```
program main
implicit none
complex*16        :: H(4,4), H2(4,4)
complex*16        :: F12(2), ChernN
double precision :: ek, kx, ky, soc, mu, Hz, Delta, dk, q1x, q1y, q2x, q2y
integer           :: ix, iy, iu, j, ih
double precision :: PI
complex*16, parameter :: CI = cmplx(0.0d0, 1.0d0)
```

= I

```
integer           :: INFO
integer           :: LWORK = 8
complex*16        :: WORK(8)
double precision :: RWORK(12)
double precision :: W(4), W2(4)
complex*16        :: tmp1, tmp2
```

→ lapack

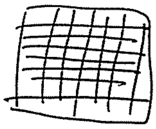
```
mu = 0.5
soc = 1.0
Hz = 0.0
Delta = 1.0
dk = 0.1
PI = 4 * atan(1.0d0)

do ih = 0, 100
Hz = 0.02 * ih

ChernN = 0.0

do ix = -50, 50
  do iy = -50, 50
```

取离散的点



```
  kx = dk * ix
  ky = dk * iy

  F12 = cmplx(1.0d0, 0.0d0)

  do iu = 1, 4
```

4个点

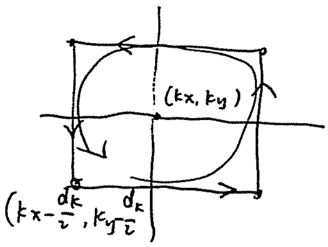
```
  if(iu .eq. 1) then
    q1x = kx - dk * 0.5
    q1y = ky - dk * 0.5
    q2x = kx + dk * 0.5
    q2y = ky - dk * 0.5
  endif

  if(iu .eq. 2) then
    q1x = kx + dk * 0.5
    q1y = ky - dk * 0.5
    q2x = kx + dk * 0.5
    q2y = ky + dk * 0.5
  endif

  if(iu .eq. 3) then
    q1x = kx + dk * 0.5
    q1y = ky + dk * 0.5
    q2x = kx - dk * 0.5
    q2y = ky + dk * 0.5
  endif

  if(iu .eq. 4) then
    q1x = kx - dk * 0.5
    q1y = ky + dk * 0.5
    q2x = kx - dk * 0.5
    q2y = ky - dk * 0.5
  endif

 H = cmplx(0.0, 0.0)
```

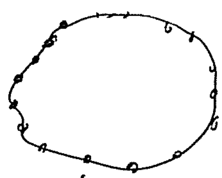


F_{ij} = 这个loop 的 overlap.

$$\oint_{\Sigma} \vec{F}\cdot d\vec{s} = \int_{\partial\Sigma} (\nabla\times\vec{F})\cdot d\vec{l}$$

= 某一个区域边界上的积分.

在一个loop上



$\prod_i \langle \phi(i) | \phi(i+1) \rangle$ is well-defined.

```
  ek = q1x * q1x + q1y * q1y - mu
  H(1, 1)  =  ek + Hz
  H(2, 2)  =  ek - Hz
  H(3, 3)  = -(ek + Hz)
  H(4, 4)  = -(ek - Hz)
  H(1, 2)  = soc * cmplx(q1x,  q1y)
  H(2, 1)  = soc * cmplx(q1x, -q1y)
  H(3, 4)  = soc * cmplx(q1x, -q1y)
  H(4, 3)  = soc * cmplx(q1x,  q1y)
  H(1, 4)  =  Delta
  H(2, 3)  = -Delta
  H(3, 2)  = -Delta
  H(4, 1)  =  Delta
```

计算 $\psi(i)$

```
  call zheev('V', 'U', 4, H, 4, W, WORK, LWORK, RWORK, INFO)
  if(INFO .ne. 0) then
    write(*, *) " Error in calculating H, INFO = ", INFO
    call abort
  endif

  H2 = cmplx(0.0, 0.0)
  ek = q2x * q2x + q2y * q2y - mu
  H2(1, 1)  =  ek + Hz
  H2(2, 2)  =  ek - Hz
  H2(3, 3)  = -(ek + Hz)
  H2(4, 4)  = -(ek - Hz)
  H2(1, 2)  = soc * cmplx(q2x,  q2y)
  H2(2, 1)  = soc * cmplx(q2x, -q2y)
  H2(3, 4)  = soc * cmplx(q2x, -q2y)
  H2(4, 3)  = soc * cmplx(q2x,  q2y)
  H2(1, 4)  =  Delta
  H2(2, 3)  = -Delta
  H2(3, 2)  = -Delta
  H2(4, 1)  =  Delta
```

$\psi(i+1)$

```
  call zheev('V', 'U', 4, H2, 4, W, WORK, LWORK, RWORK, INFO)
  if(INFO .ne. 0) then
    write(*, *) " Error in calculating H, INFO = ", INFO
    call abort
  endif

  tmp1 = cmplx(0.0, 0.0)
  tmp2 = cmplx(0.0, 0.0)
  do j=1, 4
    tmp1 = tmp1 + conjg(H(j,1)) * H2(j,1)
    tmp2 = tmp2 + conjg(H(j,2)) * H2(j,2)
  end do
  tmp1 =tmp1 /abs(tmp1)
  tmp2 =tmp2 /abs(tmp2)
```

$\langle \psi_n(i) | \psi_n(i+1) \rangle$

band index

```
  F12(1) = F12(1) * tmp1
  F12(2) = F12(2) * tmp2
```

← loop上面积分

```
  end do

  ChernN = ChernN + log(F12(1))/(2*PI*CI) + log(F12(2))/(2*PI*CI)

  end do
end do
```

2个 bands 求和.

```
write(*,'(3f14.6)')  Hz, Real(ChernN), AIMAG(ChernN)

end do

end program
```

$\boxed{\simeq 1}$ $= 0$

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我用这个方法来做

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.

KEYWORDS: Chern number, Berry connection, quantum Hall effect, lattice gauge theory
DOI: 10.1143/JPSJ.74.1674

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 ($\ell = 1,\ldots,N_1N_2$) 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 $N_\mu = q_\nu N_{\rm B}$ ($\mu \neq \nu$) so that the unit plaquette is a square of the size $2\pi/(q_1q_2N_{\rm B})$.

We first define a U(1) link variable from the wave functions of the nth band as $= e^{i\theta_{\ell\mu}}$

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

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

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

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

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

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

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

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

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

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 $(1/{\rm i})\tilde{F}_{12}(k_\ell)$ 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 $N_{\rm B} \to \infty$, where $\delta k_\mu = 2\pi/(q_1q_2N_{\rm B})$. 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 $N_{\rm B}$ and the lattice Chern number will approach the one in the continuum $\tilde{c}_n \to c_n$ in the $N_{\rm B} \to \infty$ limit. Since both $\tilde{c}_n$ and c_n are integers, we have $\tilde{c}_n = c_n$ for $N_{\rm B} > N_{\rm B}^{\rm c}$. The critical mesh size $N_{\rm B}^{\rm c}$ 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 $N_{\rm B}^{\rm c}$ 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 $4\pi^2/(q_1q_2)$, we can estimate the field strength as $F_{12}(k_\ell) \approx {\rm i}c_nq_1q_2/(2\pi)$. In this way, the critical mesh size is given by

$$N_{\rm B}^{\rm c} \approx \mathcal{O}(\sqrt{2|c_n|/(q_1q_2)}). \tag{15}$$

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*

θ_{x1} θ.