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Topological Invariant and the Quantization of the Hall Conductance

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The topological aspects of wavefunctions for electrons in a two dimensional periodic potential with a magnetic field are discussed. Special attention is paid to the linear response formula for the Hall conductance σ_{xy}. It is shown that the quantized value of σ_{xy} is related to the number of zeros of wavefunctions in the magnetic Brillouin zone. A phase of wavefunctions cannot be determined in a unique and smooth way over the entire magnetic Brillouin zone unless the magnetic subband carries no Hall current. © 1985 Academic Press, Inc.

1. INTRODUCTION

The discovery of the quantization of the Hall conductance by von Klitzing, Dorda, and Pepper [1] is one of the most important results in condensed matter physics in recent years. Since there had been no prediction of such a precise quantization, the subject has been under intensive theoretical investigation [2]. The ideal two dimensional electron system has integral values of the Hall conductance in unit of e^2/h if the Fermi energy lies in a gap between Landau levels. The experimental result is astonishing because, in a real system, we would expect corrections of various sorts, due to, for example, electron–electron interactions, impurities, quasi-two-dimensionality, substrate potentials, finite size of samples, etc.

The effects of periodic potentials have been discussed by several authors [3–6]. Spectrum of electrons in a crystal with a magnetic field can display an amazing complexity including various kinds of scaling and a Cantor set structure [7–9]. However, it was shown that the Hall conductance is still an integral multiple of e^2/h as long as the Fermi energy lies in a gap.

This paper discusses topological aspects of a two-dimensional periodic systems in a magnetic field. The Hall conductance is shown to be represented by a topological invariant which is naturally an integer. This is a sequel to Ref. [3] in a spirit similar to Laughlin's arguments [10] that an exact quantization must be a consequence of a general principle which is determined by the geometrical nature of the problem.

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This subject has been first discussed by Avron, Seiler and Simon [6] using homotopy theory. More recently, Simon [11] made a connection between this topological invariant and Berry's geometrical phase factor in the quantum adiabatic theorem [12]. The purpose of the present paper is to illustrate and explain the topological invariant of Thouless *et al.* and Avron *et al.* in a rather simple physical picture.

In Section II, some relevant features of Bloch electrons in a magnetic field are reviewed. The implications of the topological features for wavefunctions are discussed. In Section III, the linear response (Nakano–Kubo) formula for the Hall conductance is introduced. It is shown that a contribution of a single filled band to σ_{xy} is given by an integer associated with a topological invariant. In Section IV, the problem is further analyzed by the theory of fiber bundles. It is shown that the quantized Hall conductance is related to the first Chern number which characterizes a principal $U(1)$ bundle.

II. Bloch Electrons in a Uniform Magnetic Field

The Schrödinger equation for a 2–D non-interacting electron system in a uniform magnetic field perpendicular to the plane is written as

$$H\Psi = \left[\frac{1}{2m}(\mathbf{p}+e\mathbf{A}))^2 + U(x,y)\right]\Psi = E\Psi, \tag{2.1}$$

where the momentum $\mathbf{p} = -i\hbar\nabla$ and the gauge potential $\mathbf{A}$ are in the x–y plane. We consider the case where $U(x, y)$ is periodic in both the x- and y-directions, i.e.,

$$U(x+a, y) = U(x, y+b) = U(x, y). \tag{2.2}$$

The system is invariant under a translation by a along the x-direction or a translation by b along the y-direction. However, the Hamiltonian is not invariant under these translations. The reason for this is that the gauge potential $\mathbf{A}$ is not constant in spite of the fact that the magnetic field is uniform. An appropriate gauge transformation is required to make the Hamiltonian invariant. Let us introduce some formalism in order to better describe the point discussed above and also to clarify the topological aspects of the problem. Let $\mathbf{R}$ be a Bravais lattice vector, i.e.,

$$\mathbf{R} = n\mathbf{a} + m\mathbf{b},$$

where n and m are integers. For each Bravais lattice vector $\mathbf{R}$ we define a translation operator T_R which, when operating on any smooth function $f(\mathbf{r})$, shifts the argument by $\mathbf{R}$:

$$T_R f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R}). \tag{2.3}$$

This operator is explicitly written as

$$T_R = \exp\{(i/\hbar)\,\mathbf{R}\cdot\mathbf{p}\}. \tag{2.4}$$

If T_R is applied to the Hamiltonian (2.1), the potential $U(\mathbf{r})$ is left invariant. However, the gauge potential is transformed to $\mathbf{A}(\mathbf{r}+\mathbf{R})$ which is not generally equal to $\mathbf{A}(\mathbf{r})$. Instead, $\mathbf{A}(\mathbf{r})$ and $\mathbf{A}(\mathbf{r}+\mathbf{R})$ differ by a gradient of a scalar function since the magnetic field is uniform:

