Spectral Flow and Global Topology of the Hofstadter Butterfly

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We study the relation between the global topology of the Hofstadter butterfly of a multiband insulator and the topological invariants of the underlying Hamiltonian. The global topology of the butterfly, i.e., the displacement of the energy gaps as the magnetic field is varied by one flux quantum, is determined by the spectral flow of energy eigenstates crossing gaps as the field is tuned. We find that for each gap this spectral flow is equal to the topological invariant of the gap, i.e., the net number of edge modes traversing the gap. For periodically driven systems, our results apply to the spectrum of quasienergies. In this case, the spectral flow of the sum of all the quasienergies gives directly the Rudner-Lindner-Berg-Levin invariant that characterizes the topological phases of a periodically driven system.

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The Hofstadter butterfly is the self-similar structure of subgaps in the energy spectrum of a charged particle hopping on a two-dimensional lattice, as a function of a perpendicular magnetic field. Its fractal structure becomes apparent when the magnetic flux on each plaquette, \( \Phi \), is a sizable fraction of the magnetic flux quantum, \( \Phi_0 = h/Q \); i.e., the normalized flux \( \phi = \Phi/\Phi_0 \) is of the order of 1 (\( Q \) is the charge and \( h \) is the Planck constant). This is shown in Fig. 1(a). Since it was first numerically computed [1], the Hofstadter butterfly has played an instrumental role in understanding the quantum Hall effect [2,3], it has made connections between number theory and physics [4,5], and it has inspired numerous other works (see, e.g., Ref. [6]). Observation of the butterfly using traditional solid-state materials would require prohibitively strong magnetic fields (thousands of Tesla). Alternative approaches focus on enlarging the plaquette size using superlattices, or substituting the magnetic field with a synthetic implementation of a vector potential (e.g., by rotation [7] or laser-assisted tunneling [8,9]). There has recently been a renewed interest in this problem because after so many years both approaches have come close to “netting” the Hofstadter butterfly, using heterostructure superlattices [10–12] or moiré superlattices made of graphene on a substrate [13], and using ultracold atoms in “shaken” optical lattices [14,15].

The Hofstadter butterfly is known to be periodic: the spectrum is invariant under a shift of \( \phi \) by 1. This also applies to multiband insulators, e.g., if the particle has several internal states [18]. In such a multiband Hofstadter butterfly, the periodicity is trivially obeyed if each band develops its own set of minigaps, as shown with an example in Fig. 1(b). However, there exist more ways in which this constraint can be obeyed: bands can also flow into each other as \( \phi \) is tuned from 0 to 1, as shown in Fig. 1(c). We call this pattern of bands flowing into each other the global topology of the Hofstadter butterfly. An even wider variety of nontrivial global topologies can occur in a periodically driven system (Floquet system), where quasienergy replaces energy—much like quasimomentum takes the place of momentum in a lattice system. In this case, bands can even wind in quasienergy, as shown in Fig. 1(d).

FIG. 1. Examples of Hofstadter butterfly spectra for (a) a simple charged particle on an infinite square lattice (Harper model), (b) a topologically trivial multiband insulator (Qi-Wu-Zhang model with \( u = 3 \) of Ref. [16]), (c) a topological multiband insulator (same Qi-Wu-Zhang model with \( u = -1.2 \)), and (d) a topological Floquet insulator [Rudner model of Ref. [17] with \( \delta_{AB} = 0 \) and \( JT/5 \) chosen for the first four segments as \( (3/8,3/8,5/8,5/8)\pi \)]. The topological indices of a few representative band gaps are shown in the figure.
The normalized flux per plaquette is thus shown for a given quasimomentum only (spectral flow across each gap, in the limit of $N_y$). We give a direct formula for this invariant in terms of the Rudner-Lindner-Berg-Levin (RLBL) invariant [17].

We shall focus on an energy gap of the bulk Hamiltonian, which we label by an energy value $E$ well inside the gap. Eigenstates at $E$, if they exist, are edge states, with wave functions exponentially decaying towards the bulk; the maximum decay length of these states is denoted by $\lambda$. By choosing $m$ sufficiently large, we assume $N_y \gg \lambda$, so that these states can be assigned to either the upper or lower edge. Thus, edge modes, which are sections of the dispersion relation of $\tilde{H}(k_x)$ that intersect $\tilde{E}$, can correspondingly be assigned to either the upper or lower edge. We denote the edge mode energies by $E^{up}_j(k_x, \phi)$ and $E^{low}_j(k_x, \phi)$, for the upper and lower edge, respectively ($s$ and $r$ designate the indices of the edge modes). The topological invariant $\nu$ of the gap is the net number of edge modes at the upper edge, with the right- and left-propagating edge modes counted with opposite signs.

