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, Φ, 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 ϕ 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 ϕ 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).

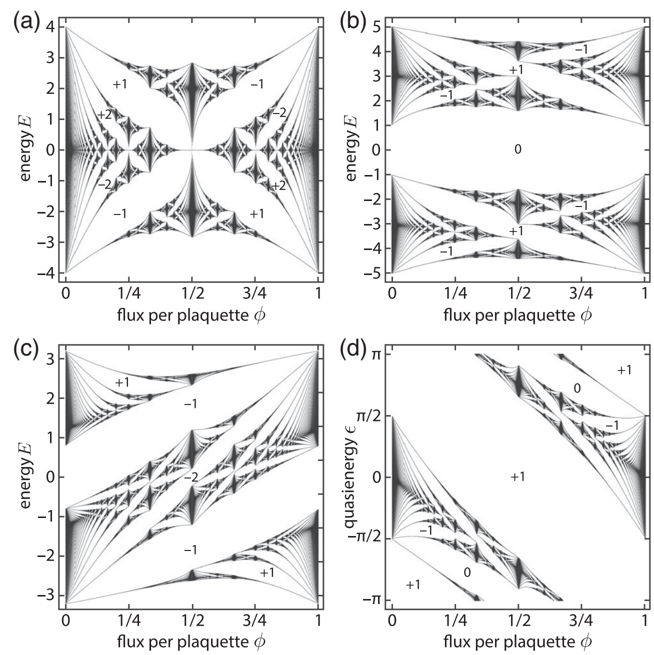

FIG. 1. Examples of Hofstadter butterfly spectra for (a) a simple charged particle on an infinite square lattice (Harper model), (b) a topologically trivial multiband insulator (Qi-Wu-Zhang model with $u = 3$ of Ref. [16]), (c) a topological multiband insulator (same Qi-Wu-Zhang model with $u = -1.2$), 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.

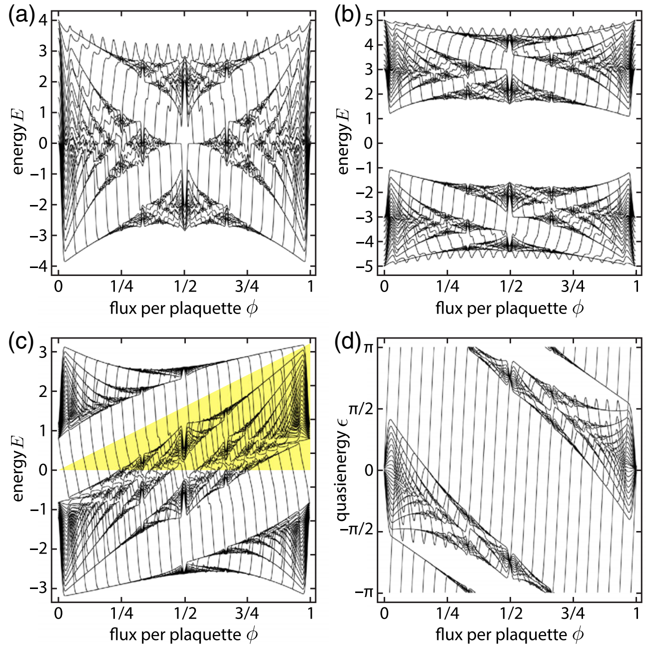

FIG. 2. Examples of Hofstadter spectra analogous to those shown in Fig. 1, but computed for a lattice of finite width along y (24 sites with periodic boundary conditions), and still infinite along x. For better visibility of the spectral flow, the spectra are shown for a given quasimomentum only ($k_x = 0$).

In this Letter, we establish a connection between the global topology of a multiband Hofstadter butterfly and the topological invariants of the underlying Hamiltonians. For periodically driven systems, in particular, we find that the winding of the Hofstadter butterfly is determined by the Rudner-Lindner-Berg-Levin (RLBL) invariant [17]. We give a direct formula for this invariant in terms of the sum of quasienergy eigenvalues.

