Chern Number and Edge States in the Integer Quantum Hall Effect

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We consider the integer quantum Hall effect on a square lattice in a uniform rational magnetic field. The relation between two different interpretations of the Hall conductance as topological invariants is clarified. One is the Thouless–Kohmoto–Nightingale–den Nijs (TKNN) integer in the infinite system and the other is a winding number of the edge state. In the TKNN form of the Hall conductance, a phase of the Bloch wave function defines U(1) vortices on the magnetic Brillouin zone and the total vorticity gives σ_{xy}. We find that these vortices are given by the edge states when they are degenerate with the bulk states.

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After the discovery of the integral quantum Hall effect, the problem of electrons in a magnetic field has been studied from a geometrical point of view [1–8]. The gauge invariance discussed by Laughlin [3] as well as the role of the edge states emphasized by Halperin [1] are central to these investigations. The Hall conductance σ_{xy} of the system has a fundamental topological meaning as first discovered by Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) [2,4,5]. Their work is performed in a system without edges and σ_{xy} is expressed as an integral that represents the Chern number of the U(1) bundle over the magnetic Brillouin zone. This is an invariant on the magnetic Brillouin zone and supports the high accuracy in the quantization of the Hall conductance. However, the topological role of the edge state is unclear since the TKNN integers are written in terms of the bulk wave functions.

Recently the Hall conductance in a system with edges has been treated from a topological point of view [6]. In the work, σ_{xy} is written as the winding number of the edge state on a complex energy surface that is a high genus ($g \geq 1$) Riemann surface. The winding number and the TKNN integer are apparently different. In this paper, we clarify the connection between these two different numbers, i.e., elucidate the relation between the Hall conductance of the infinite system without edges and that of the system with edges.

In the Landau gauge, a tight-binding Hamiltonian for electrons on a square lattice in a uniform magnetic field is given by $H = -t\sum_{m,n}(c^\dagger_{m+1,n}c_{m,n} + c^\dagger_{m,n+1}e^{i2\pi\phi m}c_{m,n} + \text{H.c.})$, where $c_{m,n}$ is the annihilation operator for a lattice fermion at site (m,n). We assume that the magnetic field per plaquette ϕ is rational; i.e., $\phi = p/q$ with mutually prime integers p and q. First we consider an infinite system [2,7]. Since the system is periodic in y direction, the single particle wave function $\Psi_{m,n}$ is written as $\Psi_{m,n} = e^{ik_yn}\Psi_m(k_y)$, $k_y \in [0,2\pi]$. The Schrödinger equation then reduces to a one-dimensional equation with a parameter k_y as

$$-t\{\Psi_{m+1}(k_y) + \Psi_{m-1}(k_y)\} - 2t\cos(k_y - 2\pi\phi m)\Psi_m(k_y) = E(k_y)\Psi_m(k_y). \quad (1)$$

This one-dimensional system has a period q. Therefore the Bloch theorem tells that the Bloch function Ψ_m satisfies $\Psi_m(k_x,k_y) = e^{ik_xm}\tilde{u}_m(k_x,k_y)$ where $\tilde{u}_{m+q}(\mathbf{k}) = \tilde{u}_m(\mathbf{k})$ and $k_x \in [0,2\pi/q]$.

The spectrum of H has been investigated extensively and it consists of q energy bands [2,7,8]. The Hall conductance σ_{xy} of the filled jth band ($j = 1,\ldots,q$) is calculated using the Kubo formula and an adiabatic approximation as [2,4,7]

$$\sigma_{xy}^{j,\text{bulk}} = -\frac{e^2}{h}\frac{1}{2\pi i}\int\int_{T^2_{\text{MBZ}}} dk_x dk_y\ [\ \nabla_k \times \mathbf{A}^j_u(\mathbf{k})\ ]_z, \quad (2)$$

