Colored Hofstadter butterflies

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ABSTRACT   I explain the thermodynamic significance, the duality and open problems associated with the two colored butterflies shown in figures 1 and 4.

1   Overview

My aim is to explain what is known about the thermodynamic significance of the two colored butterflies shown in figures 1 and 4 and what remains open. Both diagrams were made by my student, D. Osadchy [14], as part of his M.Sc. thesis. I shall explain their interpretation as the $T = 0$ phase diagrams of a two dimensional gas of charged, though non-interacting, fermions. Fig. 1 is associated with weak magnetic fields (and strong periodic potentials) while Fig. 4 with strong magnetic fields (and weak periodic potentials). The two cases are related by duality. The duality, which is further discussed below, is manifest if colors are disregarded.

The horizontal coordinate in both figures is the chemical potential μ and the vertical coordinate is proportional to the magnetic induction B in fig. 1 and $1/B$ in fig. 4. The colors represent the quantized values of the Hall conductance, i.e. represent integers [1]. Warm colors represent positive multiples and cold colors represent negative ones: Orange represents 2, red 1, white 0, blue -1 etc.

Remark: *It is problematic to represent integers by colors with good contrast between nearby integers. This is related to the fact that colors are not ordered on the line but rather are represented by the simplex (r, g, b) with $r + g + b = 1$. (Pure colors are located on the boundary of the simplex). The assignment in the figures becomes problematic for large, positive or negative, integers: Large positive integers are not represented anymore by warm colors but rather by yellow and green.*

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[1]The quantum unit of conductance, e^2/h, is $1/2\pi$, in natural units where $e = \hbar = 1$.

I shall also present an open problem. Namely, how do these diagrams change if one replaces the magnetic induction B by the magnetic field H as the thermodynamic coordinate.

2   Some history

That the Hall conductance took different signs in different metals was an embarrassment to Sommerfeld theory. Since charge is carried by the electrons one sign was predicted. The wrong sign was called the anomalous Hall effect and was explained by R. Peierls [5] who showed that the periodicity of the electron dispersion $\epsilon(k)$ plus the Pauli principle allow for either sign, depending on μ. This subsequently lead to the important concept of holes as charge carriers—a term not used by Peierls in his original work.

The electron-hole anti-symmetry of the Hall conductance is seen in Fig. 1 where cold and warm colors are interchanged upon reflection about the vertical axis. However, the figure is much more complicated than what Peierls had in mind.
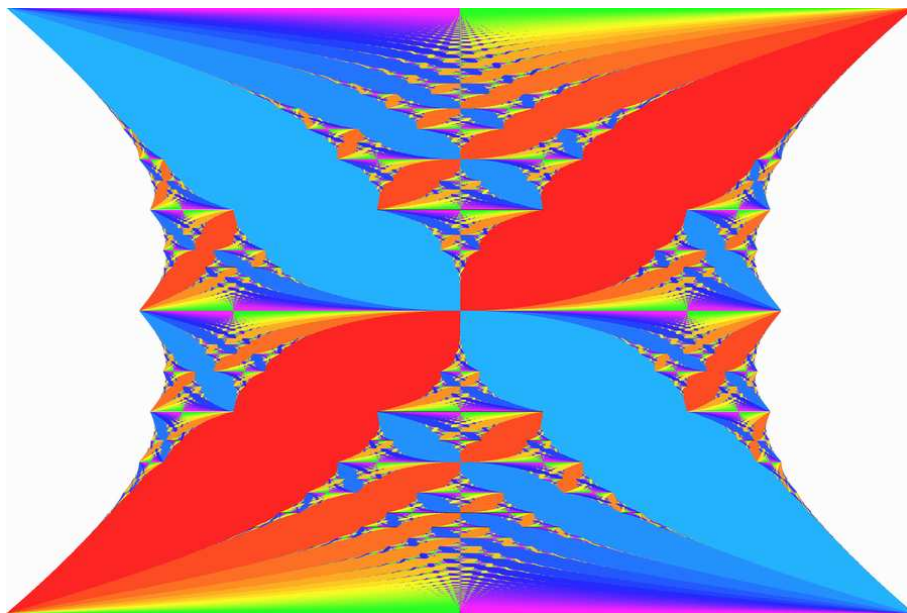

FIGURE 1. Colored Hofstadter butterfly for Bloch electrons in weak magnetic field. The horizontal axis is the chemical potential; the vertical axis is the magnetic flux through the unit cell. The diagram is periodic in the flux and one period is shown. It admits a thermodynamic interpretation of a phase diagram.

