Origin of band flatness and constraints of higher Chern numbers

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Flat bands provide a natural platform for emergent electronic states beyond Landau paradigm. Among those of particular importance are flat Chern bands, including bands of higher Chern numbers \((C>1)\). We introduce a new framework for band flatness through wave functions, and classify the existing isolated flat bands in a ”periodic table” according to tight binding features and wave function properties. Our flat band categorization encompasses seemingly different classes of flat bands ranging from atomic insulators to perfectly flat Chern bands and Landau Levels. The perfectly flat Chern bands satisfy Berry curvature condition \(F_{xy} = \text{Tr} G_{ij}\), which on the tight-binding level is fulfilled only for infinite-range models. Here \(\Lambda\) is the hopping range. Setting here lattice constant \(a\rightarrow\infty\) (or \(t_{ij}=0\)) immediately recovers the ”atomic insulator”, a system with a perfectly flat band at \(E_0=0\). The atomic insulator is the simplest perfectly flat band opening the ”periodic table” of perfectly flat bands (Table I).

Electronic band flatness is a new condensed matter paradigm. The flat bands had been studied in the context of Landau levels [1–3]; however a conceptually new approach in material science is engineering flat bands from the first principles [4–6]. To date, we have accumulated sufficient numerical evidence of flat bands formation ranging from artificial crystallographic lattices (Kagome, Lieb) to controllable flat band engineering in twisted van der Waals heterostructures [7–9]. The controllable and predictable engineering of band flatness is of strategic importance, especially for strongly correlated phases such as unconventional superconductivity [10–13], Fractional Chern Insulators [14–17], and the SYK phase [18–20], to name a few. Of particular importance are flat Chern bands, however the higher-order Chern numbers are a rare case in reality, with the majority of natural flat bands restricted to \(|C|=1\).

It is certainly surprising that in many cases we can point out on the common origin for perfectly flat bands, which is (self)-trapping in a limited coordinate region. In case of Landau levels with \(v_{\perp}\sim e^{-r^2/2t^2}\), the self-trapping occurs in the area \(\sim t^2\); for atomic insulator the self-trapping occurs on the lattice sites; for fine-tuned flat-bands (such as in Kagome, Liebe lattices) the self-trapping happens within the plaquette \(<a^2\); in twisted van der Waals heterostructures the self-trapping happens at small part of the moiré cell around high-symmetry points (AA stacking in twisted bilayer graphene). This motivates us to define the band flatness parameter through wave functions

\[
 f = \frac{\sum_{R>R_0} |\Psi(R)|^2}{\sum_{R>R_0} |\Psi(R)|^2}. \tag{1}
\]

Here \(\Lambda\) is a system-dependent real space hopping range (dimensionless). The parameter \(f\leq1\) is identifying band flatness through wave function localization. Clearly \(\delta(R)\) gives a perfectly flat band with \(f=0\), and the flatness construction at small \(\Lambda\sim1\) is intuitively clear. Let’s illustrate that definition (1) works also for \(\Lambda \to \infty\), both for the gapped trivial and topological bands.

Generic construction of flat bands.—Consider a generic tight binding Hamiltonian \(\mathcal{H} = \sum_{ij} t_{ij} \hat{c}_i^\dagger \hat{c}_j\). Here \(\Lambda\) is the hopping range. Setting here lattice constant \(a\to\infty\) (or \(t_{ij}=0\)) immediately recovers the ”atomic insulator”, a system with a perfectly flat band at \(E_0=0\). The atomic insulator is the simplest perfectly flat band opening the ”periodic table” of perfectly flat bands (Table I). We can systematically build other classes of flat bands from the tight binding. In the momentum representation the generic tight-binding Hamiltonian reads \(\mathcal{H} = \sum_k \varepsilon_{\alpha}(k) \hat{c}^\dagger_{\alpha} \hat{c}_{\alpha}\). The matrix Hamiltonian \(\mathcal{H}_{\alpha\beta}(k)\) has electronic bands \(\varepsilon_1(k), \varepsilon_2(k)\ldots \varepsilon_N(k)\). Among them, we pick up the \(n^\text{th}\) band which is dispersive, gapped out from the others, and not crossing zero. We further introduce a new Hamiltonian hosting the perfectly flat band through procedure