where $\mathbf{A}^j_u(\mathbf{k}) = \langle u^j(\mathbf{k})|\nabla_k|u^j(\mathbf{k})\rangle = \sum_{i=1}^q u^{j\,*}_m(\mathbf{k})\nabla_k u^j_m(\mathbf{k})$ and u^j_m is obtained from $\tilde{u}^j_m$ by normalizing as $\langle u^j(\mathbf{k})|u^j(\mathbf{k})\rangle = 1$. When the Fermi energy lies in the jth gap, the Hall conductance of the system is given by $\sum_{l=1}^j \sigma^l_{xy}$. The wave function $|u^j(\mathbf{k})\rangle$ forms a U(1) fiber bundle on the magnetic Brillouin zone and the integral Eq. (2) is the Chern number which is a topological invariant of the U(1) bundle. This gives a topological meaning to the Hall conductance in the infinite system (without edges). In Eq. (2), there is a gauge freedom which comes from the *phase ambiguity* of $|u(\mathbf{k})\rangle$. One can use another gauge to calculate σ^j_{xy} by the gauge transformation, $|v^j(\mathbf{k})\rangle = e^{if(\mathbf{k})}|u^j(\mathbf{k})\rangle$ (f: real). Since the Chern number is invariant under this gauge transformation, σ_{xy} is well defined. If one uses the Stokes theorem in Eq. (2), σ_{xy} is always zero since there is no boundary in the magnetic Brillouin zone T^2_{MBZ}. However, this procedure is incorrect. The phase of the wave function is not well defined globally over the magnetic Brillouin zone. Therefore one can not apply the Stokes theorem globally.

Following Ref. [4], we divide T^2_{MBZ} into several regions. We require that $\Psi^j_m(\mathbf{k})$ is an analytical function of k_x and

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k_y on the magnetic Brillouin zone and choose $\Psi_1^j = 1$, i.e., $\tilde{u}_1^j = e^{-ik_x}$. By using a geometry with edges, we give below an explicit construction for $\Psi_m^j(\mathbf{k})$ that satisfies these requirements. This convention is not compatible with the periodicity of the magnetic Brillouin zone. However, we avoid this difficulty in the following by using the freedom of the gauge transformation.

We denote the zero points of the $\Psi_q^j(\mathbf{k})$ in the magnetic Brillouin zone by $\mathbf{k} = \mathbf{k}_1^*, \ldots, \mathbf{k}_{N_j}^*$. At these points, $u_q(\mathbf{k}) = 0$ also. Then we divide the whole magnetic Brillouin zone $T^2_{\rm MBZ}$ into $N_j + 1$ parts as follows:

$$R_s^\epsilon = \{ \mathbf{k} \in T^2_{\rm MBZ} \big| \; |\mathbf{k} - \mathbf{k}_s^*| < \epsilon, \; \Psi_q^j(\mathbf{k}_s^*) = 0 \}, \tag{3}$$

$$R_0 = T^2_{\rm MBZ} \Big\backslash \bigcup_{s=1}^{N_j} R_s^\epsilon, \tag{4}$$

where $s = 1, \ldots, N_j$ and $\epsilon \ll 1$. In the local regions R_s^ϵ, we use a phase convention for $|U^j(\mathbf{k})\rangle$ to calculate $\mathbf{A}_U(\mathbf{k})$ as $U_m^j(\mathbf{k}) = u_m^j(\mathbf{k})$. In the region R_0, we use another phase convention for $|V(\mathbf{k})\rangle$ to calculate $\mathbf{A}_V(\mathbf{k})$ as $V_q(\mathbf{k})$ is real and positive. This convention in R_0 is compatible with the periodicity of the magnetic Brillouin zone, provided we choose $V_m^j(\mathbf{k}) = u_m^j(\mathbf{k}) e^{-i\xi(\mathbf{k})}$, where $\xi(\mathbf{k}) = \Im \ln u_q^j(\mathbf{k}) = \Im \ln \tilde{u}_q^j(\mathbf{k})$. This is well defined since $\Psi_q^j(\mathbf{k}) = e^{iqk_x} \tilde{u}_q(\mathbf{k}) \neq 0$ in R_0. Then using the Stokes theorem in each region, we get from Eq. (2)