Mark Azbel [2] realized that the Schrödinger equation in a periodic po-

tential and magnetic field had tantalizing spectral properties. But it was the graphic rendering of the spectrum by D. Hofstadter [9], shown in Fig. 2, (and his scaling rules,) that brought the problem into limelights. The richness of spectral properties is a result of competing area scales: One dictated by the unit cell of the underlying periodic potential and the other by the area that carries one unit of magnetic flux. When Φ is rational the two areas are commensurate, when it is irrational, they are not. At $T = 0$ the electrons gas is coherent on large distance scales and commensuration lead to interference phenomena that affect spectral properties at very small energy scales. The delicate spectral properties attracted considerable attention of a community of spectral analysts. Reference [1] is a pointer to a rich and wonderful literature on the subject.
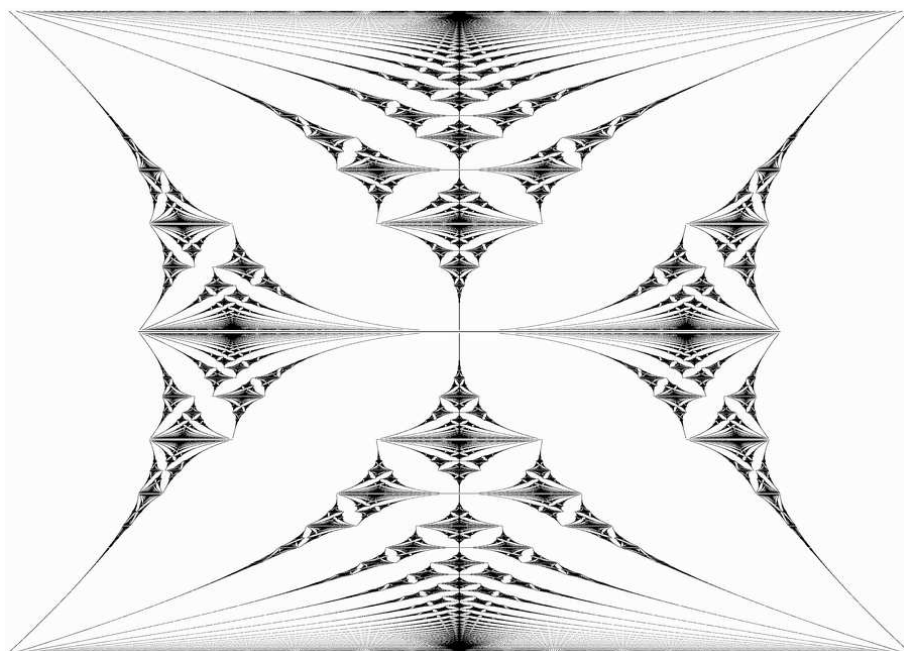

FIGURE 2. The original, monochrome, Hofstadter butterfly, shows the spectrum, on the horizontal axis, as function of the flux Φ which is the vertical axis. The spectrum is the complement of the colored set shown in fig. 1.

In a seminal work, TKNN [18] realized that the Hall conductance of the Hofstadter model admits a topological characterization in terms of Chern numbers. This discovery has an an interesting piece of lost history. In fact S. Novikov was apparently the first to realized the topological significance of the spectral gaps for Bloch electrons in magnetic fields [13]. However, he missed their significance as Hall conductance. TKNN [18] were not aware of the work of Novikov. Instead, they were motivated by a puzzle that

follow from applying the Laughlin argument for the quantization of the Hall conductance to the Hofstadter model. By essentially reinventing the proof of integrality of Chern numbers in a special case, they showed that whenever the Fermi energy is in a gap the Hall conductance is quantized.

In the two diagrams, figs. 1,4, the Hall conductance is quantized almost everywhere. The set of points where the Hall conductance is not quantized is a set of zero measure and so invisible. This is related to the fact that the spectrum is a set of measure zero (see e.g. [1] and references therein).

3   Thermodynamics considerations

It is interesting to consider the colored butterflies from the perspective of thermodynamics.

3.1   Gibbs phase rule

The first and second laws of thermodynamics constrain the shape of phase diagrams. The phase rules depend on the choice of the independent thermodynamic coordinates X be they extensive, such as $X = (E, V, N)$, or intensive, such as (P, T).