\[
 t_{ij} \rightarrow T_{ij} = \frac{E_0}{N} \sum_k \frac{\mathcal{H}(k)}{\varepsilon_n(k)} e^{-i\varepsilon_n(k) R_i R_j}. \tag{2}
\]

The new tight binding Hamiltonian with hopping (2) \(\mathcal{H}^\text{flat} = \sum_{ij} T_{ij}^\text{flat} \hat{c}_i^\dagger \hat{c}_j\) contains at least one perfectly flat band positioned at \(E = E_0\). However, this unique flat band comes at the expense that the tight-binding model becomes nonlocal \((\Lambda \to \infty)\). Of course, one can now take only the first few terms of \(T_{ij}^\text{flat}\), since they are decaying exponentially fast with distance. However any real space truncation of \(\Lambda\) inevitably introduces a ”parasitic dispersion”, so the band is no longer perfectly flat. The analysis above is useful for understanding the ”fine tuning” flat bands in Kagome, Lieb and other lattices. In the rare cases, one can find a lucky choice of fine-tuning parameter set upon truncation to nearest neighbors NN and NNN (\(\Lambda\approx2,3\)), which gives flat or perfectly flat band through destructive interference. However, this construction is a fine tuning and inclusion of further-order hop-
TABLE I: "Periodic table" for perfectly flat gapped bands categorized through criteria (1), (7), (13).

| atomic insulator | fine-tuned flat | generic trivial nonlocal | generic topological nonlocal | Landau Level | TBG chiral |
|------------------|----------------|--------------------------|-----------------------------|-------------|-----------|
| O(1)             | ∞              | ∞                        | ∞                           | ∞           | (∞); O(1) |
| - none           | any            | ~ π/a                    | ~ π/a                       | -           | (cancelled; π/Λ) |
| -                 | 0              | 0                        | | C = ±1 | C = ±1 |
| not defined      | double-periodic, meromorphic | double-periodic, non-double-periodic | holomorphic | holomorphic |
|                  | nonholomorphic, nonholomorphic | nonholomorphic | quasiperiodic | quasiperiodic |

In case of several singularities we take $h = \min[\text{Im} \, k_x]$, corresponding to the one closest to the real axis. We further use this asymptotic to derive the behavior of the flatness parameter (1) as

$$f \sim \frac{1}{\Lambda^{2(\alpha+1)}} e^{-2h\Lambda a},$$

(6)

For this, we need to use analytical estimates of the sums of form $\Sigma_n(x) = \sum_{x=0}^{\infty} x^n e^{-x}$. We rewrite this sum as $\Sigma_n(x) = e^{-x} \zeta(\frac{x}{\Lambda}, n, \Lambda)$ where $\zeta(\phi, n, \Lambda) = \sum_{x=0}^{\infty} (x + \Lambda)^{-n} e^{-2\pi i \phi x}$ is Lerch zeta function (see e.g. [24]). Up to $O(1)$ prefactor Lerch zeta function $\zeta(\frac{x}{\Lambda}, n, \Lambda)$ behaves as $1/\Lambda^n$ for $\Lambda \gg 1$, thus we obtain analytical estimate $\Sigma_n(x) \sim \Lambda^{-n} e^{-x}$ and $\Sigma_n(1) \sim O(1/\epsilon)$. The flatness parameter involves summation of form $\Sigma_n(x) = e^{-x} / (x + \Lambda)^{-n} e^{-2\pi i \phi x}$. We confirm numerically that this estimate works good even for $\Lambda \sim 2$. Taking now $n = 2(\alpha+1)$ and restoring dimensional parameters, we obtain (6). For our purposes, we are not interested here in the power-law prefactor, and factor of 2 in the exponent. It is safe to rewrite the flatness criterion as

$$f_0 = e^{-h\Lambda a},$$

(7)