$$\begin{aligned} \sigma_{xy}^{j,\rm bulk} &= -\sum_{s=1}^{N_j} \frac{1}{2\pi i} \oint_{\partial R_s} d\mathbf{k} \cdot [\mathbf{A}_U^j(\mathbf{k}) - \mathbf{A}_V^j(\mathbf{k})] \\ &= -\sum_{s=1}^{N_j} \frac{1}{2\pi} \oint_{\partial R_s} d\mathbf{k} \cdot \nabla \xi(\mathbf{k}) \\ &= -\sum_{s=1}^{N_j} \frac{1}{2\pi} \oint_{\partial R_s} d\mathbf{k} \cdot \nabla \Im \ln \Psi_q(\mathbf{k}), \end{aligned} \tag{5}$$

where we use $\oint_{\partial R_s} d\mathbf{k} \cdot \nabla \Im \ln e^{iqk_x} = 0$ in the last line. Since the zero of the wave function at $\mathbf{k} = \mathbf{k}_s^*$ gives a vortexlike structure, σ_{xy}^j is obtained as the sum of the vorticity in the magnetic Brillouin zone [4].

Now let us consider a system in a strip geometry with edges; i.e., the system size is infinite in y direction and finite in x direction [6]. We apply the method of transfer matrix and use results from the nonlinear lattice theory [6,9]. Here we only state the results of Ref. [6] relevant to our purpose. The boundary condition for the strip geometry is

$$\Psi_0^{(e)}(k_y) = \Psi_{L_x}^{(e)}(k_y) = 0. \tag{6}$$

We assume that L_x is commensurate to the flux ϕ; that is, $L_x = ql$ with some integer l. Mathematically the difference between systems with and without edges corresponds to the difference in the boundary condition. For the system without edges, the condition follows the Bloch theorem as

$$\Psi_{m+q}^{(b)}(k_y) = \rho \Psi_m^{(b)}(k_y), \;\; \rho = e^{iqk_x} \;\; (k_x \in [\,0, 2\pi/q\,]). \tag{7}$$

Now let us write Eq. (1) using the transfer matrix as

$$\begin{pmatrix} \Psi_{m+1}(\epsilon, k_y) \\ \Psi_m(\epsilon, k_y) \end{pmatrix} = \tilde{M}_m(\epsilon, k_y) \begin{pmatrix} \Psi_m(\epsilon, k_y) \\ \Psi_{m-1}(\epsilon, k_y) \end{pmatrix}, \tag{8}$$

$$\tilde{M}_m(\epsilon, k_y) = \begin{pmatrix} -\epsilon - 2\cos(k_y - 2\pi\phi m) & -1 \\ 1 & 0 \end{pmatrix}, \tag{9}$$

where $\epsilon = E/t$ is a dimensionless energy. In this formulation, all solutions are obtained by different choices of initial conditions, Ψ_0 and Ψ_1. For the boundary condition in the strip geometry, Eq. (6), we use the condition $\Psi_0^{(e)} = 0$ and $\Psi_1^{(e)} = 1$. Then the roots of the equation $\Psi_{L_x}^{(e)} = [M(\epsilon)]_{21}^l = 0$ correspond to the energy eigenvalues of the system where $M(\epsilon) = \tilde{M}(\epsilon)_q \tilde{M}(\epsilon)_{q-1} \cdots \tilde{M}(\epsilon)_2 \tilde{M}(\epsilon)_1$.

The energy eigenvalues of the strip system are classified into two classes: (i) the spectrum of the edge states which is independent of the system size L_x; (ii) the complementary point spectrum that converges into energy bands in the limit $L_x \to \infty$. There are q energy bands and each energy gap has one edge state; i.e., there are $g = q - 1$ edge states. The energy of the edge state μ_j ($j = 1, \ldots, g$) is determined by a q site problem [6],

$$M_{21}(\mu_j) = \Psi_q^{(e)}(\mu_j) = 0. \tag{10}$$

On the other hand, the Bloch function (without edges) satisfies Eq. (7). Therefore Ψ_1 and Ψ_0 form an eigenvector of M with the eigenvalue ρ as

$$M(\epsilon) \begin{pmatrix} \Psi_1^{(b)} \\ \Psi_0^{(b)} \end{pmatrix} = \begin{pmatrix} \Psi_{q+1}^{(b)}(\epsilon) \\ \Psi_q^{(b)}(\epsilon) \end{pmatrix} = \rho(\epsilon) \begin{pmatrix} \Psi_1^{(b)} \\ \Psi_0^{(b)} \end{pmatrix}. \tag{11}$$

