Quantized Hall conductivity of Bloch electrons: topology and the Dirac fermion*

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Abstract

We consider the Hall conductivity of two-dimensional non-interacting Bloch electrons when the magnetic flux per unit cell is a rational number $p/q$ where $p$ and $q$ are mutually coprime. We present a counter-example for the naive expectation that the Hall conductivity carried by a band is given by treating gap minima as Dirac fermions. Instead of the above expectation, we show that the change of the Hall conductivity at a gap-closing phenomenon is given by the Dirac fermion argument. Comparing with the Diophantine equation, our result implies that a band-gap closes at $q$ points simultaneously. Furthermore, we show that the dispersion relation is $q$-fold degenerate in the magnetic Brillouin zone.

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I. INTRODUCTION

It was a surprise that Hall conductance of two-dimensional electron system was found to be quantized in some experiments. The presence of disorder or edges are considered to be necessary for the quantization of the Hall conductance in the experiments. However, basic important facts are that there are energy gaps in the bulk system without disorder and that the Hall conductivity is quantized when the Fermi level lies in the gap. In the free electron case, it is easy to show this; eigenstates are the degenerate Landau levels separated by energy gaps, and each Landau level contributes $e^2/h$ exactly to the Hall conductivity.

When a periodic potential is present, it is a more non-trivial problem since a Landau level splits into several subbands by turning on a periodic potential, one may expect that a subband carries fractional (in units of $e^2/h$) Hall conductivity. However, Thouless, Kohmoto, Nightingale and den Nijs (TKNN) showed that the Hall conductivity carried by a magnetic subband is always an integer. This quantization comes from the topological nature; TKNN integer is a topological invariant on the magnetic Brillouin zone. Ishikawa et al. also discussed the topological aspect of the quantized Hall conductivity. Topological character of the Hall conductivity carried by edge states and its relation to the bulk TKNN integer are also discussed.

On the other hand, it has been widely accepted that low-energy behavior of a thermodynamic system is correctly described by a continuum field theory. In the present case, a minimum of a gap between magnetic bands may be described by a Dirac fermion (in 2+1 dimensions), which gives the Hall conductivity $-e^2/2h \text{sgn} m$ ($m$ is the Dirac mass.) Hence we may expect that the Hall conductivity carried by a band is given by counting only the Dirac fermions. There are several works based on this idea.

However, it is not trivial whether the Dirac fermion argument is true or not, because the Hall conductivity is given by an integral over whole Brillouin zone while the Dirac fermion argument looks only the gap minima in the Brillouin zone. Therefore, in this paper we investigate the validity of the Dirac fermion argument for Bloch electrons, and its relation to the topological TKNN integer.

Contrary to the naive expectation, we found that the Hall conductivity carried by a band cannot given by the Dirac fermion argument in general. Instead, applying the argument by Simon and others, we showed that the change of the Hall conductivity at a gap-closing point is correctly described by the Dirac fermion argument.

Comparing with the Diophantine equation, this result implies that a band-gap closes simultaneously at $q$ points. Moreover, we showed a stronger statement that the dispersion relation is $q$-fold degenerate in the magnetic Brillouin zone for general 2D Bloch electrons. This is a generalization of the result for the tight-binding model on a square lattice.

Throughout this paper, we consider two-dimensional non-interacting electron systems under a periodic potential and a uniform magnetic field at zero temperature. The flux per unit cell is assumed to be a rational number, and the Fermi level lies at a band gap except when the gap closes. We set the velocity of light $c$ to be 1 while we keep Planck’s constant $h$ or $\hbar = h/2\pi$.

The organization of this paper is as follows. In Section 1, we give a brief review on the Hall conductivity as a topological invariant. In Section 2, we review the Dirac fermion in 2 + 1 dimensions. Section 3 describes a counterexample in which Dirac fermion argument
cannot give the correct value of the Hall conductivity of Bloch electrons. In Section V, we show that the change of the Hall conductivity during a gap-closing is given by the Dirac fermion argument. A q-fold structure in the magnetic Brillouin zone is shown in Section VI. Conclusions and a discussion are given in Section VII.

II. HALL CONDUCTIVITY OF BLOCH ELECTRONS

Here we review known important facts about the quantized Hall conductivity of Bloch electrons, especially the topological aspect of the quantized Hall conductivity.

