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Topological Description of (Spin) Hall Conductances on Brillouin Zone Lattices: Quantum Phase Transitions and Topological Changes

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Abstract

It is widely accepted that topological quantities are useful to describe quantum liquids in low dimensions. The (spin) Hall conductances are typical examples. They are expressed by the Chern numbers, which are topological invariants given by the Berry connections of the ground states. We present a topological description for the (spin) Hall conductances on a discretized Brillouin Zone. At the same time, it is quite efficient in practical numerical calculations for concrete models. We demonstrate its validity in a model with quantum phase transitions. Topological changes supplemented with the transition is also described in the present lattice formulation.

Key words: Chern Number, Berry Connection, Hall Conductance, Lattice Gauge Theory

1. Introduction

Topological quantities are fundamental to describe low dimensional quantum liquids where standard symmetry breaking do not have a primal importance [1,2]. Typical examples are quantum Hall liquids [3,4,5] and anisotropic superconductors with time-reversal symmetry breaking [6,7]. Recently spin Hall conductance for semiconductors are also attracting much current interest [6,7,8,9,10]. The (spin) Hall conductance has a characteristic geometrical meaning [3,5]. In some physical units, they are given by the first Chern number of the Berry connection [4].

In practical numerical calculations, we diagonalize Hamiltonians on a set of discrete points on the Brillouin zone (BZ). It is thus crucial to develop an efficient method of revealing the topological property of infinite systems with continuum BZ from corresponding finite systems with discrete BZ. We propose an efficient method for the calculation of the Chern numbers on a discretized BZ based on a geometrical formulation of topological charges in lattice gauge theory [11,12,13]. The Chern numbers thus obtained are *manifestly gauge-invariant* and *integer-valued* even for a discretized BZ. One can compute the Chern numbers using wave functions in *any gauge* or *without specifying gauge fixing-conditions*. Details of the formulation and the basic results were published elsewhere [14].

2. Topological Description of (Spin) Hall conductances

Chern Numbers as (Spin) Hall conductances: Let us consider Chern numbers in the quantum Hall effect as a typical example. The spin Hall conductances is treated similarly. We take the BZ by $0 \le k_\mu < 2\pi/q_\mu$ ($\mu = 1$, 2 with integers q_μ). Since the Hamiltonian $H(k)$ is periodic in both k_1 and k_2 directions, the BZ is 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 [3]. The Chern number assigned to the nth band is defined by $c_n = \frac{1}{2\pi i}\int_{T^2} F$ with $F = dA$, where the Berry connection $A = A_\mu dk_\mu$ with $A_\mu = \langle n|\partial/\partial k_\mu|n\rangle$ is defined by a normalized wave function of the nth Bloch band $|n\rangle$ satisfying $H(k)|n(k)\rangle = E_n(k)|n(k)\rangle$ and $\langle n|n\rangle = 1$ [3,4,5]. The Chern number 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 local gauge (a phase convention for the wave functions) such that the gauge potential is a well defined function. In an overlap between two patches, gauge potentials defined on each patch are related by a U(1) gauge transformation: $|n\rangle \to |n\rangle\omega$ and $A \to A + \omega^\dagger d\omega$ ($|\omega| = 1$). In the continuum theory, one needs to fix this gauge freedom to perform any explicit calculations. To fix the gauge, one first selects an arbitrary state $|\phi\rangle$ which is globally well defined over the whole BZ [2]. Then the gauge can be specified by $|n^\phi\rangle = P_n|\phi\rangle/N^\phi$ (if $N^\phi \ne 0$), where $P_n = |n\rangle\langle n|$ and $N^\phi = |\langle\phi|n\rangle|$ are gauge independent. Generically, this gauge is only allowed locally because the overlap N^ϕ may vanishes. It inevitably occurs to have a non vanishing Chern number. Then one needs to use several different state $|\phi\rangle$ (gauges) in several regions of patches to cover the whole BZ.