In Eq. (11), the energy ϵ represents a real variable and we can analytically continue ϵ to a complex energy z in order to discuss a wave function of the edge state.

We get from Eq. (11)

$$\rho(z) = \tfrac{1}{2}[\Delta(z) - \sqrt{\Delta(z)^2 - 4}], \tag{12}$$

$$\Psi_q^{(b)}(z) = -\frac{\rho M_{21}(z)}{M_{22} - \rho} = \frac{1}{M_{12}}(\rho^2 - \rho M_{11}), \tag{13}$$

where $\Delta(z) = {\rm Tr} M(z)$ and we impose an initial condition $\Psi_1^{(b)} = 1$ which is compatible with the above requirements. Since the analytic structure of the wave function is determined by the function $\omega = \sqrt{\Delta(z)^2 - 4}$, let us discuss the Riemann surface of a hyperelliptic curve $\omega^2 = \Delta(z)^2 - 4$. To make the analytic structure of $\omega = \sqrt{\Delta(z)^2 - 4}$ unique, we have to specify the branch cuts which are given by $\Delta(z)^2 - 4 \leq 0$ at $\Im z = 0$. Since this condition also gives the condition for $|\rho| = 1$, the branch cuts are given by the q energy bands (see Fig. 1). Therefore $\Delta(z)^2 - 4$ can be factorized as

$$\begin{aligned} \omega &= \sqrt{\Delta(z)^2 - 4} \\ &= \sqrt{(z - \lambda_1)(z - \lambda_2) \cdots (z - \lambda_{2q-1})(z - \lambda_{2q})}, \end{aligned}$$

where λ_j, $j = 1, \ldots, 2q$ denote energies of the band edges.

Also we need two sheets (Riemann spheres R^+ and R^-)

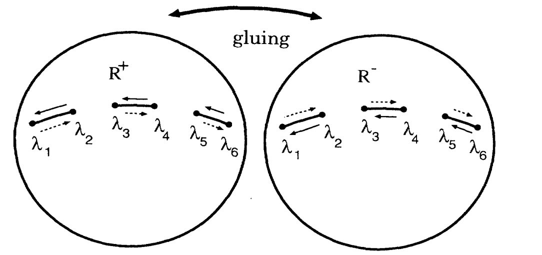

FIG. 1. Two sheets (Riemann spheres) with $q = g + 1$ cuts which correspond to the energy bands of the system.

to define the Riemann surface. (The Riemann spheres are obtained by compactifying the $|z| = \infty$ points to one point.) Finally, the Riemann surface is obtained by gluing the two Riemann spheres at these q branch cuts along the arrows in Fig. 1. After the gluing operation, the surface is topologically equivalent to the surface shown in Fig. 2. The genus of the Riemann surface is $g = q - 1$ which is the number of energy gaps. In this way, the wave function is defined on the genus g $(= q - 1)$ Riemann surface. The branch of the function is specified as $\sqrt{\Delta(z)^2 - 4} > 0$ ($z \to -\infty$ on the real axis of R^+). By this construction, it becomes clear that the complex energy surface of the one-dimensional system Eq. (1) is a genus $g = q - 1$ Riemann surface $\Sigma_g(k_y)$ for each k_y.

On the surface, the energy gaps correspond to circles around the holes of the $\Sigma_g(k_y)$ and the energy bands correspond to closed paths on $\Sigma_g(k_y)$ (see Fig. 2). The Bloch function is defined on this surface. $\Psi_q^{(b)}$ has always g zero points at μ_j $[\Psi_q^{(b)}(\mu_j) = 0]$. Since there are two real axes on the Σ_g, there are two μ_j's on the surface. However, only one of the two gives a zero of $\Psi_q^{(b)}$.