The Schrödinger equation for a two-dimensional non-interacting electron system in a uniform magnetic field is written as

$$H \psi(\vec{r}) = \left[ \frac{1}{2m} (\vec{p} + e\vec{A})^2 + U(\vec{r}) \right] \psi(\vec{r}) = E \psi(\vec{r})$$

(1)

where $\vec{p}$ is the momentum $-i\hbar \nabla$ and $\vec{A}$ is the vector potential. In our case, the potential $U(\vec{r})$ is periodic, i.e.,

$$U(\vec{r} + \vec{a}_1) = U(\vec{r} + \vec{a}_2) = U(\vec{r})$$

(2)

where $\vec{a}_1$ and $\vec{a}_2$ are linearly independent Braveis vectors. We take the symmetric gauge $\vec{A} = 1/2(\vec{B} \times \vec{r})$ for the moment. Let us define the magnetic translation operators

$$\hat{T}_{\vec{R}} = \exp \left[ \frac{i}{\hbar} \vec{R} \cdot (\vec{p} - e\vec{A}) \right].$$

(3)

In the symmetric gauge, this operator commutes with the kinetic term in the Hamiltonian, as well as with the potential term.

We consider the case where the magnetic flux per unit cell is $p/q$, where $p$ and $q$ are mutually prime integers. Namely, the magnetic flux density $\vec{B}$ satisfies

$$\vec{B} \cdot (\vec{a}_1 \times \vec{a}_2) = \frac{p \hbar}{q e}$$

(4)

Then the following relations hold:

$$[\hat{T}_{q\vec{a}_1}, \hat{T}_{\vec{a}_2}] = 0, [\hat{T}_{\vec{R}}, H] = 0$$

(5)

where $\vec{R} = n(q\vec{a}_1) + m\vec{a}_2$ and $n, m$ are integers. Thus we can apply the Bloch’s theorem if we take an enlarged unit cell (magnetic unit cell) which is $q$ times larger than the original unit cell. Correspondingly, the reciprocal space (magnetic Brillouin zone) becomes $1/q$ of the original Brillouin zone. Namely, the Schrödinger equation can be reduced as

$$\hat{H}(\vec{k}) u^i(\vec{r}) = E^i u^i(\vec{r})$$

(6)

$$\hat{H}(\vec{k}) = \frac{1}{2m} (-i\hbar \nabla + \hbar \vec{k} + e\vec{A})^2 + U(\vec{r})$$

(7)
where \( i \) is the band index, \( \vec{k} \) is the crystal momentum and \( u^i \) is a wavefunction with the generalized Bloch condition:

\[
  u^i(\vec{r}) = u^i(\vec{r} + \vec{q} \vec{a}_1) \exp \left[ -i \frac{q e}{2\hbar} \vec{B} \cdot (\vec{r} \times \vec{a}_1) \right] = u^i(\vec{r} + \vec{a}_2) \exp \left[ -i \frac{e}{2\hbar} \vec{B} \cdot (\vec{r} \times \vec{a}_2) \right].
\]  

(8)

Defining the reciprocal lattice vectors \( \vec{g}_i \) by \( \vec{g}_i \cdot \vec{a}_j = \delta_{ij} \), we have equivalence relations

\[
  \vec{k} \sim \vec{k} + 2\pi \vec{g}_1 \sim \vec{k} + 2\pi \vec{g}_2
\]

(9)

among crystal momenta \( \vec{k} \). Hence we can restrict \( \vec{k} \) to the magnetic Brillouin zone

\[
  \vec{k} = k_1 \vec{g}_1 + k_2 \vec{g}_2 \quad \left( -\frac{\pi}{q} \leq k_1 < \frac{\pi}{q}, -\pi \leq k_2 < \pi \right).
\]

(10)

From the linear response theory (Nakano-Kubo formula), the Hall conductivity of the system is given by

\[
  \sigma_{xy} = \sum_{i \mid E_i < E_F} \frac{e^2}{\hbar} \frac{1}{2\pi i} \int_{\text{MUC}} d^2k \int_{\text{MUC}} \left[ \left( \frac{\partial u^i_{k}(\vec{r})}{\partial k_y} \right)^* \frac{\partial u^i_{k}(\vec{r})}{\partial k_x} - \left( \frac{\partial u^i_{k}(\vec{r})}{\partial k_x} \right)^* \frac{\partial u^i_{k}(\vec{r})}{\partial k_y} \right].
\]

(11)

That is, the total Hall conductivity \( \sigma_{xy} \) is obtained as a sum of the contributions from all bands below the Fermi level.