The flatness parameter $f_0$ of (7) sets a fundamental scale for achievable band flatness, and covers three distinguished classes of perfectly flat nontopological bands with $f_0 = 0$:

- $a \to \infty$, atomic insulator.
- $\Lambda \to \infty$, generic flat band construction, Eq. (2).
- $h \to \infty$, singularity removed to infinity (nonsingular perfectly flat band).

The first two cases are discussed on page 1; the examples for nonsingular perfectly flat bands are listed in Ref. [6]. Cases of topologically trivial, gapped perfectly flat bands are covered by the three classes above, and constitute the topologically-trivial sector of the flat band classification (Table I). We do not have evidence of perfectly flat, gapped topologically-trivial bands which do not fit into this classification. We now proceed to the Chern bands.
Band flatness for Chern bands. We start from the construction of higher-$C$ Chern bands on the basis of double periodic meromorphic functions. The essential toolbox is built upon implementation of theta functions, Weierstrass and Jacobi functions, and their combinations [25]. Independently of the choice of the elliptic function, we can use connection between the wave function singularities (poles) and the band Chern number $C = \int_{BZ} \frac{\partial^2 \theta}{\partial y^2} dxy$, with $F_{xy} = \partial_x A_y - \partial_y A_x$, $A_k = -i(u_k \partial_k u_k)$, in the complex plane $z = (k_x, k_y)$ [26, 27].

$$C = \left[ \phi_{res} + \sum_{z_i^*} \phi \right] \frac{A_{dz} + A_{dz^*}}{4\pi} = \sum z_i^* p_i(z_i^*). \quad (8)$$

The Chern number is expressed through the sum of all poles $z_i^*$ in Brillouin zone (BZ), counting their multiplicity $p_i(z_i^*)$ [27]. The definition (8) is important since it is not connected to the band dispersion as such.

A theorem, tracing back to Thouless [28], prevents Wannierizing a Chern band along 1D; see recent discussion in [29]. However, as was pointed out by Qi, it does not prevent Wannierizing a Chern band along one of the 1D directions of a 2D Chern insulator [30]. (Moreover, in this way a duality between a Chern number is established [30].)

For our purposes, localization along 1D is a good indicator of band flatness through (1), (4). We thus proceed with Wannierizing a Chern band along 1D, and finding its asymptotic behavior. For this, it is sufficient to replace the elliptic functions with their principal behavior around poles

$$u(k) \simeq \sum_n \frac{u_0}{i(k - k_n^*)^{p_n}} + \text{Regular part}. \quad (9)$$

(here $k = k_x + ik_y$ is in the first BZ). The associated Chern number is $C = \sum_n p_n$. The main contribution to the integral (4) is given by the pole (9) of multiplicity $p_n \leq C/2$ closest to the real axis. The residue at the pole is $\text{Res} u(k) = -i u_0 x^{p_n-1} e^{ixk}/(p_n - 1)!$, with $k_n = k_0 + ih$. Using the residue theorem, and an appropriate contour, one obtains asymptote

$$W(x) \simeq \frac{2\pi u_0}{(p_n - 1)!} x^{p_n - 1} e^{-hx}. \quad (10)$$

To derive the flatness parameter, we need to evaluate sums of form $\sum_m(\lambda) = \sum_{x > \Lambda} x^m e^{-x}$ with $m = 2(p_n - 1)$. We can rewrite this sum through Lerch zeta function as

$$\sum_m(\lambda) = e^{-\Lambda} \zeta\left(\frac{p_n}{2}, -m, \lambda\right). \quad (11)$$