Changing k_y from 0 to 2π, we can consider a family of $\Sigma_g(k_y)$. $\Sigma_g(k_y)$ can be modified by this change yet all the $\Sigma_g(k_y)$ with different k_y's are topologically equivalent if there are stable energy gaps in the two-dimensional spectrum. By identifying the topologically equivalent $\Sigma_g(k_y)$, we can observe that the $\mu_j(k_y)$ moves around the holes and forms an oriented loop $C(\mu_j)$.

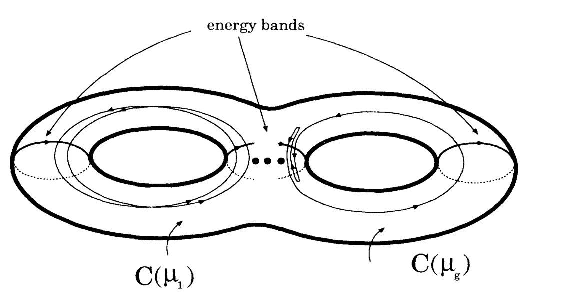

FIG. 2. Riemann surface of the Bloch function under the rational flux $\phi = p/q$. The number of the gaps, g, is the genus of the Riemann surface. $C(\mu_j)$ is a loop formed by the trace of the zero point of $\Psi_q(z)$. The energy bands are also shown by closed loops.

The winding number of the loop around the jth hole $I(C(\mu_j))$ is a well defined topological quantity. When the Fermi energy of the two-dimensional system lies in the jth energy gap, the Hall conductance is obtained by this winding number as [6]

$$\sigma_{xy}^{\rm edge} = \sum_{l=1}^{j} \sigma_{xy}^{l,{\rm edge}} = -\frac{e^2}{h} I(C(\mu_j)). \quad (14)$$

This is a second interpretation of the Hall conductance as a topological number.

Further we can determine the behavior of the edge state and the loop $C(\mu_j)$ by investigating M_{11}. When $|M_{11}(\mu_j)| < 1$, the edge state is localized at the left edge and $\Psi_q(\mu_j) = 0$ on R^+ and when $|M_{11}(\mu_j)| > 1$, they are localized at the right edge and $\Psi_q(\mu_j) = 0$ on R^-. Using this relation we can follow the movement of μ_j and assign the Hall conductance from the numerical calculation. Here we show an example in Fig. 3. From the figure and using Eq. (14), we can determine σ_{xy}.

Now we calculate the Hall conductance in Eq. (5) by using the explicit wave function Eq. (13). When we restrict the complex energy to the (real) energy bands, we obtain the Bloch function for the jth band $\Psi_q^j(\epsilon, k_y)$ on the magnetic Brillouin zone. The energy ϵ lies on the q circles S_j^1, $j = 1, \ldots, q$ which are explicitly defined on $\Sigma_q(k_y)$ (see Fig. 2). These circles are parametrized by k_x through $\rho = e^{iqk_x}$. Using a relation $-2i\sin(qk_x) = \sqrt{\Delta^2 - 4}$ and considering the branch convention for $\sqrt{\Delta^2 - 4}$, we can get an explicit parametrization of the circles $S_j^1(k_x)$. k_y also lies on the circle $S^1(k_y)$ and the product $S_j^1(k_x) \times S^1(k_y)$ is the magnetic Brillouin zone for each energy band j. The Bloch function $\Psi_q^j(\epsilon, k_y)$ is analytical in ϵ and k_y and ϵ is analytical in k_x and k_y. Therefore $\Psi_q^j(k_x, k_y)$ is also an analytical function of both k_x and k_y and $\Psi_1^j = 1$. This Bloch function satisfies the requirements discussed earlier to calculate σ_{xy}.