The contribution from a single band can be written in a compact form as follows. We will omit the band index when a single band is considered. For each band, we define a vector field in the magnetic Brillouin zone by

\[
  \hat{A}(\vec{k}) = \langle u(\vec{k}) | \nabla_k | u(\vec{k}) \rangle \equiv \int_{\text{MUC}} d^2k u^*_k(\vec{r}) \nabla_k u_k(\vec{r})
\]

(12)

where \( \nabla_k \) is a vector operator \((\partial/\partial k_x, \partial/\partial k_y)\) and MUC represents the magnetic unit cell. It should be noted that we can choose the phase of the wavefunction for each \( \vec{k} \) arbitrarily.

Transformation of the phase as

\[
  u^i_k(\vec{r}) = u^i_k(\vec{r}) e^{i f(\vec{k})}, \quad \hat{A}^i(\vec{k}) = \hat{A}(\vec{k}) + i \nabla_k f(\vec{k})
\]

(13)

is nothing but a \( U(1) \) gauge transformation; \( \hat{A}(\vec{k}) \) is a \( U(1) \) gauge field defined on the magnetic Brillouin zone. Using this gauge field, the Hall conductivity carried by a single band is written as

\[
  \sigma_{xy} = \frac{e^2}{\hbar} \frac{1}{2\pi i} \int_{\text{MBZ}} d^2k \nabla_k \times \hat{A}(\vec{k})
\]

(14)

where \( \nabla_k \times \) denotes the rotation in two-dimensional \( \vec{k} \)-space and MBZ represents the magnetic Brillouin zone.
Although a naive application of the Stokes' theorem implies that (14) is zero, a non-zero value of the hall conductivity arises from a non-trivial topology of the fiber bundle. That is, one cannot determine the phase of the wavefunction $u_{\vec{k}}$ smoothly and uniquely over the entire Brillouin zone in general. For example, one can fix the gauge by requiring that the amplitude $\langle a|u(\vec{k})\rangle$ is real ($|a\rangle$ is an arbitrary wavefunction.) Though this seems a well-defined gauge fixing, this cannot fix the gauge at the zeros of the amplitude. We must cover the region near a zero by another patch, in which a different gauge fixing is chosen. Phase mismatch between the two gauges produces a non-zero value of (14). We call a zero of the amplitude as a vortex. Uniqueness of the phase in each patch implies that the phase mismatch around a vortex should be an integral multiple of $2\pi$. This integer is called vorticity. Thus the Hall conductivity carried by a band (14) is $e^2/h$ times the total vorticity in the magnetic Brillouin zone. While the location of the vortices depends on the gauge, total vorticity is gauge invariant and is known as the first Chern number of the principal $U(1)$ bundle.

III. DIRAC FERMION IN 2+1 DIMENSIONS

To fix the convention, here we briefly review the relativistic Dirac fermion in 2 + 1 dimensions. The Lagrangian density is given by

$$\mathcal{L} = \bar{\psi}(i\hbar\partial_{\mu} - eA_\mu)\gamma^\mu \psi - m\bar{\psi}\psi$$

(15)

Where $A_\mu$ is the (background) vector potential. The $\gamma$-matrices satisfy the anticommutation relation $\{\gamma^\mu, \gamma^\nu\} = \eta^{\mu\nu}$ where $\eta^{\mu\nu}$ is the flat Minkowski metric. In the 2+1 dimensions, $\gamma$-matrices are $2 \times 2$ matrices. We choose the convention

$$\gamma^0 = \sigma^z, \gamma^1 = i\sigma^y, \gamma^2 = -i\sigma^x$$

(16)

where $\sigma^x, \sigma^y, \sigma^z$ are the standard Pauli matrices. When the electromagnetic field is absent, the 1-body Hamiltonian is derived from (14) as

$$H = m\sigma^z + p_x\sigma^x + p_y\sigma^y$$

(17)

where $(p_x, p_y)$ represents the momentum.