Let $X = (E, V, N)$ be the extensive coordinates of a simple thermodynamic system. X and λX with $\lambda > 0$ are thermodynamically equivalent systems, while X and $Y \neq \lambda X$ are not. Mixing X and Y, in any proportion, is, in general, an irreversible process. The second law then says that the entropy of the mixed system is not smaller than the sum of the entropies of its constituents. Namely, for $0 \leq \lambda \leq 1$

$$S(\lambda X + \lambda' Y) \geq S(\lambda X) + S(\lambda' Y) = \lambda S(X) + \lambda' S(Y), \quad \lambda' = 1 - \lambda \quad (1)$$

The first law, conservation of energy, (plus conservation of number of particles and additivity of volumes), was used in the first step and the extensivity of the entropy, $S(\lambda X) = \lambda S(X)$, in the second. Eq. (1) says that the entropy $S(X)$ is a concave function of its arguments. This embodies the basic laws of thermodynamics.

Equality in Eq. (1) holds if mixing is reversible which is, of course, the case if a phase is mixed with itself. It is also the case if coexisting phases are mixed: Clearly one can separate ice from water by mechanical means alone. The geometric expression of equality in Eq. (1) is that S contains linear segment: For a pure phase this is the half line $S(\lambda X) = \lambda S(X)$. When $X \neq \lambda Y$, are in coexistence S contains a two dimensional cone: $S(\lambda_1 X + \lambda_2 Y) = \lambda_1 S(X) + \lambda_2 S(Y)$, $\lambda_{12} > 0$. (This notion extends to multiple phase coexistence.)

Positivity of the temperature implies that S is an increasing function of E. Consequently, $S(E, V, N)$ can be inverted to give the internal energy
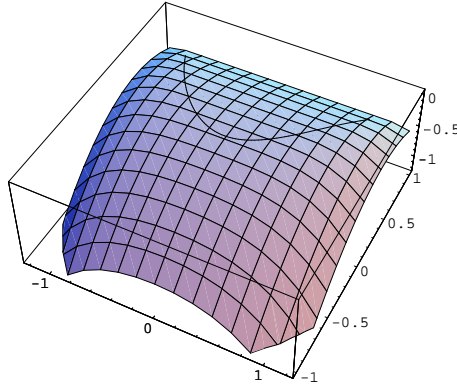
FIGURE 3. $S(E, V, N)$ is a concave function shown here for N fixed. The strictly convex pieces are associated with pure phases. The ruled piece is where two phases coexists. The boundary of the region of coexistence is shown as a black line.

$E(S, V, N)$. Since S is a concave function of its arguments $E(S, V, N)$ is a convex function of its arguments (which are the extensive state variables). Its Legendre transform with respect to all its arguments, gives a function of the intensive variables T, P and μ alone which, by scaling, must be identically zero. This is the Gibbs-Duhamel relation. It determines the pressure P as a convex function of the remaining intensive coordinates, (T, μ):

$$PV = \mu N + TS - E \tag{2}$$

The pressure is a convenient object to consider because all the terms on the rhs of Eq. (2) admit a simple representation in statistical mechanics. $-P$ is sometimes called the grand potential, e.g. [12]. Since the pressure is the Legendre transform of the internal energy with respect to S and N. The convexity of E then implies the convexity of the pressure with respect to T and μ.

Now, it is a consequence of the duality of the Legendre transform that if E has a linear segment of length ΔX then its Legendre transform P has a corresponding jump in gradient with $\Delta(\nabla P) = \Delta X$. It follows that pure phases correspond to points where $P(T, \mu)$ has a unique tangent, while two phase coexist at those points (T, μ) where P has two (linearly independent) tangents planes. (Triple points are similarly define.)

It is now a fact about convex functions that almost all points have a unique tangent while the set with multiple tangents has codimension 1 (in the sense of comparing Hausdorff dimensions). A geometric proof of this fact can be found in [6]. This gives a weak version of the Gibbs phase rule: If one considers the pressure P as function of (T, μ), (or alternatively, chemical potential μ as function of (P, t),) then pure phases are the typical sets while phases coexist on exceptional, (i.e. small), sets.

3.2 Magnetic systems

At $T = 0$ the entropy term in Eq. (2) drops. For a system of non-interacting Fermions all single particle states below μ are occupied, while those above are empty. This says that for the single particle Hamiltonian H and area A the pressure is

$$P = \lim_{A \to \infty} \frac{1}{A} Tr \left((\mu - H)_+ \chi(A) \right) \tag{3}$$

χ is the characteristic function of the area and $x_+ = x\,\theta(x)$ with θ a unit step function.