Moreover one can see that the zeros of the Bloch function $\Psi_q^j(k_x, k_y)$ are given by the zeros of M_{21} since ρ is always nonzero on the magnetic Brillouin zone and M_{12} is a polynomial in the energy variable. The zero of $M_{21}(\epsilon)$ is given by the energy of the edge state and always lies in energy gaps or at band edges. Therefore the zeros of $\Psi_q^{(b)}(k_x, k_y)$ are given by the points where the edge state is degenerate with the bulk state at the band edges (see Fig. 3).

Near the degenerate point $\mathbf{k} = (k_x^*, k_y^*)$, we expand the Ψ_q^j up to linear order in $\delta k_x = k_x - k_x^*$ and $\delta k_y = k_y - k_y^*$ to calculate σ_{xy}. For example, consider the contribution from the jth energy band (j: odd) and focus on the degenerate point at the band top A as shown in Fig. 4. Near A, μ_j moves from the upper Riemann surface R^+ to the lower Riemann surface R^-. In the jth energy gap for j: odd, one can show that $M_{11}(\mu_j(k_y)) < 0$ and $k_x^* = \pi/q$ [6]. Therefore we obtain $-1 < M_{11}(\mu_j(k_y))$ when $k_y < k_y^*$ (on the solid line in the gap), $M_{11}(\mu_j(k_y^*)) = -1$

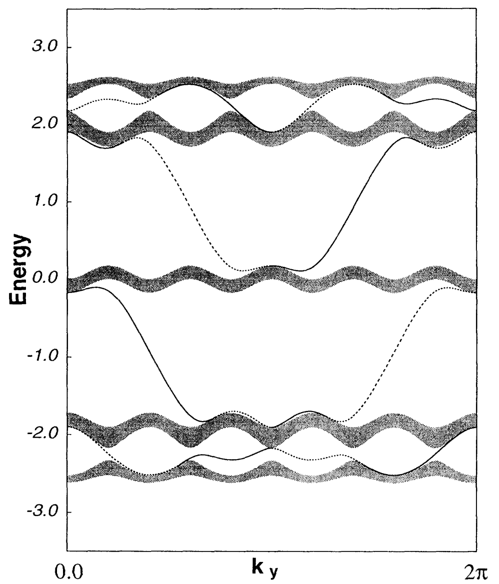

FIG. 3. Asymptotic energy spectrum of the two-dimensional tight-binding electrons with edges under the rational flux $\phi = p/q$. The number of sites along the x direction is $L_x - 1 \approx \infty$. The shaded areas are the energy bands and the lines are the spectrum of the edge states. The solid line means the energy of the edge state is on R^+ and the dotted line means it is on R^-. The numerical result is for the $\phi = 2/5$ case ($t = 1$) and the corresponding winding numbers are as follows: $I(C(\mu_1)) = -2$, $I(C(\mu_2)) = 1$, $I(C(\mu_3)) = -1$, and $I(C(\mu_4)) = 2$.

and $M_{11}(\mu_j(k_y)) < -1$ when $k_y^* < k_y$ (on the dotted line) (see Figs. 3 and 4).

Near the band edge $k_x^* = \pi/q$, the energy deviation in δk_x is proportional to $(\delta k_x)^2$. Therefore $M_{11} \approx -1 - C\delta k_y$, $C > 0$ and $\rho \approx -1 - iq\delta k_x$ up to linear in δk_x and δk_y. Then from Eq. (13), $\Psi_q^j(k_x, k_y)$ is given as $\Psi_q^j(k_x, k_y) \approx C'(-C\delta k_y + iq\delta k_x)$. From the expression, we obtain $(1/2\pi) \oint_A d\mathbf{k} \cdot \nabla \Im \ln \Psi_q = +1$. When μ_j moves from the lower Riemann surface R^- to the upper Riemann surface R^+, the vorticity is -1. On the other hand, when the degeneracy is at the band bottom (point B in Fig. 4), one can obtain similarly $(1/2\pi) \oint_B d\mathbf{k} \cdot \nabla \Im \ln \Psi_q = -1$. Near B, μ_j moves from R^- to R^+. When μ_j moves from R^+ to R^-, it gives $+1$. This consideration is for the odd j case and a similar approach is also applied to the even j case.