In the low-energy limit, the current is evaluated by several methods

$$\langle e_j^\mu \rangle = e\langle \bar{\psi}\gamma^\mu \psi \rangle = -\frac{e^2}{4\hbar} \varepsilon_{\mu\nu\sigma} F_{\nu\sigma} \text{sgn} m$$

(18)

where $F_{\nu\sigma}$ is the field strength $\partial_\nu A_\sigma - \partial_\sigma A_\nu$. Namely, the Hall conductivity carried by a Dirac fermion is $-e^2/2\hbar\text{sgn} m$.

IV. FAILURE OF THE DIRAC FERMION ARGUMENT

In many cases, the low-energy behavior of a thermodynamic system can be treated by a continuous field theory. From the field-theory point of view, this means a field theory is independent of details in the regularization.
In the case of the Bloch electron system in a magnetic field, the low-energy states near a gap minimum may be treated as a Dirac fermion\cite{15}. Thus we may expect that summing up contributions from each Dirac fermion gives the Hall conductivity of a band. Several authors made discussions based on this idea, and in fact it seems correct in some simple lattice models\cite{7,8}.

However, we show that this naive expectation is false in general. As a counterexample, we take a tight-binding model discussed in Ref.\cite{16}. We consider a isotropic square lattice with nearest-neighbor (NN) and next-nearest-neighbor (NNN) hoppings with $1/3$ magnetic flux per unit cell. Let the absolute value of the NN and NNN hoppings be $t_1$ and $t_2$, respectively.

Namely, the Hamiltonian of the system reads

$$H = \sum_{n,m} c_{n+1,m}^\dagger c_{n,m} \exp (i\theta_A) + \sum_{n,m} c_{n,m+1}^\dagger c_{n,m} \exp (i\theta_B)$$

$$+ t_2 \sum_{n,m} c_{n+1,m+1}^\dagger c_{n,m} \exp (i\theta_C)$$

$$+ t_2 \sum_{n,m} c_{n,m+1}^\dagger c_{n+1,m} \exp (i\theta_D) + \text{H.c.}$$

where

$$\theta_A = 0, \quad \theta_B = \frac{2\pi}{3} n, \quad \theta_C = \theta_D = \frac{2\pi}{3} (n + \frac{1}{2}).$$

The energy spectrum of this model is analyzed by Hatsugai and Kohmoto\cite{16}. According to them, the energy eigenvalue $E$ for each (crystal) momentum $\vec{k}$ is determined by the equation

$$F(E) = f(\vec{k})$$

where $F(E)$ is some polynomial of $E$ and $f(\vec{k})$ is given by

$$f(\vec{k}) = 2 \cos (3k_x)[1 - 3t_c^2] + 2 \cos (3k_y)[1 - 3t_c^2]$$

$$- 2t_c^3 \{ \cos [3(k_x + k_y)] + \cos [3(k_x - k_y)] \}.$$  

Precisely speaking, a minimum of an energy gap cannot always be regarded exactly as a Dirac fermion. In general Bloch electron systems, there are several bands separated by the energy gaps. If the gap is very small compared with other gaps, we can ignore other bands. Then the low-energy states near a gap minimum can be considered as one-particle states of a Dirac fermion. It is possible that a gap-closing point become singular; in this case the dispersion of the low-energy states is not relativistic. We have checked this is not the case in our counter-example. We will make a detailed discussion on this point in the next section.

In our model, the first gap closes simultaneously at three points when $t_c \sim 0.268$. An extremal point of an energy band is given by an extremal point of $f(\vec{k})$, and it is easy to show that the first gap has three minima in the neighborhood of the gap-closing point $t_c \sim 0.268$. Thus there are just three Dirac fermions in this region, if the Fermi level lies in the first gap. The dispersion relation of the model $t_c = 0.25$, which is near the gap-closing point, is shown in Fig. 1. 

Since a Dirac fermion contributes $\pm e^2/2h$ to the Hall conductivity $\sigma_{xy}$, it should be half-odd-integral multiple of $e^2/h$ from the Dirac fermion argument. However it should be an
integral multiple of $e^2/h$ according to the general theory of TKNN. Hence the naive Dirac
fermion argument is incorrect. In other words, there is no ‘anomaly-cancelling partner’ in
our model.

V. CHANGE OF THE HALL CONDUCTIVITY AND THE DIRAC FERMION

The naive expectation that the Dirac fermion argument gives the Hall conductivity
carried by a band is disproved in the last section. Nevertheless, the Dirac fermion argument
still makes sense for our problem. We proved the following proposition.