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}(\mathbf{r}+\mathbf{R}) + \nabla g(\mathbf{r}). \tag{2.5}$$

Let us consider the magnetic translation operators [13–15]

$$\begin{aligned}\hat{T}_R &= \exp\{(i/\hbar)\,\mathbf{R}\cdot[\mathbf{p}+e(\mathbf{r}\times\mathbf{B})/2]\}\\ &= T_R \exp\{(ie/\hbar)(\mathbf{B}\times\boldsymbol{R})\cdot\mathbf{r}/2\}.\end{aligned} \tag{2.6}$$

If the symmetric gauge $\mathbf{A} = (\mathbf{B}\times\mathbf{r})/2$ is taken, $\hat{T}_R$ leaves the Hamiltonian invariant, i.e.,

$$[\hat{T}_R, H] = 0.$$

Now, we look for eigenstates which simultaneously diagonalize $\hat{T}_R$ and H. However, note that the magnetic translations do not commute with each other in general since

$$\hat{T}_a\hat{T}_b = \exp(2\pi i\phi)\,\hat{T}_b\hat{T}_a, \tag{2.7}$$

where $\phi = (eB/h)\,ab$ is a number of magnetic flux in the unit cell. When ϕ is a rational number, $\phi = p/q$ (p and q are integers which are relatively prime), we have a subset of translations which commute with each other. We take an enlarged unit cell (magnetic unit cell) which an integral multiple of magnetic flux goes through. For example, if the Bravais latice vectors of the form

$$\mathbf{R}' = n(q\mathbf{a}) + m\mathbf{b} \tag{2.8}$$

are taken, then p magnetic flux quanta are in the magnetic unit cell which is formed by the vectors $q\mathbf{a}$ and $\mathbf{b}$. The magnetic translation operators $\hat{T}_{R'}$ which correspond to these new Bravais lattice vectors commute with each other.

Let ψ be an eigenfunction which diagonalizes H and $\hat{T}_{R'}$ simultaneously, then it is easy to show that the eigenvalues of $\hat{T}_{qa}$ and $\hat{T}_b$ are given by

$$\begin{aligned}\hat{T}_{qa}\psi &= e^{ik_1qa}\psi,\\ \hat{T}_b\psi &= e^{ik_2b}\psi,\end{aligned} \tag{2.9}$$

where k_1 and k_2 are generalized crystal momenta and can be restricted in the magnetic Brillouin zone: $0 \leqslant k_1 \leqslant 2\pi/qa$, $0 \leqslant k_2 \leqslant 2\pi/b$. The eigenfunctions are

labeled by k_1 and k_2 in addition to a band index α and are written in a Bloch form as

$$\psi^{(\alpha)}_{k_1k_2}(x, y) = e^{ik_1x + ik_2y} u^{(\alpha)}_{k_1k_2}(x, y). \tag{2.10}$$

Equations (2.9) with (2.6) give the property of $u^{(\alpha)}_{k_1k_2}(x, y)$

$$\begin{aligned} u^{(\alpha)}_{k_1k_2}(x + qa, y) &= e^{-i\pi py/b} u^{(\alpha)}_{k_1k_2}(x, y), \\ u^{(\alpha)}_{k_1k_2}(x, y + b) &= e^{i\pi px/qa} u^{(\alpha)}_{k_1k_2}(x, y), \end{aligned} \tag{2.11}$$