We study how the spectrum of the edge states depends on the magnetic flux, as this flux is tuned from one commensurate value to the next. We parametrize this process by $\beta$ as

$$\phi = \frac{p}{q} + \frac{\beta}{N_y}, \quad \beta \in [0, 1].$$

At the bottom edge, in a region of width $\lambda$, the change in $\phi$ induces a change in the vector potential $A$, which with the chosen Landau gauge is of the order of $\beta \lambda / N_y$, and vanishes in the limit $N_y \to \infty$. Thus, bottom edge states are essentially unaffected. At the top edge, in a region of width $\lambda$, however, $A_x$ is increased approximately uniformly by $\beta \Phi_0$, up to corrections of the order of $\lambda / N_y$. As a result, the upper edge modes are cycled across the whole Brillouin zone:

$$E^{up}_r(k_x, \phi) \approx E^{up}_r(k_x - 2\pi \beta p/q).$$

We define the spectral flow across the gap as the net number of times the energy eigenvalues of $\tilde{H}(k_x)$ cross the value $\tilde{E}$, as $\phi$ is tuned from $\phi = p/q$ to $\phi = p/q + 1/N_y$, for sufficiently large $N_y$ (so the bulk gap remains open).

Using the notation $F^{p/q+1/N_y}_p(E; \{E_j(k_x, \phi)\}, \phi)$ for this spectral flow, we have...
\[ \mathcal{F}_{p/q}^{p/q+1/q}(\tilde{E}; \{E_j(k_x, \phi)\}, \phi) \]
\[ = \int_{p/q}^{p/q+1/q} d\phi \sum_j \frac{\partial E_j(k_x, \phi)}{\partial \phi} \delta(E_j(k_x, \phi) - \tilde{E}). \]  

(3)

For a generic \( k_x \), edge states at the lower edge give no contribution to this spectral flow since their spectrum is only changed by \( O(1/N_y) \). Bulk states also do not contribute, since the bulk gap remains open. Hence, the spectral flow is given by the flow of the upper edge states:

\[ \mathcal{F}_{p/q}^{p/q+1/q}(\tilde{E}; \{E_j(k_x, \phi)\}, \phi) \]
\[ = \mathcal{F}_{0/q}^{p/q+1/q}(\tilde{E}; \{E_j^{\text{up}}(k_x, \phi)\}, \phi). \]  

(4)

A nonzero spectral flow across a gap indicates, as the flux is tuned according to Eq. (1), some bulk states are transformed into upper edge states, are shifted in energy across the gap, and eventually become bulk states again at the end of the cycle.

Hence, we obtain our first result: the spectral flow across a gap is equal to the topological invariant \( \nu \) of the gap. This follows from Eqs. (2) and (4), which together give

\[ \mathcal{F}_{p/q}^{p/q+1/q}(\tilde{E}; \{E_j(k_x, \phi)\}, \phi) \]
\[ = \mathcal{F}_{0/q}^{p/q+1/q}(\tilde{E}; \{E_j^{\text{up}}(k_x, \phi)\}, k_x). \]  

(5)

where the right-hand side of the equation follows the definition in Eq. (3) with the integration variable \( k_x \) in lieu of \( \phi \). This quantity is the net number of edge states \( E_j^{\text{up}}(k_x, \phi) \) crossing the midgap energy \( \tilde{E} \), as a function of \( k_x \). The latter is by definition the topological invariant \( \nu \) of the gap. This also proves that the spectral flow is independent of the choice of the generic quasimomentum \( k_x \).

