2\tilde{A}_1(k_\ell) + 2\pi\mathrm{i} n_{12}(k_\ell), \tag{11}$$

where Δ_μ is the forward difference operator on the lattice, $\Delta_\mu f(k_\ell) = f(k_\ell + \hat{\mu}) - f(k_\ell)$, and $n_{12}(k_\ell)$ is an *integer-valued* field, which is chosen such that $(1/\mathrm{i})\tilde{F}_{12}(k_\ell)$ takes a value within the principal branch. By definition, $|n_{12}(k_\ell)| \leq 2$. From eqs. (9) and (11), we have

$$\tilde{c}_n = \sum_\ell n_{12}(k_\ell), \tag{12}$$

which shows that the lattice Chern number $\tilde{c}_n$ is an integer.

The field strength on the lattice $\tilde{F}_{12}(k_\ell)$ in eq. (8) reduces to the one in the continuum $F_{12}(k)\delta k_1\delta k_2$ in the limit $N_{\mathrm{B}} \to \infty$, where $\delta k_\mu = 2\pi/(q_1 q_2 N_{\mathrm{B}})$. Generically, the continuum field strength $F_{12}(k)$ has no singularity when the nth band is well separated from the neighboring ones; that is, the energy gaps between them do not close,

$$|E_n(k) - E_{n\pm1}(k)| \neq 0, \tag{13}$$

for any value of $k \in T^2$. This is the *gap-opening condition*.[2,3] One can expect, in general, that the problem is regular if the above gap-opening condition is satisfied. Then, the lattice field strength $\tilde{F}_{12}$ will be small enough for a sufficiently large N_{B} and the lattice Chern number will approach the one in the continuum $\tilde{c}_n \to c_n$ in the $N_{\mathrm{B}} \to \infty$ limit. Since both $\tilde{c}_n$ and c_n are integers, we have $\tilde{c}_n = c_n$ for $N_{\mathrm{B}} > N_{\mathrm{B}}^{\mathrm{c}}$. The critical mesh size $N_{\mathrm{B}}^{\mathrm{c}}$ may be estimated by a breaking of the admissibility condition[12–16]

$$|F_{12}(k_\ell)|\delta k_1\delta k_2 \approx |\tilde{F}_{12}(k_\ell)| < \pi \quad \text{for all } k_\ell. \tag{14}$$

It is expected that this $N_{\mathrm{B}}^{\mathrm{c}}$ is not very large for a standard generic problem with the Chern number $c_n \approx \mathcal{O}(1)$. Since the area of the Brillouin zone is $4\pi^2/(q_1 q_2)$, we can estimate the field strength as $F_{12}(k_\ell) \approx i c_n q_1 q_2/(2\pi)$. In this way, the critical mesh size is given by

$$N_{\mathrm{B}}^{c} \approx \mathcal{O}(\sqrt{2|c_n|/(q_1 q_2)}). \tag{15}$$

That is, we can expect that our method reproduces correct Chern numbers of the continuum even for a coarsely discretized Brillouin zone. This is another advantage of the present method.

As a function of U(1) link variables which satisfy the admissibility (14), the Chern number on the lattice $\tilde{c}_n$ is a constant function. To verify this, we note that a possible discontinuity of $\tilde{c}_n$ as a function of link variables $U_{\mu(k_\ell)}$ occurs only when $|\tilde{F}_{12}(^\exists k_\ell)| = \pi$. Since $\tilde{c}_n$ is an integer which cannot continuously change, $\tilde{c}_n$ remains the same as long as a configuration is smoothly varied under the admissibility (14). In other words, under the admissibility, the space of U(1) link variables is divided into disconnected sectors and the topological number $\tilde{c}_n$ is uniquely assigned to each sector. This is the basic idea behind the present construction.[12)] The Chern number $\tilde{c}_n$ is, moreover, a *unique* gauge-invariant topological integer which can be assigned to admissible U(1) link variables.[17,18)]