Let B denote the magnetic induction (i.e. the macroscopic average of the local magnetic field [11]). The Hamiltonian is a function of B and so is the pressure. The density ρ and the (specific) magnetization M are then given by [11]

$$\rho = \frac{\partial P}{\partial \mu}, \quad M = \frac{\partial P}{\partial B} . \tag{4}$$

The Hall conductance is thermodynamically defined by

$$\sigma_H = \frac{\partial \rho}{\partial B} = \frac{\partial M}{\partial \mu} . \tag{5}$$

It follows that, in the the wings of the butterflies where the Hall conductance is quantized P is given by:

$$P(\mu, B) = \sigma_g B(\mu - \mu_g) , \tag{6}$$

where g is a discrete wing label. The wings represent pure phases since P has a unique tangent in the gaps.

3.3 The order of the transitions

P, ρ and M are bi-linear in μ and B in the gaps. P and ρ are actually also continuous functions of μ on the spectrum. For rational flux this is a consequence of Floquet theory. For irrational flux this can be seen by a limiting argument.

At the same time, the Hall conductance, being integer valued on a set of full measure, can not be extended to a continuous function [2]. (If fact, it is not even bounded.) The continuity of the first derivative and the discontinuity of the second derivatives, makes the phase transitions in μ second order according to the Ehrenfest classification [3].

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[2]The magnetization does not extend to a continuous function on the spectrum for rational fluxes [7].

3.4 Phases and their boundaries

In the colored Hofstadter butterflies pure phases are open sets. The boundary of a given phase, say the red wing, is a curve; It is not a smooth curve as at rational values of B is has distinct tangents, but it is still a curve of Hausdorf dimensions one [15]. This is reminiscent of the Gibbs phase rule. Note, however, that the notion of the boundary of a pure phase, and the notion of phase coexistence, are distinct. The phase with Hall conductance 1 meets the phase 0 at a single point, at the tip of the butterfly, not on a line, as one might expect by the Gibbs phase rule. This holds in general: The boundary of the phases i intersects the boundary of the phase j on a set of codimension 2, not 1 [15]. Moreover, any small disc that contains two distinct phases of the butterfly contain infinitely many other phases.

3.5 Magnetic domains and phase coexistence

Is the fractal phase diagram of the butterfly in conflict with basic thermodynamic principles?

The Gibbs phase rule one finds in classical thermodynamics [3] says that two phases meet on a smooth curve which is clearly not the case for the butterfly. However, this strong version of Gibbs rule involves assumptions of smoothness of free energies that may or may not hold. Convexity alone gives a weaker version of the Gibbs phase rule, which we briefly discussed in section 3.1, which allows for all kind of wild behaviors, and does not rule out fractal phase diagrams like the butterfly. [3].

More worrisome is the lack of convexity of the pressure, $P(\mu, B)$ which is manifest in the periodicity of Fig. 1 in B. This raises the question if this reflects a problem with the Hofstadter model. It does not. A little reflection shows that rather, it a consequence of choosing B, the magnetic induction, as the thermodynamic coordinate. In the remaining part of this section I shall explain why it is actually more natural to choose for the independent thermodynamic variable the magnetic field H and the difficulties in drawing the butterflies in the $\mu - H$ plane.

Imagine a two dimensional system with finite width which is broken to domains. Assume that the magnetic field in each of the domains is perpendicular to the plane and is constant through the given domain. Since $\nabla \times H = 0$, the magnetic field H must be the same in adjacent domains. Hence the notion of constant magnetic field is constant H, while B will not be constant if the system breaks into domain. The problem with H constant is more difficult because it is B, not H, that enters in the Hamiltonian [11].

Given the colored butterfly as function of B what can one say about the

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[3]Instructive examples are given in p.8 of [17]. I thank Aernout van Enter for pointing out this example to me and for a clarifying discussion on the Gibbs phase rule.

colored butterfly as a function of H? Recall that B, H and the magnetization M are related by

$$B = H + 4\pi M \qquad (7)$$

Since M is a function of B so is H. However, B may fail to be a (univalued) function of H. This is the case if $-4\pi \partial_B M \geq 1$; If the magnetic susceptibility is sufficiently negative. When this happens, the relation $H(B)$ can not be inverted to a function $B(H)$. Domains with different values of M and B may then form and coexist [11, 4].

The condition for coexistence is a stability condition: The system will pick a value of B, consistent with H, that will minimize the entropy. However, at $T = 0$ the entropy of a gas of Fermions vanishes, so the different solutions $B_j(H, \mu)$ all give the same entropy, zero. This suggests that all the B_j represent phases at coexistence.