Topological Description on a discretized BZ: We now switch to the finite systems with discrete BZ. A naive replacement of the differential operator to the difference operator breaks the gauge invariance and topological characters of the Chern numbers. Here we propose an explicitly gauge invariant and topological definition of the Chern number on a lattice. Let us denote lattice points k_ℓ ($\ell = 1, \ldots, N_1N_2$) on the discrete BZ as $k_\ell = (k_{j_1}, k_{j_2})$, $k_{j_\mu} = \frac{2\pi j_\mu}{q_\mu N_\mu}$, ($j_\mu = 0, \ldots, N_\mu - 1$). 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 $2\pi/(q_\mu N_\mu)$. We first define a U(1) link variable from the wave functions

$$U_\mu(k_\ell) \equiv \mathrm{N}_\mu^{-1}(k_\ell)\langle n(k_\ell)|n(k_\ell + \hat{\mu})\rangle,$$

where $\mathrm{N}_\mu(k_\ell) \equiv |\langle n(k_\ell)|n(k_\ell + \hat{\mu})\rangle|$. It is well defined as long as $\mathrm{N}_\mu(k_\ell) \ne 0$. (It is always assumed by an infinitesimal shift of the lattice.) Next we define a lattice field strength by

$$\tilde{F}_{12}(k_\ell) \equiv \ln U_1(k_\ell)U_2(k_\ell + \hat{1})U_1(k_\ell + \hat{2})^{-1}U_2(k_\ell)^{-1},$$

($-\pi < \frac{1}{i}\tilde{F}_{12}(k_\ell) \le \pi$). The field strength is defined within the principal branch of the logarithm. Finally, we define the Chern number on the lattice as

$$\tilde{c}_n \equiv \frac{1}{2\pi i}\sum\nolimits_\ell \tilde{F}_{12}(k_\ell).$$

We stress here that $\tilde{c}_n$ is manifestly *gauge-invariant* and *strictly an integer* for arbitrary lattice spacings. To demonstrate it, let us introduce a gauge potential

$$\tilde{A}_\mu(k_\ell) = \ln U_\mu(k_\ell),$$

($-\pi < \frac{1}{i}\tilde{A}_\mu(k_\ell) \le \pi$) which is periodic on the lattice: $\tilde{A}_\mu(k_\ell + N_\mu\hat{\mu}) = \tilde{A}_\mu(k_\ell)$. By definition, one finds

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

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 $(1/i)\tilde{F}_{12}(k_\ell)$ takes a value within the principal branch. Now we have

$$\tilde{c}_n = \sum\nolimits_\ell n_{12}(k_\ell).$$

It shows that the lattice Chern number $\tilde{c}_n$ is an integer. To avoid ambiguities we assume that there are no exceptional configurations in the system under consideration, $|\tilde{F}_{12}(k_\ell)| \ne \pi$ for all k_ℓ [12]. This condition will be referred to as *admissibility*. Under this condition, the Chern number is uniquely determined. Since our lattice formulation recovers the continuum one in the limit $N_\mu \to \infty$, we expect the lattice field strength $\tilde{F}_{12}$ will be small enough for a sufficiently large N_μ and the lattice Chern number will approach the one in the continuum $\tilde{c}_n \to c_n$ in the this limit. Since both $\tilde{c}_n$ and c_n are integers, we have $\tilde{c}_n = c_n$ for meshes of appropriate sizes. As far as the system is regular, our lattice formulation could reproduce correct Chern numbers of the continuum theory even for a coarsely discretized BZ, $N_1N_2 \sim O(|\tilde{c}_n|)$ [14].

Also our method can be extended [14] to the case of the non-Abelian Berry connection $A = \psi^\dagger d\psi$, which is a matrix-valued one-form associated with a multi-dimensional multiplet ψ [2,15].

Uniqueness of the description: It turns out that the description presented so far proves to be *unique* for discretized BZ. Namely, 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. The Chern number $\tilde{c}_n$ is, moreover, a *unique* gauge-invariant topological integer which can be assigned to admissible U(1) link variables. The proof of this statement has been given by Lüscher [11].