We next show that the spectral flow is equal to \( \nu \) also in a system with periodic boundaries along the \( y \) axis. We therefore introduce an extra hopping amplitude \( \gamma \) connecting opposite edges of the strip directly, with \( 0 \leq \gamma \leq 1 \). This results in a single defect along the stitching line, instead of two separate edges. Moreover, at \( \gamma = 1 \) and commensurate values of \( \phi \), this defect line entirely disappears, since the strip contains an integer number of magnetic unit cells, and thus the spectrum is completely gapped around \( \tilde{E} \) for all \( k_x \). Regardless of the value of \( \gamma \), the spectral flow is always an integer, since it counts the number of states crossing \( \tilde{E} \). Bulk states do not contribute to it since their spectrum is independent of \( \gamma \), and the bulk gap stays open. The only contribution is thus from states localized near the defect line. For small \( \gamma \), these can be seen as hybridized edge states, as shown with an example in Fig. 3.

**Global topology of the Hofstadter butterfly.**— We now use Eq. (5) to study the global topological features of multiband Hofstadter butterflies. To begin with, we address the case of time-independent Hamiltonians. Consider one of the bulk gaps of the Hofstadter butterfly among those that stay open for all values of the magnetic flux \( \phi \). At \( \phi = 0 \), this corresponds to the \( n_0 \)th gap, meaning that there are \( n_0 \) bands with energy below it. As \( \phi \) is continuously tuned from 0 to 1, the gap must flow into one of the gaps of the spectrum at \( \phi = 1 \), say, the \( n_1 \)th gap. We shall prove that the shift of the gap \( n_1 - n_0 \) is given by its topological invariant:

\[ n_1 - n_0 = \nu. \]  

(6)

Note that while the spectral flow in Eq. (4) relies on the Landau gauge, the result in Eq. (6) is gauge independent.

To prove Eq. (6), we keep the same setting as above with boundary conditions along the \( y \) axis freely chosen and \( N_y \) sufficiently large to guarantee a bulk for all \( \phi \). As \( \phi \) is varied, we keep track of the gap by introducing a continuous function \( \tilde{E}(\phi) \) taking midgap energies. We proceed by showing that the number of states in the spectrum at \( \phi = 1 \), in the energy interval bounded by \( \tilde{E}(0) \) and \( \tilde{E}(1) \), is given by \( \nu \). This number is equal to the net spectral flow of eigenvalues into the energy region bounded by \( \tilde{E}(\phi) \) on one side and by the constant value \( \tilde{E}(0) \) on the other side, as indicated by the highlighted region in the example in Fig. 2(c). The net flow across the constant \( \tilde{E}(0) \) is zero, since the total spectral flow across any fixed energy value \( \tilde{E} \) must always vanish,

\[ \mathcal{F}_{0/q}(\tilde{E}; \{E_j\}, \phi) = 0, \]  

(7)

a direct consequence of the periodicity of the spectrum in the variable \( \phi \). The net flow across \( \tilde{E}(\phi) \), however, can be nonzero, as is the case for a gap with a nontrivial topological invariant \( \nu \). In fact, decomposing the shift in \( \phi \) from 0 to 1 into \( N_y \) small steps, Eq. (5) shows that \( N_y \nu \) eigenvalues flow across \( \tilde{E}(\phi) \). Thus, at \( \phi = 1 \), the interval between \( \tilde{E}(0) \) and \( \tilde{E}(1) \) contains \( \nu \) energy bands; moreover, the sign of the spectral flow \( \nu \) of the band tells us...
where $\tilde{E}(1)$ is larger or smaller than $\tilde{E}(0)$, thus concluding the proof of Eq. (6).

**Floquet insulators.**—We next study the spectral flow and the Hofstadter butterfly in periodically driven (i.e., Floquet) multiband insulators. The Floquet insulator is a lattice Hamiltonian, with some of its parameters depending explicitly on time, periodically with period $T$. To define the Hofstadter butterfly, we include a time-independent magnetic field through Peierls phases, as for static Hamiltonians above. Hence, the time-dependent Hamiltonian $\hat{H}(\phi, \tau)$ is periodic both in time and in the magnetic flux,

$$
\hat{H}(\phi, \tau) = \hat{H}(\phi, \tau + 1) = \hat{H}(\phi + 1, \tau),
$$

where $\tau = t/T$ represents time $t$ in rescaled dimensionless units. The time evolution over one period of the drive is given by the Floquet operator, $\hat{U}(\phi) = T \exp[-i T/h \int_0^1 \hat{H}(\phi, \tau) d\tau]$, where $T$ denotes time ordering. The eigenvalues of the Floquet operator $\hat{U}$ read $\exp(-i\epsilon_j)_{\phi}$, with the quasienergies $\epsilon$ playing the role of the energy in a static Hamiltonian. They are defined in the interval $[\pi, \pi]$, with the end point $\epsilon = \pi$ identified with $\epsilon = -\pi$. We call this interval the Floquet zone of quasienergies, in analogy to the Brillouin zone of quasimomenta. As an example of the Floquet Hofstadter butterfly, Fig. 1(d) shows the spectrum of quasienergies as a function of the flux $\phi$ in the case of the model introduced in Ref. [17].