When a parameter in the Hamiltonian is varied, the Hall conductivity changes
only where the gap closes. This change of the Hall conductivity is correctly given
by the Dirac fermion argument; the Hall conductivity decreases by $e^2/h$ if the
Dirac mass changes from negative to positive, and increases by $e^2/h$ if it changes
from positive to negative. If the gap closes at several points simultaneously, the
change of the Hall conductivity is given by summing up the contributions from
each gap-closing point.

The above proposition is shown by mapping of the low-energy states to the Dirac fermion
and calculation of the change of the Chern number. The important point is that the change
of the Chern number is determined only by the neighborhood of the gap-closing point.
This fact was noticed by Simon, and also by Avron et al. in the context of the network
problem. We also note that the proof has similar structure to the “intuitive topological
proof” of the Nielsen-Ninomiya theorem in $3+1$ dimensions.

To discuss the change of the Hall conductivity, the Hamiltonian is assumed to vary
smoothly. Namely, we discuss a family of Hamiltonians labelled by a parameter $\lambda$. The
reduced Hamiltonian $\hat{H}$ also should be parameterized by $\lambda$ in the reduced Schrödinger equation. Thus $\hat{H}$ depends on three parameters, $k_x, k_y$, and $\lambda$; it can be said that $\hat{H}$ is defined
in a three-dimensional space whose coordinates are $k_x, k_y$ and $\lambda$.

First let us focus on the gap-closing phenomena. Assume that there is a gap-closing point
$(\vec{k}^*, \lambda^*)$ where energies of two bands are degenerate. Here we consider the generic case in
which only two bands touch at this point. We can neglect other bands near this gap-closing
point. Furthermore, we expand the Hamiltonian to the first order in

$$p = (p_x, p_y, p_z) = (\hbar (k_x - k_x^*), \hbar (k_y - k_y^*), \lambda - \lambda^*)$$ (22)

where $p$ is a three-dimensional vector. Since the effective Hamiltonian for the two bands is
$2 \times 2$ Hermitian matrix for each $p$, the most general form of the expansion is

$$\hat{H} = E^* + b \cdot p + V_{\mu}^\nu \sigma^\mu p_\nu + O(p^2)$$ (23)

where $\mu, \nu = 1, 2, 3$ and $\sigma^{1,2,3} = \sigma^{x,y,z}$. If $V$ is singular ($\det V = 0$), the dispersion relation
near the gap-closing point is not Dirac-fermion like. We don’t consider such non-generic
cases in this paper.

In order to see this is a Hamiltonian of the Dirac fermion, we make a unitary transfor-
mation and a redefinition of $(p_x, p_y)$. Since the term proportional to the identity matrix
can be absorbed to the redefinition of the energy and hence irrelevant, we only consider the terms containing a Pauli matrix. It is noted that a SU(2) transformation $U$ induces the transformation on the Pauli matrices as

$$U\sigma^\mu U^{-1} = R^\mu_\nu \sigma^\nu$$

(24)

where $R^\mu_\nu$ is a SO(3) matrix. There is always an appropriate SU(2) matrix $U$ corresponds to some given $R$. Any regular matrix $V$ can be decomposed as (Gram-Schmidt decomposition)

$$V = OT$$

(25)

where $O$ is an orthogonal matrix and $T$ is an upper triangle matrix with positive diagonal elements. Let us choose $R^{-1} = OW$ where $W = \text{diag}(1, 1, \text{sgn}(\det V))$. Then $U$ transforms the Hamiltonian as

$$U\hat{H}U^{-1} \sim \sigma^\mu T^\rho_\mu W^\nu_\rho p^\nu$$

(26)

where the terms proportional to the identity matrix are omitted. Let us define

$$\tilde{p}_\mu = (\tilde{p}_x, \tilde{p}_y, \tilde{p}_z) = T^\nu_\mu p^\nu.$$

(27)

Since $T$ is an upper triangle matrix with positive diagonal elements, this is a parity-conserving Affine transformation on $p_x, p_y$ and a scale transformation on $p_z$: $\tilde{p}_z = (\text{positive constant}) \times p_z$.

By this redefinition, the Hamiltonian becomes

$$\hat{H} \sim \text{sgn}(\det V)\tilde{p}_z \sigma_z + \tilde{p}_x \sigma_x + \tilde{p}_y \sigma_y,$$

(28)

which is nothing but the Dirac Hamiltonian $[17]$ with the mass $\text{sgn}(\det V)\tilde{p}_z$.