In the present context of the Berry connection, a gauge-invariant content of link variables is completely governed by the k dependence of the Hamiltonian $H(k)$. Each of the topological ordered states with a nontrivial Chern number corresponds to the above nontrivial topological sector specified by the admissibility. It is characterized by the lattice Chern number $\tilde{c}_n$. In the continuum, on the other hand, the topological stability of the Chern number is assured by the gap-opening condition (13). The topological quantum phase transitions are thus characterized by the gap closing. Namely, nontrivial topological sectors of the continuum, each of which is a topological ordered state, are separated by the gaps. Correspondingly the Chern number of the total bands, which is described by the non-Abelian Chern number, vanishes.[2,3)] At the critical point at which the gap-opening condition breaks down, the field strength $F_{12}(k)$ becomes singular at the gap-closing momentum. From a correspondence to the lattice case, we conclude that the admissibility condition cannot be satisfied by any finite $N_{\rm B}$ at that critical point.

Our method can be extended to the case of the non-Abelian Berry connection $\mathcal{A} = \psi^\dagger d\psi$, which is an $M \times M$ matrix-valued one-form associated with a multiplet $\psi = (|n_1\rangle, \ldots, |n_M\rangle)$.[2,3,19)] The associated Chern number is defined by $c_\psi = \int_S \mathrm{tr}\, \mathrm{d}\mathcal{A}/(2\pi\mathrm{i})$, an integral over a two-dimensional surface S with a generic (relaxed) gap-opening condition; $E_n(k) \neq E_{n'}(k)$ for all k, where $n \in I$ and $n' \notin I$ for $I = \{n_1, \ldots, n_M\}$.[2,3)] It turns out that the present lattice prescription is valid if one substitutes the U(1) link variable by

$$U_\mu(k_\ell) = \frac{1}{\mathcal{N}_\mu(k_\ell)} \det \psi^\dagger(k_\ell)\psi(k_\ell + \hat{\mu}) \tag{16}$$

with the normalization constant $\mathcal{N}_\mu(k_\ell) \equiv |\det \psi^\dagger(k_\ell)\psi(k_\ell + \hat{\mu})|$. We define the associated field strength and the Chern number on the lattice $\tilde{c}_\psi$ by the same expressions as those for the Abelian case, eqs. (8) and (9). This $\tilde{c}_\psi$ shares the features of the Chern number in the Abelian case $\tilde{c}_n$. For regular problems, we have $\tilde{c}_\psi = c_\psi$ for a sufficiently fine discretization $N_{\rm B} > N_{\rm B}^c$.

Having observed desired properties of our definition of the lattice Chern number, we now demonstrate how it works in a definite model. We consider the Hamiltonian for spinless fermions in an external magnetic field: $H = -t\sum_{\langle i,j\rangle} c_i^\dagger \mathrm{e}^{\mathrm{i}\theta_{i,j}} c_j$, where the flux per plaquette on the coordinate lattice $\phi = \sum_\Box \theta_{i,j}/(2\pi)$ is p/q.[4)] For mutually prime integers p and q, the spectrum splits into q subbands. In the Landau gauge in the x-direction, the Hamiltonian in the k-space is given by $H_{ij}(k) = -2t\delta_{ij}\cos(k_y - 2\pi\phi j) - t(\delta_{i+1,j} + \delta_{i,j+1}) - t\delta_{i+q-1,j}\mathrm{e}^{-\mathrm{i}qk_x} - t\delta_{i,j+q-1}\mathrm{e}^{\mathrm{i}qk_x}$, $(i,j = 1, \ldots, q)$ with $q_1 = q$ and $q_2 = 1$. Bellow, we will present some results of applying our method to the middle subband of the $\phi = 1/3$ (that is, $q = 3$) system.

In Fig. 1(a), we show the lattice field strength $\tilde{F}_{12}(k)$ in eq. (8). The (magnetic) Brillouin zone in the Landau gauge $[0, 2\pi/3) \times [0, 2\pi)$ is discretized by 3×9 meshes. Note that the asymmetry of the Brillouin zone is simply due to the gauge choice; there is no x–y anisotropy in the present problem. The sum of $\tilde{F}_{12}(k)$ over the mesh points gives