There is no reason why this degeneracy will hold if T is not strictly 0. Then, for most values of H a distinguished solution of $B_0(H, \mu)$ will be picked. The simple scenario is that that $B_0(H, \mu)$ will depend, for most H, continuously on H. In these intervals, the phases of the colored butterfly in (μ, H) will be a deformed version of the phases in (μ, B). However, since a values of $B_0(H, \mu)$ is picked by a minimization procedure, there is no guarantee for continuity and $B_0(H, \mu)$ will be, in general, a discontinuous function of its arguments. At the discontinuities, major qualitative changes in the diagram will take place and it is interesting to investigate the colored butterfly in the $\mu - H$ plane.

Another open problem in this context is to analyze the domain structure for coexisting phases. The quasi-periodic character of the electronic problem for irrational fluxes suggest that the domain structure could be rich and interesting as well, (e.g. a quasi-periodic domain structure for irrational fluxes).

4 Duality

We now turn to the duality relating the two diagrams.

4.1 Weak magnetic fields

Consider the "Bloch band" dispersion relation

$$\epsilon(k) = \cos(k \cdot a) + \cos(k \cdot b) \qquad (8)$$

on the two dimensional Brillouin zone. a, b are the unit lattice vectors. The Hamiltonian describing a weak external magnetic field is obtained by imposing the canonical commutation relation

$$[k \cdot a, k \cdot b] = ia \times b \cdot B \ = i \, \Phi. \qquad (9)$$

This procedure is known as the Peierls substitution [16]. The model is known as the Harper model, after a student of Peierls. The spectrum, plotted in fig. 2, is a set of measure zero and so invisible in fig. 1. Figs. 1,2 describe disjoint and complementary sets, whose union is the plane.

Although there is considerable interest in Hofstadter model for its own sake (see e.g. [1] and references therein) its physical significance to the two dimensional electron gas is limited. One reason is that the flux Φ, even for the strongest available magnetic fields, is tiny and only a horizontal sliver of the diagram in Fig. 1 near zero flux can be realized. Moreover, Φ of order one is presumably outside the region of weak field for which the model approximates the Schrödinger equation.

By gauge invariance, time-reversal and electron-hole symmetry, the pressure satisfies [7]

$$P(\mu, \Phi) = P(\mu, -\Phi) = P(\mu, \Phi + 1) = -\mu + P(-\mu, \Phi) \qquad (10)$$

This give Fig. 1 its symmetry.

4.2   Strong magnetic fields

A classical charged particle in homogeneous magnetic field moves or a circle. The center of the circle is, classically,

$$c = x + \frac{v \times B}{B^2} \qquad (11)$$

c commutes with v, but the components of the center do not commute, rather they satisfy the canonical commutation relations

$$[c \cdot a^*, c \cdot b^*] = -i \frac{B \cdot a^* \times b^*}{B^2} = -i \frac{(2\pi)^2}{\Phi} \ . \qquad (12)$$

(a^*, b^*) are dual vectors to (a, b).

If the wave function ψ belongs to a given Landau level then the shifts $e^{ic \cdot \alpha} \psi$, for $\alpha \in \mathbb{R}^2$, span the spectral subspace of that level. This means that the Hamiltonian

$$\cos(c \cdot a^*) + \cos(c \cdot b^*), \qquad (13)$$

acts within Landau levels. For large B it approximates the periodic potential $\cos(x \cdot a^*) + \cos(x \cdot b^*)$, which couples different Landau levels. This is seen from the fact that in a given Landau level $v = O(\sqrt{B})$ hence , by Eq. (11), $c \approx x$ for large B. The Hamiltonian in Eq. (12) is the same as that of Eq. (8), except that in the commutator $\Phi/2\pi$ of Eq. (9) is replaced by $2\pi/\Phi$ of Eq. (12).

Although the spectral problem of the two models is essentially the same the phase diagrams are different. This is explained in the next subsection.

Unlike the tight-binding model which is mostly of academic interest, the model of a split Landau level can be realized in artificial superlattices that accommodate a unit of quantum flux at attainable fields.