In this way, the neighborhood of a gap-closing point can be regarded as a Dirac fermion and the sign of the mass is opposite before and after the gap-closing. In Ref. [17] the Hamiltonian which is formally same as (28) represents the one-body Weyl Hamiltonian in 3+1 dimensions. In this case, $\tilde{p}_z$ denotes the third momentum, and the Weyl fermion is left-handed (right-handed) if $\det V > 0$ ($\det V < 0$). The similarity between our argument and that of Ref. [17] is based on the formal similarity between the one-body Dirac Hamiltonian in 2+1 dimensions and the one-body Weyl Hamiltonian in 3+1 dimensions. However, for our proof we should be careful not to mix the parameter $\lambda$ with the momenta $k_x, k_y$ during the transformation. This point has been solved by the Gram-Schmidt decomposition.

However, in our problem, we should be careful not to mix the parameter $\lambda$ with the momenta $k_x, k_y$ during the transformation because each section for constant $\lambda$ represents a physical model. This point has been cleared by use of the Gram-Schmidt decomposition $[25]$.

Next, we calculate the change of the Chern number as discussed in Refs. [11][12]. We introduce vortex lines in the three-dimensional parameter space. The vortex lines are defined by

$$\{(k_x, k_y, \lambda) | \exists j : \langle a | u^j(\vec{k}; \lambda) \rangle = 0\}$$

(29)
with respect to some reference vector (in the reduced Hilbert space) \(|a\rangle\). The real part and the imaginary part of the above condition fix two degrees of freedom. Thus (29) defines a set of curves (vortex lines) in the three-dimensional parameter space. When a vortex line satisfies \( \langle a|u^i(\vec{k}; \lambda) \rangle = 0 \) for the band \( i \), the vortex line is said to be in the \( i \)-th band.

It should be noted that the definition of the vortex lines is similar to that of the vortices. In fact, a section of the three-dimensional parameter space for a certain constant \( \lambda \) represents the magnetic Brillouin zone, and its intersection with the vortex lines are vortices. We define the orientation of a vortex line as shown in Fig. 2. it is taken in such a way that \( \lambda \) increases (decreases) if the vorticity at the section is positive (negative).

The following propositions are central for our result.

- For each gap-closing point, there is always a vortex line passes through it.
- The vortex line passes through the gap-closing point upward (i.e. from the lower band to the upper band) along the defined orientation if \( \det V > 0 \) and downward if \( \det V < 0 \).

Now we are going to examine the change of the Hall conductivity at the gap-closing point. We assume that the Fermi energy always lies in the gap except when it closes. We consider the case \( \det V > 0 \). Let us consider the vortex line which passes through the gap-closing point. If the orientation of the vortex line at the gap-closing point is in the direction that \( \lambda \) increases, the local vorticity is +1. According to the above proposition, the vortex line lies in the lower band when \( \lambda < \lambda^* \) and in the upper when \( \lambda > \lambda^* \). (See Fig. 3.)

If the orientation of the vortex line at the gap-closing point is the reverse, i.e. in the direction that \( \lambda \) decreases, the vorticity is \(-1\). Thus in this case the vortex line lies in the upper band when \( \lambda < \lambda^* \) and in the lower when \( \lambda > \lambda^* \). When \( \lambda \) is increased through the gap-closing value \( \lambda^* \), the total vorticity of the lower band decreases by 1 in the cases; the Hall conductivity decreases by \( e^2/h \) irrespective of the direction of the vortex line.

On the other hand, the mass of the Dirac fermion is negative when \( \lambda < \lambda^* \). If \( \lambda \) is increased, the mass become positive when \( \lambda > \lambda^* \). The prediction of the Dirac fermion argument is that the Hall conductivity decreases by \( e^2/h \) when \( \lambda \) is increased through the gap-closing value \( \lambda^* \). Now we can see it gives the correct change of the Hall conductivity. Similar arguments can be applied for a gap-closing point with \( \det V < 0 \). It is also easy to see that the change of the Hall conductivity is given by summing up the contributions from each gap-closing point when the two bands touch simultaneously at several points.