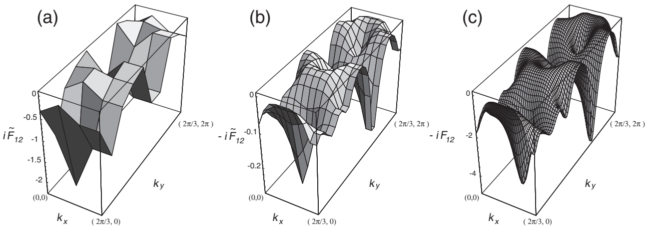

Fig. 1. (a) Field strength $-\mathrm{i}\tilde{F}_{12}(k)$ of middle band for $\phi = 1/3$ system in 3×9 lattice Brillouin zone ($N_{\rm B} = 3$), (b) the same result in 9×27 lattice ($N_{\rm B} = 9$), and (c) field strength $-\mathrm{i}F_{12}(k)$ of the same band in the continuum which is approximated by $\mathrm{Im}\,(\delta_1 A_2 - \delta_2 A_1)$ for $|\delta k_1| = |\delta k_2| = 2\pi/90$.

$\tilde{c}_n = -2$, which coincides with the known result for the present case. The same calculation but with 9×27 meshes is shown in Fig. 1(b). It indeed gives the identical Chern number $\tilde{c}_n = -2$. Figure 1(c) shows the field strength F_{12} of the continuum. As expected, it is regular and of the order of unity. Comparing these figures, one can see that the field strength of the lattice system $\tilde{F}_{12}$ converges to the one in the continuum F_{12} up to a proportionality constant. Since the problem is regular, the field strength of the lattice system $\tilde{F}_{12}$ decreases as $N_{\rm B}$ increases. The admissibility is safely satisfied in Fig. 1(b) ($N_{\rm B} = 9$), but $N_{\rm B} = 3$ is close to the critical $N_{\rm B}^c$. (Note the scales in the figures.)

It should be stressed again that the above lattice calculations can be performed in *any gauge*. We do *not* need specific gauge-fixing to make the gauge connection smooth. An *arbitrary* gauge (*e.g.*, a phase choice of eigenvectors given by a numerical library) can be adopted to compute the Chern number.

As we have discussed, the lattice Chern number $\tilde{c}_n$ is closely related to the integer field $n_{12}(k_\ell)$ in eq. (11). To illustrate this point explicitly, we next plot the field $n_{12}(k_\ell)$. Since we must specify the gauge to do so ($n_{12}(k_\ell)$ itself is *not* gauge-invariant), we briefly describe the method of gauge-fixing adopted here.[2,3)] One first selects an arbitrary state $|\phi\rangle$ which is globally well defined over the whole Brillouin zone. Then the gauge can be specified by $|n^\phi\rangle = P_n|\phi\rangle/N^\phi = |n\rangle \cdot \langle n|\phi\rangle/N^\phi$, where $P_n = |n\rangle\langle n|$ is a gauge-invariant projection and $N^\phi = |\langle\phi|n\rangle|$ is a gauge-invariant normalization which ensures $\langle n^\phi|n^\phi\rangle = 1$. A typical example of $|\phi\rangle$ is a constant state, but it can be a varying state as well.

The integer fields $n_{12}(k_\ell)$ in several different gauges are depicted in Fig. 2, where the black and white circles denote $n_{12} = -1$ and 1, respectively, whereas a blank implies $n_{12} = 0$. It is clear that any of them gives the correct Chern number $\tilde{c}_n = -2$, that is, the number of black circles minus that of white ones is always two. The field $n_{12}(k_\ell)$ is gauge-dependent, but their sum is gauge-invariant. The figures clearly show the gauge-independence of the lattice Chern number. In Figs. 2(a) and 2(b), we used the global gauges specified by the states $|\phi_{g_1}\rangle = \mathrm{e}^{\mathrm{i}q(k_x+k_y)}(1,-1,0)^T$ and $|\phi_{g_2}\rangle = \mathrm{e}^{\mathrm{i}q(k_x+k_y)}(1,1,0)^T$, respectively. The term "global" means that the gauge-fixing condition $|\langle\phi_{g_i}(k_\ell)|n(k_\ell)\rangle| \neq 0$ is satisfied at all lattice points k_ℓ.