4.3 Thermodynamic duality

The pressure of a split Landau level, P_l, and split Bloch band P_b, for any temperature T, are related by [7]

$$P_l(T, \mu, \Phi/2\pi) = \frac{\Phi}{2\pi} P_b(T, \mu, 2\pi/\Phi) \tag{14}$$

This is a duality transformation: It is symmetric under the interchange $b \longleftrightarrow l$. It implies that the thermodynamics of the split Bloch band determine the thermodynamics of a split Landau level and vice versa. The factor Φ on the right is the reason that P_l is not periodic, although P_b is.

A check on the factor $\Phi/2\pi$ comes by considering large μ. Then, the tight binding model has all sites occupied and the electron density is $\rho_b \to 1$. This implies $P_b \to \mu$. In contrast, a full Landau level, has electron density that is proportional to the flux through unit area: $\rho_l \to \Phi/2\pi$ so $P_l \to \Phi\mu/2\pi$.

The magnetization and the Hall conductances of the two models are therefore related by:

$$
\begin{aligned}
m_l(\mu, T, 2\pi/\Phi) &= -\frac{1}{2\pi} P_b(\mu, T, \Phi/2\pi) - \frac{\Phi}{2\pi} m_b(\mu, T, \Phi/2\pi); \\
\sigma_l(\mu, T, 2\pi/\Phi) &= \frac{1}{2\pi} \rho_b(\mu, T, \Phi/2\pi) - \frac{\Phi}{2\pi} \sigma_b(\mu, T, \Phi/2\pi)
\end{aligned}
\tag{15}
$$

When μ is large, $\sigma_b = 0$, since a full band is an insulator. At the same time, a full Landau level has a unit of quantum conductance, $\sigma_l = 1/2\pi$, in agreement with the Eq. (15).

5 Appendix: Diophantine equation

Let me finally describe the algorithm of [18] for coloring the gaps in the butterfly fig. 1. Suppose that the magnetic flux through a unit cell is $\frac{p}{q}$. For p and q relatively prime, define the conjugate pair (m, n) as the solutions of

$$pm - qn = 1 \tag{16}$$

m is determined by this equation modulo q and n modulo p. The algorithm for solving Eq. (16) is the division algorithm of Euclid. (Standard computer packages for finding the greatest common divisor of p and q, yield also m and n such that $pm + qn = \gcd(p, q)$.) The Hall conductance k_j, associated with the j-th gap, in the tight binding case, is given by [18]

$$k_j = jm \ mod \ q, \quad |k_j| \le q/2 \tag{17}$$

In the case of split Landau band, Eq. (17) again determines k_j provided p and q are interchanged.

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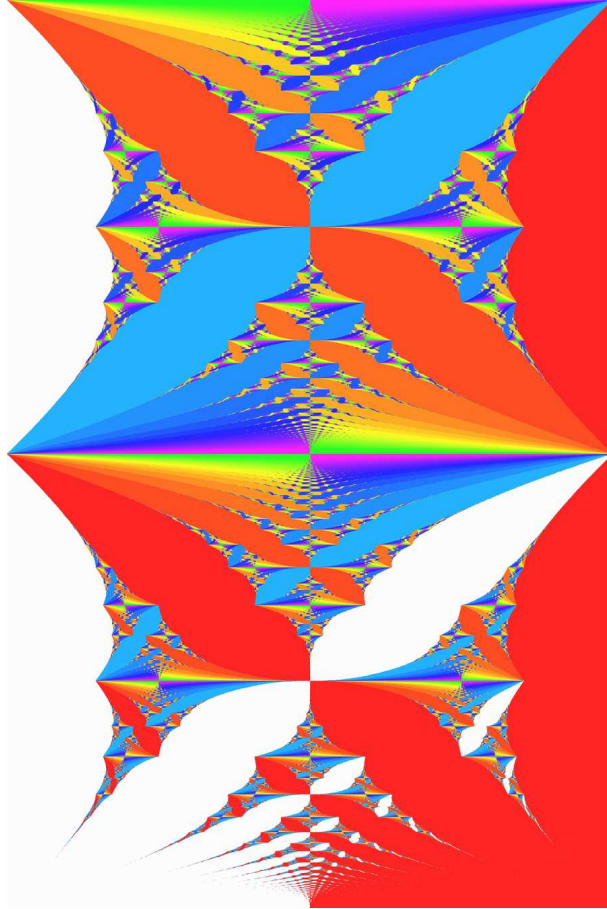
FIGURE 4. Colored Hofstadter butterfly for Landau level split by a super-lattice periodic potential. The horizontal axis is the chemical potential; the vertical axis is the average number of unit cells associated with a unit of quantum flux. As the number increase by one the pattern repeats but with a different coloring codes.