We also note that, the vortex only moves to another band and never appear or disappear when two bands touch. This implies that the sum of the Hall conductivity carried by two bands is conserved in a gap-closing. This is a simple illustration for the conservation law first discussed by Avron, Seiler and Simon.

Let us show how our result applies to the example presented in Section IV. The first gap closes simultaneously at three points when \( t_c = t_c^* \sim 0.268 \). The matrix \( V \) for these points can be calculated numerically and we obtain \( \det V \sim 7.2 > 0 \) for each point (see also the next section). Thus the Dirac mass is negative when \( t_c < t_c^* \) and positive when \( t_c > t_c^* \), and the Hall conductivity of the fist band decreases by \( 3e^2/h \) when \( t_c \) is increased through \( t_c^* \). This is consistent with the result \( \sigma_{xy} \) changes from \( e^2/h \) to \(-2e^2/h \) obtained by Hatsugai and Kohmoto.
VI. PERIODIC STRUCTURE IN THE MAGNETIC BRILLOUIN ZONE

It is known that the Hall conductivity of the Bloch electrons satisfies the Diophantine equation

\[ r = qs_r + pt_r \]  

(30)

where the Fermi level lies at the \( r \)-th gap, \( s_r \) is an integer and the total Hall conductivity is \( t_re^2/h \). A gap-closing does not affect the value of \( p, q \) and \( r \). Thus if \( t'_re^2/h \) is the Hall conductivity after the gap-closing, we have

\[ q(s_r - s'_r) + p(t_r - t'_r) = 0 \]  

(31)

for an integer \( s'_r \); the change of the Hall conductivity should be an integral multiple of \( qe^2/h \).

Comparing with this, our result implies that two bands touch simultaneously at multiple of \( q \) points. In fact, in our example shown in Section IV the first gap closes simultaneously at \( q = 3 \) points. For the tight-binding model on a square lattice, Kohmoto showed that the dispersion relation is \( q \)-fold in the magnetic Brillouin zone, combining a duality transformation and a gauge transformation. Although it seems difficult to extend the duality transformation to general models, we show that the \( q \)-fold structure is common in general Bloch electron systems.

For convenience, we make a gauge transformation in the reduced Schrödinger equation (6) to a Landau-like gauge as

\[
\begin{align*}
    u'_k(\vec{r}) &= \exp \left[ -i\pi \frac{p}{q} (\vec{r} \cdot \vec{g}_1)(\vec{r} \cdot \vec{g}_2) \right] u_k(\vec{r}) \\
    \vec{A}' &= \frac{1}{2} (\vec{B} \times \vec{r}) - \frac{1}{2} [\vec{r} \cdot (\vec{B} \times \vec{a}_2)\vec{g}_2 - \vec{r} \cdot (\vec{B} \times \vec{a}_1)\vec{g}_1] \\
    &= [(\vec{B} \times \vec{r}) \cdot \vec{a}_2] \vec{g}_2.
\end{align*}
\]  

(32)

(33)

If we shift the momentum by \( \vec{k} \to \vec{k} + 2\pi (p/q)\vec{g}_2 \), the kinetic term changes as

\[
\frac{1}{2m} (-ie\hbar \nabla + \hbar \vec{k} + e\vec{A})^2 \to \frac{1}{2m} (-ie\hbar \nabla + \hbar \vec{k} + e\frac{p}{q} \vec{g}_2 + e\vec{A})^2.
\]  

(34)

This can be absorbed by the shift \( \vec{r} \to \vec{r} - \vec{a}_1 \), which changes the vector potential as

\[
\begin{align*}
    \vec{A} &\to \vec{A} - [(\vec{a}_1 \times \vec{a}_2) \cdot \vec{B}]\vec{g}_2 \\
    &= \vec{A} - \frac{1}{e} \frac{p}{q} \vec{g}_2
\end{align*}
\]  

(35)

This shift does not change the potential term. Thus we see that \( E(\vec{k} + 2\pi (p/q)\vec{g}_2) = E(\vec{k}) \) since \( p \) and \( q \) are coprimes, for an arbitrary integer \( m \) there is always an integer \( n \) so that

\[ np \equiv m \pmod{q}. \]  

(36)

This leads to the symmetry
\[ E(\vec{k} + \frac{2\pi m}{q} \vec{g}_2) = E(\vec{k}). \] (37)

Hence the above symmetry means that the dispersion relation is \( q \)-fold; the magnetic Brillouin zone (10) consists of \( q \) sub-zones which have the same dispersion relation.