The meaning of the field $n_{12}(k_\ell)$ and the relationship between the present lattice formulation and the continuum one become much clearer by adopting a "patchwork gauge". To be specific, let us take a gauge convention specified by

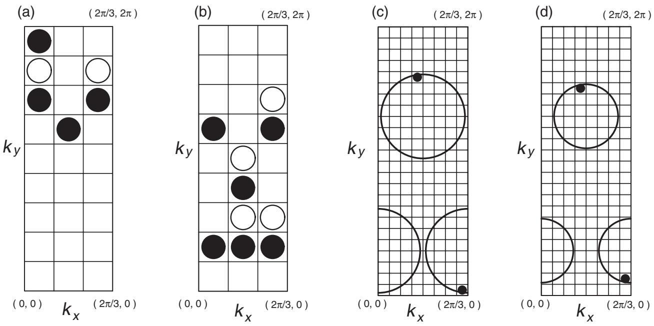

Fig. 2. Configuration of integer field $n_{12}(k_\ell)$ in gauge specified by state $|\phi\rangle$ (see text) over discretized Brillouin zones. (a) $N_B = 3$, $|\phi\rangle = |\phi_{g_1}\rangle$ (b) $N_B = 3$, $|\phi\rangle = |\phi_{g_2}\rangle$ (c) $N_B = 8$ and $|\phi\rangle = |\phi(R_{\pi/3.2})\rangle$, and (d) $N_B = 8$ and $|\phi\rangle = |\phi(R_{\pi/4.2})\rangle$. Black (white) circles denote $n_{12} = -1$ (1).

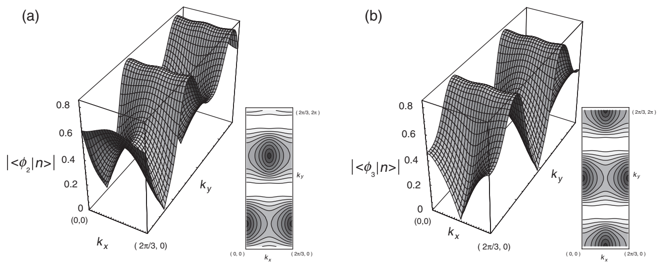

Fig. 3. Amplitude of overlap $|\langle\phi_i|n\rangle|$ between wave function $|n\rangle$ and trial state $|\phi_i\rangle$: (a) for trial state $\phi_2 = (0,1,0)^T$, and (b) for trial state $\phi_3 = (0,0,1)^T$.

$|\phi_2\rangle = (0,1,0)^T$, but another gauge specified by $|\phi_3\rangle = (0,0,1)^T$ in some regions where the former is ill-defined. We show in Fig. 3 the amplitude of the overlap between the wave function and trial states $|\phi_2\rangle$ and $|\phi_3\rangle$. Figure 3(a) shows that the gauge specified by $|\phi_2\rangle$ becomes ill-defined at two points near $k^1 = (2\pi/3, \pi/3)$ and $k^2 = (\pi/3, 4\pi/3)$. Therefore, we first define, around these points, circular regions $R_r = \{k||k - k^1| < r\} \cup \{k||k - k^2| < r\}$ with an appropriate radius r, and we next check in Fig. 3(b) that we can indeed take the second gauge specified by $|\phi_3\rangle$ safely in R_r. This patchwork gauge choice is referred to as the gauge specified by $|\phi(R_r)\rangle$. With this gauge, the wave functions $|n^\phi(k_\ell)\rangle$ and the corresponding gauge potential $\tilde{A}^\phi_\mu(k_\ell)$ are smooth if lattice points are sufficiently fine. This implies that the integer field $n_{12}(k_\ell)$ is vanishing within each region. Nonzero values of $n_{12}(k_\ell)$ are only allowed at plaquettes existing at the boundary of the regions.

The field $n_{12}(k_\ell)$ computed with the above local gauge is shown in Figs. 2(c) and 2(d) for two different radiuses r. The figures clearly show that the integer field $n_{12}(k_\ell)$ indeed acquires nonzero values only at boundaries of separated regions. The lattice field $n_{12}(k_\ell)$ carries information corresponding to the winding number of the gauge transformation along the boundary of a patch in the continuum.

In this letter, we presented our method as an efficient technique for calculating the Chern numbers in an infinite system on the basis of a discretized Brillouin zone. In finite systems, however, the Brillouin zones are discrete from the onset. Therefore, the present method will also be useful for revealing topological orders of *finite systems* with possible many-body interactions.[2,3)]

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