All our results hinge on the fact that in a lattice of fixed width N_y, tuning the magnetic flux from one commensurate value to the next (by an increase in ϕ of $1/N_y$) induces a *spectral flow* of energy eigenvalues. We will prove that the spectral flow across each gap, in the limit of $N_y \to \infty$, is equal to the topological invariant ν of the gap, i.e., the net number of edge modes traversing this gap at an edge. Figure 2 presents four different examples of Hofstadter butterfly spectra computed for a lattice of finite width, which show the spectral flow of eigenvalues across gaps with nonzero ν. Our result is consistent with the Streda formula [3] and Wannier's Diophantine equation [4]. However, it also applies to periodically driven systems, where the spectral flow of quasienergy (rather than energy) eigenvalues is considered.

Time-independent Hamiltonians.—We consider a two-dimensional band insulator on a square lattice, where each site can host N internal states. A perpendicular magnetic field B couples to the particle via Peierls phases, with the vector potential $A = (By, 0, 0)$ chosen in a Landau gauge. The normalized flux per plaquette is thus $\phi = B/\Phi_0$. The magnetic field is initially set to produce a flux with a rational value, $\phi = p/q$, with p and q relative prime.

We restrict our lattice to a strip that is infinite along the x axis and of finite width N_y along the y axis with open boundary conditions. The sites are labeled by position indices $n_x n_y \in \mathbb{N}$, with $1 \leq n_y \leq N_y$. We choose $N_y = mq$ for some $m \in \mathbb{N}$. This makes the initial value of the flux *commensurate* with the system size, in the sense that the width N_y incorporates an integer number of magnetic unit cells, each of width q. Because of translational invariance along x, the system is described by a single-particle Hamiltonian $\hat{H}(k_x)$ that is periodic in k_x with period 2π. Its eigenvalues are $E_j(k_x, \phi)$, with $j = 1, \ldots, NN_y$.

We shall focus on an energy gap of the bulk Hamiltonian, which we label by an energy value $\tilde{E}$ well inside the gap. Eigenstates at $\tilde{E}$, if they exist, are edge states, with wave functions exponentially decaying towards the bulk; the maximum decay length of these states is denoted by λ. 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 $\hat{H}(k_x)$ which intersect $\tilde{E}$, can correspondingly be assigned to either the upper or lower edge. We denote the edge mode energies by $E_r^{\mathrm{up}}(k_x, \phi)$ and $E_s^{\mathrm{low}}(k_x, \phi)$, for the upper and lower edge, respectively (s and r designate the indices of the edge modes). The topological invariant ν 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 β as

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

At the bottom edge, in a region of width λ, the change in ϕ 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 λ, however, A_x is increased approximately uniformly by $\beta\Phi_0$, up to corrections of the order of λ/N_y. As a result, the upper edge modes are cycled across the whole Brillouin zone:

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

We define the spectral flow across the gap as the net number of times the energy eigenvalues of $\hat{H}(k_x)$ cross the value $\tilde{E}$, as ϕ 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 $\mathcal{F}_{p/q}^{p/q+1/N_y}(\tilde{E}; \{E_j(k_x, \phi)\}, \phi)$ for this spectral flow, we have

$$\mathcal{F}_{p/q}^{p/q+1/N_y}(\tilde{E};\{E_j(k_x,\phi)\},\phi) = \int_{p/q}^{p/q+1/N_y} d\phi \sum_j \frac{\partial E_j(k_x,\phi)}{\partial \phi}\delta(E_j(k_x,\phi)-\tilde{E}). \quad (3)$$

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 $\mathcal{O}(1/N_y)$. 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:

$$\mathcal{F}_{p/q}^{p/q+1/N_y}(\tilde{E};\{E_j(k_x,\phi)\},\phi) = \mathcal{F}_{p/q}^{p/q+1/N_y}(\tilde{E};\{E_j^{\mathrm{up}}(k_x,\phi)\},\phi). \quad (4)$$