These are the generalized Bloch conditions. Note that a gauge transformation $\mathbf{A}' = \mathbf{A} + \nabla f$ changes the phase of a wavefunction, $\psi' = e^{-ie/\hbar f}\psi$. A gauge invariant, hence meaningful quantity, is the phase change around the boundary of the magnetic unit cell. From Eq. (2.11), the phase change is given by $2\pi p$. Writing the wavefunctions as

$$u_{k_1k_2}(x, y) = |u_{k_1k_2}(x, y)| \exp[i\theta_{k_1k_2}(x, y)], \tag{2.12}$$

then one has

$$p = \frac{-1}{2\pi} \int dl \cdot \frac{\partial \theta_{k_1k_2}(x, y)}{dl}, \tag{2.13}$$

where $\int dl$ represents a counterclockwise line integral around the boundary of the magnetic unit cell. As we will see below, Eq. (2.13) is gauge-invariant although $\theta_{k_1k_2}(x, y)$ depends on a gauge. This equation represents an important topological feature of the system. Consider an arrow whose directional angles are given by the phase $\theta_{k_1k_2}(x, y)$ of the wavefunction. The arrow rotates p times as we go around the boundary. This gives a topological constraint to the wavefunction. Consider a zero of the wavefunction. If we go around clockwise a small circle which contains the zero, the corresponding arrow rotates once either clockwise or counterclockwise. Therefore we can regard a zero of a wavefunction as a vortex which has a vorticity either 1 or -1 corresponding to clockwise or counterclockwise rotation of the arrow, respectively. Cases where we have a multiple rotation are considered to be special ones of having several vortices at the same point. The magnetic field forces a wavefunction to have $-p$ vorticity in the magnetic unit cell. This is a topological constraint because the total vorticity in the magnetic unit cell is independent of a particular potential chosen.

III. Linear Response Formula for the Hall Conductance

It is useful to write the Schrödinger equation (2.1) in a form

$$\hat{H}(k_1, k_2)\, u^{\alpha}_{k_1k_2} = E^{\alpha} u^{\alpha}_{k_1k_2}, \tag{3.1}$$

with

$$\hat{H}(k_1, k_2) = \frac{1}{2m}(-i\hbar\nabla + \hbar\mathbf{k} + e\mathbf{A})^2 + U(x, y), \tag{3.2}$$

where $\mathbf{k}$ is a vector whose x- and y-components are k_1 and k_2, respectively. Note that the eigenvalue E^α depends on $\mathbf{k}$ continuously. For a fixed band index α, a set of possible values of E^α with $\mathbf{k}$ varying in the magnetic Brillouin zone forms a band (magnetic subband).

When a small electric field is applied, a resulting current may be given by the linear response (Nakano–Kubo) formula. A linear response of current in the perpendicular direction to the applied electric field is represented by the Hall conductance

$$\sigma_{xy} = \frac{e^2\hbar}{i} \sum_{E^\alpha < E_F < E^\beta} \frac{(v_y)_{\alpha\beta}(v_x)_{\beta\alpha} - (v_x)_{\alpha\beta}(v_y)_{\beta\alpha}}{(E^\alpha - E^\beta)^2}, \tag{3.3}$$

where E_F is a Fermi energy and the summation implies the sum over all the states below and above the Fermi energy. The indices α and β label bands. One needs $\mathbf{k}$ to specify a state in addition to the band index. The existence of the index $\mathbf{k}$ must implicitly be understood wherever the band index appears. To obtain the matrix elements of the velocity operator $\mathbf{v} = (-i\hbar\nabla + e\mathbf{A})/m$, it is sufficient to integrate over one magnetic unit cell

$$(\mathbf{v})_{\alpha\beta} = \delta_{k_1k_1'}\delta_{k_2k_2'} \int_0^{qa} dx \int_0^b dy\, u^{\alpha *}_{k_1k_2} \mathbf{v} u^\beta_{k_1k_2}, \tag{3.4}$$

where the states are normalized as $\int_0^{qa} dx \int_0^b \mathrm{d}y\, |u|^2 = 1$. In Eq. (3.3) the velocity operators can be replaced by partial derivatives of the $\mathbf{k}$-dependent Hamiltonian (3.2), since only off-diagonal matrix elements are considered

$$\begin{aligned} (v_x)_{\alpha\beta} &= \frac{1}{\hbar}\left\langle \alpha \left| \frac{\partial \hat{H}}{\partial k_1} \right| \beta \right\rangle, \\ (v_y)_{\alpha\beta} &= \frac{1}{\hbar}\left\langle \alpha \left| \frac{\partial \hat{H}}{\partial k_2} \right| \beta \right\rangle. \end{aligned} \tag{3.5}$$