For $\Lambda \rightarrow \infty$, this results into a higher Chern number $C_{2N} = 2N \Lambda + 1$ restring band flatness as $f \sim \Lambda^{C_{2N} - 2} e^{-2ha\Lambda}$. To have a topological band, the wave function singularity must reside inside the BZ. This leads to the limitation $h \leq \pi/a$ (square lattice), or $ha \sim 1$ independently of $a$ and lattice symmetries. The flatness parameter is

$$f \sim \Lambda^{C_{2N} - 2} e^{-\Lambda}. \quad (11)$$

The only way to have a perfectly flat Chern band (f=0) is for $\Lambda \rightarrow \infty$. We come to the same conclusion if we consider a higher $C=N$ Chern band constructed through adding $N$ poles of multiplicity 1 (or any other combination). In this case we need to replace $C_{2N}$ with $2N C_1$, $C_1 = 1$ in (11), however the same argument holds: the Chern band is perfectly flat only for $\Lambda \rightarrow \infty$. We cannot fine-tune local tight-binding with NN and NNN hoppings in order to have perfectly flat Chern band on the lattice, as we did in the topologically-trivial case. The band flatness constraint in this case yields from the inevitable singularity of the wave functions of form $1/(k-k_n)^m$, which is irremovable by definition, and is the source for the Berry curvature.

Thus we come to the conclusion that the Chern bands cannot be perfectly flat unless in the case of infinite hopping range $\Lambda$. This observation is consistent with Chen theorem (2014), stating that in the double-periodic system the perfectly flat Chern bands are accessible only for $\Lambda = \infty$ [33].

**Flat Chern bands with $C=1$.**—Now we can relax some
of the conditions imposed in Eqs. (9), (8) on the flat band wave function. This can be done in two ways: by relaxing double periodicity or by relaxing holomorphicity conditions. First, we can relax condition of double-periodicity, but still require the flat band state to be a function of \( z = k_x + i k_y \). In this way we unlock all the odd Chern numbers in (8), including unitary \(|C| = 1\). In this case the contribution along the BZ boundary, which vanishes due to double-periodicity in (8), may itself contribute to the Chern number. Interestingly, we can go even further by canceling the remaining singularity(-ies) inside the BZ and producing an effective magnetic flux; in this case the Chern number is given purely by the circulation around the effective magnetic fields which produce Berry curvature for further details. In both cases we are dealing with flat bands, since further dropping both the condition of periodicity and holomorphicity breaks down the concept of Chern number as an integer topological invariant on the tight-binding level.

Independently of the method the flat Chern band has been composed, it is safe to rewrite the flatness criterion as

\[
f_0 = \Lambda^2 e^{-F(\Lambda)}, \quad \text{for topological bands}, \tag{13}
\]

where \( S[C] \propto |C|, F(\Lambda) \propto \Lambda, \Lambda^2 \) with system-dependent coefficients which reflect the way the Chern number \( C \) is constructed. The higher Chern number is, the harder is to make a good flat band. The topological bands can be perfectly flat only at infinite hopping range.

Comparing criterion (13) with the \( f_0 \) criterion for trivial bands (7), we notice that criterion (13) is not reducible to the atomic insulator. This is because the Chern insulator and atomic insulator belong to different topological classes, and cannot be adiabatically connected [40].

**Microscopic analysis and hopping range bounds.**—We now look deeper into the microscopic details of topological constraints (Fig. 2). A representative parameter is the hopping range scale, defined for an isolated band as

\[
r_{\text{hop}} = \left( \sum_{i,j=0}^{\infty} (x_i - x_j)^2 W(x_i) W(x_j) \right)^{1/2}
\]

For definiteness, we use the construction of higher-Chern flat band as in Eqs.(10-11). We observe numerically that \( r_{\text{hop}}^2 \) behaves monotonically with \( \hbar = h/a \); for \( ha \lesssim 1 \) we have \( r_{\text{hop}}^2 \sim 1/\hbar^2 \); \( r_{\text{hop}}^2 \sim C \). To understand this asymptotically, we replace sum with integrals in definition above, \( r_{\text{hop}}^2 \sim h^{-2} I[p_n-1,2]/I[p_n-1,0] \), with

\[
I[q,s] = \int_0^\infty dx_1 dx_2 (x_1 - x_2)^q (x_1 - x_2)^s e^{-(x_1+x_2)}. \tag{15}
\]