A nonzero spectral flow across a gap indicates that, 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 ν of the gap. This follows from Eqs. (2) and (4), which together give

$$\mathcal{F}_{p/q}^{p/q+1/N_y}(\tilde{E};\{E_j(k_x,\phi)\},\phi) = \mathcal{F}_0^{2\pi}(\tilde{E};\{E_j^{\mathrm{up}}(k_x,\phi)\},k_x), \quad (5)$$

where the right-hand side of the equation follows the definition in Eq. (3) with the integration variable k_x in lieu of ϕ. This quantity is the net number of edge states $E_r^{\mathrm{up}}(k_x,\phi)$ crossing the midgap energy $\tilde{E}$, as a function of k_x. The latter is by definition the topological invariant ν 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 ν also in a system with periodic boundaries along the y axis. We therefore introduce an extra hopping amplitude γ 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 ϕ, 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 γ, 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 γ, and the bulk gap stays open. The only contribution is thus from states localized near the defect line. For small γ, 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

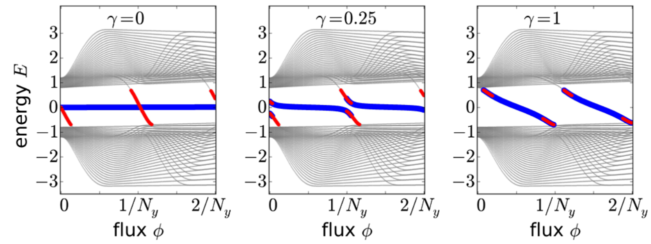

FIG. 3. Spectra of the Qi-Wu-Zhang model as a function of the magnetic flux (two cycles shown), computed on a lattice of finite width (36 sites) along y and for a fixed quasimomentum ($k_x = 0$). γ indicates the hopping amplitude at the edge ($\gamma = 0$ for open and $\gamma = 1$ for periodic boundary conditions). States with more than 30% weight in the first two rows at the top (bottom) edge are marked by thick red (blue) lines.

of the bulk gaps of the Hofstadter butterfly among those that stay open for all values of the magnetic flux ϕ. At $\phi = 0$, this corresponds to the n_0th gap, meaning that there are n_0 bands with energy below it. As ϕ 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_1th gap. We shall prove that the shift of the gap $n_1 - n_0$ is given by its topological invariant:

$$n_1 - n_0 = \nu. \quad (6)$$

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 ϕ. As ϕ 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 ν. 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 $\bar{E}$ must always vanish,

$$\mathcal{F}_0^1(\bar{E};\{E_j\},\phi) = 0, \quad (7)$$

a direct consequence of the periodicity of the spectrum in the variable ϕ. The net flow across $\tilde{E}(\phi)$, however, can be nonzero, as is the case for a gap with a nontrivial topological invariant ν. In fact, decomposing the shift in ϕ 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 ν of the band tells us whether $\tilde{E}(1)$ 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,

$$\hat{H}(\phi,\tau)=\hat{H}(\phi,\tau+1)=\hat{H}(\phi+1,\tau), \tag{8}$$

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, $\hat{U}(\phi)=\mathcal{T}\exp[-iT/\hbar\int_0^1\hat{H}(\phi,\tau)d\tau]$, where $\mathcal{T}$ denotes time ordering. The eigenvalues of the Floquet operator $\hat{U}$ read $\exp(-i\epsilon_j)$, with the *quasienergies* ϵ 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 ϕ 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 of quasienergies across it. (ii) The global topology of a Floquet Hofstadter butterfly can also be related to the topological invariants of the gaps as in Eq. (6). Concerning (ii), however, some remarks are in order.