Next, we show how to adapt our results on time-independent Hamiltonians to Floquet systems. (i) Equation (5) directly carries over to the quasienergies of a Floquet system: The topological invariant of each gap is equal to the spectral flow across a fixed quasienergy gap is given by

$$
\hat{V}(\tau, k_x, k_y) = e^{i \hat{H}_{\text{eff}} T} e^{-i \int_0^1 \hat{H}(\tau', k_x, k_y) d\tau}'.
$$

and $\hat{H}_{\text{eff}} = i \log \hat{U}$ is the effective Hamiltonian, with the branch cut of the logarithm along the negative real axis. Note that $\hat{H}_{\text{eff}}$ is time independent, unlike $\hat{H}$, and its spectrum consists of the quasienergies $\epsilon_j$.

Based on the spectral flow, we take a direct physical approach to the RLBL invariant, and obtain a simple formula for it. To show this, we consider the determinant of $\hat{U}(\phi)$, which can be expressed as

$$
\det \hat{U}(\phi) = \lim_{M \to \infty} \prod_{j=1}^M \exp[-i \text{tr} \hat{H}(\phi, j/M)/M].
$$

Each factor in the product is independent of $\phi$, since the Peierls substitution only modifies off-diagonal matrix elements of the instantaneous Hamiltonian. Thus, $\det \hat{U}(\phi)$ itself is independent of $\phi$, and the sum of quasienergies $\sum \epsilon_j(\phi)$ can only increase or decrease as a function of $\phi$ in steps of $2\pi$. A step change in this sum happens whenever a quasienergy value flows across the boundary of the first Floquet zone, $\epsilon = \pm \pi$, in the positive or negative direction. Using the relation between spectral flow and the topological invariant of the gap, Eq. (5), the net number of such crossings as $\phi$ is tuned from one commensurate value to the next is given by the topological invariant of the quasienergy gap comprising $\epsilon = \pi$. Thus, we obtain the RLBL invariant as

$$
R = \frac{1}{2\pi} \left\{ \sum_j \epsilon_j(k_x, \phi + 1/N_y) - \sum_j \epsilon_j(k_x, \phi) \right\},
$$

where $\phi = n/N_y$ with $n \in \mathbb{N}$, and $k_x$ is chosen arbitrary. Equation (12) might also be more efficient to compute than
Eq. (9), as its computation does not require numerical derivation.

Discussion and conclusions.—We introduced spectral flow as the change of the (quasi)energy eigenvalues of a charged particle on a two-dimensional finite-width lattice strip in response to an increment in a homogeneous magnetic field perpendicular to the strip. Our definition of spectral flow differs from that used in Laughlin’s argument [19,20], where the strip is rolled into a cylinder, and the increment is in an additional magnetic field threading the whole cylinder. In our case, the spectral flow is well defined only in the limit of large \( N_y \) (i.e., wide strip), when it becomes a powerful tool, allowing us to connect the topological invariants of the gaps to the global topology (connectedness) of the Hofstadter butterfly.

In periodically driven systems, our concept of spectral flow has led us to a physically intuitive and direct expression, Eq. (12), for the RLBL topological invariant. Our formula shows that, although the bulk Floquet operator is not sufficient to obtain the Rudner invariant, its evaluation at two commensurate values of the magnetic flux is. A caveat is that this formula relies on the spectral flow computed for a fixed quasimomentum \( k_x \), as in Eq. (3), which is ensured to be independent of \( k_x \) only in the Landau gauge we have chosen. Gauge invariant formulas for the spectral flow as well as for the RLBL invariant can be obtained by averaging over all values of \( k_x \). We remark, finally, that our theoretical results could find application in artificial matter experiments over all values of \( k_x \) as well as for the RLBL invariant can be obtained by averaging over all values of \( k_x \).

Recently, we became aware of related work [23].

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[18] Assuming we have a simple lattice, and the magnetic field couples only to the motion via Peierls phases, and not to the internal states.