In this way, we can derive a formula for the general case. The sum of the vorticities at the band top is written as $I(C_j)$ by using the winding number of the edge state and that at the band bottom is $-I(C_{j-1})$. Therefore the Hall conductance of the filled jth band is

$$\sigma_{xy}^{j,\mathrm{bulk}} = -\frac{e^2}{h}[\, I(C_j) - I(C_{j-1})\,] = \sigma_{xy}^{j,\mathrm{edge}}, \qquad (15)$$

because $I(C_0) = 0$.

This expression shows the relation between the TKNN number for the bulk state and the winding number of the edge state. It clarifies the relation between the two interpretations of the Hall conductance with and without edges. Nontrivial contribution to the Hall conductance in the TKNN formula comes from the degeneracy of the edge states with the bulk state. We establish a direct connection between the Hall conductance in the bulk system and that due to the edge states.

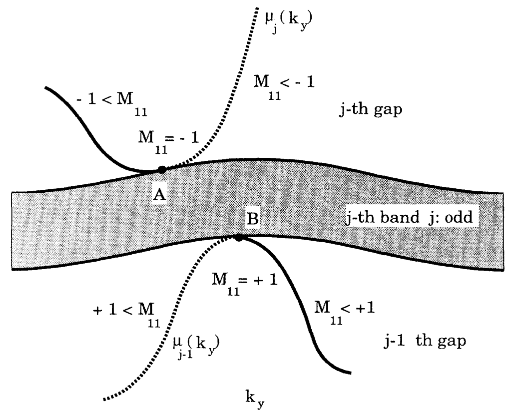

FIG. 4. A typical example for the degeneracy of the edge state with the bulk state.

Even in the case with a weak disorder, the quantization of the Hall conductance due to the edge states is stable since they are chiral. When ϕ is not commensurate, we cannot use the analytic analysis directly. However, the physics behind it is the same as discussed in Ref. [6]. When ϕ is irrational, we have to consider a sequence of the fluxes converging to the irrational flux and, correspondingly, a sequence of the Riemann surfaces.

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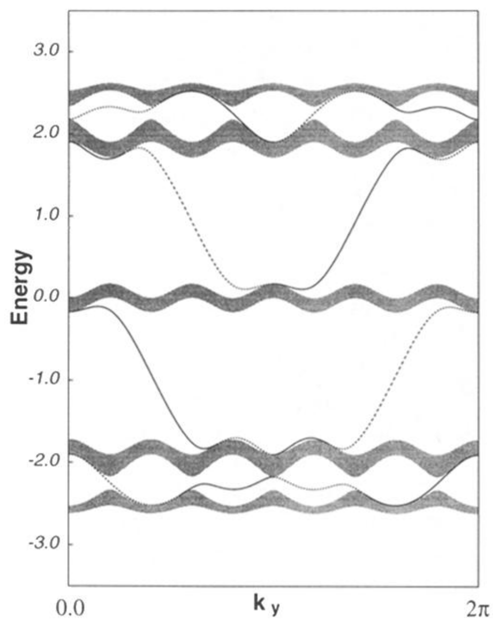

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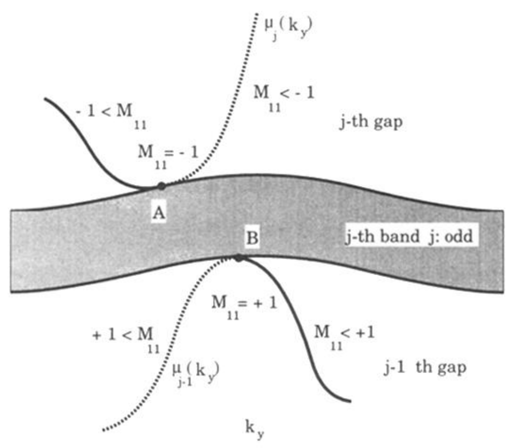

FIG. 4. A typical example for the degeneracy of the edge state with the bulk state.