First, we need to show that the total spectral flow of quasienergies across a constant $\bar{\epsilon}$ vanishes; see Eq. (7). To prove this, we deform $\hat{U}(\phi)$ continuously to $\hat{1}$ (the unity operator) by replacing $\hat{H}(\phi,t)$ with $\eta\hat{H}(\phi,t)$, where $\eta\in[0,1]$. Since the total spectral flow across a fixed quasienergy $\bar{\epsilon}$ is an integer-valued, continuous function of η, its value must be independent of η. At $\eta=0$, the total spectral flow vanishes because $\hat{U}(\phi)=\hat{1}$; thus, it also vanishes at $\eta=1$.

Second, it is convenient to describe the spectral flow of quasienergies in a scheme of repeated Floquet zones (in analogy to the repeated Brillouin zones of quasimomentum). Quasienergies can flow from one Floquet zone into a neighboring one, as ϕ is tuned. However, since the total spectral flow vanishes, they must return to the original zone at $\phi=1$. Hence, the same arguments used to prove Eq. (6) apply: gaps that stay open for all values of ϕ must be shifted by ν energy bands as ϕ is tuned from 0 to 1. Note that the difference n_1-n_0 is well defined in the repeated Floquet zone scheme, although n_0 and n_1 individually are not. Once quasienergies are "folded back" into the first zone, the flow of quasienergy gaps into neighboring Floquet zones can result in the Floquet Hofstadter butterfly winding in quasienergy, as shown by the example in Fig. 2(d).

Physical approach to the RLBL topological invariant.—The net number of edge states traversing the quasienergy gap at the edge of the Floquet zone is the RLBL topological invariant R, which is unique to periodically driven systems. It modifies the bulk-edge correspondence of the effective Hamiltonian [17]: The net number of edge states traversing the nth quasienergy gap is given by $\nu_n=R+\sum_{m<n}C_m$, where C_m is the Chern number of the mth quasienergy band. Unlike the Chern numbers, R cannot be obtained from the bulk Floquet operator $\hat{U}(k_x,k_y)$ as a function of the quasimomenta k_x, k_y, but instead was identified by Rudner *et al.* [17] with a winding number,

$$R=\int_0^1 d\tau\int_{\mathrm{BZ}}d^2k\,\mathrm{tr}\{\hat{V}^\dagger\partial_\tau\hat{V}[\hat{V}^\dagger\partial_{k_x}\hat{V},\hat{V}^\dagger\partial_{k_y}\hat{V}]\}, \tag{9}$$

where $\hat{V}$ is the "periodized" operator

$$\hat{V}(\tau,k_x,k_y)=e^{i\hat{H}_{\mathrm{eff}}\tau}\mathcal{T}e^{-i\int_0^\tau\hat{H}(\tau',k_x,k_y)d\tau'} \tag{10}$$

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

$$\det\hat{U}(\phi)=\lim_{M\to\infty}\prod_{j=1}^{M}\exp[-i\mathrm{tr}\hat{H}(\phi,j/M)/M]. \tag{11}$$

Each factor in the product is independent of ϕ, since the Peierls substitution only modifies off-diagonal matrix elements of the instantaneous Hamiltonian. Thus, $\det\hat{U}(\phi)$ itself is independent of ϕ, and the sum of quasienergies $\sum_j\epsilon_j(\phi)$ can only increase or decrease as a function of ϕ in steps of 2π. 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 ϕ is tuned from one commensurate value to the next is given by the topological invariant of the quasienergy gap comprising $\varepsilon=\pi$. Thus, we obtain the RLBL invariant as

$$R=\frac{1}{2\pi}\left\{\sum_j\epsilon_j(k_x,\phi+1/N_y)-\sum_j\epsilon_j(k_x,\phi)\right\}, \tag{12}$$

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 aiming to explore the Hofstadter butterfly and Floquet topological phases using periodic driving [21] (where gauge-dependent quantities can be directly accessed [22]).

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

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