Furthermore the matrix elements of the partial derivatives of $\hat{H}$ are written as

$$\begin{aligned} \left\langle \alpha \left| \frac{\partial \hat{H}}{\partial k_j} \right| \beta \right\rangle &= (E^\beta - E^\alpha)\left\langle \alpha \left| \frac{\partial u^\beta}{\partial k_j} \right\rangle \right. \\ &= -(E^\beta - E^\alpha)\left\langle \frac{\partial u^\alpha}{\partial k_j} \middle| \beta \right\rangle, \qquad j = 1 \text{ or } 2. \end{aligned} \tag{3.6}$$

From Eqs. (3.5) and (3.6), Eq. (3.3) is written as

$$\sigma_{xy}=\frac{e^2}{i\hbar}\sum_{E^\alpha<E_F<E^\beta}\left(\left\langle\frac{\partial u^\alpha}{\partial k_2}\middle|\beta\right\rangle\left\langle\beta\middle|\frac{\partial u^\alpha}{\partial k_2}\right\rangle-\left\langle\frac{\partial u^\alpha}{\partial k_1}\middle|\beta\right\rangle\left\langle\beta\middle|\frac{\partial u^\alpha}{\partial k_1}\right\rangle\right).$$

Using the identity $\sum_{E^\alpha<E_F<E^\beta}(|\alpha\rangle\langle\alpha|+|\beta\rangle\langle\beta|)=1$, we have

$$\sigma_{xy}^{(\alpha)}=\frac{e^2}{h}\frac{1}{2\pi i}\int d^2k\int d^2r\left(\frac{\partial u_{k_1k_2}^{\alpha *}}{\partial k_2}\frac{\partial u_{k_1k_2}^{\alpha}}{\partial k_1}-\frac{\partial u_{k_1k_2}^{\alpha *}}{\partial k_1}\frac{\partial u_{k_1k_2}^{\alpha}}{\partial k_2}\right), \tag{3.7}$$

where $\sigma_{xy}^{(\alpha)}$ is a contribution of the Hall conductance from a completely filled band α. Let us define a vector field in the magnetic Brillouin zone by

$$\hat{\mathbf{A}}(k_1,k_2)=\int d^2r u_{k_1k_2}^{*}\nabla_k u_{k_1k_2}=\langle u_{k_1k_2}|\,\nabla_k\,|u_{k_1k_2}\rangle, \tag{3.8}$$

where ∇_k is a vector operator whose components are $\partial/\partial k_1$ and $\partial/\partial k_2$. The band index α is omitted from the wavefunction, since we will consider only a contribution from a single band only. The contribution is written from Eqs. (3.7) and (3.8) as

$$\sigma_{xy}^{(\alpha)}=\frac{e^2}{h}\frac{1}{2\pi i}\int d^2k[\nabla_k\times\hat{\mathbf{A}}(k_1,k_2)]_3, \tag{3.9}$$

where, $[\ ]_3$ represents the third component of the vector.

The integration is over the magnetic Brillouin zone: $0\leqslant k_1\leqslant 2\pi/qa$, $0\leqslant k_2\leqslant 2\pi/b$. An important observation here is that the magnetic Brillouin zone is topologically a torus T^2 rather than a rectangular in **k**-space. The two points in **k**-space $k_1=0$ and $2\pi/qa$ (or, $k_2=0$ and $2\pi/b$) must be identified as the same point. Since a torus does not have a boundary, the application of Stokes' theorem to Eq. (3.9) would give $\sigma_{xy}^{(\alpha)}=0$ if $\hat{\mathbf{A}}(k_1,k_2)$ is uniquely defined on the entire torus T^2. A possible non-zero value of $\sigma_{xy}^{(\alpha)}$ is a consequence of a non-trivial topology of $\hat{\mathbf{A}}(k_1,k_2)$. Note that the identification of the magnetic Brillouin zone as a torus T^2 is essential here. Non-trivial $\hat{\mathbf{A}}(k_1,k_2)$ can only be constructed when the global topology of the base space is non-contractible.