A key ingredient of his proof is that any U(1) link variable can be decomposed uniquely into $U_\mu(k_\ell) = e^{iA_\mu^{[\tilde{c}_n]}(k_\ell)+iA_\mu^{\mathrm{T}}(k_\ell)}\Lambda(k_\ell)U_\mu^{[w]}(k_\ell)\Lambda(k_\ell+\hat{\mu})$, where $A_\mu^{[\tilde{c}_n]}(k_\ell)$ is a gauge field giving rise to the Chern number; $\Delta_1 A_2^{[\tilde{c}_n]}(k_\ell) - \Delta_2 A_1^{[\tilde{c}_n]}(k_\ell) = 2\pi i\tilde{c}_n/(N_1N_2)$, $A_\mu^{\mathrm{T}}(k_\ell)$ is a periodic transverse field, $\Lambda(k_\ell)$ is a gauge transformation, and $U_\mu^{[w]}(k_\ell)$ is a gauge field giving nontrivial Wilson lines but giving zero field strength. Once $A_\mu^{[\tilde{c}_n]}(k_\ell)$ is found, $A_\mu^{\mathrm{T}}(k_\ell)$ can be determined uniquely by the relation $\tilde{F}_{12}(k_\ell) = \Delta_1 A_2^{\mathrm{T}}(k_\ell) - \Delta_2 A_1^{\mathrm{T}}(k_\ell) + 2\pi i\tilde{c}_n/(N_1N_2)$. Readers who are interested in the proof should refer Lüscher's paper.

The admissibility condition is important for the present lattice formulation and its breakdown is closely related to a singular behavior of the Berry connection, that is, it is supplemented with a quantum phase transition. In the present context of the Berry connection, a distribution of the gauge invariant field $\tilde{F}_{12}$ is completely governed by the k dependence of the Hamiltonian. Each of the topological ordered states with a nontrivial Chern number corresponds to nontrivial topological sector specified by the admissibility and also characterized by the lattice Chern number $\tilde{c}_n$. In the continuum, on the other hand, the topological stability of the Chern number is assured by the gap-opening condition [2]. The topological quantum phase transitions are thus characterized by the gap closing. Namely, nontrivial topological sectors of the continuum, each of which is a topological ordered state, are separated by the gaps.

In passing, we would like to mention the Kubo formula which is often used in numerical calculations: $\bar{F}_{12}(k) = 2i\sum_{m(\neq n)} \frac{\mathrm{Im}\langle n(k)|\partial_1 H(k)|m(k)\rangle\langle m(k)|\partial_2 H(k)|n(k)\rangle}{[E_n(k)-E_m(k)]^2}$. This formula is equivalent the field strength $F_{12}(k)$ in the continuum BZ, but *not* to $\tilde{F}_{12}(k_\ell)$ in the discretized BZ. In the latter case, $\sum_\ell \bar{F}_{12}(k_\ell)$ is no longer topological, although the gauge-invariance remains. Therefore, our topological and gauge-invariant formulation for discrete BZ should have strong advantages, especially of describing regions where topological transitions occur.

3. Quantum Phase Transition and Topological Change

To demonstrate the present scheme, we take the Hamiltonian for spinless fermions in an external magnetic field: $H = -\sum_{\langle i,j\rangle} t_{ij}c_i^\dagger e^{i\theta_{i,j}}c_j$, where the flux per plaquette on the coordinate lattice $\phi = \sum_\square \theta_{i,j}/(2\pi)$ is p/q. We consider a model with quantum phase transition, that is, with next nearest neighbor (NNN) hopping t' (nearest neighbor hopping is t). The Hamiltonian in the k-space is given by $H_{ij}(k) = -2t\delta_{ij}\cos(k_y - 2\pi\phi j) - B_i\delta_{i+1,j} - B_j^*\delta_{i,j+1} - B_q^*\delta_{i+q-1,j}e^{-iqk_x} - B_q\delta_{i,j+q-1}e^{iqk_x}$, where $B_j = t + 2t'\cos\left(k_y - 2\pi\phi(j+1/2)\right)$ $(i,\, j = 1,\, \ldots,\, q)$ with $q_1 = q$ and $q_2 = 1$ [16]. Bellow, we will present some results of applying our method to the middle subband of the $\phi = 1/3$ (that is, $q = 3$) system. For simplicity, we set $N_1 = N_{\mathrm{B}}$ and $N_2 = qN_{\mathrm{B}}$ $(= 3N_{\mathrm{B}})$.

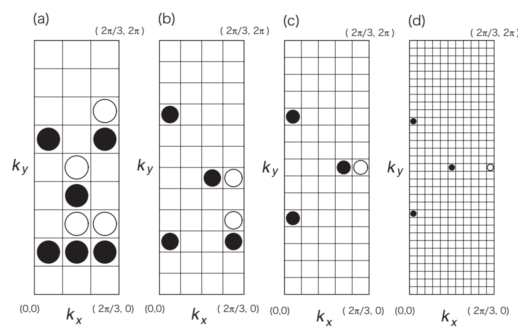

Fig. 1. Configuration of integer field $n_{12}(k_\ell)$ of the NN model ($t' = 0$) in a gauge specified by state $|\phi_g\rangle$ over discretized Brillouin zones. $N_{\mathrm{B}} = 3(a), 4(b), 5(c)$ and $11(d)$. Black (white) circles denote $n_{12} = -1$ (1).