We arrive to the analytical expression \( r_{\text{hop}}^2 = 2\pi (p_n + 1)/h^2 \Gamma(p_n) \). Since in this case \( p_n \) are integers, we have \( r_{\text{hop}}^2 \approx 2p_n/h^2 \). Restoring connection between the poles and the Chern number as in Eq.(11), we obtain

\[
r_{\text{hop}} \approx \frac{1}{\hbar} \sqrt{C}. \tag{14}
\]

Hence the higher-C bands require longer-range hopping.

The wave function singularity position \( h = h_{\text{max}} \) results into the **lower bound** for hopping range (14). For the Chern bands, it is impossible to remove this singularity to infinity, thus \( h_{\text{max}} \) is bounded from above. For a square lattice, the first estimate on \( h_{\text{max}} \) gives as \( \pi/a \). Independently of lattice symmetries, we can use \( h_{\text{max}} = 1 \), hence the lower bound for hopping range in case of topological bands scales as (Fig.2a)

\[
r_{\text{hop}} \approx \sqrt{C}a. \tag{15}
\]

This disagrees with Ref.[26]. Note that the actual hopping range cutoff \( \Delta_n \) required to stabilize the band of desirable flatness \( f_0 \) with respect to next-order hoppings can be much higher than the lower bound (15) scaling as \( \sqrt{C}a \) (Fig.2b).
TOPOLOGICAL CONSTRAINTS ON HOPPING RANGE

FIG. 2. Microscopical analysis of topological constraints on the band flatness. (a) Characteristic hopping range scale \( r_{\text{hop}} \) demonstrates the lower bound \( \simeq \sqrt{C/a} \), Eqs.(14-15). This lower bound is fundamental [26], (b) Required tight-binding cut-off \( \Lambda_{t} \) to stabilize band flatness \( f_{x}\ll1 \) is higher than the hopping range lower bound \( r_{0} \). For all data points, we take \( h=1 \) and \( f_{\Lambda}(\Lambda_{t})=0.1 \). For higher-Chern flat bands, both (a,b) require precise experimental control of multiple hopping parameters beyond NN and NNN, thus restricting realizations of \( |C|\gg1 \) flat bands. The strategy to bypass this limitation is proposed in the main text.

Bypassing higher Chern constraints.—We notice that the microscopic constraints of form (14),(15), which were derived assuming higher-order poles of multiplicity \( N=C/2 \), could be bypassed in the experiment. Instead, we can take (a physically reasonable number) \( N \) of simple poles to construct \( C=N\times C_{1} \) flat band using \( C_{1}=1 \). In this case \( W(x)\sim x^{C_{1}-1}e^{-ha} \), hence we need to replace \( C \) with \( C_{1} \) in (15), and the lower bound \( \sqrt{C_{1}a} \sim a \) remains fixed on the lattice size for all the Chern numbers. Consider a thin film material (e.g. a monolayer or bilayer) with its band structure hosting a flat Chern band of unit \( |C_{1}|=1 \). We can stack \( N \) such layers into a multilayer heterostructure, represented by matrix Hamiltonian \( \mathcal{H} \) with monolayer Hamiltonians on the main diagonal and interlayer coupling terms placed on the diagonals just below and above. The topological invariant of this composition can be found through computing \( C[\mathcal{G}]=\frac{1}{3!} \sum_{ijk} \epsilon_{ijk} \text{Tr} \mathcal{G}_{i} \mathcal{G}_{j}^{-1} \mathcal{G}_{k}^{-1} \) where \( i,j,k=w,k_{x},k_{y} \) and \( \mathcal{G}=(\omega-\mathcal{H})^{-1} \) is matrix Green’s function [41]. Consider a case of vanishingly weak interlayer interaction; in this case the Hamiltonian approximately factorizes into matrix tensor product. If the Chern number, associated with a single layer is \( C_{1} \), the \( N \) layers in this case give

\[
C[\mathcal{G}_{N}]=N \times C_{1}, \quad \rightarrow \quad r_{\text{hop}} \sim a. \tag{16}
\]