In order to understand the topology of $\hat{\mathbf{A}}(k_1,k_2)$, let us first discuss a "gauge transformation" of a special kind. Suppose $u_{k_1k_2}(x,y)$ satisfies the Schrödinger equation (3.1), then so does $u_{k_1k_2}(x,y)\,e^{if(k_1,k_2)}$, where $f(k_1,k_2)$ is an arbitrary smooth function of k_1 and k_2 and is independent of x and y.

This introduces a transformation

$$u'_{k_1k_2}(x,y)=u_{k_1k_2}(x,y)\exp[if(k_1,k_2)]. \tag{3.10}$$

Since this is a change of the overall phase of the wavefunction, any physical quan-

tity remains invariant under this transformation. From Eq. (3.8) the corresponding transformation of $\hat{\mathbf{A}}(k_1, k_2)$ is given by

$$\hat{\mathbf{A}}'(k_1, k_2) = \hat{\mathbf{A}}(k_1, k_2) + i\nabla_k f(k_1, k_2). \tag{3.11}$$

It is easy to see from Eqs. (3.9) and (3.11) that $\sigma_{xy}^{(\alpha)}$ is invariant under the transformation (3.10).

The non-trivial topology arises when the phase of the wavefunction cannot be determined uniquely and smoothly in the entire magnetic Brillouin zone. The transformation (3.10) implies that the overall phase factor for each state vector $|u_{k_1k_2}\rangle$ can be chosen arbitrary. This phase can be determined, for example, by demanding that a component of the state vector $u_{k_1k_2}(x^{(0)}, y^{(0)}) = \langle x^{(0)}, y^{(0)}|u_{k_1k_2}\rangle$ is real. However, this convention is not enough to fix the phase on the entire magnetic Brillouin zone, since $u_{k_1k_2}(x^{(0)}, y^{(0)})$ vanishes for some (k_1, k_2). The existence of zeros of $u_{k_1k_2}(x, y)$ has been shown in Section II. For the sake of simplicity, consider the case where $u_{k_1k_2}(x^{(0)}, y^{(0)})$ vanishes only at one point $(k_1^{(0)}, k_2^{(0)})$ in the magnetic Brillouin zone. See Fig. 1. Divide T^2 into two pieces H_{I} and H_{II} such that H_{I} contains $(k_1^{(0)}, k_2^{(0)})$. We adopt a different convention in H_{I} so that another component of the state vector $u_{k_1k_2}(x^{(1)}, y^{(1)}) = \langle x^{(1)}, y^{(1)}|u_{k_1k_2}\rangle$ is real, where $(x^{(1)}, y^{(1)})$ and H_{I} are chosen such that $u_{k_1k_2}(x^{(1)}, y^{(1)})$ does not vanish in H_{I}. Thus the overall phase is uniquely determined on the entrie T^2. In Fig. 1, a phase of one component of the state vector $u_{k_1k_2}(x^{(0)}, y^{(0)}) = \langle x^{(0)}y^{(0)}|u_{k_1k_2}\rangle$ is schematically drawn.

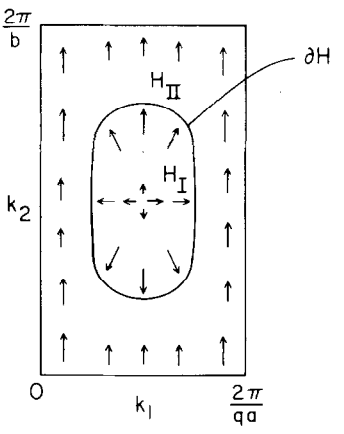

FIG. 1. Schematic diagram of a phase of a wavefunction in the magnetic Brillouin zone. The Brillouin zone is actually a torus, so the edges $(k_1, k_2) = (0, k_2)$ and $(2\pi/qa, k_2)$; and also the edges $(k_1, 0)$ and $(k_1, 2\pi/b)$ must be identified.