We show the integer field $n_{12}(k_\ell)$ in Figs. 1(a)-(d), where we use the global gauge specified by the states $|\phi_g\rangle = e^{iq(k_x+k_y)}(1,1,0)^T$. The black and white circles denote $n_{12} = -1$ and 1, respectively, whereas a blank implies $n_{12} = 0$. It is clear that any of them gives the correct Chern number $\tilde{c}_n = -2$. The field $n_{12}(k_\ell)$ is gauge-dependent, but their sum is gauge-invariant. It also shows a convergence of the gauge dependent field n_{12} in the limit $N_{\mathrm{B}} \to \infty$. Although we have fixed the gauge to calculate the field n_{12}, calculations of the Chern numbers are performed in *any gauge*. We do *not* need specific gauge-fixing to make the gauge connection smooth. An *arbitrary* gauge (e.g., a phase choice of eigenvectors given by a numerical library) can be also adopted to compute the Chern number.

Now let us change a ratio t'/t in the NNN model. In Figs. 2, we show the energy spectra of the NNN models. They are modified Hofstadter's butterfly diagrams. The integers in the figures are the Hall conductances when the fermi energy lies in the gap, that is, it is a sum of the Chern numbers below the energy gap. Due to the sum rule of the Chern number [2], the Chern number of the specific energy band is given by a difference of two integers, above and below the band. As is known [16], the NNN model shows a topological quantum phase transition accompanying a discrete change of the Chern numbers. For example, an increase of t'/t causes a rearrangement of the gap connectivity near $t'/t = 0.26$ at $\phi = 1/3$. One can see that the energy gap just above the second band at $\phi = 1/3$ is rearranged by the small change of t'/t. It is associated with a change of the gap labeling from -1 to $+2$. Since the large energy gap just below the middle band is stable and the gap is labeled as $+1$, the Chern number of the middle band changes from -2 to $+1$. This topological change of the Chern number is confirmed by a calculation of the gauge dependent field n_{12} in Figs.3(b) and (d). The field strength $\tilde{F}_{12}$ just before and the after the quantum transition in also shown in (a) and (c). A small

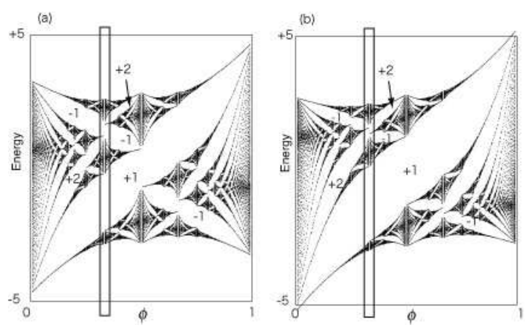

Fig. 2. Energy spectra of the NNN models as a function of the flux per plaquette ϕ. (a) $t' = 0.18t$ and (b) $t' = 0.32t$. Rearrangement of the gap connectivity is observed at the second gap near $\phi = 1/3$.

change of the parameter t'/t does not change the spectrum so much. On the other hand, the field strength $\tilde{F}_{12}$ is singular at the critical point. It is consistent with the breakdown of the admissibility as expected. That is, the quantum phase transition (of the present lattice

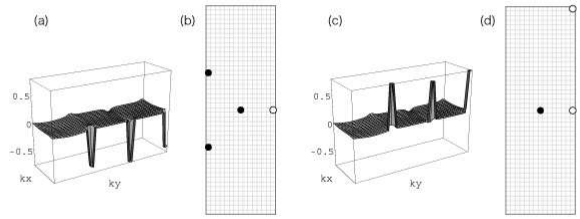

Fig. 3. (a):lattice field strength $\tilde{F}_{12}$ and (b): configuration of integer field $n_{12}(k_\ell)$ of the NNN model with $t' = 0.267t$, $N_{\rm B} = 15$. (c) and (d) the same for parameters $t' = 0.268t$.

model) occurs at $t' = t_c$ ($0.267 < t'_c/t < 0.268$). This quantum phase transition is associated with a topological change of the integer value field n_{12} as shown.

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