The fact that two bands should touch simultaneously at multiple of \( q \) points follows from this proposition. Moreover, we can also see that the Dirac masses (if they are well-defined) are the same for the \( q \) Dirac fermions connected by the shift \( \vec{k} \rightarrow \vec{k} + 2\pi(m/q)\vec{g}_2 \).

The above result shows the consistency between the Dirac fermion argument and the Diophantine equation. We note that, in general, the Diophantine equation (30) implies that the Hall conductivity is not an integral multiple of \( qe^2/h \) nor \( qe^2/(2h) \), although the dispersion is \( q \)-fold. Hence a Dirac fermion argument cannot give the correct Hall conductivity as long as one defines Dirac fermions with respect to the dispersion relation. The \( q \)-fold structure restricts only the change of the Hall conductivity to be a multiple of \( qe^2/h \). While the Dirac fermion argument can determine the precise value of the change of the Hall conductivity, the Diophantine equation restricts also the value of the total Hall conductivity; they are consistent and complementary results.

VII. CONCLUSIONS AND DISCUSSION

We discussed two-dimensional non-interacting Bloch electrons in a uniform magnetic field. The naive expectation that the Hall conductivity carried by a band is given by treating gap minima as Dirac fermions was found to be false. Instead of the naive expectation, we showed that the change of the Hall conductivity when the band gap closes is correctly given by the Dirac fermion argument. Comparing with the Diophantine equation, our result implies that the gap-closing occurs simultaneously at multiple of \( q \) points. We proved a stronger statement that the magnetic Brillouin zone consists of \( q \) sub-zones that have the same dispersion relation.

Although there is no reason that a naive field-theory prediction should be always true, one may ask why it fails in the present case. Our answer is that the failure is already implicit in the (naive) Dirac fermion argument itself. The Hall conductivity of a Dirac fermion depends only on the sign of the Dirac mass. That is, a Dirac fermion with arbitrary large mass contributes to the Hall conductivity. However, the large Dirac mass corresponds to the large gap between the bands in the Bloch electrons. When the gap is not small compared with other gaps, the identification between the Dirac fermion and the gap minimum becomes ambiguous.

On the other hand, since the Hall conductivity is given by an integral over the whole magnetic Brillouin zone, it seems impossible to determine the value only from gap minima. However, the Hall conductivity is not an ordinary integral but a topological invariant and cannot change except when the gap closes. Hence we can expect that the change of the Hall conductivity can be described by the local neighborhood of the gap-closing point. This expectation is realized in the proof.

Finally, we comment on the Dirac fermion argument\[ E(\vec{k} + \frac{2\pi m}{q} \vec{g}_2) = E(\vec{k}). \] using the Widom-Streda formula. It is summarized as follows. The Hall conductivity is related to the change of the charge density in an infinitesimal extra magnetic field. In a constant magnetic field, the energy
levels of a Dirac fermion form Landau levels. There are zero modes, whose energy depends on the Dirac mass, among the Landau levels. Since the spectrum besides the zero modes is symmetric for the Dirac fermion, the Hall conductivity is determined by the zero modes as $-e^2/(2h)\text{sgn}m$ for each Dirac fermion. However, in a general Bloch electron system, the spectrum is not symmetric about the Fermi level; the Dirac fermion argument is not reliable to obtain the Hall conductivity. Nevertheless, we can expect that only the contribution from the zero modes will change at a gap-closing point. This is consistent with our result that the Dirac fermion argument gives only the correct change of the Hall conductivity.

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Figure 1: The energy bands for the whole magnetic Brillouin zone of the tight-binding model on the square lattice with the NN and NNN hoppings. Here the NNN hopping $t_c = 0.25$, which is slightly less than the gap-closing point $t_c \sim 0.268$. If the Fermi level lies in the first gap, there are three (approximate) Dirac fermions corresponding to the minima of the gap.
Figure 2: The definition of the orientation of a vortex line. The plane represents a section of the three-dimensional parameter space. The orientation is defined by the vorticity of the vortex which is the section of the vortex line.
Figure 3: An example for the neighborhood of a gap-closing point with $\det V > 0$. The motion of the vortex line implies that the change of the Hall conductivity agrees with the change of the sign of the Dirac mass.