Note that the overall phase of the state vector is well defined at $(k_1^{(0)}, k_2^{(0)})$ even though a phase of a single component $u_{k_1k_2}(x^{(0)}, y^{(0)}) = \langle x^{(0)}, y^{(0)} | u_{k_1k_2} \rangle$ cannot be defined there. At the boundary ∂H of H_{I} and H_{II}, we have a phase mismatch

$$|u_{k_1k_2}^{\mathrm{II}}\rangle = \exp[i\chi(k_1, k_2)]\,|u_{k_1k_2}^{\mathrm{I}}\rangle, \tag{3.12}$$

where $\chi(k_1, k_2)$ is a smooth function of (k_1, k_2) on ∂H.

This non-trivial topology of $|u_{k_1k_2}\rangle$ is simply carried over to that of $\hat{\mathbf{A}}(k_1, k_2)$. Smooth vector fields $\hat{\mathbf{A}}_{\mathrm{I}}(k_1, k_2)$ and $\hat{\mathbf{A}}_{\mathrm{II}}(k_1, k_2)$ are defined on H_{I} and H_{II}, respectively, by Eq. (3.8). The phase mismatch of the state vector given by Eq. (3.12) induces the following relation between $\hat{\mathbf{A}}_{\mathrm{I}}(k_1, k_2)$ and $\hat{\mathbf{A}}_{\mathrm{II}}(k_1, k_2)$ on ∂H:

$$\hat{\mathbf{A}}_{\mathrm{II}}(k_1, k_2) = \hat{\mathbf{A}}_{\mathrm{I}}(k_1, k_2) + i\nabla_k \chi(k_1, k_2). \tag{3.13}$$

Now, in Eq. (3.9) we can apply Stokes' theorem to H_{I} and H_{II} separately

$$\begin{aligned}\sigma_{xy}^{(\alpha)} &= \frac{e^2}{h}\frac{1}{2\pi i}\left\{\int_{H_I} d^2k[\nabla_k \times \hat{\mathbf{A}}_{\mathrm{I}}(k_1, k_2)]_3 + \int_{H_{\mathrm{II}}} d^2k[\nabla_k \times \hat{\mathbf{A}}_{\mathrm{II}}(k_1 k_2)]_3\right\} \\ &= \frac{e^2}{h}\frac{1}{2\pi i}\int_{\partial H} d\mathbf{k}\cdot[\hat{\mathbf{A}}_{\mathrm{I}}(k_1, k_2) - \hat{\mathbf{A}}_{\mathrm{II}}(k_1, k_2)],\end{aligned} \tag{3.13}$$

where $\int_{\partial H} d\mathbf{k}$ represents a line integral on ∂H and the sign change occurs because ∂H has the opposite orientation for H_{I} and H_{II}. Using the relation between $\hat{\mathbf{A}}_{\mathrm{I}}$ and $\hat{\mathbf{A}}_{\mathrm{II}}$, Eq. (3.12), we find

$$\sigma_{xy}^{(\alpha)} = \frac{e^2}{h} n, \tag{3.14}$$

with

$$n = \frac{1}{2\pi}\int_{\partial H} d\mathbf{k}\cdot\nabla_k \chi(k_1, k_2). \tag{3.15}$$

n must be an integer for each of the state vectors must fit together exactly when we complete a full revolution around ∂H.

A generalization of the above argument which allows $u_{k_1k_2}(x^{(0)}, y^{(0)})$ to have more than one zero can be done using the theory of fiber bundles [16]. This will be discussed in the following section.

In Section II, it was shown that the vorticity of a wavefunction $u_{k_1k_2}(x, y)$ for a fixed (k_1, k_2) in a magnetic unit cell is given by an integer $-p$. There is a similar structure in the dual space, i.e., the magnetic Brillouin zone T^2. Consider a wavefunction $u_{k_1k_2}(x, y)$ for a fixed (x, y). This wavefunction has a number of zeros in the magnetic Brillouin zone. As in Section II, we can assign vorticities 1 or -1 to each zero by considering the phase in the neighborhood of a zero. The quantized value of $\sigma_{xy}^{(\alpha)}$ is given by the total vorticity of the wavefunction in the magnetic Brillouin zone.

IV. Fiber Bundle and Chern Class

The topological structure discussed in Section III has a close resemblance to that of the Dirac magnetic monopole bundle which is a principal $U(1)$ bundle over a sphere S^2 [16].