This argument is expected to be valid when the weak interlayer interactions are switched on while preserving the finite gap; a similar algorithm was implemented by Trescher and Bergholtz [42]. Importantly, the construction (16) does not obstruct the band flatness, i.e. the flat Chern bands can be constructed for any number of layers \( N \). Clearly, this argument is also valid for constructing higher Chern numbers by bringing together \( 2n \) (gapped) Dirac cones in van der Waals multilayers for reaching \( C=1,2,3\ldots \) nearly flat Chern bands [43].

Quantum geometry and flatness constraints.—Finally, we make connection between the band geometry and flatness criterion (1). The band topology and geometry is described by the “quantum geometric” tensor [44, 45]:

\[
\Theta_{ij} = \langle \partial_{i} u_{k} | (1 - |u_{k}\rangle\langle u_{k}|) | \partial_{j} u_{k} \rangle,
\]

where \( \partial_{i} = \frac{\partial}{\partial k_{i}} \). The imaginary part of \( \Theta \) is responsible for topology, and gives (off-diagonal) Berry curvature \( F_{ij} = \text{Im} \Theta_{ij} \); the real part \( G_{ij} = \text{Re} \Theta_{ij} \) is Fubini-Study metrics and is responsible for the band geometry and its flatness. The ideal flat Chern bands satisfy the Berry-geometric condition \( F_{xy} = \text{Tr} G_{ij} \) (see Refs.[17, 44, 46]). The holomorphic (and meromorphic) perfectly flat Chern bands automatically satisfy this criterion [47]. This identity requires \( \Lambda = \infty \), thus consistent with our classification of Table I. We can further rewrite

\[
F_{xy} = \text{Tr} G_{ij} = \langle u_{k} | \hat{r}^{2} | u_{k} \rangle, \tag{17}
\]

where \( \hat{r} \) is the generalized position operator. Integrating (17) over Brillouin zone, one obtains \( r_{0}^{2} \propto C \), hence the localization length is \( r_{0} \sim \sqrt{C/a} \). For the Chern bands it is impossible to minimize localization length \( r_{0} \) independently from the hopping range bound (15); thus the flatness parameter (1) cannot be made arbitrary small for any finite \( \Lambda \), there are always finite tails. The Chern bands can be made perfectly flat only for \( \Lambda = \infty \), as was demonstrated through Eq. (13). This is an intuitive interpretation of Chen theorem [33]. Clearly now, the higher Berry fluxes in (17), hence the higher Chern numbers \( |C|\gg1 \), present stronger constraints on electronic band flatness.

Conclusions.—To conclude, the new criterion for band flatness (1) allows us to derive two concise cases \( f_{0}=e^{-ha} \) for trivial bands and \( f_{0}=\Lambda^{S[C]}e^{-F[A]} \) for topological bands of Chern number \( C \). The criteria allows us to systematize the known classes of perfectly flat bands (Table I) as the fundamental building blocks for realistic nearly flat bands. The large Chern number presents an obstruction to the band flatness, which can be seen in e.g. in the required range \( \propto \sqrt{C/a} \). The most feasible route for overcoming this obstruction is using multilayers for gluing together higher Chern numbers. We can hope that the strategy for building higher-\( C \) bands with proposed pathways (16) shall become a route towards realizing elusive Kitaev \( F_{g} \) state, a bosonic Quantum Hall phase which can be build on the \( C=8n \) flat band [49].
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