We have been considering the normalized eigenstate $|u_{k_1k_2}\rangle$. Since $\exp[if(k_1, k_2)]|u_{k_1k_2}\rangle$ is also a normalized eigenstate, it is natural to consider a principal $U(1)$ bundle over T^2. A torus is covered by four neighborhoods $\{H_i\}$, $i = 1,..., 4$ where each H_i is a subspace of R^2. For example, if we define four regions by

$$\begin{aligned} H'_1 &= \{(k_1, k_2)|\, 0 < k_1 < \pi/qa,\, 0 < k_2 < \pi/b\}, \\ H'_2 &= \{(k_1, k_2)|\, \pi/qa < k_1 < 2\pi/qa,\, 0 < k_2 < \pi/b\}, \\ H'_3 &= \{(k_1, k_2)|\, \pi/qa < k_1 < 2\pi/qa,\, \pi/b < k_2 < 2\pi/b\}, \\ H'_4 &= \{(k_1, k_2)|\, 0 < k_1 < \pi/qa,\, \pi/b < k_2 < 2\pi/b\}, \end{aligned} \tag{4.1}$$

then we can choose H_i $(i = 1,..., 4)$ to be slightly larger regions each of which completely includes H'_i $(i = 1,..., 4)$. A principal $U(1)$ bundle is a topological space which is locally isomorphic to $H_i \times U(1)$ in each neighborhood H_i. We consider a specific fiber whose global topology is determined by the eigenstate $|u_{k_1k_2}\rangle$. A construction of a fiber bundle is as follows: Take a component of the state vector $u_{k_1k_2}(x^{(0)}, y^{(0)}) = \langle x^{(0)}y^{(0)}|u_{k_1k_2}\rangle$ which does not vanish in the overlaps of H_i. Since H_i is contractible, it is possible to choose a phase convention such that the phase factor $\exp[i\theta^{(i)}(k_1, k_2)] = u^{(i)}_{k_1k_2}(x^{(0)}, y^{(0)})/|u^{(i)}_{k_1k_2}(x^{(0)}, y^{(0)})|$ is smooth in each neighborhood H_i except at zeros of $u_{k_1k_2}(x^{(0)}, y^{(0)})$. As exemplified in Section III, it is not possible in general to have a global phase convention which is good to all the neighborhoods. As a result, we have a transition function Φ_{ij} in the overlap between two neighborhoods, $H_i \cap H_j$:

$$\Phi_{ij} = \exp i[\theta^{(i)}(k_1k_2) - \theta^{(j)}(k_1, k_2)] = \exp[if^{(ij)}(k_1k_2)]. \tag{4.2}$$

If we regard Φ_{ij} to be a map Φ_{ij}: $U(1) \to U(1)$, a principal $U(1)$ bundle over T^2 is completely specified by this transition function.

Thus, we have constructed a nontrivial fiber bundle. Fiber bundles are classified by certain integers characterizing the transition functions. These integers also correspond to integrals involving a bundle curvature when we put connections on the bundles. We may write a connection 1-form as

$$\begin{aligned} \omega &= g^{-1}Ag + g^{-1}dg \\ &= A + id\chi, \end{aligned} \tag{4.3}$$

where $g = e^{i\chi} \in U(1)$ is a fiber. We choose a 1-form A by

$$A(k_1, k_2) = \hat{A}_\mu(k_1, k_2)\, dk_\mu = \langle u_{k_1k_2}|\, \frac{\partial}{\partial k_\mu}\, |u_{k_1k_2}\rangle\, dk_\mu. \tag{4.4}$$

The transition functions of the form (4.2) act on fibers by left multiplication. In an overlap of two neighborhoods H_i and H_j, a transition function $\Phi = \Phi_{ij}$ relates the local fiber coordinated g and g' in H_j and H_i as

$$g' = \Phi g. \tag{4.5}$$

This is equivalent to the "gauge transformation" Eq. (3.10). From Eqs. (3.11), (4.2) and (4.5), a transformation of $A(k_1, k_2)$ is given by

$$A' = \Phi A \Phi^{-1} + \Phi d\Phi^{-1} = A - i \frac{\partial f}{\partial k_\mu} dk_\mu. \tag{4.6}$$

It can be shown that ω is invariant under the transformations (4.5) and (4.6). So, ω is indeed a legitimate connection 1-form with a choice of A in Eq. (4.4).

Since a connection is given, we have a differential geometry on the topological space. The curvature is given by

$$F = dA = \frac{\partial \hat{A}_\mu}{\partial k_\nu} dk_\nu \wedge dk_\mu. \tag{4.7}$$

Since $c_1 = (i/2\pi) F$ is the first Chern form, an integral of c_1 over the entire manifold T^2,

$$C_1 = \frac{i}{2\pi} \int F = \frac{i}{2\pi} \int dA = \frac{i}{2\pi} \int \frac{\partial \hat{A}_\mu}{\partial k_\nu} dk_\nu \wedge dk_\mu, \tag{4.8}$$

is the first Chern number. This number is an integer which is independent of a particular connection chosen. It is only given by the topology of the principal $U(1)$ bundle which is constructed from the state vector $|u_{k_1 k_2}\rangle$.

A comparison of Eqs. (3.9) and (4.8) gives

$$\sigma_{xy}^{(\alpha)} = -\frac{e^2}{h} C_1, \tag{4.9}$$

i.e., a contribution to the Hall conductance from a single filled band in unit of e^2/h is given by minus the first Chern number.

V. Concluding Remarks

The methods of differential geometry have been essential in modern gauge theory as well as in Einstein's theory of gravity. Maxwell's electromagnetism is nothing but an Abelian gauge theory. The differential geometry in the real physical space is given by a gauge potential.

In the present problem of two dimensional periodic potentials with a uniform magnetic field, we have a differential geometry on the reciprocal k-space (magnetic

Brillouin zone) which is a torus T^2. A connection is given by $\hat{\mathbf{A}}(k_1, k_2)$ (see Eqs. (3.8) and (4.3)). The phase factor of the state vector in the magnetic Brillouin zone is a section of a principal $U(1)$ bundle. The first Chern number characterizing this fiber bundle is an integer and is given by a certain integral involving $\hat{\mathbf{A}}(k_1, k_2)$. It is remarkable that this integral can be identified as the linear response formula for $\sigma_{xy}^{(\alpha)}$: a contribution to the Hall conductance from a single band. There is no higher order Chern number associated with the $U(1)$ bundle since the base space is two dimensional. Therefore $\alpha_{xy}^{(\alpha)}$ is the only quantized quantity of this kind.

The quantized value of $\alpha_{xy}^{(\alpha)}$ is related to zeros of wavefunction in the magnetic Brillouin zone. An integer vorticity can be assigned to each of the zeros from a local structure around it. The total vorticity in the magnetic Brillouin zone gives $\alpha_{xy}^{(\alpha)}$. Therefore if the topological structures of wavefunctions are known, we do not have to perform the four dimensional integration in Eq. (3.7) to calculate $\alpha_{xy}^{(\alpha)}$.

When $\sigma_{xy}^{(\alpha)}$ takes a non-zero value, wavefunctions have a non-trivial topological structure in the magnetic Brillouin zone. This means that a phase of wavefunctions cannot be determined globally. We need several different phase conventions to cover the entire magnetic Brillouin zone.

The topological nature of the formula for $\alpha_{xy}^{(\alpha)}$ implies that it will be unchanged when the potential is varied in a way that the band α remains non-degenerate. This gives a convenient calculational method since we can take the most convenient form of a potential to obtain $\alpha_{xy}^{(\alpha)}$ [3].

In case two bands touch each other while a potential is varied, we can still expect that the sum of the Hall conductances remains unchanged. However, each conductance may not be conserved when the bands split again. This has been proved by Avron *et al.* [6].

The linear response (Nakano–Kubo) formula for the Hall conductance has played a crucial role in relating an abstract mathematical quantity (the Chern number) to the quantity of physical interests. There are serious foundational questions regarding this formula [17]. The physical system we have considered is dissipationless. There is no longitudinal current [18] when the Fermi energy lies in a gap. In this case, it is possible to have an alternative derivation of the formula which is free from the criticisms of van Kampen and others.

The topological aspects of the quantized Hall effect in periodic potentials have been discussed. It will be of great interest to generalize the above arguments to more realistic models of the experimental systems which should include the effects of disorder and/or electron–electron interactions.

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